



## Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 02:14 AM UTC

PDB ID : 9WD5 / pdb\_00009wd5  
EMDB ID : EMD-65883  
Title : Cryo-EM structure of PSI-CpcL  
Authors : Mao, Z.Y.; Li, Z.H.; Han, G.Y.  
Deposited on : 2025-08-18  
Resolution : 2.98 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

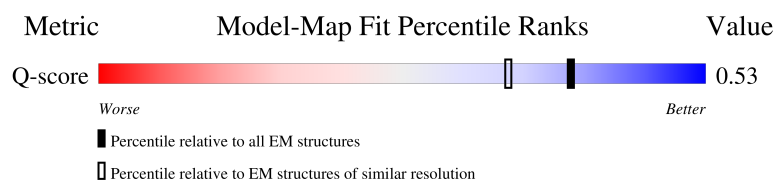
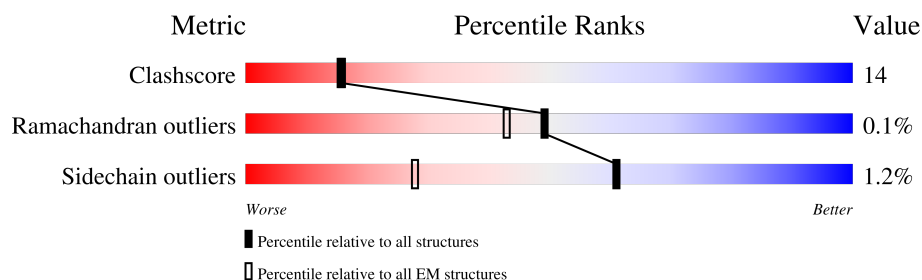
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




























| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|--|
| Clashscore            | 229148                      | 23984                       | -  |
| Ramachandran outliers | 224038                      | 23583                       | -  |
| Sidechain outliers    | 223484                      | 23102                       | -  |
| Q-score               | -                           | 25397                       | 13236 ( 2.48 - 3.48 )                                    |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                           |
|-----|-------|--------|--|
| 1   | 1     | 237    | <div> <div>9%</div> <div>86%</div> </div>  |
| 2   | A     | 752    | <div> <div>73%</div> <div>25%</div> </div> |
| 2   | G     | 752    | <div> <div>73%</div> <div>25%</div> </div> |
| 2   | a     | 752    | <div> <div>74%</div> <div>24%</div> </div> |


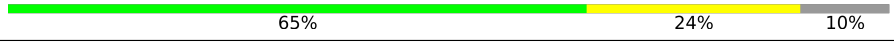
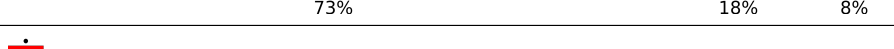
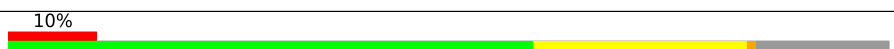



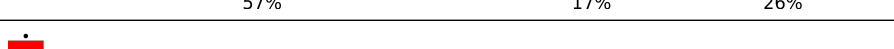



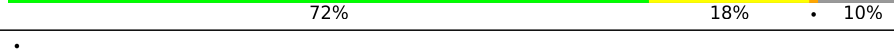

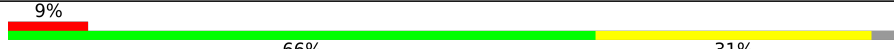


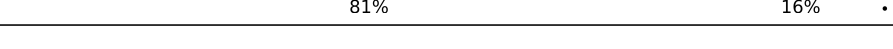
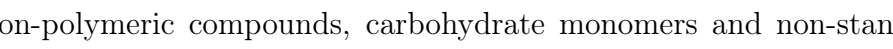

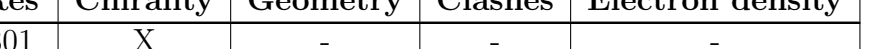
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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 2   | g     | 752    |    |
| 3   | H     | 44     |    |
| 3   | X     | 44     |    |
| 3   | h     | 44     |    |
| 3   | x     | 44     |    |
| 4   | B     | 741    |    |
| 4   | N     | 741    |    |
| 4   | b     | 741    |    |
| 4   | n     | 741    |    |
| 5   | C     | 81     |    |
| 5   | P     | 81     |    |
| 5   | c     | 81     |    |
| 5   | p     | 81     |  |
| 6   | D     | 139    |  |
| 6   | Q     | 139    |  |
| 6   | d     | 139    |  |
| 6   | q     | 139    |  |
| 7   | E     | 70     |  |
| 7   | R     | 70     |  |
| 7   | e     | 70     |  |
| 7   | r     | 70     |  |
| 8   | F     | 164    |  |
| 8   | S     | 164    |  |
| 8   | f     | 164    |  |
| 8   | s     | 164    |  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 9   | J     | 49     |    |
| 9   | T     | 49     |    |
| 9   | j     | 49     |    |
| 9   | t     | 49     |    |
| 10  | K     | 86     |    |
| 10  | U     | 86     |    |
| 10  | k     | 86     |    |
| 10  | u     | 86     |    |
| 11  | I     | 46     |    |
| 11  | V     | 46     |   |
| 11  | i     | 46     |  |
| 11  | v     | 46     |  |
| 12  | L     | 172    |  |
| 12  | W     | 172    |  |
| 12  | l     | 172    |  |
| 12  | w     | 172    |  |
| 13  | M     | 32     |  |
| 13  | Y     | 32     |  |
| 13  | m     | 32     |  |
| 13  | y     | 32     |  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14  | CLA  | A     | 801 | X         | -        | -       | -                |
| 14  | CLA  | A     | 802 | X         | -        | -       | -                |
| 14  | CLA  | A     | 803 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14  | CLA  | A     | 804 | X         | -        | -       | -                |
| 14  | CLA  | A     | 805 | X         | -        | -       | -                |
| 14  | CLA  | A     | 806 | X         | -        | -       | -                |
| 14  | CLA  | A     | 807 | X         | -        | -       | -                |
| 14  | CLA  | A     | 808 | X         | -        | -       | -                |
| 14  | CLA  | A     | 809 | X         | -        | -       | -                |
| 14  | CLA  | A     | 810 | X         | -        | -       | -                |
| 14  | CLA  | A     | 811 | X         | -        | -       | -                |
| 14  | CLA  | A     | 812 | X         | -        | -       | -                |
| 14  | CLA  | A     | 813 | X         | -        | -       | -                |
| 14  | CLA  | A     | 814 | X         | -        | -       | -                |
| 14  | CLA  | A     | 815 | X         | -        | -       | -                |
| 14  | CLA  | A     | 816 | X         | -        | -       | -                |
| 14  | CLA  | A     | 817 | X         | -        | -       | -                |
| 14  | CLA  | A     | 818 | X         | -        | -       | -                |
| 14  | CLA  | A     | 819 | X         | -        | -       | -                |
| 14  | CLA  | A     | 820 | X         | -        | -       | -                |
| 14  | CLA  | A     | 821 | X         | -        | -       | -                |
| 14  | CLA  | A     | 822 | X         | -        | -       | -                |
| 14  | CLA  | A     | 823 | X         | -        | -       | -                |
| 14  | CLA  | A     | 824 | X         | -        | -       | -                |
| 14  | CLA  | A     | 825 | X         | -        | -       | -                |
| 14  | CLA  | A     | 826 | X         | -        | -       | -                |
| 14  | CLA  | A     | 827 | X         | -        | -       | -                |
| 14  | CLA  | A     | 828 | X         | -        | -       | -                |
| 14  | CLA  | A     | 829 | X         | -        | -       | -                |
| 14  | CLA  | A     | 830 | X         | -        | -       | -                |
| 14  | CLA  | A     | 831 | X         | -        | -       | -                |
| 14  | CLA  | A     | 832 | X         | -        | -       | -                |
| 14  | CLA  | A     | 833 | X         | -        | -       | -                |
| 14  | CLA  | A     | 834 | X         | -        | -       | -                |
| 14  | CLA  | A     | 835 | X         | -        | -       | -                |
| 14  | CLA  | A     | 836 | X         | -        | -       | -                |
| 14  | CLA  | A     | 837 | X         | -        | -       | -                |
| 14  | CLA  | A     | 838 | X         | -        | -       | -                |
| 14  | CLA  | A     | 839 | X         | -        | -       | -                |
| 14  | CLA  | A     | 840 | X         | -        | -       | -                |
| 14  | CLA  | A     | 841 | X         | -        | -       | -                |
| 14  | CLA  | A     | 853 | X         | -        | -       | -                |
| 14  | CLA  | A     | 854 | X         | -        | -       | -                |
| 14  | CLA  | A     | 855 | X         | -        | X       | -                |
| 14  | CLA  | A     | 857 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14  | CLA  | B     | 803 | X         | -        | -       | -                |
| 14  | CLA  | B     | 804 | X         | -        | -       | -                |
| 14  | CLA  | B     | 805 | X         | -        | -       | -                |
| 14  | CLA  | B     | 806 | X         | -        | -       | -                |
| 14  | CLA  | B     | 807 | X         | -        | -       | -                |
| 14  | CLA  | B     | 808 | X         | -        | -       | -                |
| 14  | CLA  | B     | 809 | X         | -        | -       | -                |
| 14  | CLA  | B     | 810 | X         | -        | -       | -                |
| 14  | CLA  | B     | 811 | X         | -        | -       | -                |
| 14  | CLA  | B     | 812 | X         | -        | -       | -                |
| 14  | CLA  | B     | 813 | X         | -        | -       | -                |
| 14  | CLA  | B     | 814 | X         | -        | -       | -                |
| 14  | CLA  | B     | 815 | X         | -        | -       | -                |
| 14  | CLA  | B     | 816 | X         | -        | -       | -                |
| 14  | CLA  | B     | 817 | X         | -        | -       | -                |
| 14  | CLA  | B     | 818 | X         | -        | -       | -                |
| 14  | CLA  | B     | 819 | X         | -        | -       | -                |
| 14  | CLA  | B     | 820 | X         | -        | -       | -                |
| 14  | CLA  | B     | 821 | X         | -        | -       | -                |
| 14  | CLA  | B     | 822 | X         | -        | -       | -                |
| 14  | CLA  | B     | 823 | X         | -        | -       | -                |
| 14  | CLA  | B     | 824 | X         | -        | -       | -                |
| 14  | CLA  | B     | 825 | X         | -        | -       | -                |
| 14  | CLA  | B     | 826 | X         | -        | -       | -                |
| 14  | CLA  | B     | 827 | X         | -        | -       | -                |
| 14  | CLA  | B     | 828 | X         | -        | -       | -                |
| 14  | CLA  | B     | 829 | X         | -        | -       | -                |
| 14  | CLA  | B     | 830 | X         | -        | -       | -                |
| 14  | CLA  | B     | 831 | X         | -        | -       | -                |
| 14  | CLA  | B     | 832 | X         | -        | -       | -                |
| 14  | CLA  | B     | 833 | X         | -        | -       | -                |
| 14  | CLA  | B     | 834 | X         | -        | -       | -                |
| 14  | CLA  | B     | 835 | X         | -        | -       | -                |
| 14  | CLA  | B     | 836 | X         | -        | -       | -                |
| 14  | CLA  | B     | 837 | X         | -        | -       | -                |
| 14  | CLA  | B     | 838 | X         | -        | -       | -                |
| 14  | CLA  | B     | 839 | X         | -        | -       | -                |
| 14  | CLA  | B     | 840 | X         | -        | -       | -                |
| 14  | CLA  | B     | 841 | X         | -        | -       | -                |
| 14  | CLA  | B     | 850 | X         | -        | -       | -                |
| 14  | CLA  | F     | 201 | X         | -        | -       | -                |
| 14  | CLA  | F     | 202 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14  | CLA  | G     | 801 | X         | -        | -       | -                |
| 14  | CLA  | G     | 802 | X         | -        | -       | -                |
| 14  | CLA  | G     | 803 | X         | -        | -       | -                |
| 14  | CLA  | G     | 804 | X         | -        | -       | -                |
| 14  | CLA  | G     | 805 | X         | -        | -       | -                |
| 14  | CLA  | G     | 806 | X         | -        | -       | -                |
| 14  | CLA  | G     | 807 | X         | -        | -       | -                |
| 14  | CLA  | G     | 808 | X         | -        | -       | -                |
| 14  | CLA  | G     | 809 | X         | -        | -       | -                |
| 14  | CLA  | G     | 810 | X         | -        | -       | -                |
| 14  | CLA  | G     | 811 | X         | -        | -       | -                |
| 14  | CLA  | G     | 812 | X         | -        | -       | -                |
| 14  | CLA  | G     | 813 | X         | -        | -       | -                |
| 14  | CLA  | G     | 814 | X         | -        | -       | -                |
| 14  | CLA  | G     | 815 | X         | -        | -       | -                |
| 14  | CLA  | G     | 816 | X         | -        | -       | -                |
| 14  | CLA  | G     | 817 | X         | -        | -       | -                |
| 14  | CLA  | G     | 818 | X         | -        | -       | -                |
| 14  | CLA  | G     | 819 | X         | -        | -       | -                |
| 14  | CLA  | G     | 820 | X         | -        | -       | -                |
| 14  | CLA  | G     | 821 | X         | -        | -       | -                |
| 14  | CLA  | G     | 822 | X         | -        | -       | -                |
| 14  | CLA  | G     | 823 | X         | -        | -       | -                |
| 14  | CLA  | G     | 824 | X         | -        | -       | -                |
| 14  | CLA  | G     | 825 | X         | -        | -       | -                |
| 14  | CLA  | G     | 826 | X         | -        | -       | -                |
| 14  | CLA  | G     | 827 | X         | -        | -       | -                |
| 14  | CLA  | G     | 828 | X         | -        | -       | -                |
| 14  | CLA  | G     | 829 | X         | -        | -       | -                |
| 14  | CLA  | G     | 830 | X         | -        | -       | -                |
| 14  | CLA  | G     | 831 | X         | -        | -       | -                |
| 14  | CLA  | G     | 832 | X         | -        | -       | -                |
| 14  | CLA  | G     | 833 | X         | -        | -       | -                |
| 14  | CLA  | G     | 834 | X         | -        | -       | -                |
| 14  | CLA  | G     | 835 | X         | -        | -       | -                |
| 14  | CLA  | G     | 836 | X         | -        | -       | -                |
| 14  | CLA  | G     | 837 | X         | -        | -       | -                |
| 14  | CLA  | G     | 838 | X         | -        | -       | -                |
| 14  | CLA  | G     | 839 | X         | -        | -       | -                |
| 14  | CLA  | G     | 840 | X         | -        | -       | -                |
| 14  | CLA  | G     | 852 | X         | -        | X       | -                |
| 14  | CLA  | G     | 853 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CLA  | H     | 1701 | X         | -        | -       | -                |
| 14  | CLA  | J     | 101  | X         | -        | -       | -                |
| 14  | CLA  | J     | 102  | X         | -        | -       | -                |
| 14  | CLA  | K     | 101  | X         | -        | -       | -                |
| 14  | CLA  | L     | 1501 | X         | -        | -       | -                |
| 14  | CLA  | L     | 1502 | X         | -        | -       | -                |
| 14  | CLA  | L     | 1503 | X         | -        | -       | -                |
| 14  | CLA  | N     | 801  | X         | -        | -       | -                |
| 14  | CLA  | N     | 803  | X         | -        | -       | -                |
| 14  | CLA  | N     | 804  | X         | -        | -       | -                |
| 14  | CLA  | N     | 805  | X         | -        | -       | -                |
| 14  | CLA  | N     | 806  | X         | -        | -       | -                |
| 14  | CLA  | N     | 807  | X         | -        | -       | -                |
| 14  | CLA  | N     | 808  | X         | -        | -       | -                |
| 14  | CLA  | N     | 809  | X         | -        | -       | -                |
| 14  | CLA  | N     | 810  | X         | -        | -       | -                |
| 14  | CLA  | N     | 811  | X         | -        | -       | -                |
| 14  | CLA  | N     | 812  | X         | -        | -       | -                |
| 14  | CLA  | N     | 813  | X         | -        | -       | -                |
| 14  | CLA  | N     | 814  | X         | -        | -       | -                |
| 14  | CLA  | N     | 815  | X         | -        | -       | -                |
| 14  | CLA  | N     | 816  | X         | -        | -       | -                |
| 14  | CLA  | N     | 817  | X         | -        | -       | -                |
| 14  | CLA  | N     | 818  | X         | -        | -       | -                |
| 14  | CLA  | N     | 819  | X         | -        | -       | -                |
| 14  | CLA  | N     | 820  | X         | -        | -       | -                |
| 14  | CLA  | N     | 821  | X         | -        | -       | -                |
| 14  | CLA  | N     | 822  | X         | -        | -       | -                |
| 14  | CLA  | N     | 823  | X         | -        | -       | -                |
| 14  | CLA  | N     | 824  | X         | -        | -       | -                |
| 14  | CLA  | N     | 825  | X         | -        | -       | -                |
| 14  | CLA  | N     | 826  | X         | -        | -       | -                |
| 14  | CLA  | N     | 827  | X         | -        | -       | -                |
| 14  | CLA  | N     | 828  | X         | -        | -       | -                |
| 14  | CLA  | N     | 829  | X         | -        | -       | -                |
| 14  | CLA  | N     | 830  | X         | -        | -       | -                |
| 14  | CLA  | N     | 831  | X         | -        | -       | -                |
| 14  | CLA  | N     | 832  | X         | -        | -       | -                |
| 14  | CLA  | N     | 833  | X         | -        | -       | -                |
| 14  | CLA  | N     | 834  | X         | -        | -       | -                |
| 14  | CLA  | N     | 835  | X         | -        | -       | -                |
| 14  | CLA  | N     | 836  | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CLA  | N     | 837  | X         | -        | -       | -                |
| 14  | CLA  | N     | 838  | X         | -        | -       | -                |
| 14  | CLA  | N     | 839  | X         | -        | -       | -                |
| 14  | CLA  | N     | 840  | X         | -        | -       | -                |
| 14  | CLA  | N     | 841  | X         | -        | -       | -                |
| 14  | CLA  | N     | 842  | X         | -        | -       | -                |
| 14  | CLA  | N     | 851  | X         | -        | -       | -                |
| 14  | CLA  | S     | 201  | X         | -        | -       | -                |
| 14  | CLA  | S     | 203  | X         | -        | -       | -                |
| 14  | CLA  | T     | 101  | X         | -        | -       | -                |
| 14  | CLA  | T     | 102  | X         | -        | -       | -                |
| 14  | CLA  | U     | 101  | X         | -        | -       | -                |
| 14  | CLA  | U     | 102  | X         | -        | -       | -                |
| 14  | CLA  | W     | 202  | X         | -        | -       | -                |
| 14  | CLA  | W     | 203  | X         | -        | -       | -                |
| 14  | CLA  | W     | 204  | X         | -        | -       | -                |
| 14  | CLA  | X     | 1701 | X         | -        | -       | -                |
| 14  | CLA  | a     | 801  | X         | -        | -       | -                |
| 14  | CLA  | a     | 802  | X         | -        | -       | -                |
| 14  | CLA  | a     | 803  | X         | -        | -       | -                |
| 14  | CLA  | a     | 804  | X         | -        | -       | -                |
| 14  | CLA  | a     | 805  | X         | -        | -       | -                |
| 14  | CLA  | a     | 806  | X         | -        | -       | -                |
| 14  | CLA  | a     | 807  | X         | -        | -       | -                |
| 14  | CLA  | a     | 808  | X         | -        | -       | -                |
| 14  | CLA  | a     | 809  | X         | -        | -       | -                |
| 14  | CLA  | a     | 810  | X         | -        | -       | -                |
| 14  | CLA  | a     | 811  | X         | -        | -       | -                |
| 14  | CLA  | a     | 812  | X         | -        | -       | -                |
| 14  | CLA  | a     | 813  | X         | -        | -       | -                |
| 14  | CLA  | a     | 814  | X         | -        | -       | -                |
| 14  | CLA  | a     | 815  | X         | -        | -       | -                |
| 14  | CLA  | a     | 816  | X         | -        | -       | -                |
| 14  | CLA  | a     | 817  | X         | -        | -       | -                |
| 14  | CLA  | a     | 818  | X         | -        | -       | -                |
| 14  | CLA  | a     | 819  | X         | -        | -       | -                |
| 14  | CLA  | a     | 820  | X         | -        | -       | -                |
| 14  | CLA  | a     | 821  | X         | -        | -       | -                |
| 14  | CLA  | a     | 822  | X         | -        | -       | -                |
| 14  | CLA  | a     | 823  | X         | -        | -       | -                |
| 14  | CLA  | a     | 824  | X         | -        | -       | -                |
| 14  | CLA  | a     | 825  | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14  | CLA  | a     | 826 | X         | -        | -       | -                |
| 14  | CLA  | a     | 827 | X         | -        | -       | -                |
| 14  | CLA  | a     | 828 | X         | -        | -       | -                |
| 14  | CLA  | a     | 829 | X         | -        | -       | -                |
| 14  | CLA  | a     | 830 | X         | -        | -       | -                |
| 14  | CLA  | a     | 831 | X         | -        | -       | -                |
| 14  | CLA  | a     | 832 | X         | -        | -       | -                |
| 14  | CLA  | a     | 833 | X         | -        | -       | -                |
| 14  | CLA  | a     | 834 | X         | -        | -       | -                |
| 14  | CLA  | a     | 835 | X         | -        | -       | -                |
| 14  | CLA  | a     | 836 | X         | -        | -       | -                |
| 14  | CLA  | a     | 837 | X         | -        | -       | -                |
| 14  | CLA  | a     | 838 | X         | -        | -       | -                |
| 14  | CLA  | a     | 839 | X         | -        | -       | -                |
| 14  | CLA  | a     | 840 | X         | -        | -       | -                |
| 14  | CLA  | a     | 852 | X         | -        | -       | -                |
| 14  | CLA  | a     | 853 | X         | -        | -       | -                |
| 14  | CLA  | a     | 854 | X         | -        | -       | -                |
| 14  | CLA  | b     | 802 | X         | -        | -       | -                |
| 14  | CLA  | b     | 803 | X         | -        | -       | -                |
| 14  | CLA  | b     | 804 | X         | -        | -       | -                |
| 14  | CLA  | b     | 805 | X         | -        | -       | -                |
| 14  | CLA  | b     | 806 | X         | -        | -       | -                |
| 14  | CLA  | b     | 807 | X         | -        | -       | -                |
| 14  | CLA  | b     | 808 | X         | -        | -       | -                |
| 14  | CLA  | b     | 809 | X         | -        | -       | -                |
| 14  | CLA  | b     | 810 | X         | -        | -       | -                |
| 14  | CLA  | b     | 811 | X         | -        | -       | -                |
| 14  | CLA  | b     | 812 | X         | -        | -       | -                |
| 14  | CLA  | b     | 813 | X         | -        | -       | -                |
| 14  | CLA  | b     | 814 | X         | -        | -       | -                |
| 14  | CLA  | b     | 815 | X         | -        | -       | -                |
| 14  | CLA  | b     | 816 | X         | -        | -       | -                |
| 14  | CLA  | b     | 817 | X         | -        | -       | -                |
| 14  | CLA  | b     | 818 | X         | -        | -       | -                |
| 14  | CLA  | b     | 819 | X         | -        | -       | -                |
| 14  | CLA  | b     | 820 | X         | -        | -       | -                |
| 14  | CLA  | b     | 821 | X         | -        | -       | -                |
| 14  | CLA  | b     | 822 | X         | -        | -       | -                |
| 14  | CLA  | b     | 823 | X         | -        | -       | -                |
| 14  | CLA  | b     | 824 | X         | -        | -       | -                |
| 14  | CLA  | b     | 825 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 14  | CLA  | b     | 826 | X         | -        | -       | -                |
| 14  | CLA  | b     | 827 | X         | -        | -       | -                |
| 14  | CLA  | b     | 828 | X         | -        | -       | -                |
| 14  | CLA  | b     | 829 | X         | -        | -       | -                |
| 14  | CLA  | b     | 830 | X         | -        | -       | -                |
| 14  | CLA  | b     | 831 | X         | -        | -       | -                |
| 14  | CLA  | b     | 832 | X         | -        | -       | -                |
| 14  | CLA  | b     | 833 | X         | -        | -       | -                |
| 14  | CLA  | b     | 834 | X         | -        | -       | -                |
| 14  | CLA  | b     | 835 | X         | -        | -       | -                |
| 14  | CLA  | b     | 836 | X         | -        | -       | -                |
| 14  | CLA  | b     | 837 | X         | -        | -       | -                |
| 14  | CLA  | b     | 838 | X         | -        | -       | -                |
| 14  | CLA  | b     | 839 | X         | -        | -       | -                |
| 14  | CLA  | b     | 840 | X         | -        | -       | -                |
| 14  | CLA  | b     | 841 | X         | -        | -       | -                |
| 14  | CLA  | b     | 851 | X         | -        | -       | -                |
| 14  | CLA  | b     | 853 | X         | -        | -       | -                |
| 14  | CLA  | f     | 201 | X         | -        | -       | -                |
| 14  | CLA  | f     | 202 | X         | -        | -       | -                |
| 14  | CLA  | g     | 801 | X         | -        | -       | -                |
| 14  | CLA  | g     | 802 | X         | -        | -       | -                |
| 14  | CLA  | g     | 803 | X         | -        | -       | -                |
| 14  | CLA  | g     | 804 | X         | -        | -       | -                |
| 14  | CLA  | g     | 805 | X         | -        | -       | -                |
| 14  | CLA  | g     | 806 | X         | -        | -       | -                |
| 14  | CLA  | g     | 807 | X         | -        | -       | -                |
| 14  | CLA  | g     | 808 | X         | -        | -       | -                |
| 14  | CLA  | g     | 809 | X         | -        | -       | -                |
| 14  | CLA  | g     | 810 | X         | -        | -       | -                |
| 14  | CLA  | g     | 811 | X         | -        | -       | -                |
| 14  | CLA  | g     | 812 | X         | -        | -       | -                |
| 14  | CLA  | g     | 813 | X         | -        | -       | -                |
| 14  | CLA  | g     | 814 | X         | -        | -       | -                |
| 14  | CLA  | g     | 815 | X         | -        | -       | -                |
| 14  | CLA  | g     | 816 | X         | -        | -       | -                |
| 14  | CLA  | g     | 817 | X         | -        | -       | -                |
| 14  | CLA  | g     | 818 | X         | -        | -       | -                |
| 14  | CLA  | g     | 819 | X         | -        | -       | -                |
| 14  | CLA  | g     | 820 | X         | -        | -       | -                |
| 14  | CLA  | g     | 821 | X         | -        | -       | -                |
| 14  | CLA  | g     | 822 | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CLA  | g     | 823  | X         | -        | -       | -                |
| 14  | CLA  | g     | 824  | X         | -        | -       | -                |
| 14  | CLA  | g     | 825  | X         | -        | -       | -                |
| 14  | CLA  | g     | 826  | X         | -        | -       | -                |
| 14  | CLA  | g     | 827  | X         | -        | -       | -                |
| 14  | CLA  | g     | 828  | X         | -        | -       | -                |
| 14  | CLA  | g     | 829  | X         | -        | -       | -                |
| 14  | CLA  | g     | 830  | X         | -        | -       | -                |
| 14  | CLA  | g     | 831  | X         | -        | -       | -                |
| 14  | CLA  | g     | 832  | X         | -        | -       | -                |
| 14  | CLA  | g     | 833  | X         | -        | -       | -                |
| 14  | CLA  | g     | 834  | X         | -        | -       | -                |
| 14  | CLA  | g     | 835  | X         | -        | -       | -                |
| 14  | CLA  | g     | 836  | X         | -        | -       | -                |
| 14  | CLA  | g     | 837  | X         | -        | -       | -                |
| 14  | CLA  | g     | 838  | X         | -        | -       | -                |
| 14  | CLA  | g     | 839  | X         | -        | -       | -                |
| 14  | CLA  | g     | 840  | X         | -        | -       | -                |
| 14  | CLA  | g     | 852  | X         | -        | -       | -                |
| 14  | CLA  | g     | 853  | X         | -        | -       | -                |
| 14  | CLA  | g     | 854  | X         | -        | -       | -                |
| 14  | CLA  | h     | 1701 | X         | -        | -       | -                |
| 14  | CLA  | j     | 101  | X         | -        | -       | -                |
| 14  | CLA  | j     | 102  | X         | -        | -       | -                |
| 14  | CLA  | k     | 101  | X         | -        | -       | -                |
| 14  | CLA  | l     | 202  | X         | -        | -       | -                |
| 14  | CLA  | l     | 203  | X         | -        | -       | -                |
| 14  | CLA  | l     | 204  | X         | -        | -       | -                |
| 14  | CLA  | n     | 802  | X         | -        | -       | -                |
| 14  | CLA  | n     | 803  | X         | -        | -       | -                |
| 14  | CLA  | n     | 804  | X         | -        | -       | -                |
| 14  | CLA  | n     | 805  | X         | -        | -       | -                |
| 14  | CLA  | n     | 806  | X         | -        | -       | -                |
| 14  | CLA  | n     | 807  | X         | -        | -       | -                |
| 14  | CLA  | n     | 808  | X         | -        | -       | -                |
| 14  | CLA  | n     | 809  | X         | -        | -       | -                |
| 14  | CLA  | n     | 810  | X         | -        | -       | -                |
| 14  | CLA  | n     | 811  | X         | -        | -       | -                |
| 14  | CLA  | n     | 812  | X         | -        | -       | -                |
| 14  | CLA  | n     | 813  | X         | -        | -       | -                |
| 14  | CLA  | n     | 814  | X         | -        | -       | -                |
| 14  | CLA  | n     | 815  | X         | -        | -       | -                |

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| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 14  | CLA  | n     | 816  | X         | -        | -       | -                |
| 14  | CLA  | n     | 817  | X         | -        | -       | -                |
| 14  | CLA  | n     | 818  | X         | -        | -       | -                |
| 14  | CLA  | n     | 819  | X         | -        | -       | -                |
| 14  | CLA  | n     | 820  | X         | -        | -       | -                |
| 14  | CLA  | n     | 821  | X         | -        | -       | -                |
| 14  | CLA  | n     | 822  | X         | -        | -       | -                |
| 14  | CLA  | n     | 823  | X         | -        | -       | -                |
| 14  | CLA  | n     | 824  | X         | -        | -       | -                |
| 14  | CLA  | n     | 825  | X         | -        | -       | -                |
| 14  | CLA  | n     | 826  | X         | -        | -       | -                |
| 14  | CLA  | n     | 827  | X         | -        | -       | -                |
| 14  | CLA  | n     | 828  | X         | -        | -       | -                |
| 14  | CLA  | n     | 829  | X         | -        | -       | -                |
| 14  | CLA  | n     | 830  | X         | -        | -       | -                |
| 14  | CLA  | n     | 831  | X         | -        | -       | -                |
| 14  | CLA  | n     | 832  | X         | -        | -       | -                |
| 14  | CLA  | n     | 833  | X         | -        | -       | -                |
| 14  | CLA  | n     | 834  | X         | -        | -       | -                |
| 14  | CLA  | n     | 835  | X         | -        | -       | -                |
| 14  | CLA  | n     | 836  | X         | -        | -       | -                |
| 14  | CLA  | n     | 837  | X         | -        | -       | -                |
| 14  | CLA  | n     | 838  | X         | -        | -       | -                |
| 14  | CLA  | n     | 839  | X         | -        | -       | -                |
| 14  | CLA  | n     | 840  | X         | -        | -       | -                |
| 14  | CLA  | n     | 850  | X         | -        | -       | -                |
| 14  | CLA  | n     | 852  | X         | -        | -       | -                |
| 14  | CLA  | s     | 201  | X         | -        | -       | -                |
| 14  | CLA  | s     | 202  | X         | -        | -       | -                |
| 14  | CLA  | t     | 101  | X         | -        | -       | -                |
| 14  | CLA  | t     | 102  | X         | -        | -       | -                |
| 14  | CLA  | u     | 101  | X         | -        | -       | -                |
| 14  | CLA  | u     | 102  | X         | -        | -       | -                |
| 14  | CLA  | w     | 203  | X         | -        | -       | -                |
| 14  | CLA  | w     | 204  | X         | -        | -       | -                |
| 14  | CLA  | w     | 205  | X         | -        | -       | -                |
| 14  | CLA  | x     | 1701 | X         | -        | -       | -                |
| 17  | BCR  | N     | 852  | -         | -        | X       | -                |
| 19  | CL0  | A     | 852  | X         | -        | -       | -                |
| 19  | CL0  | G     | 851  | X         | -        | -       | -                |
| 19  | CL0  | a     | 851  | X         | -        | -       | -                |
| 19  | CL0  | g     | 851  | X         | -        | -       | -                |

## 2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 98661 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I-associated linker protein CpcL.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 1   | 1     | 33       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 247   | 166 | 36 | 44 | 1 |         |       |

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

| Mol | Chain | Residues | Atoms |      |      |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|----|---------|-------|
| 2   | G     | 741      | Total | C    | N    | O   | S  | 0       | 0     |
|     |       |          | 5814  | 3814 | 1001 | 978 | 21 |         |       |
| 2   | g     | 742      | Total | C    | N    | O   | S  | 0       | 0     |
|     |       |          | 5823  | 3820 | 1003 | 979 | 21 |         |       |
| 2   | A     | 742      | Total | C    | N    | O   | S  | 0       | 0     |
|     |       |          | 5823  | 3820 | 1003 | 979 | 21 |         |       |
| 2   | a     | 742      | Total | C    | N    | O   | S  | 0       | 0     |
|     |       |          | 5823  | 3820 | 1003 | 979 | 21 |         |       |

- Molecule 3 is a protein called Photosystem I 4.8 kDa protein.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 3   | H     | 31       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 257   | 179 | 40 | 38 |         |       |
| 3   | h     | 30       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 248   | 174 | 38 | 36 |         |       |
| 3   | X     | 31       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 257   | 179 | 40 | 38 |         |       |
| 3   | x     | 31       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 257   | 179 | 40 | 38 |         |       |

- Molecule 4 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 1.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 4   | N     | 739      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5913  | 3902 | 990 | 1003 | 18 |         |       |

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| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 4   | n     | 738      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5906  | 3898 | 989 | 1001 | 18 |         |       |
| 4   | B     | 740      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5918  | 3905 | 991 | 1004 | 18 |         |       |
| 4   | b     | 740      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5918  | 3905 | 991 | 1004 | 18 |         |       |

- Molecule 5 is a protein called Photosystem I iron-sulfur center.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 5   | P     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 598   | 367 | 103 | 117 | 11 |         |       |
| 5   | p     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 598   | 367 | 103 | 117 | 11 |         |       |
| 5   | C     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 598   | 367 | 103 | 117 | 11 |         |       |
| 5   | c     | 80       | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 598   | 367 | 103 | 117 | 11 |         |       |

- Molecule 6 is a protein called Photosystem I reaction center subunit II.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | Q     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1040  | 666 | 179 | 194 | 1 |         |       |
| 6   | q     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1047  | 670 | 180 | 196 | 1 |         |       |
| 6   | D     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1040  | 666 | 179 | 194 | 1 |         |       |
| 6   | d     | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1047  | 670 | 180 | 196 | 1 |         |       |

- Molecule 7 is a protein called Photosystem I reaction center subunit IV.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 7   | R     | 61       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 490   | 313 | 84 | 93 |         |       |
| 7   | r     | 60       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 481   | 308 | 83 | 90 |         |       |
| 7   | E     | 61       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 490   | 313 | 84 | 93 |         |       |
| 7   | e     | 61       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 490   | 313 | 84 | 93 |         |       |

- Molecule 8 is a protein called Photosystem I reaction center subunit III.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | S     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 690 | 184 | 204 | 2 |         |       |
| 8   | s     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 690 | 184 | 204 | 2 |         |       |
| 8   | F     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 690 | 184 | 204 | 2 |         |       |
| 8   | f     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1080  | 690 | 184 | 204 | 2 |         |       |

- Molecule 9 is a protein called Photosystem I reaction center subunit IX.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 9   | T     | 44       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 354   | 241 | 53 | 60 |         |       |
| 9   | t     | 45       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 359   | 244 | 54 | 61 |         |       |
| 9   | J     | 45       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 359   | 244 | 54 | 61 |         |       |
| 9   | j     | 45       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 359   | 244 | 54 | 61 |         |       |

- Molecule 10 is a protein called Photosystem I reaction center subunit PsaK 1.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10  | U     | 73       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 537   | 357 | 89 | 90 | 1 |         |       |
| 10  | u     | 78       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 568   | 376 | 94 | 97 | 1 |         |       |
| 10  | K     | 73       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 537   | 357 | 89 | 90 | 1 |         |       |
| 10  | k     | 78       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 568   | 376 | 94 | 97 | 1 |         |       |

- Molecule 11 is a protein called Photosystem I reaction center subunit VIII.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 11  | V     | 33       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 268   | 184 | 37 | 47 |         |       |
| 11  | v     | 34       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 275   | 189 | 38 | 48 |         |       |
| 11  | I     | 34       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 275   | 189 | 38 | 48 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 11  | i     | 34       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 275   | 189 | 38 | 48 |         |       |

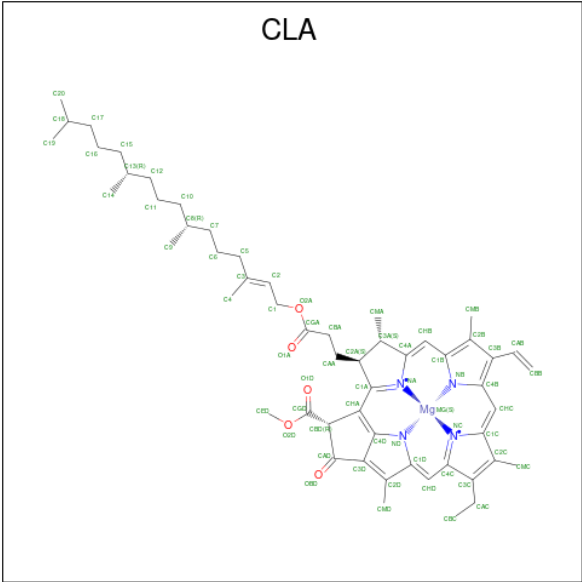
- Molecule 12 is a protein called Photosystem I reaction center subunit XI.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | W     | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1163  | 763 | 197 | 202 | 1 |         |       |
| 12  | w     | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1163  | 763 | 197 | 202 | 1 |         |       |
| 12  | L     | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1163  | 763 | 197 | 202 | 1 |         |       |
| 12  | l     | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1163  | 763 | 197 | 202 | 1 |         |       |

- Molecule 13 is a protein called Photosystem I reaction center subunit XII.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 13  | Y     | 31       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 241   | 160 | 37 | 44 |         |       |
| 13  | y     | 31       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 241   | 160 | 37 | 44 |         |       |
| 13  | M     | 31       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 241   | 160 | 37 | 44 |         |       |
| 13  | m     | 31       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 241   | 160 | 37 | 44 |         |       |

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | H     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |
| 14  | N     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14  | N     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | N     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | N     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | N     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | N     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | N     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | N     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | N     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | S     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | S     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | T     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | T     | 1        | Total<br>37 | C<br>31 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 14  | U     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 14  | U     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | W     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | W     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | W     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14  | g     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | g     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | h     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14  | n     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | n     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 47    | 37 | 1  | 4 | 5 |         |
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |
| 14  | n     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 14  | s     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 14  | s     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | t     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14  | t     | 1        | Total<br>37 | C<br>31 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 14  | u     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 14  | u     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | w     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | w     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | w     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | A     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 14  | X     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 50    | 40 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 55    | 45 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 58    | 48 | 1  | 4 | 5 |         |
| 14  | B     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | B     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | F     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | F     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | J     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | J     | 1        | Total<br>37 | C<br>31 | Mg<br>1 | N<br>4 | O<br>1 | 0       |
| 14  | K     | 1        | Total<br>41 | C<br>33 | Mg<br>1 | N<br>4 | O<br>3 | 0       |
| 14  | L     | 1        | Total<br>51 | C<br>41 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | L     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | L     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | a     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | a     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | a     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 59    | 49 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 54    | 44 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 51    | 41 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 14  | x     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 49    | 39 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 14  | b     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

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| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>50 | C<br>40 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>49 | C<br>39 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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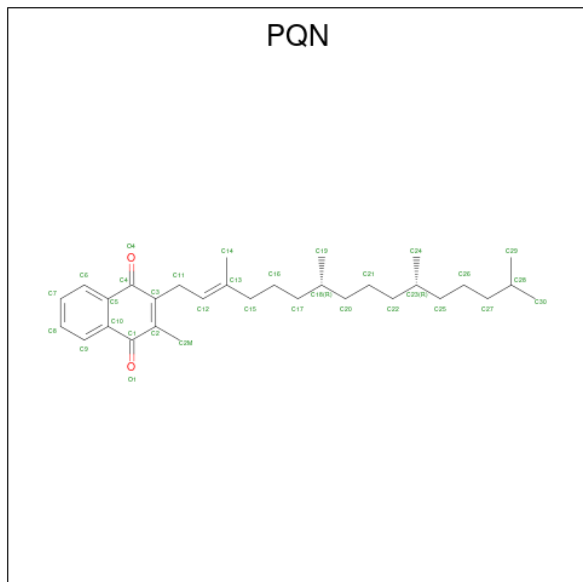
| Mol | Chain | Residues | Atoms       |         |         |        |        | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>54 | C<br>44 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>60 | C<br>50 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>47 | C<br>37 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>65 | C<br>55 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>58 | C<br>48 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | b     | 1        | Total<br>55 | C<br>45 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | f     | 1        | Total<br>59 | C<br>49 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | f     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |
| 14  | j     | 1        | Total<br>45 | C<br>35 | Mg<br>1 | N<br>4 | O<br>5 | 0       |

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| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 14  | j     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 37    | 31 | 1  | 4 | 1 |         |
| 14  | k     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 41    | 33 | 1  | 4 | 3 |         |
| 14  | l     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 14  | l     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 60    | 50 | 1  | 4 | 5 |         |
| 14  | l     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 15  | G     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 15  | N     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 15  | g     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 15  | n     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 15  | A     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 15  | B     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |

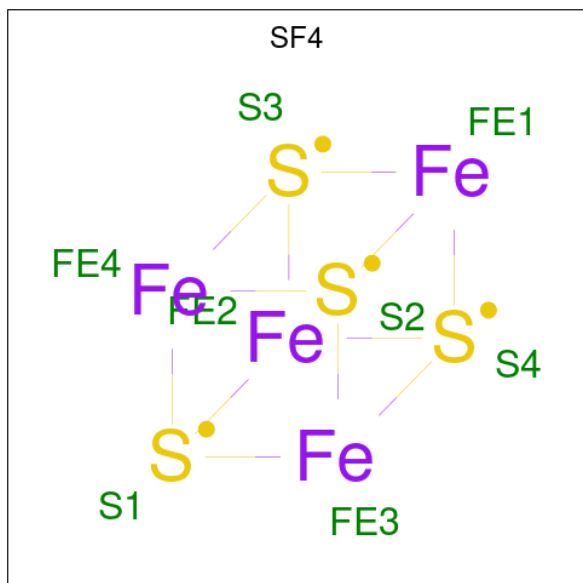
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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 15  | a     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |
| 15  | b     | 1        | Total | C  | O | 0       |
|     |       |          | 33    | 31 | 2 |         |

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



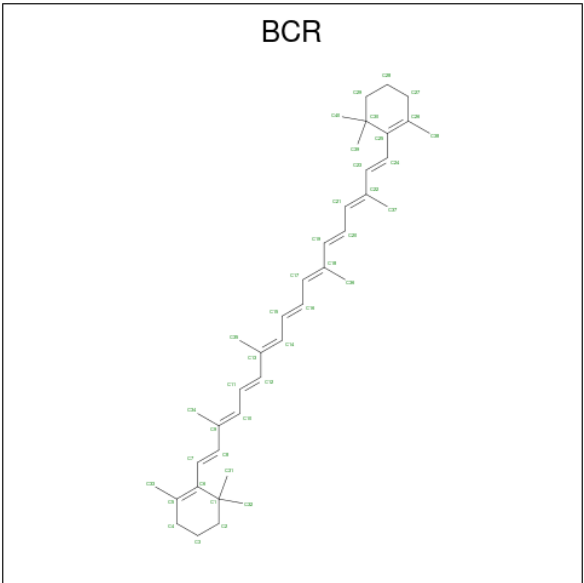
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 16  | G     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | P     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | P     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | g     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | p     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | p     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | A     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | C     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

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| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 16  | a     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | c     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |
| 16  | c     | 1        | Total | Fe | S | 0       |
|     |       |          | 8     | 4  | 4 |         |

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 17  | G     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | G     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | G     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | G     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | G     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | G     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | N     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |
| 17  | N     | 1        | Total | C  | 0       |
|     |       |          | 40    | 40 |         |

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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 17  | N     | 1        | Total C<br>40 40 | 0       |
| 17  | N     | 1        | Total C<br>40 40 | 0       |
| 17  | N     | 1        | Total C<br>40 40 | 0       |
| 17  | N     | 1        | Total C<br>40 40 | 0       |
| 17  | N     | 1        | Total C<br>40 40 | 0       |
| 17  | N     | 1        | Total C<br>40 40 | 0       |
| 17  | S     | 1        | Total C<br>40 40 | 0       |
| 17  | T     | 1        | Total C<br>40 40 | 0       |
| 17  | T     | 1        | Total C<br>40 40 | 0       |
| 17  | U     | 1        | Total C<br>40 40 | 0       |
| 17  | V     | 1        | Total C<br>40 40 | 0       |
| 17  | W     | 1        | Total C<br>40 40 | 0       |
| 17  | W     | 1        | Total C<br>40 40 | 0       |
| 17  | W     | 1        | Total C<br>40 40 | 0       |
| 17  | Y     | 1        | Total C<br>40 40 | 0       |
| 17  | g     | 1        | Total C<br>40 40 | 0       |
| 17  | g     | 1        | Total C<br>40 40 | 0       |
| 17  | g     | 1        | Total C<br>40 40 | 0       |
| 17  | g     | 1        | Total C<br>40 40 | 0       |
| 17  | g     | 1        | Total C<br>40 40 | 0       |
| 17  | g     | 1        | Total C<br>40 40 | 0       |

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| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 17  | n     | 1        | Total C<br>40 40 | 0       |
| 17  | n     | 1        | Total C<br>40 40 | 0       |
| 17  | n     | 1        | Total C<br>40 40 | 0       |
| 17  | n     | 1        | Total C<br>40 40 | 0       |
| 17  | n     | 1        | Total C<br>40 40 | 0       |
| 17  | n     | 1        | Total C<br>40 40 | 0       |
| 17  | n     | 1        | Total C<br>40 40 | 0       |
| 17  | n     | 1        | Total C<br>40 40 | 0       |
| 17  | s     | 1        | Total C<br>40 40 | 0       |
| 17  | t     | 1        | Total C<br>40 40 | 0       |
| 17  | t     | 1        | Total C<br>40 40 | 0       |
| 17  | u     | 1        | Total C<br>40 40 | 0       |
| 17  | v     | 1        | Total C<br>40 40 | 0       |
| 17  | w     | 1        | Total C<br>40 40 | 0       |
| 17  | w     | 1        | Total C<br>40 40 | 0       |
| 17  | w     | 1        | Total C<br>40 40 | 0       |
| 17  | y     | 1        | Total C<br>40 40 | 0       |
| 17  | A     | 1        | Total C<br>40 40 | 0       |
| 17  | A     | 1        | Total C<br>40 40 | 0       |
| 17  | A     | 1        | Total C<br>40 40 | 0       |
| 17  | A     | 1        | Total C<br>40 40 | 0       |

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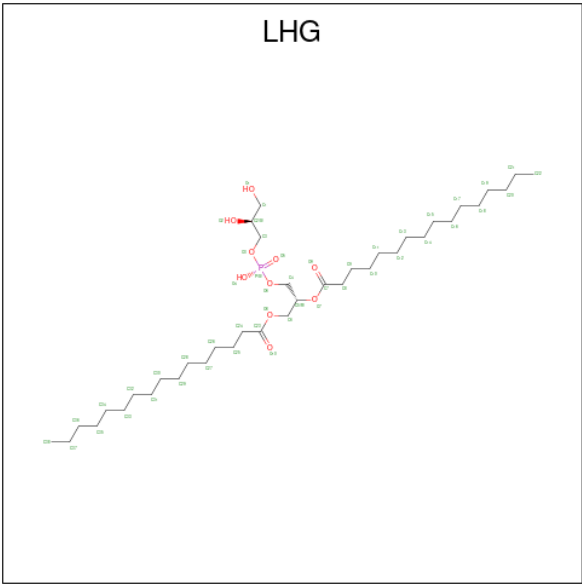
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 17  | A     | 1        | Total C<br>40 40 | 0       |
| 17  | A     | 1        | Total C<br>40 40 | 0       |
| 17  | A     | 1        | Total C<br>40 40 | 0       |
| 17  | B     | 1        | Total C<br>40 40 | 0       |
| 17  | B     | 1        | Total C<br>40 40 | 0       |
| 17  | B     | 1        | Total C<br>40 40 | 0       |
| 17  | B     | 1        | Total C<br>40 40 | 0       |
| 17  | B     | 1        | Total C<br>40 40 | 0       |
| 17  | B     | 1        | Total C<br>40 40 | 0       |
| 17  | B     | 1        | Total C<br>40 40 | 0       |
| 17  | B     | 1        | Total C<br>40 40 | 0       |
| 17  | B     | 1        | Total C<br>40 40 | 0       |
| 17  | F     | 1        | Total C<br>40 40 | 0       |
| 17  | J     | 1        | Total C<br>40 40 | 0       |
| 17  | K     | 1        | Total C<br>40 40 | 0       |
| 17  | I     | 1        | Total C<br>40 40 | 0       |
| 17  | I     | 1        | Total C<br>40 40 | 0       |
| 17  | I     | 1        | Total C<br>40 40 | 0       |
| 17  | L     | 1        | Total C<br>40 40 | 0       |
| 17  | M     | 1        | Total C<br>40 40 | 0       |
| 17  | a     | 1        | Total C<br>40 40 | 0       |
| 17  | a     | 1        | Total C<br>40 40 | 0       |

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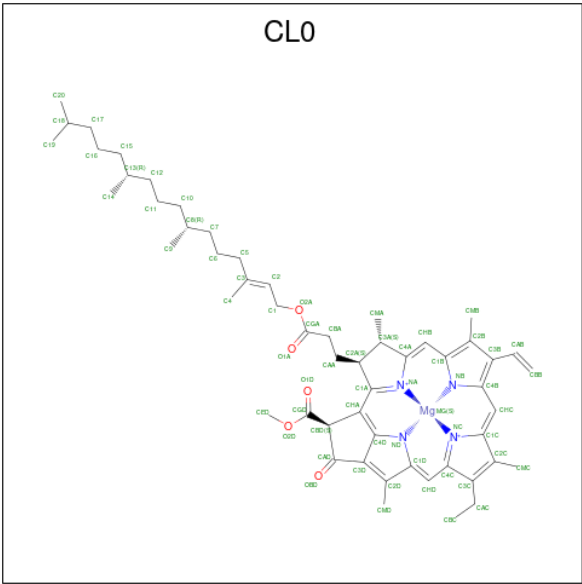
| Mol | Chain | Residues | Atoms            | AltConf |
|-----|-------|----------|------------------|---------|
| 17  | a     | 1        | Total C<br>40 40 | 0       |
| 17  | a     | 1        | Total C<br>40 40 | 0       |
| 17  | a     | 1        | Total C<br>40 40 | 0       |
| 17  | a     | 1        | Total C<br>40 40 | 0       |
| 17  | b     | 1        | Total C<br>40 40 | 0       |
| 17  | b     | 1        | Total C<br>40 40 | 0       |
| 17  | b     | 1        | Total C<br>40 40 | 0       |
| 17  | b     | 1        | Total C<br>40 40 | 0       |
| 17  | b     | 1        | Total C<br>40 40 | 0       |
| 17  | b     | 1        | Total C<br>40 40 | 0       |
| 17  | b     | 1        | Total C<br>40 40 | 0       |
| 17  | b     | 1        | Total C<br>40 40 | 0       |
| 17  | b     | 1        | Total C<br>40 40 | 0       |
| 17  | f     | 1        | Total C<br>40 40 | 0       |
| 17  | j     | 1        | Total C<br>40 40 | 0       |
| 17  | j     | 1        | Total C<br>40 40 | 0       |
| 17  | k     | 1        | Total C<br>40 40 | 0       |
| 17  | i     | 1        | Total C<br>40 40 | 0       |
| 17  | i     | 1        | Total C<br>40 40 | 0       |
| 17  | l     | 1        | Total C<br>40 40 | 0       |
| 17  | l     | 1        | Total C<br>40 40 | 0       |
| 17  | m     | 1        | Total C<br>40 40 | 0       |

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 18  | G     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 18  | G     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 18  | S     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |
| 18  | g     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 18  | g     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 18  | v     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |
| 18  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 18  | A     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 18  | X     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |
| 18  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 18  | a     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 49    | 38 | 10 | 1 |         |
| 18  | m     | 1        | Total | C  | O  | P | 0       |
|     |       |          | 43    | 32 | 10 | 1 |         |

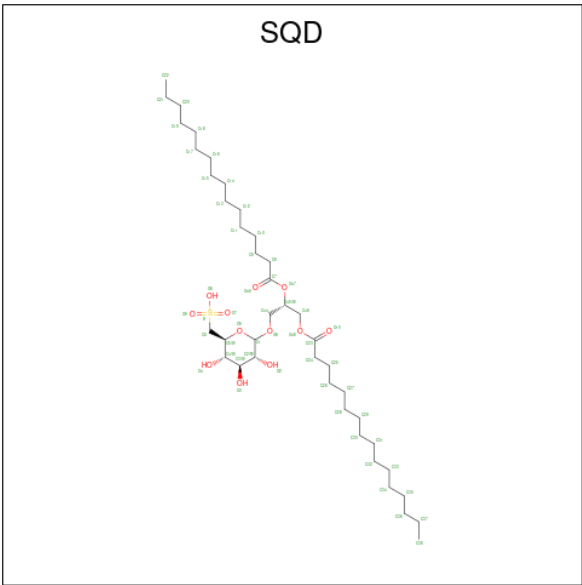
- Molecule 19 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |    |   |   | AltConf |
|-----|-------|----------|-------|----|----|---|---|---------|
| 19  | G     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | g     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |
| 19  | A     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 45    | 35 | 1  | 4 | 5 |         |
| 19  | a     | 1        | Total | C  | Mg | N | O | 0       |
|     |       |          | 65    | 55 | 1  | 4 | 5 |         |

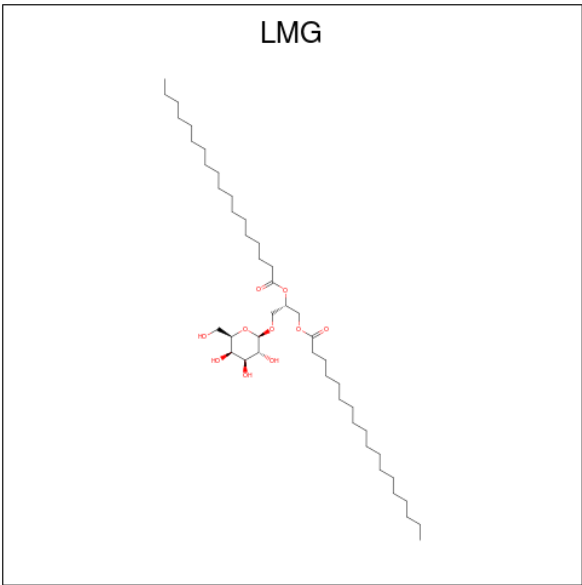
- Molecule 20 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ) (labeled as "Ligand of Interest" by depositor).





| Mol | Chain | Residues | Atoms |    |    |   | AltConf |
|-----|-------|----------|-------|----|----|---|---------|
| 20  | H     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 20  | h     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 20  | n     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 20  | w     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 20  | B     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 20  | x     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 20  | b     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |
| 20  | l     | 1        | Total | C  | O  | S | 0       |
|     |       |          | 54    | 41 | 12 | 1 |         |

- Molecule 21 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).

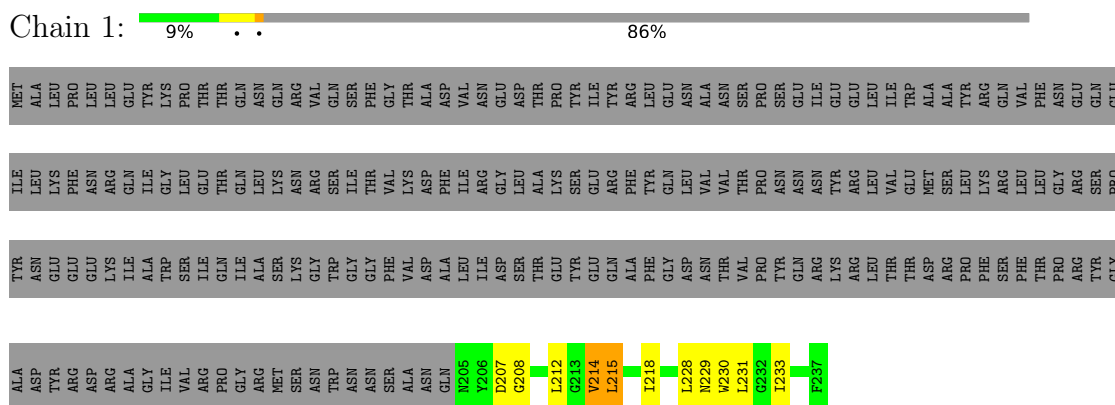


| Mol | Chain | Residues | Atoms |    |    | AltConf |
|-----|-------|----------|-------|----|----|---------|
| 21  | N     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 25 | 10 |         |
| 21  | N     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |
| 21  | n     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |
| 21  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 35    | 25 | 10 |         |
| 21  | B     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |
| 21  | b     | 1        | Total | C  | O  | 0       |
|     |       |          | 55    | 45 | 10 |         |

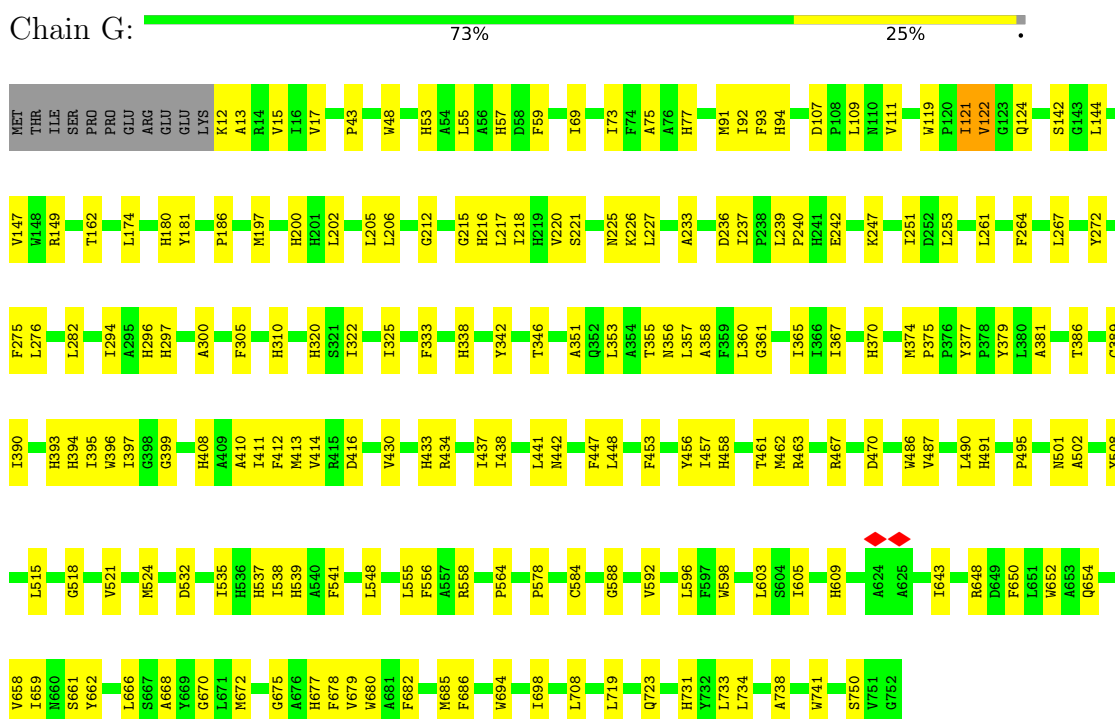
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

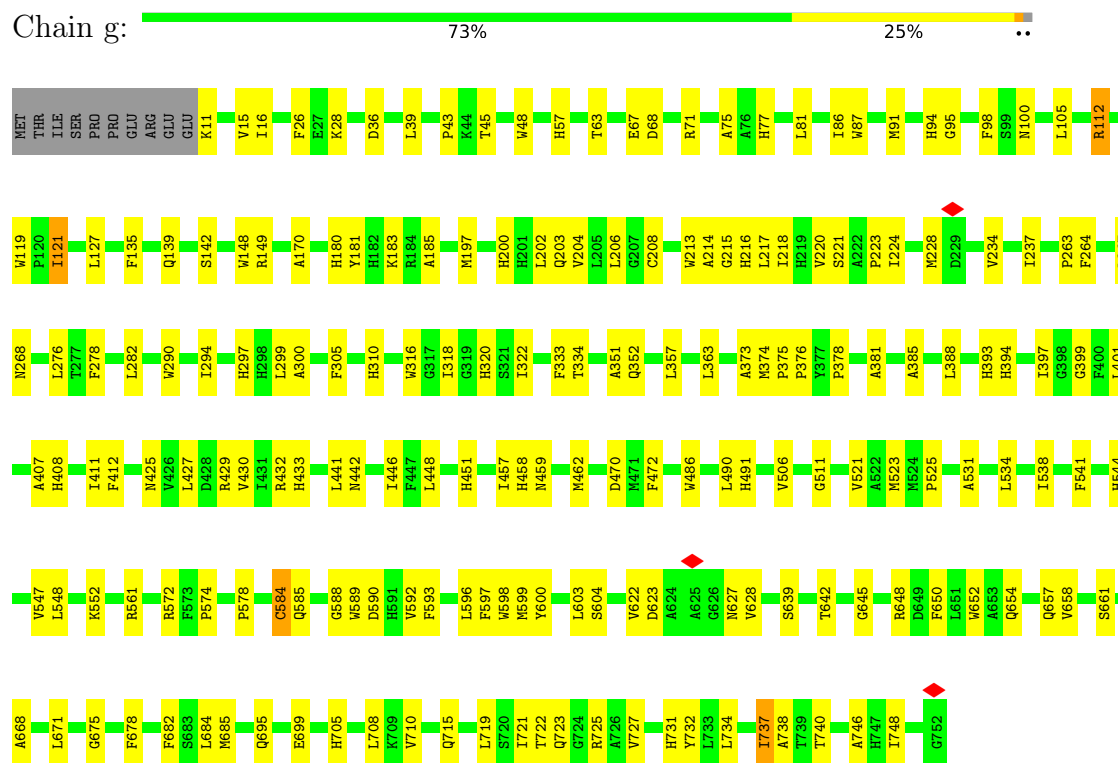
#### • Molecule 1: Photosystem I-associated linker protein CpcL



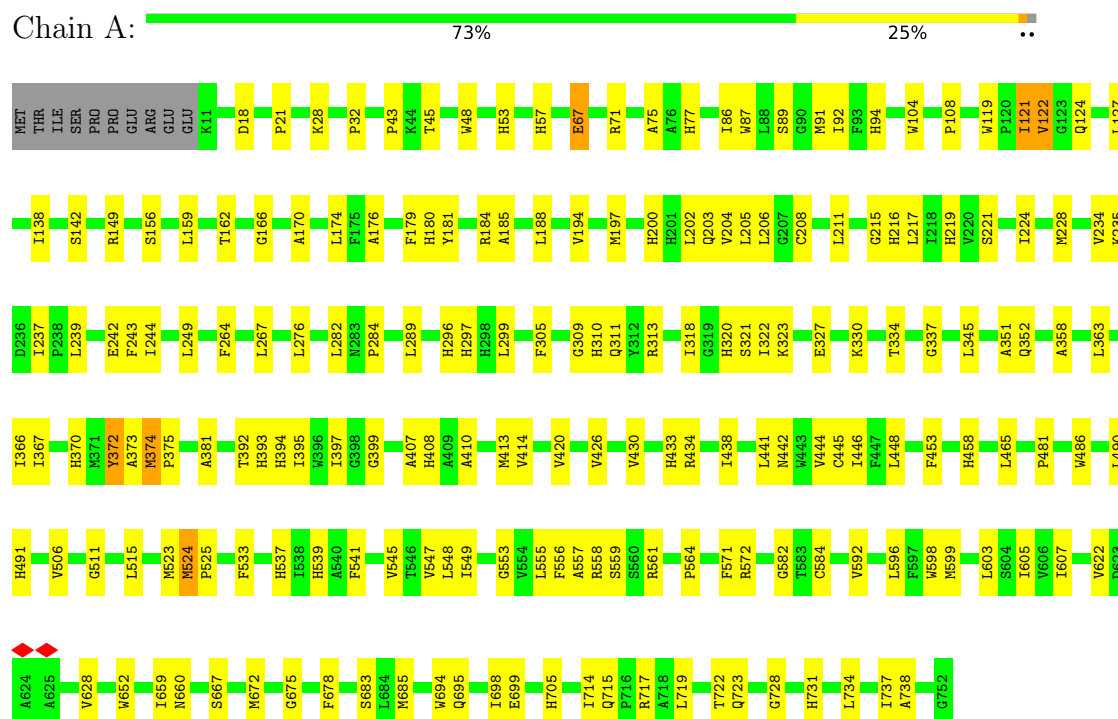
#### • Molecule 2: Photosystem I P700 chlorophyll a apoprotein A1



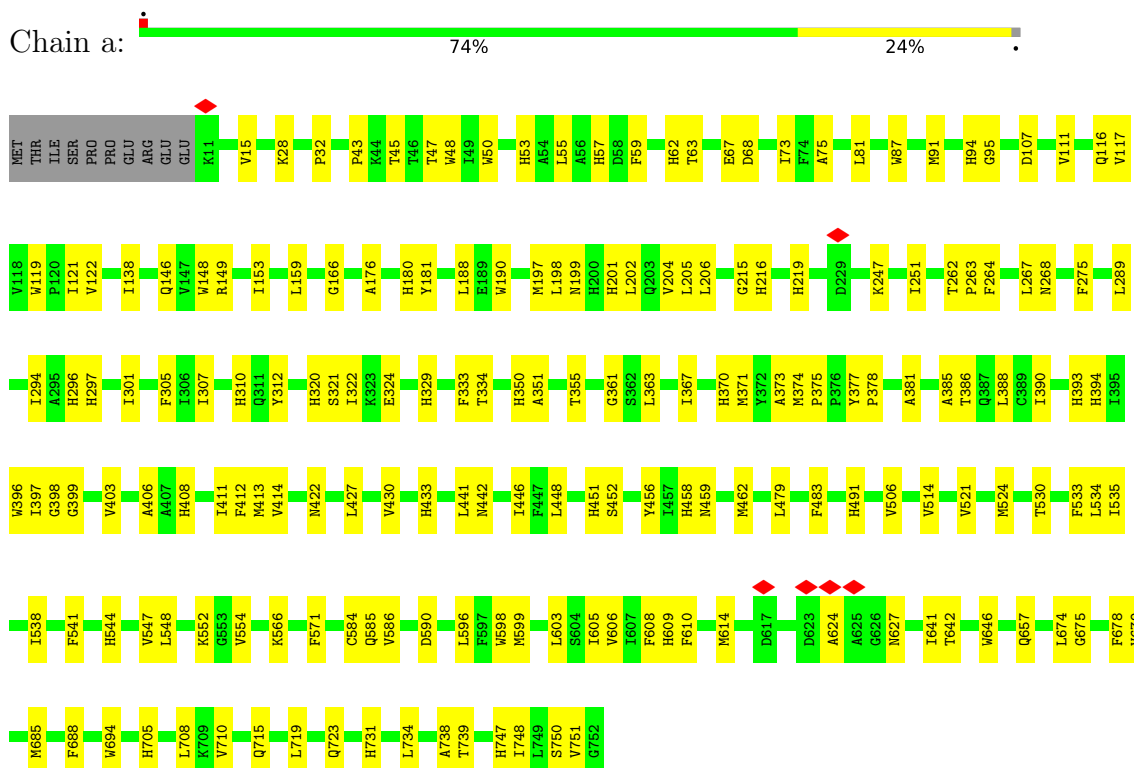
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A1



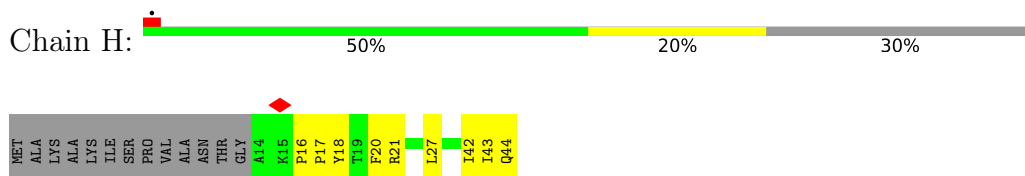
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A1



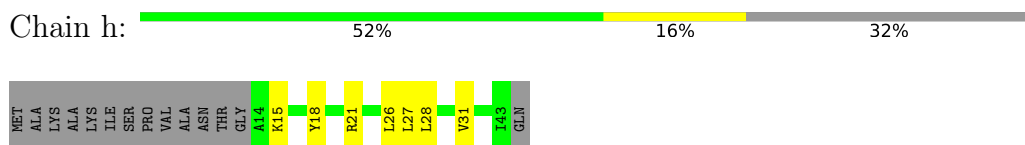
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A1



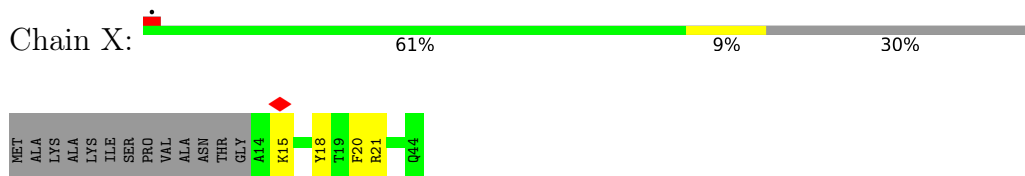
• Molecule 3: Photosystem I 4.8 kDa protein



• Molecule 3: Photosystem I 4.8 kDa protein




• Molecule 3: Photosystem I 4.8 kDa protein

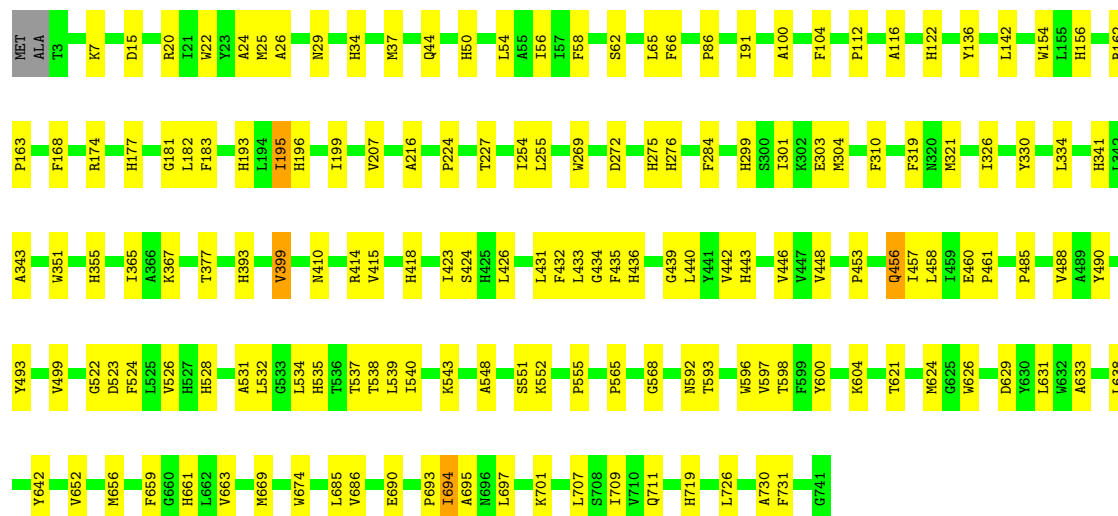


• Molecule 3: Photosystem I 4.8 kDa protein



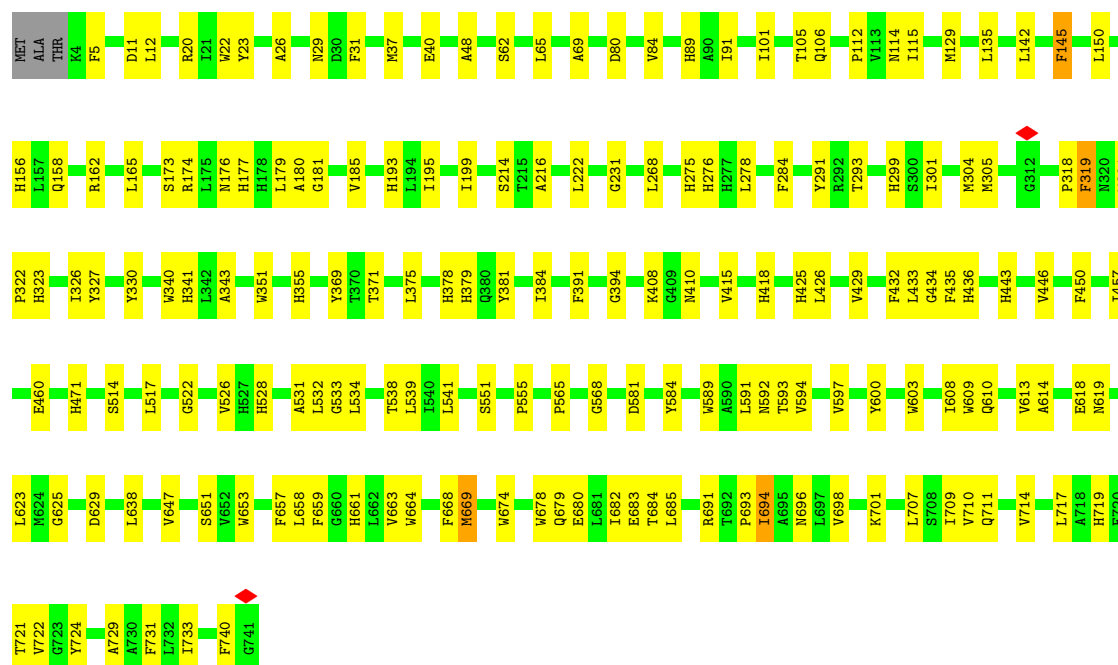
- Molecule 4: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain N:  78% 21%



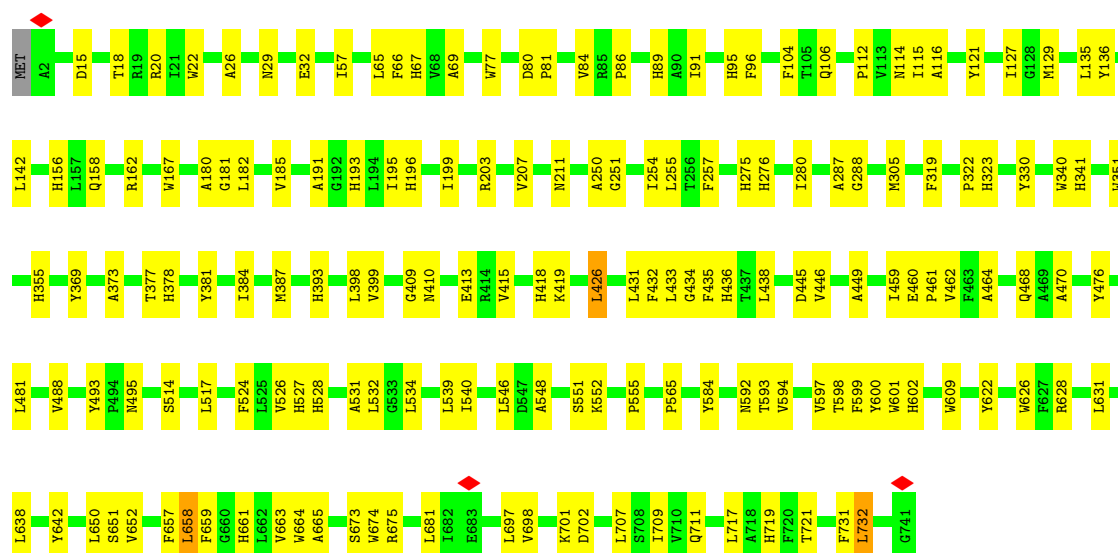
- Molecule 4: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain n:  76% 23%



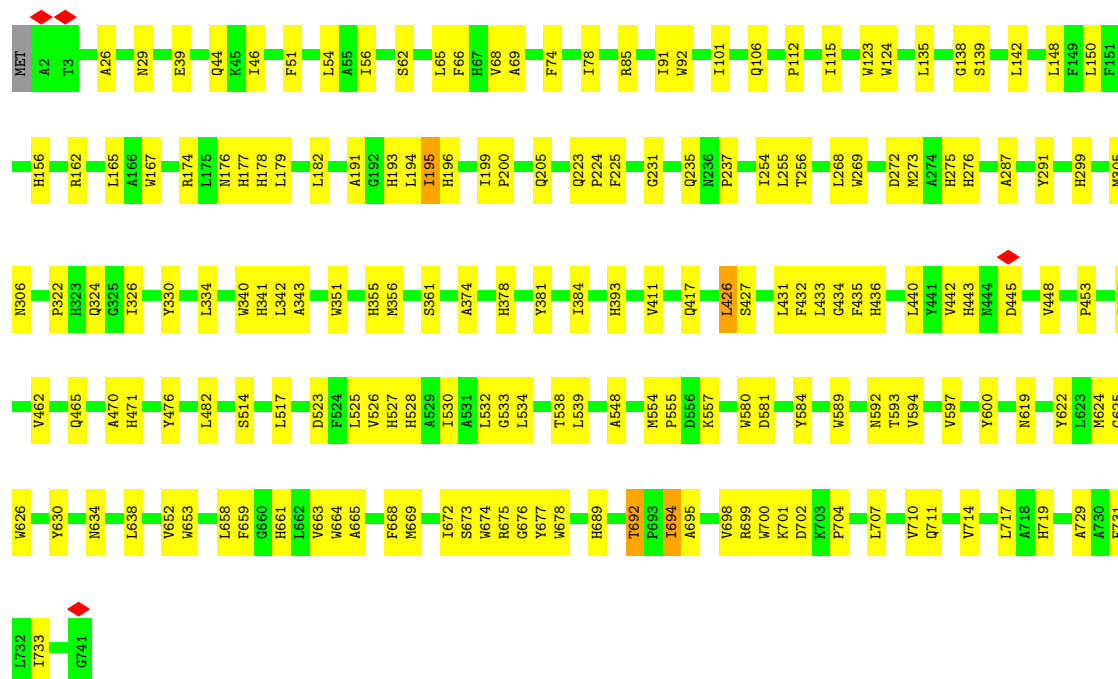
- Molecule 4: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain B:  77% 22%



• Molecule 4: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain b: 76% 24%




• Molecule 5: Photosystem I iron-sulfur center

Chain P: 85% 14%



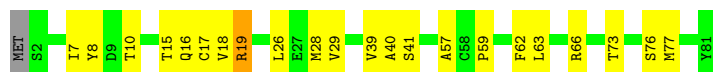
• Molecule 5: Photosystem I iron-sulfur center

Chain p:  78% 21% .




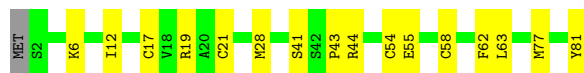
- Molecule 5: Photosystem I iron-sulfur center

Chain C:  72% 26% ..




- Molecule 5: Photosystem I iron-sulfur center

Chain c:  79% 20% .




- Molecule 6: Photosystem I reaction center subunit II

Chain Q:  81% 17% .




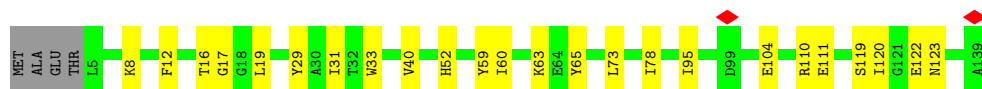
- Molecule 6: Photosystem I reaction center subunit II

Chain q:  90% 8% .




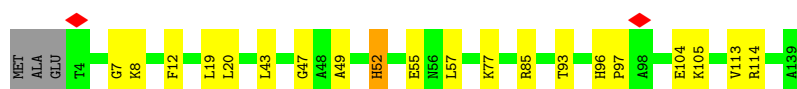
- Molecule 6: Photosystem I reaction center subunit II

Chain D:  80% 17% .



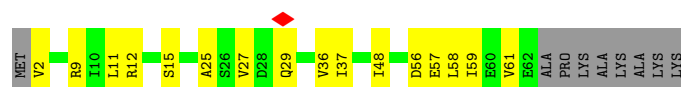
- Molecule 6: Photosystem I reaction center subunit II

Chain d:  83% 14% ..



- Molecule 7: Photosystem I reaction center subunit IV





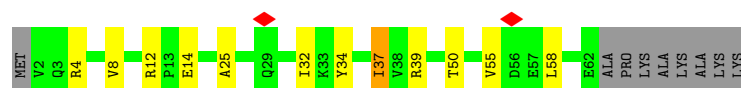
- Molecule 7: Photosystem I reaction center subunit IV



- Molecule 7: Photosystem I reaction center subunit IV



- Molecule 7: Photosystem I reaction center subunit IV



- Molecule 8: Photosystem I reaction center subunit III

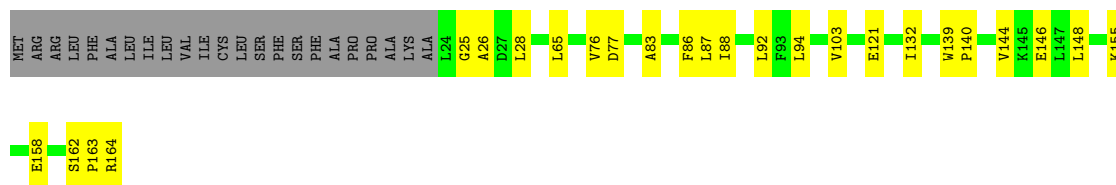


- Molecule 8: Photosystem I reaction center subunit III



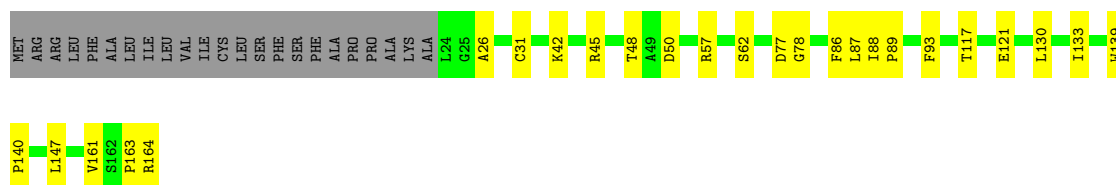
- Molecule 8: Photosystem I reaction center subunit III

Chain F:  71% 15% 14%



- Molecule 8: Photosystem I reaction center subunit III

Chain f:  71% 15% 14%



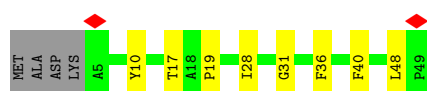
- Molecule 9: Photosystem I reaction center subunit IX

Chain T:  65% 24% 10%



- Molecule 9: Photosystem I reaction center subunit IX

Chain t:  76% 16% 8%



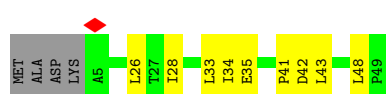
- Molecule 9: Photosystem I reaction center subunit IX

Chain J:  73% 18% 8%

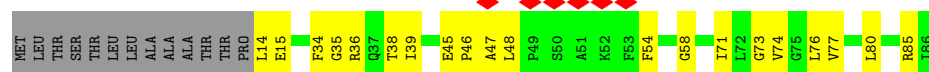


- Molecule 9: Photosystem I reaction center subunit IX

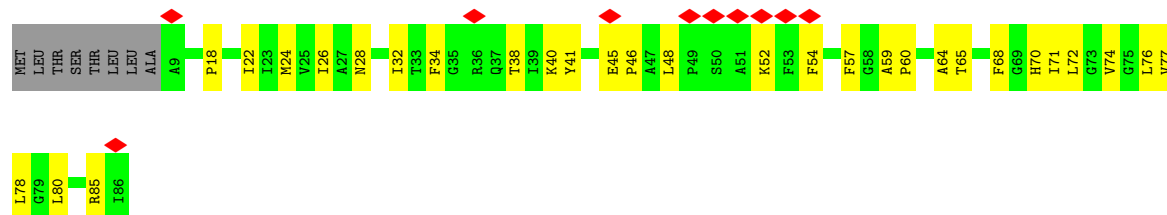
Chain j:  73% 18% 8%



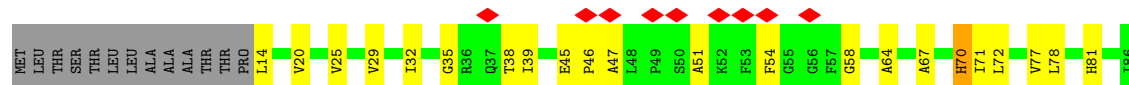
- Molecule 10: Photosystem I reaction center subunit PsaK 1



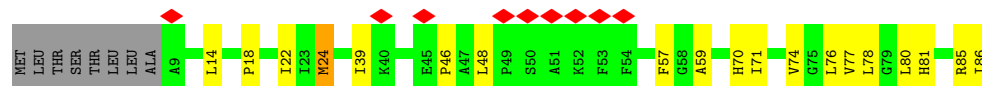
• Molecule 10: Photosystem I reaction center subunit PsaK 1



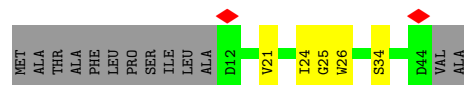
• Molecule 10: Photosystem I reaction center subunit PsaK 1



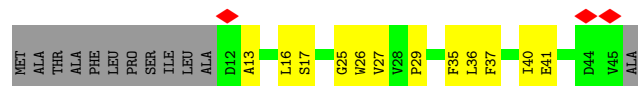
• Molecule 10: Photosystem I reaction center subunit PsaK 1



• Molecule 11: Photosystem I reaction center subunit VIII

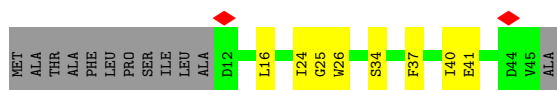


• Molecule 11: Photosystem I reaction center subunit VIII

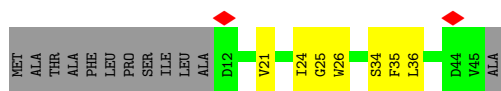


• Molecule 11: Photosystem I reaction center subunit VIII





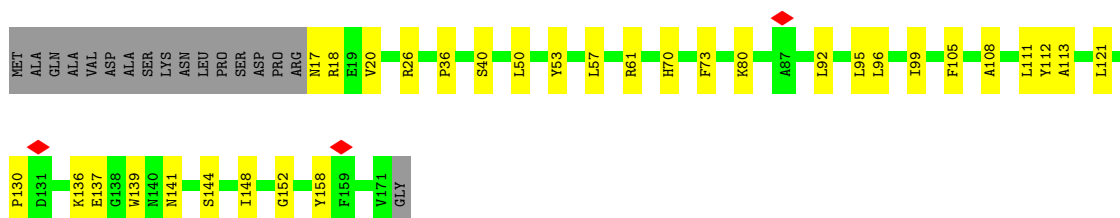
- Molecule 11: Photosystem I reaction center subunit VIII



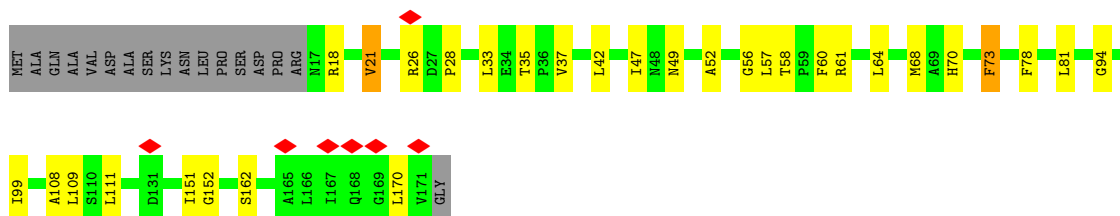
- Molecule 12: Photosystem I reaction center subunit XI



- Molecule 12: Photosystem I reaction center subunit XI

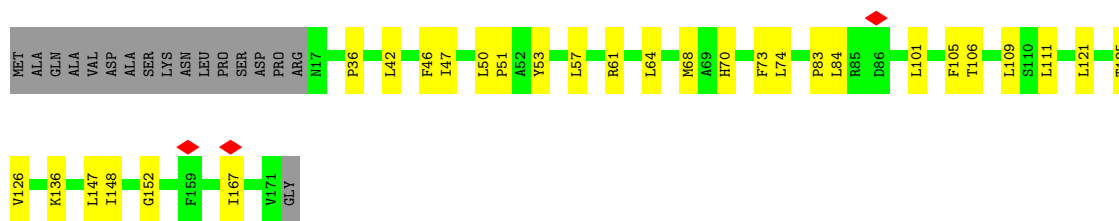


- Molecule 12: Photosystem I reaction center subunit XI

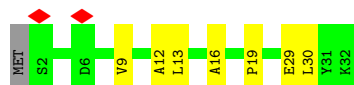
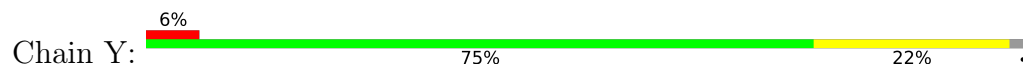


- Molecule 12: Photosystem I reaction center subunit XI

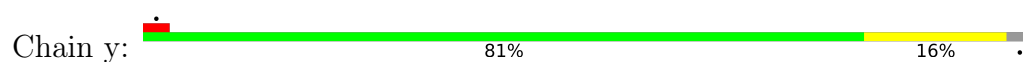




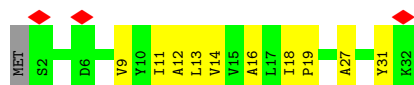
- Molecule 13: Photosystem I reaction center subunit XII



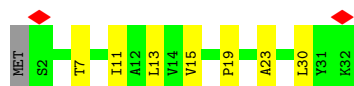
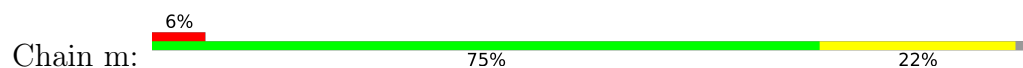
- Molecule 13: Photosystem I reaction center subunit XII



- Molecule 13: Photosystem I reaction center subunit XII



- Molecule 13: Photosystem I reaction center subunit XII



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 120345                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 60                                      | Depositor |
| Minimum defocus (nm)                 | 1000                                    | Depositor |
| Maximum defocus (nm)                 | 2000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 BIOCONTINUUM (6k x 4k)         | Depositor |
| Maximum map value                    | 1.126                                   | Depositor |
| Minimum map value                    | -0.389                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.022                                   | Depositor |
| Recommended contour level            | 0.185                                   | Depositor |
| Map size (Å)                         | 686.39996, 686.39996, 686.39996         | wwPDB     |
| Map dimensions                       | 660, 660, 660                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.04, 1.04, 1.04                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, SF4, BCR, CL0, LHG, CLA, PQN, LMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 1   | 1     | 0.14         | 0/252   | 0.43        | 0/341   |
| 2   | A     | 0.13         | 0/6022  | 0.28        | 0/8214  |
| 2   | G     | 0.15         | 0/6013  | 0.31        | 0/8203  |
| 2   | a     | 0.13         | 0/6022  | 0.29        | 0/8214  |
| 2   | g     | 0.13         | 0/6022  | 0.29        | 0/8214  |
| 3   | H     | 0.14         | 0/267   | 0.36        | 0/366   |
| 3   | X     | 0.16         | 0/267   | 0.39        | 0/366   |
| 3   | h     | 0.14         | 0/258   | 0.31        | 0/354   |
| 3   | x     | 0.13         | 0/267   | 0.32        | 0/366   |
| 4   | B     | 0.14         | 0/6142  | 0.31        | 0/8396  |
| 4   | N     | 0.13         | 0/6137  | 0.29        | 0/8389  |
| 4   | b     | 0.12         | 0/6142  | 0.28        | 0/8396  |
| 4   | n     | 0.13         | 0/6130  | 0.28        | 0/8379  |
| 5   | C     | 0.14         | 0/608   | 0.32        | 0/825   |
| 5   | P     | 0.14         | 0/608   | 0.31        | 0/825   |
| 5   | c     | 0.14         | 0/608   | 0.39        | 0/825   |
| 5   | p     | 0.13         | 0/608   | 0.28        | 0/825   |
| 6   | D     | 0.10         | 0/1064  | 0.26        | 0/1436  |
| 6   | Q     | 0.15         | 0/1064  | 0.31        | 0/1436  |
| 6   | d     | 0.12         | 0/1071  | 0.38        | 0/1446  |
| 6   | q     | 0.10         | 0/1071  | 0.26        | 0/1446  |
| 7   | E     | 0.20         | 0/499   | 0.35        | 0/677   |
| 7   | R     | 0.12         | 0/499   | 0.28        | 0/677   |
| 7   | e     | 0.12         | 0/499   | 0.28        | 0/677   |
| 7   | r     | 0.11         | 0/490   | 0.30        | 0/665   |
| 8   | F     | 0.14         | 0/1104  | 0.31        | 0/1500  |
| 8   | S     | 0.12         | 0/1104  | 0.29        | 0/1500  |
| 8   | f     | 0.12         | 0/1104  | 0.33        | 0/1500  |
| 8   | s     | 0.12         | 0/1104  | 0.30        | 0/1500  |
| 9   | J     | 0.10         | 0/371   | 0.23        | 0/509   |
| 9   | T     | 0.12         | 0/366   | 0.27        | 0/502   |
| 9   | j     | 0.13         | 0/371   | 0.28        | 0/509   |

| Mol | Chain | Bond lengths |         | Bond angles |          |
|-----|-------|--------------|---------|-------------|----------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5  |
| 9   | t     | 0.12         | 0/371   | 0.26        | 0/509    |
| 10  | K     | 0.14         | 0/551   | 0.40        | 0/750    |
| 10  | U     | 0.18         | 0/551   | 0.46        | 0/750    |
| 10  | k     | 0.15         | 0/583   | 0.41        | 0/796    |
| 10  | u     | 0.23         | 0/583   | 0.54        | 0/796    |
| 11  | I     | 0.14         | 0/284   | 0.31        | 0/388    |
| 11  | V     | 0.16         | 0/277   | 0.37        | 0/378    |
| 11  | i     | 0.15         | 0/284   | 0.28        | 0/388    |
| 11  | v     | 0.14         | 0/284   | 0.29        | 0/388    |
| 12  | L     | 0.13         | 0/1198  | 0.30        | 0/1642   |
| 12  | W     | 0.12         | 0/1198  | 0.27        | 0/1642   |
| 12  | l     | 0.11         | 0/1198  | 0.26        | 0/1642   |
| 12  | w     | 0.14         | 0/1198  | 0.32        | 0/1642   |
| 13  | M     | 0.10         | 0/245   | 0.23        | 0/334    |
| 13  | Y     | 0.13         | 0/245   | 0.27        | 0/334    |
| 13  | m     | 0.12         | 0/245   | 0.24        | 0/334    |
| 13  | y     | 0.13         | 0/245   | 0.23        | 0/334    |
| All | All   | 0.13         | 0/73694 | 0.30        | 0/100525 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 1     | 247   | 0        | 250      | 11      | 0            |
| 2   | A     | 5823  | 0        | 5696     | 188     | 0            |
| 2   | G     | 5814  | 0        | 5684     | 176     | 0            |
| 2   | a     | 5823  | 0        | 5696     | 180     | 0            |
| 2   | g     | 5823  | 0        | 5697     | 180     | 0            |
| 3   | H     | 257   | 0        | 261      | 11      | 0            |
| 3   | X     | 257   | 0        | 261      | 5       | 0            |
| 3   | h     | 248   | 0        | 253      | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | x     | 257   | 0        | 261      | 6       | 0            |
| 4   | B     | 5918  | 0        | 5671     | 159     | 0            |
| 4   | N     | 5913  | 0        | 5666     | 157     | 0            |
| 4   | b     | 5918  | 0        | 5671     | 171     | 0            |
| 4   | n     | 5906  | 0        | 5659     | 165     | 0            |
| 5   | C     | 598   | 0        | 574      | 16      | 0            |
| 5   | P     | 598   | 0        | 574      | 9       | 0            |
| 5   | c     | 598   | 0        | 574      | 12      | 0            |
| 5   | p     | 598   | 0        | 574      | 13      | 0            |
| 6   | D     | 1040  | 0        | 1043     | 18      | 0            |
| 6   | Q     | 1040  | 0        | 1043     | 15      | 0            |
| 6   | d     | 1047  | 0        | 1050     | 13      | 0            |
| 6   | q     | 1047  | 0        | 1050     | 9       | 0            |
| 7   | E     | 490   | 0        | 484      | 8       | 0            |
| 7   | R     | 490   | 0        | 484      | 8       | 0            |
| 7   | e     | 490   | 0        | 484      | 9       | 0            |
| 7   | r     | 481   | 0        | 478      | 13      | 0            |
| 8   | F     | 1080  | 0        | 1078     | 20      | 0            |
| 8   | S     | 1080  | 0        | 1078     | 16      | 0            |
| 8   | f     | 1080  | 0        | 1078     | 20      | 0            |
| 8   | s     | 1080  | 0        | 1078     | 20      | 0            |
| 9   | J     | 359   | 0        | 364      | 11      | 0            |
| 9   | T     | 354   | 0        | 359      | 9       | 0            |
| 9   | j     | 359   | 0        | 364      | 10      | 0            |
| 9   | t     | 359   | 0        | 364      | 6       | 0            |
| 10  | K     | 537   | 0        | 562      | 19      | 0            |
| 10  | U     | 537   | 0        | 562      | 15      | 0            |
| 10  | k     | 568   | 0        | 593      | 15      | 0            |
| 10  | u     | 568   | 0        | 593      | 23      | 0            |
| 11  | I     | 275   | 0        | 268      | 6       | 0            |
| 11  | V     | 268   | 0        | 259      | 4       | 0            |
| 11  | i     | 275   | 0        | 268      | 9       | 0            |
| 11  | v     | 275   | 0        | 268      | 13      | 0            |
| 12  | L     | 1163  | 0        | 1166     | 29      | 0            |
| 12  | W     | 1163  | 0        | 1166     | 28      | 0            |
| 12  | l     | 1163  | 0        | 1166     | 23      | 0            |
| 12  | w     | 1163  | 0        | 1166     | 32      | 0            |
| 13  | M     | 241   | 0        | 256      | 8       | 0            |
| 13  | Y     | 241   | 0        | 256      | 7       | 0            |
| 13  | m     | 241   | 0        | 256      | 7       | 0            |
| 13  | y     | 241   | 0        | 256      | 4       | 0            |
| 14  | A     | 2631  | 0        | 2625     | 202     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14  | B     | 2345  | 0        | 2344     | 156     | 0            |
| 14  | F     | 104   | 0        | 91       | 1       | 0            |
| 14  | G     | 2451  | 0        | 2445     | 197     | 0            |
| 14  | H     | 49    | 0        | 39       | 3       | 0            |
| 14  | J     | 82    | 0        | 58       | 3       | 0            |
| 14  | K     | 41    | 0        | 29       | 2       | 0            |
| 14  | L     | 156   | 0        | 133      | 8       | 0            |
| 14  | N     | 2495  | 0        | 2526     | 179     | 0            |
| 14  | S     | 104   | 0        | 91       | 3       | 0            |
| 14  | T     | 82    | 0        | 58       | 2       | 0            |
| 14  | U     | 90    | 0        | 68       | 1       | 0            |
| 14  | W     | 156   | 0        | 133      | 17      | 0            |
| 14  | X     | 49    | 0        | 39       | 3       | 0            |
| 14  | a     | 2501  | 0        | 2483     | 190     | 0            |
| 14  | b     | 2495  | 0        | 2528     | 181     | 0            |
| 14  | f     | 104   | 0        | 91       | 7       | 0            |
| 14  | g     | 2542  | 0        | 2562     | 182     | 0            |
| 14  | h     | 49    | 0        | 39       | 4       | 0            |
| 14  | j     | 82    | 0        | 58       | 6       | 0            |
| 14  | k     | 41    | 0        | 29       | 0       | 0            |
| 14  | l     | 150   | 0        | 125      | 11      | 0            |
| 14  | n     | 2430  | 0        | 2450     | 177     | 0            |
| 14  | s     | 104   | 0        | 91       | 3       | 0            |
| 14  | t     | 82    | 0        | 58       | 2       | 0            |
| 14  | u     | 90    | 0        | 68       | 0       | 0            |
| 14  | w     | 150   | 0        | 125      | 11      | 0            |
| 14  | x     | 49    | 0        | 39       | 2       | 0            |
| 15  | A     | 33    | 0        | 46       | 5       | 0            |
| 15  | B     | 33    | 0        | 46       | 5       | 0            |
| 15  | G     | 33    | 0        | 46       | 10      | 0            |
| 15  | N     | 33    | 0        | 46       | 6       | 0            |
| 15  | a     | 33    | 0        | 46       | 4       | 0            |
| 15  | b     | 33    | 0        | 46       | 4       | 0            |
| 15  | g     | 33    | 0        | 46       | 4       | 0            |
| 15  | n     | 33    | 0        | 46       | 4       | 0            |
| 16  | A     | 8     | 0        | 0        | 0       | 0            |
| 16  | C     | 16    | 0        | 0        | 1       | 0            |
| 16  | G     | 8     | 0        | 0        | 0       | 0            |
| 16  | P     | 16    | 0        | 0        | 1       | 0            |
| 16  | a     | 8     | 0        | 0        | 0       | 0            |
| 16  | c     | 16    | 0        | 0        | 1       | 0            |
| 16  | g     | 8     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16  | p     | 16    | 0        | 0        | 1       | 0            |
| 17  | A     | 280   | 0        | 392      | 45      | 0            |
| 17  | B     | 320   | 0        | 448      | 51      | 0            |
| 17  | F     | 40    | 0        | 56       | 1       | 0            |
| 17  | G     | 240   | 0        | 336      | 35      | 0            |
| 17  | I     | 120   | 0        | 168      | 21      | 0            |
| 17  | J     | 40    | 0        | 56       | 6       | 0            |
| 17  | K     | 40    | 0        | 56       | 3       | 0            |
| 17  | L     | 40    | 0        | 56       | 5       | 0            |
| 17  | M     | 40    | 0        | 56       | 4       | 0            |
| 17  | N     | 320   | 0        | 448      | 63      | 0            |
| 17  | S     | 40    | 0        | 56       | 4       | 0            |
| 17  | T     | 80    | 0        | 112      | 12      | 0            |
| 17  | U     | 40    | 0        | 56       | 2       | 0            |
| 17  | V     | 40    | 0        | 56       | 2       | 0            |
| 17  | W     | 120   | 0        | 168      | 18      | 0            |
| 17  | Y     | 40    | 0        | 56       | 4       | 0            |
| 17  | a     | 240   | 0        | 336      | 33      | 0            |
| 17  | b     | 320   | 0        | 448      | 49      | 0            |
| 17  | f     | 40    | 0        | 56       | 4       | 0            |
| 17  | g     | 240   | 0        | 336      | 35      | 0            |
| 17  | i     | 80    | 0        | 112      | 15      | 0            |
| 17  | j     | 80    | 0        | 112      | 8       | 0            |
| 17  | k     | 40    | 0        | 56       | 2       | 0            |
| 17  | l     | 80    | 0        | 112      | 9       | 0            |
| 17  | m     | 40    | 0        | 56       | 3       | 0            |
| 17  | n     | 320   | 0        | 448      | 52      | 0            |
| 17  | s     | 40    | 0        | 56       | 4       | 0            |
| 17  | t     | 80    | 0        | 112      | 14      | 0            |
| 17  | u     | 40    | 0        | 56       | 2       | 0            |
| 17  | v     | 40    | 0        | 56       | 7       | 0            |
| 17  | w     | 120   | 0        | 168      | 19      | 0            |
| 17  | y     | 40    | 0        | 56       | 2       | 0            |
| 18  | A     | 98    | 0        | 148      | 7       | 0            |
| 18  | G     | 98    | 0        | 148      | 10      | 0            |
| 18  | S     | 43    | 0        | 59       | 4       | 0            |
| 18  | X     | 43    | 0        | 59       | 2       | 0            |
| 18  | a     | 98    | 0        | 148      | 14      | 0            |
| 18  | g     | 98    | 0        | 148      | 8       | 0            |
| 18  | m     | 43    | 0        | 59       | 6       | 0            |
| 18  | v     | 43    | 0        | 59       | 3       | 0            |
| 19  | A     | 45    | 0        | 33       | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19  | G     | 65    | 0        | 72       | 7       | 0            |
| 19  | a     | 65    | 0        | 70       | 4       | 0            |
| 19  | g     | 65    | 0        | 72       | 7       | 0            |
| 20  | B     | 54    | 0        | 78       | 4       | 0            |
| 20  | H     | 54    | 0        | 78       | 3       | 0            |
| 20  | b     | 54    | 0        | 78       | 6       | 0            |
| 20  | h     | 54    | 0        | 78       | 7       | 0            |
| 20  | l     | 54    | 0        | 78       | 4       | 0            |
| 20  | n     | 54    | 0        | 78       | 0       | 0            |
| 20  | w     | 54    | 0        | 78       | 3       | 0            |
| 20  | x     | 54    | 0        | 78       | 4       | 0            |
| 21  | B     | 90    | 0        | 126      | 6       | 0            |
| 21  | N     | 90    | 0        | 126      | 8       | 0            |
| 21  | b     | 55    | 0        | 86       | 3       | 0            |
| 21  | n     | 55    | 0        | 86       | 3       | 0            |
| All | All   | 98661 | 0        | 99030    | 2867    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (2867) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:G:852:CLA:CED  | 17:N:852:BCR:H401 | 1.27                     | 1.58              |
| 14:G:852:CLA:CED  | 17:N:852:BCR:C40  | 2.02                     | 1.37              |
| 14:G:852:CLA:HED2 | 17:N:852:BCR:C40  | 1.54                     | 1.33              |
| 2:A:442:ASN:OD1   | 14:A:855:CLA:HED1 | 1.35                     | 1.25              |
| 2:A:541:PHE:CZ    | 14:A:855:CLA:O1A  | 1.79                     | 1.25              |
| 14:G:852:CLA:HED1 | 17:N:852:BCR:H291 | 1.27                     | 1.16              |
| 14:G:852:CLA:CED  | 17:N:852:BCR:C29  | 2.26                     | 1.14              |
| 14:G:852:CLA:HED1 | 17:N:852:BCR:C29  | 1.79                     | 1.12              |
| 14:G:852:CLA:HMD3 | 4:N:540:ILE:HG12  | 1.30                     | 1.10              |
| 2:a:685:MET:HG3   | 14:a:852:CLA:NC   | 1.68                     | 1.07              |
| 14:b:820:CLA:NC   | 14:b:825:CLA:H141 | 1.72                     | 1.04              |
| 14:A:855:CLA:HBB2 | 4:B:665:ALA:HB1   | 1.33                     | 1.02              |
| 14:A:801:CLA:CBB  | 14:A:855:CLA:O1A  | 2.07                     | 1.01              |
| 14:A:855:CLA:HED2 | 17:B:848:BCR:H401 | 1.40                     | 1.01              |
| 14:G:852:CLA:CED  | 17:N:852:BCR:H291 | 1.87                     | 1.00              |
| 14:G:852:CLA:HED1 | 17:N:852:BCR:C30  | 1.92                     | 0.98              |
| 2:a:694:TRP:HZ3   | 14:a:852:CLA:O1D  | 1.46                     | 0.98              |
| 14:a:852:CLA:HED3 | 4:b:539:LEU:CD2   | 1.93                     | 0.98              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:G:852:CLA:CED  | 17:N:852:BCR:C30  | 2.43                     | 0.97              |
| 2:A:442:ASN:OD1   | 14:A:855:CLA:CED  | 2.15                     | 0.94              |
| 14:A:855:CLA:HBB2 | 4:B:665:ALA:CB    | 1.98                     | 0.93              |
| 4:N:534:LEU:HD12  | 14:N:827:CLA:NC   | 1.83                     | 0.93              |
| 14:G:852:CLA:HED3 | 17:N:852:BCR:C29  | 1.98                     | 0.92              |
| 14:a:852:CLA:HED3 | 4:b:539:LEU:HD21  | 1.50                     | 0.91              |
| 14:A:801:CLA:HBB2 | 14:A:855:CLA:O1A  | 1.68                     | 0.91              |
| 14:G:808:CLA:HBB1 | 17:T:103:BCR:HC8  | 1.56                     | 0.88              |
| 2:a:685:MET:HG3   | 14:a:852:CLA:C4C  | 2.03                     | 0.88              |
| 14:g:807:CLA:HBB1 | 17:t:103:BCR:HC8  | 1.58                     | 0.84              |
| 5:C:17:CYS:HB3    | 16:C:102:SF4:S4   | 2.18                     | 0.83              |
| 14:G:852:CLA:HED3 | 17:N:852:BCR:H292 | 1.61                     | 0.83              |
| 10:U:35:GLY:HA2   | 10:U:39:ILE:HD13  | 1.60                     | 0.82              |
| 14:N:828:CLA:H152 | 17:N:848:BCR:H17C | 1.59                     | 0.82              |
| 14:a:807:CLA:HBB1 | 17:j:103:BCR:HC8  | 1.60                     | 0.82              |
| 2:A:541:PHE:HZ    | 14:A:855:CLA:O1A  | 0.93                     | 0.82              |
| 14:A:855:CLA:CBB  | 4:B:665:ALA:HB1   | 2.10                     | 0.81              |
| 14:G:832:CLA:HBB1 | 14:G:833:CLA:H2   | 1.63                     | 0.81              |
| 4:b:555:PRO:HB3   | 8:f:163:PRO:HG2   | 1.63                     | 0.81              |
| 14:g:819:CLA:NB   | 14:g:825:CLA:H122 | 1.94                     | 0.81              |
| 12:W:108:ALA:HB1  | 17:W:205:BCR:H19C | 1.61                     | 0.81              |
| 2:g:71:ARG:HD2    | 2:g:185:ALA:HB1   | 1.62                     | 0.81              |
| 17:I:103:BCR:H19C | 12:L:108:ALA:HB1  | 1.63                     | 0.80              |
| 2:a:694:TRP:CZ3   | 14:a:852:CLA:O1D  | 2.33                     | 0.80              |
| 10:u:45:GLU:HG3   | 10:u:46:PRO:HD3   | 1.61                     | 0.80              |
| 4:N:255:LEU:HB3   | 4:N:275:HIS:HB2   | 1.63                     | 0.80              |
| 14:B:820:CLA:H2A  | 14:B:820:CLA:HED3 | 1.62                     | 0.80              |
| 14:G:852:CLA:HED1 | 17:N:852:BCR:C39  | 2.12                     | 0.80              |
| 2:a:678:PHE:HB2   | 14:b:803:CLA:HBA2 | 1.62                     | 0.79              |
| 4:b:719:HIS:NE2   | 14:b:841:CLA:NA   | 2.31                     | 0.79              |
| 4:n:591:LEU:HD11  | 4:n:721:THR:HG22  | 1.65                     | 0.79              |
| 4:b:254:ILE:HG13  | 4:b:255:LEU:HG    | 1.65                     | 0.79              |
| 14:G:852:CLA:HED3 | 17:N:852:BCR:C40  | 2.13                     | 0.79              |
| 14:G:852:CLA:HBB1 | 14:N:803:CLA:C4B  | 2.13                     | 0.79              |
| 7:R:11:LEU:HD11   | 7:R:59:ILE:HG13   | 1.64                     | 0.78              |
| 14:n:806:CLA:H162 | 14:n:828:CLA:HBB2 | 1.64                     | 0.78              |
| 14:N:842:CLA:H193 | 17:V:101:BCR:H271 | 1.66                     | 0.78              |
| 14:G:852:CLA:HED1 | 17:N:852:BCR:H391 | 1.65                     | 0.77              |
| 9:T:23:THR:HG21   | 17:T:104:BCR:H21C | 1.65                     | 0.77              |
| 4:b:669:MET:HG3   | 14:b:805:CLA:NC   | 1.98                     | 0.77              |
| 14:N:822:CLA:HBB1 | 17:N:844:BCR:H14C | 1.67                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:652:VAL:HG22  | 14:B:810:CLA:HAC1 | 1.65                     | 0.76              |
| 14:n:819:CLA:HBB1 | 14:n:824:CLA:H61  | 1.67                     | 0.76              |
| 19:a:851:CL0:H15  | 19:a:851:CL0:H2   | 1.68                     | 0.76              |
| 17:g:843:BCR:H19C | 10:u:71:ILE:HD11  | 1.67                     | 0.76              |
| 4:b:669:MET:HB2   | 14:b:805:CLA:C1C  | 2.15                     | 0.76              |
| 14:A:811:CLA:HBC3 | 14:A:812:CLA:HAB  | 1.68                     | 0.76              |
| 14:n:825:CLA:HMA1 | 17:n:846:BCR:H14C | 1.67                     | 0.76              |
| 17:a:843:BCR:H19C | 10:k:71:ILE:HD11  | 1.66                     | 0.75              |
| 13:m:13:LEU:HB3   | 17:m:102:BCR:H21C | 1.67                     | 0.75              |
| 14:f:202:CLA:HMB2 | 9:j:33:LEU:HD21   | 1.67                     | 0.75              |
| 1:l:214:VAL:HG22  | 20:b:801:SQD:H141 | 1.68                     | 0.75              |
| 14:b:821:CLA:HBB1 | 17:b:843:BCR:H14C | 1.68                     | 0.75              |
| 14:a:853:CLA:C1B  | 14:b:805:CLA:HBB1 | 2.15                     | 0.74              |
| 2:a:599:MET:HG3   | 14:a:824:CLA:HBC1 | 1.70                     | 0.74              |
| 17:B:846:BCR:H282 | 17:B:847:BCR:H23C | 1.70                     | 0.74              |
| 4:N:535:HIS:NE2   | 14:N:840:CLA:NA   | 2.36                     | 0.74              |
| 2:A:320:HIS:CE1   | 14:A:821:CLA:NA   | 2.56                     | 0.74              |
| 2:A:524:MET:HE1   | 2:A:628:VAL:HG11  | 1.70                     | 0.73              |
| 9:J:28:ILE:HA     | 14:J:101:CLA:HBB2 | 1.70                     | 0.73              |
| 19:g:851:CL0:H2   | 19:g:851:CL0:H15  | 1.69                     | 0.73              |
| 8:S:100:ILE:HG12  | 14:S:203:CLA:ND   | 2.02                     | 0.73              |
| 17:n:845:BCR:H21C | 17:n:845:BCR:H361 | 1.68                     | 0.73              |
| 15:G:841:PQN:H172 | 17:N:852:BCR:H382 | 1.68                     | 0.73              |
| 14:b:826:CLA:HMA1 | 17:b:847:BCR:H14C | 1.70                     | 0.73              |
| 2:g:678:PHE:HB2   | 14:n:802:CLA:HBA2 | 1.71                     | 0.73              |
| 14:G:852:CLA:HBA2 | 4:N:431:LEU:HD23  | 1.71                     | 0.73              |
| 4:N:534:LEU:HD12  | 14:N:827:CLA:C1C  | 2.18                     | 0.73              |
| 14:n:840:CLA:HBB1 | 17:n:847:BCR:H363 | 1.71                     | 0.73              |
| 2:g:448:LEU:HD11  | 14:g:836:CLA:HMB2 | 1.72                     | 0.72              |
| 14:N:816:CLA:H3A  | 17:N:846:BCR:H272 | 1.72                     | 0.72              |
| 2:A:652:TRP:HD1   | 14:B:804:CLA:HBC1 | 1.54                     | 0.72              |
| 14:A:821:CLA:HBD  | 10:K:39:ILE:HG22  | 1.72                     | 0.72              |
| 2:a:584:CYS:HB2   | 4:b:674:TRP:HB3   | 1.72                     | 0.72              |
| 14:N:851:CLA:HBB2 | 17:N:852:BCR:HC31 | 1.72                     | 0.71              |
| 12:W:73:PHE:HZ    | 14:W:203:CLA:HBB1 | 1.55                     | 0.71              |
| 4:N:426:LEU:HD13  | 4:N:539:LEU:HA    | 1.73                     | 0.71              |
| 12:W:152:GLY:HA3  | 17:W:206:BCR:H312 | 1.72                     | 0.71              |
| 2:A:373:ALA:HB1   | 14:A:826:CLA:HMC2 | 1.70                     | 0.71              |
| 2:a:63:THR:HG21   | 2:a:68:ASP:HB3    | 1.73                     | 0.71              |
| 14:b:807:CLA:H162 | 14:b:829:CLA:HBB2 | 1.72                     | 0.71              |
| 10:k:86:ILE:H     | 10:k:86:ILE:HD12  | 1.55                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:N:812:CLA:HAB  | 11:V:25:GLY:HA3   | 1.71                     | 0.71              |
| 14:N:807:CLA:NC   | 14:N:831:CLA:HMB3 | 2.05                     | 0.71              |
| 2:g:204:VAL:HB    | 14:g:811:CLA:HAB  | 1.72                     | 0.70              |
| 4:n:460:GLU:HG3   | 8:s:28:LEU:HD11   | 1.73                     | 0.70              |
| 4:n:661:HIS:NE2   | 14:n:803:CLA:NB   | 2.39                     | 0.70              |
| 14:N:834:CLA:H51  | 17:N:852:BCR:H312 | 1.73                     | 0.70              |
| 13:Y:13:LEU:HB3   | 17:Y:101:BCR:H21C | 1.73                     | 0.70              |
| 4:n:707:LEU:HB3   | 4:n:711:GLN:HG2   | 1.74                     | 0.70              |
| 2:A:320:HIS:HE1   | 14:A:821:CLA:NA   | 1.89                     | 0.70              |
| 14:B:827:CLA:H152 | 17:B:846:BCR:H373 | 1.73                     | 0.70              |
| 4:b:707:LEU:HD22  | 4:b:711:GLN:HE22  | 1.57                     | 0.70              |
| 2:g:596:LEU:HD21  | 14:g:828:CLA:HBC1 | 1.73                     | 0.70              |
| 4:b:669:MET:HG3   | 14:b:805:CLA:C4C  | 2.21                     | 0.70              |
| 4:N:25:MET:HE1    | 15:N:843:PQN:H291 | 1.72                     | 0.69              |
| 14:n:831:CLA:H61  | 8:s:147:LEU:HD12  | 1.74                     | 0.69              |
| 14:n:837:CLA:H203 | 17:s:203:BCR:H272 | 1.75                     | 0.69              |
| 2:A:678:PHE:HB2   | 14:B:803:CLA:HBA2 | 1.72                     | 0.69              |
| 4:N:707:LEU:HB3   | 4:N:711:GLN:HG2   | 1.74                     | 0.69              |
| 14:B:808:CLA:H62  | 17:I:101:BCR:HC32 | 1.74                     | 0.69              |
| 4:n:696:ASN:HB3   | 12:w:121:LEU:HB2  | 1.75                     | 0.69              |
| 2:a:267:LEU:HD13  | 10:k:77:VAL:HG21  | 1.74                     | 0.69              |
| 4:b:176:ASN:HD21  | 4:b:291:TYR:HB2   | 1.57                     | 0.69              |
| 14:G:827:CLA:H142 | 14:G:827:CLA:H72  | 1.75                     | 0.69              |
| 4:N:656:MET:HG2   | 4:N:730:ALA:HB2   | 1.74                     | 0.69              |
| 14:A:805:CLA:H151 | 14:A:828:CLA:HBB2 | 1.74                     | 0.68              |
| 4:N:669:MET:HB2   | 14:N:805:CLA:C1C  | 2.23                     | 0.68              |
| 14:g:854:CLA:H152 | 12:w:108:ALA:HB2  | 1.75                     | 0.68              |
| 14:A:853:CLA:HBB1 | 14:B:803:CLA:C4B  | 2.22                     | 0.68              |
| 2:g:352:GLN:HG3   | 14:g:823:CLA:H152 | 1.76                     | 0.68              |
| 18:S:202:LHG:HC5  | 18:S:202:LHG:H261 | 1.74                     | 0.68              |
| 2:a:586:VAL:HG22  | 4:b:676:GLY:HA3   | 1.74                     | 0.68              |
| 2:A:685:MET:HB2   | 14:A:853:CLA:C1C  | 2.23                     | 0.68              |
| 4:n:69:ALA:HB2    | 4:n:135:LEU:HB2   | 1.76                     | 0.68              |
| 4:N:254:ILE:HG13  | 4:N:255:LEU:HD12  | 1.76                     | 0.68              |
| 10:U:47:ALA:HA    | 10:U:58:GLY:HA2   | 1.76                     | 0.68              |
| 2:A:370:HIS:NE2   | 14:A:826:CLA:NB   | 2.42                     | 0.68              |
| 2:g:45:THR:HG22   | 2:g:715:GLN:HB2   | 1.76                     | 0.68              |
| 2:a:197:MET:HB2   | 14:a:811:CLA:HBC2 | 1.75                     | 0.68              |
| 14:N:808:CLA:H41  | 21:N:850:LMG:H321 | 1.76                     | 0.67              |
| 8:F:92:LEU:HG     | 14:J:102:CLA:HAB  | 1.75                     | 0.67              |
| 2:G:91:MET:HE1    | 14:G:807:CLA:H2A  | 1.76                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:W:153:GLY:HA2  | 17:W:206:BCR:H10C | 1.75                     | 0.67              |
| 14:n:814:CLA:H3A  | 17:n:844:BCR:H272 | 1.76                     | 0.67              |
| 14:B:811:CLA:HAB  | 11:I:25:GLY:HA3   | 1.76                     | 0.67              |
| 15:A:842:PQN:H111 | 17:B:851:BCR:H393 | 1.76                     | 0.67              |
| 14:a:852:CLA:CED  | 4:b:539:LEU:CD2   | 2.72                     | 0.67              |
| 4:N:142:LEU:HG    | 17:N:846:BCR:H382 | 1.77                     | 0.67              |
| 2:G:69:ILE:O      | 2:G:73:ILE:HG12   | 1.94                     | 0.67              |
| 2:a:448:LEU:HB3   | 2:a:541:PHE:HB2   | 1.77                     | 0.67              |
| 19:g:851:CL0:H29  | 19:g:851:CL0:H40  | 1.77                     | 0.67              |
| 10:k:80:LEU:HB3   | 10:k:85:ARG:HB2   | 1.77                     | 0.67              |
| 4:n:40:GLU:HG3    | 4:n:165:LEU:HB2   | 1.76                     | 0.67              |
| 14:N:823:CLA:HBA2 | 17:N:844:BCR:H282 | 1.75                     | 0.67              |
| 14:b:809:CLA:H121 | 14:b:809:CLA:H2   | 1.77                     | 0.67              |
| 4:B:91:ILE:HB     | 4:B:112:PRO:HB2   | 1.77                     | 0.66              |
| 14:B:815:CLA:H3A  | 17:B:845:BCR:H272 | 1.76                     | 0.66              |
| 14:N:828:CLA:H151 | 17:N:847:BCR:H373 | 1.77                     | 0.66              |
| 4:n:305:MET:HG3   | 4:n:327:TYR:HB2   | 1.75                     | 0.66              |
| 2:G:217:LEU:HA    | 2:G:221:SER:HB2   | 1.77                     | 0.66              |
| 2:A:366:ILE:HD12  | 14:A:825:CLA:HED2 | 1.77                     | 0.66              |
| 14:b:802:CLA:H172 | 14:b:840:CLA:H171 | 1.76                     | 0.66              |
| 12:W:49:ASN:HB3   | 14:W:202:CLA:HAC1 | 1.77                     | 0.66              |
| 2:g:320:HIS:HE1   | 14:g:820:CLA:NA   | 1.94                     | 0.66              |
| 9:J:19:PRO:O      | 9:J:23:THR:HG23   | 1.96                     | 0.66              |
| 2:G:121:ILE:HD12  | 17:T:104:BCR:H313 | 1.78                     | 0.66              |
| 2:a:491:HIS:NE2   | 14:a:833:CLA:NA   | 2.43                     | 0.66              |
| 4:b:448:VAL:HG23  | 4:b:453:PRO:HB3   | 1.76                     | 0.66              |
| 4:b:699:ARG:HD3   | 12:l:121:LEU:HD21 | 1.77                     | 0.66              |
| 10:K:25:VAL:O     | 10:K:29:VAL:HG23  | 1.96                     | 0.66              |
| 4:b:195:ILE:HA    | 4:b:199:ILE:HD12  | 1.78                     | 0.66              |
| 15:B:842:PQN:H301 | 17:I:103:BCR:H321 | 1.78                     | 0.66              |
| 6:d:96:HIS:HB3    | 6:d:97:PRO:HD3    | 1.77                     | 0.66              |
| 14:G:812:CLA:HHC  | 14:G:812:CLA:HBB1 | 1.77                     | 0.66              |
| 14:A:831:CLA:HBC2 | 14:A:838:CLA:HMC2 | 1.78                     | 0.66              |
| 4:N:460:GLU:HG3   | 8:S:28:LEU:HD11   | 1.78                     | 0.65              |
| 2:A:549:ILE:HG12  | 14:A:855:CLA:HMD3 | 1.78                     | 0.65              |
| 17:A:849:BCR:H362 | 14:B:803:CLA:H51  | 1.77                     | 0.65              |
| 2:a:374:MET:HE2   | 14:a:825:CLA:HMC2 | 1.78                     | 0.65              |
| 17:W:201:BCR:C10  | 14:W:203:CLA:HAB  | 2.26                     | 0.65              |
| 2:a:452:SER:HB2   | 2:a:538:ILE:HG12  | 1.78                     | 0.65              |
| 14:a:839:CLA:HBB2 | 17:a:848:BCR:H19C | 1.78                     | 0.65              |
| 4:N:719:HIS:NE2   | 14:N:842:CLA:NA   | 2.45                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:B:181:GLY:HA3   | 14:B:814:CLA:HBB1 | 1.78                     | 0.65              |
| 2:G:596:LEU:HD21  | 14:G:829:CLA:HBC1 | 1.78                     | 0.65              |
| 2:A:67:GLU:HB2    | 2:A:188:LEU:HB2   | 1.76                     | 0.65              |
| 2:A:205:LEU:HD11  | 14:A:812:CLA:H42  | 1.77                     | 0.65              |
| 14:N:803:CLA:HMA1 | 14:N:804:CLA:H171 | 1.78                     | 0.65              |
| 4:n:176:ASN:HD21  | 4:n:291:TYR:HB2   | 1.60                     | 0.65              |
| 14:b:832:CLA:HBC2 | 14:b:839:CLA:HMC2 | 1.76                     | 0.65              |
| 14:n:832:CLA:HBB2 | 17:n:849:BCR:HC31 | 1.79                     | 0.65              |
| 2:A:598:TRP:CH2   | 14:A:801:CLA:HAB  | 2.32                     | 0.65              |
| 2:A:598:TRP:HE1   | 14:A:855:CLA:C1D  | 2.08                     | 0.65              |
| 14:B:826:CLA:HMA1 | 17:B:847:BCR:H14C | 1.79                     | 0.65              |
| 12:l:152:GLY:HA3  | 17:l:206:BCR:H312 | 1.79                     | 0.65              |
| 2:a:483:PHE:HB3   | 14:a:835:CLA:H2   | 1.78                     | 0.65              |
| 4:b:231:GLY:HA2   | 14:b:817:CLA:HAA2 | 1.79                     | 0.65              |
| 14:b:803:CLA:HMA3 | 14:b:804:CLA:H71  | 1.79                     | 0.65              |
| 2:A:399:GLY:HA3   | 2:A:603:LEU:HD11  | 1.79                     | 0.65              |
| 4:b:694:ILE:HD12  | 14:l:203:CLA:H42  | 1.79                     | 0.65              |
| 2:A:564:PRO:HG3   | 6:D:65:TYR:HD1    | 1.62                     | 0.65              |
| 2:g:506:VAL:HG21  | 14:g:825:CLA:HAB  | 1.78                     | 0.64              |
| 14:G:852:CLA:HBB1 | 14:N:803:CLA:CHC  | 2.27                     | 0.64              |
| 2:g:320:HIS:CE1   | 14:g:820:CLA:NA   | 2.64                     | 0.64              |
| 10:u:76:LEU:O     | 10:u:80:LEU:HD12  | 1.98                     | 0.64              |
| 2:A:584:CYS:HB2   | 4:B:674:TRP:HB3   | 1.79                     | 0.64              |
| 2:a:458:HIS:CE1   | 14:a:832:CLA:NA   | 2.66                     | 0.64              |
| 2:G:121:ILE:HG12  | 2:G:122:VAL:HG23  | 1.80                     | 0.64              |
| 14:a:830:CLA:HBC2 | 14:a:837:CLA:HMC2 | 1.78                     | 0.64              |
| 14:g:824:CLA:H52  | 18:g:850:LHG:H201 | 1.79                     | 0.64              |
| 4:n:526:VAL:HG11  | 4:n:600:TYR:HB2   | 1.79                     | 0.64              |
| 2:A:448:LEU:HB3   | 2:A:541:PHE:HB2   | 1.78                     | 0.64              |
| 4:B:319:PHE:HB2   | 14:B:824:CLA:HMA1 | 1.79                     | 0.64              |
| 2:a:685:MET:HB2   | 14:a:852:CLA:C1C  | 2.28                     | 0.64              |
| 10:u:28:ASN:O     | 10:u:32:ILE:HD12  | 1.98                     | 0.64              |
| 14:a:837:CLA:H203 | 17:a:846:BCR:H312 | 1.78                     | 0.64              |
| 10:k:76:LEU:O     | 10:k:80:LEU:HD12  | 1.97                     | 0.64              |
| 2:G:462:MET:HE1   | 2:G:467:ARG:HH21  | 1.63                     | 0.64              |
| 17:A:849:BCR:H23C | 14:A:853:CLA:H111 | 1.80                     | 0.64              |
| 5:c:17:CYS:HB3    | 16:c:102:SF4:S4   | 2.37                     | 0.64              |
| 14:B:807:CLA:HED1 | 14:B:830:CLA:H2   | 1.79                     | 0.63              |
| 14:b:820:CLA:C4C  | 14:b:825:CLA:H141 | 2.28                     | 0.63              |
| 4:N:652:VAL:HG22  | 14:N:811:CLA:HAC1 | 1.80                     | 0.63              |
| 4:n:683:GLU:HG2   | 5:p:81:TYR:HE1    | 1.63                     | 0.63              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:l:214:VAL:HG13   | 20:b:801:SQD:H152 | 1.79                     | 0.63              |
| 20:h:1702:SQD:H383 | 14:n:825:CLA:H141 | 1.80                     | 0.63              |
| 14:A:855:CLA:HED2  | 17:B:848:BCR:C40  | 2.21                     | 0.63              |
| 4:b:355:HIS:CE1    | 14:b:827:CLA:NB   | 2.67                     | 0.63              |
| 4:N:26:ALA:HA      | 14:N:831:CLA:H43  | 1.81                     | 0.63              |
| 2:g:734:LEU:HD11   | 17:g:848:BCR:HC8  | 1.80                     | 0.63              |
| 14:A:806:CLA:H2    | 14:A:808:CLA:H2   | 1.80                     | 0.63              |
| 14:A:827:CLA:H203  | 17:J:103:BCR:H12C | 1.80                     | 0.63              |
| 2:g:28:LYS:HB2     | 14:g:809:CLA:HAA2 | 1.81                     | 0.63              |
| 2:A:204:VAL:O      | 2:A:208:CYS:HB2   | 1.99                     | 0.63              |
| 11:I:40:ILE:HG13   | 11:I:41:GLU:HG2   | 1.80                     | 0.63              |
| 2:a:204:VAL:HB     | 14:a:811:CLA:HAB  | 1.79                     | 0.63              |
| 2:a:355:THR:HG22   | 17:a:846:BCR:HC7  | 1.78                     | 0.63              |
| 14:a:830:CLA:H2    | 14:l:203:CLA:H43  | 1.81                     | 0.63              |
| 14:b:853:CLA:HMA2  | 13:m:30:LEU:HD22  | 1.80                     | 0.63              |
| 10:u:72:LEU:O      | 10:u:76:LEU:HD12  | 1.99                     | 0.63              |
| 2:A:374:MET:HE1    | 14:A:826:CLA:HHC  | 1.81                     | 0.63              |
| 14:B:850:CLA:HBB1  | 14:B:850:CLA:HHC  | 1.80                     | 0.63              |
| 10:U:14:LEU:HD11   | 10:U:77:VAL:HG22  | 1.80                     | 0.63              |
| 14:g:838:CLA:HBC2  | 17:n:849:BCR:H21C | 1.80                     | 0.63              |
| 2:A:596:LEU:HD21   | 14:A:829:CLA:HBC1 | 1.80                     | 0.63              |
| 14:N:832:CLA:HAB   | 14:N:840:CLA:HBB2 | 1.80                     | 0.62              |
| 14:A:804:CLA:HBA1  | 14:A:812:CLA:HBA1 | 1.81                     | 0.62              |
| 2:A:53:HIS:HE1     | 14:A:802:CLA:ND   | 1.98                     | 0.62              |
| 10:k:46:PRO:HB2    | 10:k:59:ALA:HB3   | 1.82                     | 0.62              |
| 2:G:652:TRP:HD1    | 14:N:804:CLA:HBC1 | 1.63                     | 0.62              |
| 14:B:827:CLA:H13   | 17:B:847:BCR:H351 | 1.80                     | 0.62              |
| 14:G:817:CLA:HBC1  | 14:G:820:CLA:H161 | 1.81                     | 0.62              |
| 14:G:852:CLA:HBB1  | 14:N:803:CLA:C1C  | 2.30                     | 0.62              |
| 5:C:62:PHE:HD2     | 6:D:120:ILE:HB    | 1.63                     | 0.62              |
| 14:a:804:CLA:H151  | 14:a:827:CLA:HBB2 | 1.81                     | 0.62              |
| 14:n:824:CLA:H71   | 14:n:826:CLA:H42  | 1.82                     | 0.62              |
| 2:A:284:PRO:HA     | 2:A:515:LEU:HD21  | 1.82                     | 0.62              |
| 4:B:254:ILE:HG13   | 4:B:255:LEU:HD12  | 1.82                     | 0.62              |
| 4:b:237:PRO:HB3    | 4:b:256:THR:HG21  | 1.81                     | 0.62              |
| 14:G:806:CLA:H2    | 14:G:808:CLA:H2   | 1.81                     | 0.62              |
| 11:v:27:VAL:HG13   | 20:w:202:SQD:H322 | 1.80                     | 0.62              |
| 13:y:13:LEU:HB3    | 17:y:101:BCR:H21C | 1.81                     | 0.62              |
| 2:A:414:VAL:HG21   | 2:A:571:PHE:HB2   | 1.80                     | 0.62              |
| 13:M:13:LEU:HB3    | 17:M:101:BCR:H21C | 1.82                     | 0.62              |
| 2:a:413:MET:HA     | 2:a:413:MET:HE3   | 1.82                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 12:w:152:GLY:HA3  | 17:w:207:BCR:H312  | 1.82                     | 0.62              |
| 3:X:15:LYS:HE2    | 3:X:15:LYS:N       | 2.14                     | 0.62              |
| 2:G:53:HIS:HE1    | 14:G:802:CLA:ND    | 1.99                     | 0.61              |
| 2:G:399:GLY:HA3   | 2:G:603:LEU:HD11   | 1.82                     | 0.61              |
| 14:G:852:CLA:HBB1 | 14:N:803:CLA:NC    | 2.15                     | 0.61              |
| 7:r:7:LYS:HE3     | 7:r:23:THR:HG22    | 1.82                     | 0.61              |
| 2:A:217:LEU:HA    | 2:A:221:SER:HB3    | 1.81                     | 0.61              |
| 4:b:342:LEU:HD21  | 14:b:830:CLA:HAB   | 1.81                     | 0.61              |
| 17:G:843:BCR:H291 | 10:U:39:ILE:HD11   | 1.81                     | 0.61              |
| 2:A:18:ASP:HB2    | 2:A:71:ARG:HH12    | 1.65                     | 0.61              |
| 14:B:840:CLA:HBB2 | 15:B:842:PQN:H141  | 1.82                     | 0.61              |
| 4:b:174:ARG:HB2   | 14:b:814:CLA:HBC2  | 1.81                     | 0.61              |
| 12:l:57:LEU:HD22  | 12:l:61:ARG:HG2    | 1.80                     | 0.61              |
| 4:b:123:TRP:HH2   | 14:b:829:CLA:H2    | 1.66                     | 0.61              |
| 2:G:491:HIS:NE2   | 14:G:834:CLA:NA    | 2.48                     | 0.61              |
| 14:G:852:CLA:CBB  | 14:N:803:CLA:NC    | 2.63                     | 0.61              |
| 4:B:322:PRO:HB2   | 4:B:410:ASN:HA     | 1.82                     | 0.61              |
| 8:F:103:VAL:HG13  | 8:F:132:ILE:HG22   | 1.81                     | 0.61              |
| 17:a:848:BCR:H362 | 14:b:803:CLA:H51   | 1.83                     | 0.61              |
| 11:i:36:LEU:HD11  | 18:m:101:LHG:H302  | 1.83                     | 0.61              |
| 2:G:267:LEU:HD13  | 10:U:77:VAL:HG11   | 1.82                     | 0.61              |
| 14:g:816:CLA:H111 | 14:g:834:CLA:HBA1  | 1.83                     | 0.61              |
| 2:a:708:LEU:HD21  | 14:b:832:CLA:H3A   | 1.81                     | 0.61              |
| 2:G:457:ILE:HG22  | 14:G:833:CLA:HBC2  | 1.81                     | 0.61              |
| 14:G:807:CLA:HBB2 | 14:G:827:CLA:H193  | 1.81                     | 0.61              |
| 14:A:855:CLA:HBC3 | 4:B:673:SER:HB3    | 1.83                     | 0.61              |
| 2:a:399:GLY:HA3   | 2:a:603:LEU:HD11   | 1.81                     | 0.61              |
| 19:g:851:CL0:H21  | 14:n:803:CLA:HBC3  | 1.82                     | 0.61              |
| 5:c:41:SER:HB2    | 6:d:113:VAL:H      | 1.66                     | 0.61              |
| 4:N:355:HIS:CE1   | 14:N:828:CLA:NB    | 2.69                     | 0.61              |
| 2:A:228:MET:HE2   | 2:A:234:VAL:HG23   | 1.83                     | 0.61              |
| 4:B:180:ALA:HB2   | 4:B:288:GLY:HA3    | 1.82                     | 0.61              |
| 12:L:152:GLY:HA2  | 17:L:1504:BCR:HC42 | 1.82                     | 0.61              |
| 14:b:815:CLA:H3A  | 17:b:845:BCR:H272  | 1.82                     | 0.60              |
| 2:A:156:SER:HA    | 2:A:159:LEU:HD12   | 1.81                     | 0.60              |
| 14:B:820:CLA:H152 | 14:B:825:CLA:H202  | 1.83                     | 0.60              |
| 5:c:28:MET:HA     | 5:c:28:MET:HE3     | 1.83                     | 0.60              |
| 14:n:852:CLA:H52  | 18:v:102:LHG:H262  | 1.83                     | 0.60              |
| 2:a:28:LYS:HB2    | 14:a:809:CLA:HAA2  | 1.82                     | 0.60              |
| 2:G:448:LEU:HB3   | 2:G:541:PHE:HB2    | 1.83                     | 0.60              |
| 17:G:848:BCR:H362 | 14:N:803:CLA:H51   | 1.82                     | 0.60              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:g:685:MET:HG3    | 14:g:852:CLA:NC   | 2.16                     | 0.60              |
| 2:g:204:VAL:HA     | 2:g:208:CYS:HB2   | 1.84                     | 0.60              |
| 4:B:701:LYS:HG3    | 14:B:840:CLA:HED2 | 1.82                     | 0.60              |
| 14:a:810:CLA:HBB2  | 14:a:818:CLA:H62  | 1.81                     | 0.60              |
| 8:f:78:GLY:HA2     | 8:f:87:LEU:HD11   | 1.82                     | 0.60              |
| 14:G:805:CLA:HMA2  | 14:G:805:CLA:H2   | 1.83                     | 0.60              |
| 4:N:399:VAL:HG23   | 4:N:548:ALA:HB1   | 1.83                     | 0.60              |
| 2:g:374:MET:HE2    | 14:g:825:CLA:HMC2 | 1.83                     | 0.60              |
| 14:a:828:CLA:H42   | 18:a:849:LHG:H251 | 1.84                     | 0.60              |
| 7:e:32:ILE:HG22    | 7:e:34:TYR:H      | 1.66                     | 0.60              |
| 2:G:661:SER:HB2    | 2:G:666:LEU:HB2   | 1.84                     | 0.60              |
| 14:G:816:CLA:CHD   | 14:G:817:CLA:HBB2 | 2.32                     | 0.60              |
| 14:N:818:CLA:CHD   | 14:N:819:CLA:HBB2 | 2.31                     | 0.60              |
| 20:h:1702:SQD:H351 | 17:n:845:BCR:H333 | 1.84                     | 0.60              |
| 4:b:65:LEU:HD11    | 17:b:845:BCR:H281 | 1.84                     | 0.60              |
| 4:b:729:ALA:HB2    | 14:b:828:CLA:HBB1 | 1.82                     | 0.60              |
| 14:B:850:CLA:HBB2  | 17:B:851:BCR:HC31 | 1.83                     | 0.60              |
| 14:n:818:CLA:H8    | 14:n:818:CLA:HAB  | 1.82                     | 0.60              |
| 2:A:367:ILE:HD12   | 14:A:828:CLA:HAC2 | 1.83                     | 0.60              |
| 15:g:841:PQN:H111  | 17:n:849:BCR:H393 | 1.83                     | 0.60              |
| 14:A:854:CLA:H71   | 14:B:850:CLA:H11  | 1.84                     | 0.60              |
| 4:B:373:ALA:HB1    | 4:B:732:LEU:HD11  | 1.84                     | 0.60              |
| 2:a:719:LEU:HB3    | 2:a:723:GLN:HG2   | 1.84                     | 0.60              |
| 14:a:805:CLA:H2    | 14:a:807:CLA:H52  | 1.84                     | 0.60              |
| 14:b:805:CLA:HBC2  | 14:b:805:CLA:HHH  | 1.82                     | 0.60              |
| 4:N:528:HIS:CD2    | 17:N:853:BCR:HC21 | 2.37                     | 0.59              |
| 4:n:528:HIS:CD2    | 17:n:851:BCR:HC21 | 2.36                     | 0.59              |
| 2:A:53:HIS:NE2     | 14:A:802:CLA:NB   | 2.49                     | 0.59              |
| 3:x:27:LEU:O       | 3:x:31:VAL:HG23   | 2.02                     | 0.59              |
| 4:b:351:TRP:HE1    | 4:b:355:HIS:CE1   | 2.19                     | 0.59              |
| 8:F:155:LYS:HB2    | 8:F:158:GLU:HG3   | 1.83                     | 0.59              |
| 1:1:208:GLY:O      | 1:1:212:LEU:HD22  | 2.02                     | 0.59              |
| 2:g:408:HIS:HE1    | 14:g:828:CLA:NA   | 2.00                     | 0.59              |
| 4:b:51:PHE:CZ      | 14:b:812:CLA:HBB1 | 2.38                     | 0.59              |
| 2:A:537:HIS:HE1    | 14:A:837:CLA:ND   | 2.01                     | 0.59              |
| 4:B:69:ALA:HB2     | 4:B:135:LEU:HB2   | 1.83                     | 0.59              |
| 14:B:810:CLA:H111  | 14:B:828:CLA:H18  | 1.85                     | 0.59              |
| 7:E:10:ILE:HG22    | 7:E:12:ARG:H      | 1.67                     | 0.59              |
| 4:b:29:ASN:HD21    | 14:b:853:CLA:C1C  | 2.15                     | 0.59              |
| 2:g:121:ILE:HB     | 17:t:104:BCR:H322 | 1.83                     | 0.59              |
| 2:G:77:HIS:NE2     | 14:G:804:CLA:ND   | 2.50                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 3:h:21:ARG:HB3     | 20:h:1702:SQD:H45 | 1.85                     | 0.59              |
| 4:n:638:LEU:HD22   | 4:n:731:PHE:HA    | 1.84                     | 0.59              |
| 12:L:35:THR:HG22   | 12:L:37:VAL:H     | 1.67                     | 0.59              |
| 2:g:63:THR:HG21    | 2:g:68:ASP:HB3    | 1.84                     | 0.59              |
| 2:A:289:LEU:HD21   | 2:A:374:MET:HB3   | 1.84                     | 0.59              |
| 2:a:53:HIS:HE1     | 14:a:801:CLA:ND   | 2.00                     | 0.59              |
| 14:g:832:CLA:HBB1  | 17:v:101:BCR:H282 | 1.85                     | 0.59              |
| 4:N:156:HIS:CE1    | 14:N:813:CLA:NA   | 2.71                     | 0.59              |
| 14:g:819:CLA:C1B   | 14:g:825:CLA:H122 | 2.32                     | 0.59              |
| 7:R:27:VAL:HG23    | 7:R:36:VAL:HG22   | 1.85                     | 0.59              |
| 20:h:1702:SQD:H332 | 17:n:845:BCR:H333 | 1.85                     | 0.59              |
| 14:A:802:CLA:H43   | 14:A:839:CLA:H102 | 1.83                     | 0.59              |
| 8:F:28:LEU:HD22    | 8:F:65:LEU:HB3    | 1.85                     | 0.59              |
| 14:G:805:CLA:H151  | 14:G:828:CLA:HBB2 | 1.85                     | 0.58              |
| 10:u:22:ILE:O      | 10:u:26:ILE:HD12  | 2.03                     | 0.58              |
| 18:X:1702:LHG:H322 | 14:B:831:CLA:H43  | 1.84                     | 0.58              |
| 4:N:321:MET:HA     | 4:N:321:MET:HE3   | 1.83                     | 0.58              |
| 14:N:832:CLA:H3A   | 14:N:833:CLA:OBD  | 2.03                     | 0.58              |
| 12:W:68:MET:HE3    | 17:W:206:BCR:H311 | 1.84                     | 0.58              |
| 14:B:824:CLA:H93   | 14:B:825:CLA:H162 | 1.83                     | 0.58              |
| 2:a:685:MET:HB2    | 14:a:852:CLA:CHC  | 2.33                     | 0.58              |
| 4:b:85:ARG:HB3     | 4:b:115:ILE:HD12  | 1.84                     | 0.58              |
| 14:b:807:CLA:HED1  | 14:b:830:CLA:H2   | 1.85                     | 0.58              |
| 2:G:438:ILE:HG13   | 2:G:556:PHE:HE2   | 1.68                     | 0.58              |
| 14:G:801:CLA:HBA2  | 14:G:801:CLA:HED3 | 1.85                     | 0.58              |
| 14:a:833:CLA:H2    | 17:a:847:BCR:H383 | 1.86                     | 0.58              |
| 12:l:50:LEU:HG     | 12:l:51:PRO:HD2   | 1.85                     | 0.58              |
| 14:N:832:CLA:H43   | 18:S:202:LHG:H321 | 1.85                     | 0.58              |
| 2:g:408:HIS:CE1    | 14:g:828:CLA:NA   | 2.71                     | 0.58              |
| 4:n:355:HIS:NE2    | 14:n:826:CLA:NC   | 2.51                     | 0.58              |
| 6:q:31:ILE:HG21    | 6:q:69:LEU:HD23   | 1.85                     | 0.58              |
| 17:B:851:BCR:H23C  | 17:B:851:BCR:H383 | 1.86                     | 0.58              |
| 2:a:688:PHE:HB2    | 14:a:852:CLA:HBC2 | 1.85                     | 0.58              |
| 4:b:433:LEU:HD11   | 14:b:838:CLA:HMB2 | 1.86                     | 0.58              |
| 4:b:527:HIS:HE1    | 14:b:837:CLA:ND   | 2.01                     | 0.58              |
| 2:A:267:LEU:HD13   | 10:K:77:VAL:HG11  | 1.84                     | 0.58              |
| 2:a:53:HIS:NE2     | 14:a:801:CLA:NB   | 2.51                     | 0.58              |
| 2:a:598:TRP:CH2    | 14:a:853:CLA:HAB  | 2.39                     | 0.58              |
| 14:G:831:CLA:H52   | 14:W:203:CLA:H43  | 1.86                     | 0.58              |
| 2:g:388:LEU:HD23   | 2:g:748:ILE:HG21  | 1.85                     | 0.58              |
| 17:g:848:BCR:H362  | 14:n:802:CLA:H51  | 1.84                     | 0.58              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:A:393:HIS:O      | 2:A:397:ILE:HD12  | 2.04                     | 0.58              |
| 14:B:824:CLA:H42   | 17:B:846:BCR:H10C | 1.85                     | 0.58              |
| 6:D:73:LEU:HD22    | 6:D:78:ILE:HD12   | 1.84                     | 0.58              |
| 2:a:738:ALA:HB2    | 17:a:848:BCR:H322 | 1.86                     | 0.58              |
| 4:b:106:GLN:HG3    | 4:b:115:ILE:HD11  | 1.85                     | 0.58              |
| 2:A:564:PRO:HG3    | 6:D:65:TYR:CD1    | 2.38                     | 0.58              |
| 9:J:30:ALA:O       | 9:J:34:ILE:HG13   | 2.03                     | 0.58              |
| 2:a:734:LEU:HD11   | 17:a:848:BCR:HC8  | 1.85                     | 0.58              |
| 2:g:333:PHE:HE2    | 12:w:36:PRO:HG3   | 1.69                     | 0.58              |
| 4:n:694:ILE:HD12   | 14:w:204:CLA:H42  | 1.86                     | 0.58              |
| 2:a:675:GLY:HA2    | 17:a:848:BCR:H17C | 1.85                     | 0.58              |
| 14:a:815:CLA:CHD   | 14:a:816:CLA:HBB2 | 2.34                     | 0.58              |
| 9:j:28:ILE:HG12    | 14:j:101:CLA:HBB2 | 1.86                     | 0.58              |
| 2:G:142:SER:HA     | 14:G:827:CLA:HMA2 | 1.86                     | 0.58              |
| 2:a:320:HIS:NE2    | 14:a:820:CLA:ND   | 2.51                     | 0.58              |
| 4:b:445:ASP:OD1    | 4:b:622:TYR:HB2   | 2.04                     | 0.58              |
| 14:n:806:CLA:HED1  | 14:n:829:CLA:H2   | 1.86                     | 0.58              |
| 7:r:12:ARG:HD2     | 7:r:15:SER:HB2    | 1.86                     | 0.58              |
| 4:B:719:HIS:NE2    | 14:B:841:CLA:NA   | 2.52                     | 0.58              |
| 17:L:1504:BCR:H321 | 12:l:148:ILE:HD12 | 1.86                     | 0.58              |
| 14:b:803:CLA:HMB2  | 14:b:804:CLA:H191 | 1.86                     | 0.58              |
| 2:G:142:SER:HB3    | 14:G:827:CLA:HAA2 | 1.86                     | 0.57              |
| 14:N:827:CLA:HAA2  | 14:N:828:CLA:OBD  | 2.04                     | 0.57              |
| 4:n:321:MET:HE3    | 14:n:823:CLA:HAB  | 1.86                     | 0.57              |
| 2:A:420:VAL:HG22   | 6:D:40:VAL:HB     | 1.86                     | 0.57              |
| 4:B:15:ASP:HB3     | 4:B:20:ARG:HB2    | 1.85                     | 0.57              |
| 14:B:807:CLA:H161  | 14:B:829:CLA:HBB2 | 1.85                     | 0.57              |
| 5:C:19:ARG:HD3     | 6:D:104:GLU:HG2   | 1.86                     | 0.57              |
| 2:G:397:ILE:HD12   | 14:G:805:CLA:H143 | 1.86                     | 0.57              |
| 2:g:684:LEU:HB2    | 14:g:852:CLA:HMC2 | 1.87                     | 0.57              |
| 14:g:815:CLA:CHD   | 14:g:816:CLA:HBB2 | 2.33                     | 0.57              |
| 11:i:24:ILE:HD12   | 17:i:101:BCR:H333 | 1.86                     | 0.57              |
| 2:G:708:LEU:HD21   | 14:N:833:CLA:H3A  | 1.85                     | 0.57              |
| 4:B:470:ALA:HB1    | 4:B:481:LEU:HD12  | 1.86                     | 0.57              |
| 12:L:170:LEU:HD22  | 12:l:84:LEU:HD13  | 1.86                     | 0.57              |
| 4:b:46:ILE:HD11    | 14:b:806:CLA:HMC2 | 1.86                     | 0.57              |
| 14:G:852:CLA:CMD   | 4:N:540:ILE:HG12  | 2.21                     | 0.57              |
| 2:g:448:LEU:HB3    | 2:g:541:PHE:HB2   | 1.84                     | 0.57              |
| 5:C:7:ILE:HD13     | 5:C:41:SER:HA     | 1.86                     | 0.57              |
| 14:a:801:CLA:H2    | 14:a:801:CLA:HED2 | 1.85                     | 0.57              |
| 14:H:1701:CLA:HBC3 | 14:N:840:CLA:HBC2 | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:g:75:ALA:HB2    | 2:g:181:TYR:HB2   | 1.86                     | 0.57              |
| 5:p:29:VAL:HG12   | 6:q:110:ARG:HB3   | 1.87                     | 0.57              |
| 6:D:8:LYS:HB2     | 6:D:52:HIS:CD2    | 2.39                     | 0.57              |
| 2:a:458:HIS:HE1   | 14:a:832:CLA:C1A  | 2.17                     | 0.57              |
| 18:a:850:LHG:HC82 | 18:a:850:LHG:H252 | 1.86                     | 0.57              |
| 2:g:441:LEU:HG    | 2:g:548:LEU:HB2   | 1.87                     | 0.57              |
| 2:g:642:THR:HG23  | 2:g:645:GLY:H     | 1.68                     | 0.57              |
| 14:B:826:CLA:HAA2 | 14:B:827:CLA:OBD  | 2.02                     | 0.57              |
| 2:a:351:ALA:O     | 2:a:355:THR:HG23  | 2.05                     | 0.57              |
| 15:G:841:PQN:H111 | 17:N:852:BCR:H393 | 1.85                     | 0.57              |
| 14:A:802:CLA:HBB2 | 14:A:810:CLA:H112 | 1.87                     | 0.57              |
| 4:b:527:HIS:CE1   | 14:b:837:CLA:ND   | 2.72                     | 0.57              |
| 4:b:673:SER:HB3   | 4:b:678:TRP:HE1   | 1.70                     | 0.57              |
| 7:e:39:ARG:HG2    | 7:e:50:THR:HG22   | 1.87                     | 0.57              |
| 14:G:802:CLA:HBB2 | 14:G:810:CLA:H112 | 1.86                     | 0.57              |
| 14:G:839:CLA:HAC1 | 15:G:841:PQN:H171 | 1.86                     | 0.57              |
| 4:N:435:PHE:HZ    | 17:N:852:BCR:H20C | 1.69                     | 0.57              |
| 3:h:27:LEU:O      | 3:h:31:VAL:HG23   | 2.04                     | 0.57              |
| 2:A:599:MET:HG2   | 14:A:825:CLA:HBC1 | 1.87                     | 0.57              |
| 2:G:731:HIS:CE1   | 14:G:839:CLA:NA   | 2.73                     | 0.57              |
| 14:G:818:CLA:H92  | 14:G:828:CLA:H91  | 1.87                     | 0.57              |
| 7:R:2:VAL:HG11    | 7:R:58:LEU:HD23   | 1.87                     | 0.57              |
| 14:n:832:CLA:HBB1 | 17:n:849:BCR:H323 | 1.86                     | 0.57              |
| 2:A:197:MET:HB2   | 14:A:812:CLA:HBC2 | 1.85                     | 0.57              |
| 4:B:22:TRP:CG     | 4:B:711:GLN:HE22  | 2.23                     | 0.57              |
| 17:I:103:BCR:HC8  | 17:I:103:BCR:H331 | 1.87                     | 0.57              |
| 14:a:826:CLA:HBC2 | 17:a:848:BCR:H332 | 1.87                     | 0.57              |
| 2:G:375:PRO:HG2   | 2:G:381:ALA:HB2   | 1.87                     | 0.57              |
| 2:G:413:MET:HE3   | 2:G:558:ARG:HG3   | 1.87                     | 0.57              |
| 2:G:686:PHE:HA    | 15:G:841:PQN:H9   | 1.86                     | 0.57              |
| 4:N:301:ILE:HA    | 4:N:304:MET:HB2   | 1.86                     | 0.57              |
| 2:A:441:LEU:HG    | 2:A:548:LEU:HB2   | 1.87                     | 0.57              |
| 14:a:822:CLA:HBB  | 14:a:840:CLA:HAB  | 1.87                     | 0.57              |
| 2:G:396:TRP:CD1   | 14:G:827:CLA:HAB  | 2.40                     | 0.56              |
| 8:S:155:LYS:HB2   | 8:S:158:GLU:HG3   | 1.85                     | 0.56              |
| 14:g:801:CLA:H91  | 17:t:104:BCR:H21C | 1.86                     | 0.56              |
| 2:a:15:VAL:HG11   | 14:a:808:CLA:HAA2 | 1.87                     | 0.56              |
| 14:a:837:CLA:H93  | 17:a:846:BCR:H14C | 1.85                     | 0.56              |
| 17:a:843:BCR:H391 | 10:k:39:ILE:HD11  | 1.87                     | 0.56              |
| 17:a:848:BCR:H281 | 17:b:850:BCR:H14C | 1.87                     | 0.56              |
| 7:e:25:ALA:HB3    | 7:e:37:ILE:HG23   | 1.87                     | 0.56              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 14:G:802:CLA:H43   | 14:G:839:CLA:H102 | 1.86                     | 0.56              |
| 4:N:174:ARG:HB2    | 14:N:815:CLA:HBC2 | 1.86                     | 0.56              |
| 14:h:1701:CLA:HBC3 | 14:n:838:CLA:HBC2 | 1.87                     | 0.56              |
| 2:A:363:LEU:HD12   | 14:A:826:CLA:H52  | 1.87                     | 0.56              |
| 2:a:514:VAL:HG13   | 2:a:524:MET:HB3   | 1.87                     | 0.56              |
| 2:A:194:VAL:HG13   | 14:A:824:CLA:HMD1 | 1.87                     | 0.56              |
| 2:A:734:LEU:HD11   | 17:A:849:BCR:HC8  | 1.87                     | 0.56              |
| 14:B:805:CLA:HBD   | 14:B:805:CLA:HBA1 | 1.87                     | 0.56              |
| 12:L:58:THR:HG22   | 12:L:60:PHE:H     | 1.71                     | 0.56              |
| 20:b:801:SQD:H161  | 14:b:812:CLA:HAC1 | 1.85                     | 0.56              |
| 14:b:810:CLA:H91   | 14:b:841:CLA:H12  | 1.86                     | 0.56              |
| 4:N:697:LEU:HD21   | 12:W:52:ALA:HB1   | 1.87                     | 0.56              |
| 2:g:429:ARG:HG2    | 2:g:432:ARG:HH21  | 1.70                     | 0.56              |
| 2:A:299:LEU:HG     | 14:A:816:CLA:HAB  | 1.87                     | 0.56              |
| 14:A:802:CLA:H8    | 9:J:23:THR:HG22   | 1.87                     | 0.56              |
| 14:B:808:CLA:HMB2  | 17:I:101:BCR:H322 | 1.86                     | 0.56              |
| 2:a:403:VAL:HG11   | 2:a:596:LEU:HG    | 1.87                     | 0.56              |
| 2:a:458:HIS:HE1    | 14:a:832:CLA:NA   | 2.02                     | 0.56              |
| 14:b:807:CLA:H2    | 14:b:807:CLA:HED3 | 1.87                     | 0.56              |
| 4:N:177:HIS:NE2    | 14:N:814:CLA:NA   | 2.54                     | 0.56              |
| 4:N:458:LEU:HD23   | 4:N:621:THR:HG21  | 1.88                     | 0.56              |
| 12:W:24:ALA:HB2    | 12:W:32:ASN:HB3   | 1.87                     | 0.56              |
| 4:n:719:HIS:NE2    | 14:n:840:CLA:NA   | 2.54                     | 0.56              |
| 8:s:141:ALA:O      | 8:s:145:LYS:HG2   | 2.05                     | 0.56              |
| 14:A:804:CLA:H162  | 17:A:845:BCR:HC8  | 1.88                     | 0.56              |
| 4:B:136:TYR:HE1    | 13:M:12:ALA:HB2   | 1.70                     | 0.56              |
| 2:a:119:TRP:HB3    | 17:j:104:BCR:HC21 | 1.87                     | 0.56              |
| 2:a:385:ALA:HA     | 2:a:748:ILE:HD13  | 1.88                     | 0.56              |
| 4:b:471:HIS:NE2    | 14:b:834:CLA:NA   | 2.54                     | 0.56              |
| 2:G:322:ILE:HG21   | 14:G:824:CLA:HAC1 | 1.86                     | 0.56              |
| 14:G:837:CLA:HBB2  | 14:G:838:CLA:HBC3 | 1.87                     | 0.56              |
| 14:N:841:CLA:HBB2  | 15:N:843:PQN:H141 | 1.86                     | 0.56              |
| 2:a:305:PHE:CE1    | 14:a:819:CLA:HAB  | 2.40                     | 0.56              |
| 2:a:305:PHE:HE1    | 14:a:819:CLA:HAB  | 1.70                     | 0.56              |
| 14:a:822:CLA:HAC1  | 17:a:846:BCR:HC8  | 1.88                     | 0.56              |
| 4:b:178:HIS:NE2    | 14:b:814:CLA:NA   | 2.54                     | 0.56              |
| 5:c:17:CYS:HB2     | 5:c:54:CYS:HB2    | 1.87                     | 0.56              |
| 2:G:233:ALA:HB3    | 2:G:236:ASP:HB2   | 1.88                     | 0.56              |
| 2:G:564:PRO:HG3    | 6:Q:65:TYR:CD2    | 2.41                     | 0.56              |
| 14:g:822:CLA:HAC2  | 14:g:837:CLA:H202 | 1.87                     | 0.56              |
| 14:g:854:CLA:H142  | 14:n:839:CLA:H71  | 1.88                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:B:830:CLA:H141 | 14:B:841:CLA:HBA1  | 1.87                     | 0.56              |
| 2:a:67:GLU:HG2    | 2:a:188:LEU:HB2    | 1.86                     | 0.56              |
| 2:a:199:ASN:HD21  | 2:a:312:TYR:HB2    | 1.71                     | 0.56              |
| 15:a:841:PQN:H161 | 17:b:850:BCR:H382  | 1.86                     | 0.56              |
| 18:a:850:LHG:H331 | 18:a:850:LHG:H152  | 1.87                     | 0.56              |
| 10:u:46:PRO:HB2   | 10:u:59:ALA:HB3    | 1.88                     | 0.56              |
| 4:B:181:GLY:O     | 4:B:185:VAL:HB     | 2.04                     | 0.56              |
| 12:L:56:GLY:HA3   | 12:l:136:LYS:HD2   | 1.87                     | 0.56              |
| 2:a:53:HIS:CE1    | 14:a:801:CLA:NA    | 2.73                     | 0.56              |
| 4:b:299:HIS:NE2   | 14:b:822:CLA:ND    | 2.54                     | 0.56              |
| 13:m:7:THR:O      | 13:m:11:ILE:HG23   | 2.06                     | 0.56              |
| 2:G:91:MET:HB3    | 2:G:144:LEU:HD21   | 1.88                     | 0.56              |
| 2:G:355:THR:HG22  | 17:G:846:BCR:HC7   | 1.86                     | 0.56              |
| 12:W:77:PRO:HB3   | 14:W:204:CLA:HBB1  | 1.88                     | 0.56              |
| 2:g:202:LEU:HD23  | 2:g:206:LEU:HD12   | 1.86                     | 0.56              |
| 4:n:319:PHE:CD1   | 14:n:822:CLA:HAB   | 2.40                     | 0.56              |
| 4:n:623:LEU:HD11  | 14:n:803:CLA:H193  | 1.88                     | 0.56              |
| 2:A:127:LEU:HB3   | 2:A:138:ILE:HD11   | 1.88                     | 0.56              |
| 4:B:460:GLU:HG3   | 8:F:28:LEU:HD11    | 1.87                     | 0.56              |
| 14:a:805:CLA:H101 | 17:j:104:BCR:H373  | 1.87                     | 0.56              |
| 14:b:811:CLA:HAB  | 11:i:25:GLY:HA3    | 1.87                     | 0.56              |
| 4:N:711:GLN:HB2   | 21:N:850:LMG:H111  | 1.87                     | 0.56              |
| 2:g:511:GLY:HA2   | 2:g:525:PRO:HG3    | 1.86                     | 0.56              |
| 14:g:819:CLA:C4C  | 14:g:825:CLA:H152  | 2.36                     | 0.56              |
| 14:g:822:CLA:HAC1 | 17:g:846:BCR:H323  | 1.87                     | 0.56              |
| 2:A:675:GLY:HA2   | 17:A:849:BCR:H17C  | 1.86                     | 0.56              |
| 14:B:809:CLA:H122 | 14:B:828:CLA:H152  | 1.88                     | 0.56              |
| 2:G:358:ALA:HB1   | 17:G:847:BCR:H343  | 1.89                     | 0.55              |
| 2:g:310:HIS:CE1   | 17:g:843:BCR:H363  | 2.42                     | 0.55              |
| 4:n:729:ALA:HB2   | 14:n:827:CLA:HBB1  | 1.87                     | 0.55              |
| 2:A:549:ILE:CG1   | 14:A:855:CLA:HMD3  | 2.36                     | 0.55              |
| 2:A:598:TRP:HE1   | 14:A:855:CLA:CHD   | 2.20                     | 0.55              |
| 14:A:818:CLA:H111 | 14:A:818:CLA:HAB   | 1.87                     | 0.55              |
| 17:A:856:BCR:H312 | 9:J:38:ARG:HD3     | 1.89                     | 0.55              |
| 12:L:152:GLY:HA3  | 17:L:1504:BCR:H312 | 1.88                     | 0.55              |
| 4:b:534:LEU:HD23  | 4:b:593:THR:HG21   | 1.89                     | 0.55              |
| 4:N:488:VAL:HG23  | 4:N:493:TYR:HB3    | 1.88                     | 0.55              |
| 4:n:65:LEU:HD11   | 17:n:844:BCR:H281  | 1.88                     | 0.55              |
| 4:n:435:PHE:HZ    | 17:n:849:BCR:H372  | 1.71                     | 0.55              |
| 2:A:375:PRO:HG2   | 2:A:381:ALA:HB2    | 1.87                     | 0.55              |
| 2:a:441:LEU:HG    | 2:a:548:LEU:HB2    | 1.88                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:g:719:LEU:HB3   | 2:g:723:GLN:HG2   | 1.88                     | 0.55              |
| 2:A:434:ARG:HB2   | 2:A:555:LEU:HD13  | 1.89                     | 0.55              |
| 2:a:45:THR:HG22   | 2:a:715:GLN:HB2   | 1.88                     | 0.55              |
| 4:b:69:ALA:HB2    | 4:b:135:LEU:HB2   | 1.88                     | 0.55              |
| 2:G:733:LEU:HD12  | 18:G:849:LHG:H342 | 1.89                     | 0.55              |
| 14:G:824:CLA:HBA1 | 14:G:828:CLA:H191 | 1.89                     | 0.55              |
| 14:N:815:CLA:H11  | 17:N:845:BCR:H21C | 1.88                     | 0.55              |
| 8:S:100:ILE:HG12  | 14:S:203:CLA:C4D  | 2.36                     | 0.55              |
| 17:B:846:BCR:H272 | 17:B:847:BCR:H282 | 1.89                     | 0.55              |
| 14:b:830:CLA:H11  | 21:b:849:LMG:H301 | 1.87                     | 0.55              |
| 5:c:81:TYR:HB3    | 6:d:20:LEU:HD12   | 1.89                     | 0.55              |
| 2:G:682:PHE:HZ    | 14:G:839:CLA:HBC2 | 1.71                     | 0.55              |
| 6:Q:5:LEU:HB3     | 6:Q:57:LEU:HD11   | 1.89                     | 0.55              |
| 14:n:810:CLA:H93  | 17:w:201:BCR:HC42 | 1.89                     | 0.55              |
| 14:n:825:CLA:HAA2 | 14:n:826:CLA:OBD  | 2.07                     | 0.55              |
| 14:A:805:CLA:HED1 | 14:A:829:CLA:H2   | 1.89                     | 0.55              |
| 14:A:820:CLA:NB   | 14:A:826:CLA:C12  | 2.69                     | 0.55              |
| 12:L:99:ILE:HD12  | 12:L:151:ILE:HD13 | 1.88                     | 0.55              |
| 2:a:598:TRP:CZ2   | 14:a:853:CLA:HAB  | 2.42                     | 0.55              |
| 2:g:598:TRP:CZ2   | 14:g:853:CLA:HAB  | 2.42                     | 0.55              |
| 4:n:340:TRP:CH2   | 17:n:845:BCR:H20C | 2.42                     | 0.55              |
| 2:A:320:HIS:NE2   | 14:A:821:CLA:ND   | 2.55                     | 0.55              |
| 4:B:528:HIS:CD2   | 17:B:852:BCR:HC21 | 2.42                     | 0.55              |
| 5:C:62:PHE:CD2    | 6:D:120:ILE:HB    | 2.41                     | 0.55              |
| 14:b:828:CLA:HBC3 | 21:b:849:LMG:H442 | 1.89                     | 0.55              |
| 12:W:58:THR:HG23  | 12:W:61:ARG:H     | 1.70                     | 0.55              |
| 14:g:838:CLA:H92  | 17:n:849:BCR:H17C | 1.88                     | 0.55              |
| 4:n:701:LYS:HG3   | 14:n:839:CLA:HED2 | 1.89                     | 0.55              |
| 14:A:820:CLA:HBA2 | 14:A:826:CLA:H142 | 1.89                     | 0.55              |
| 14:B:808:CLA:HBB2 | 14:B:808:CLA:H142 | 1.88                     | 0.55              |
| 10:K:14:LEU:HD13  | 10:K:81:HIS:HB2   | 1.88                     | 0.55              |
| 14:b:835:CLA:HBB1 | 17:b:847:BCR:HC32 | 1.88                     | 0.55              |
| 14:g:817:CLA:HAB  | 14:g:817:CLA:H121 | 1.88                     | 0.55              |
| 14:A:802:CLA:H102 | 14:A:807:CLA:H172 | 1.88                     | 0.55              |
| 4:n:659:PHE:O     | 4:n:663:VAL:HG23  | 2.08                     | 0.54              |
| 8:f:48:THR:HG23   | 8:f:50:ASP:H      | 1.71                     | 0.54              |
| 17:W:206:BCR:H323 | 12:w:148:ILE:HG23 | 1.89                     | 0.54              |
| 17:n:849:BCR:H312 | 14:n:850:CLA:H52  | 1.90                     | 0.54              |
| 15:A:842:PQN:H141 | 14:F:201:CLA:HBB2 | 1.89                     | 0.54              |
| 14:B:833:CLA:H52  | 17:B:851:BCR:H312 | 1.89                     | 0.54              |
| 4:N:269:TRP:HB2   | 4:N:272:ASP:HB2   | 1.90                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:n:156:HIS:CE1   | 14:n:811:CLA:NA   | 2.75                     | 0.54              |
| 6:d:43:LEU:HD12   | 6:d:47:GLY:HA3    | 1.89                     | 0.54              |
| 6:q:120:ILE:HG22  | 7:r:14:GLU:HG3    | 1.89                     | 0.54              |
| 19:A:852:CL0:H14  | 14:B:804:CLA:C1A  | 2.37                     | 0.54              |
| 10:K:45:GLU:HG2   | 10:K:46:PRO:HD2   | 1.88                     | 0.54              |
| 2:G:678:PHE:HB2   | 14:N:803:CLA:HBA2 | 1.90                     | 0.54              |
| 14:N:815:CLA:H111 | 14:N:820:CLA:H92  | 1.88                     | 0.54              |
| 2:g:685:MET:HG3   | 14:g:852:CLA:C4C  | 2.38                     | 0.54              |
| 4:B:514:SER:HA    | 4:B:517:LEU:HD21  | 1.90                     | 0.54              |
| 2:a:350:HIS:HD2   | 2:a:408:HIS:HD1   | 1.56                     | 0.54              |
| 14:a:852:CLA:O2A  | 4:b:532:LEU:HD11  | 2.07                     | 0.54              |
| 4:b:393:HIS:HE1   | 14:b:830:CLA:NA   | 2.05                     | 0.54              |
| 4:N:592:ASN:HB2   | 14:N:803:CLA:HBC2 | 1.88                     | 0.54              |
| 2:g:215:GLY:HA3   | 14:g:813:CLA:HAB  | 1.89                     | 0.54              |
| 4:n:29:ASN:HD21   | 14:n:852:CLA:C1C  | 2.20                     | 0.54              |
| 4:n:142:LEU:HG    | 17:n:844:BCR:H382 | 1.88                     | 0.54              |
| 2:A:719:LEU:HB3   | 2:A:723:GLN:HG2   | 1.88                     | 0.54              |
| 4:B:351:TRP:CE2   | 14:B:827:CLA:HAA1 | 2.43                     | 0.54              |
| 4:B:707:LEU:HB3   | 4:B:711:GLN:HG2   | 1.89                     | 0.54              |
| 14:B:827:CLA:H13  | 17:B:847:BCR:H15C | 1.90                     | 0.54              |
| 2:G:441:LEU:HG    | 2:G:548:LEU:HB2   | 1.90                     | 0.54              |
| 2:G:584:CYS:HB2   | 4:N:674:TRP:HB3   | 1.90                     | 0.54              |
| 14:n:810:CLA:HAB  | 11:v:25:GLY:HA3   | 1.88                     | 0.54              |
| 14:A:855:CLA:CED  | 17:B:848:BCR:H401 | 2.28                     | 0.54              |
| 2:G:521:VAL:HG11  | 2:G:524:MET:HG2   | 1.89                     | 0.54              |
| 2:G:731:HIS:NE2   | 14:G:839:CLA:NB   | 2.56                     | 0.54              |
| 14:N:801:CLA:HBC1 | 15:N:843:PQN:H191 | 1.89                     | 0.54              |
| 7:R:25:ALA:HB3    | 7:R:37:ILE:HG13   | 1.89                     | 0.54              |
| 2:g:87:TRP:HA     | 14:g:805:CLA:HBB2 | 1.89                     | 0.54              |
| 5:C:29:VAL:HG12   | 6:D:110:ARG:HB3   | 1.90                     | 0.54              |
| 2:a:406:ALA:HB2   | 17:a:847:BCR:H323 | 1.89                     | 0.54              |
| 14:g:807:CLA:HBC2 | 4:n:450:PHE:HE1   | 1.72                     | 0.54              |
| 4:n:351:TRP:HE1   | 4:n:355:HIS:CE1   | 2.25                     | 0.54              |
| 14:n:806:CLA:H143 | 14:n:828:CLA:HBB2 | 1.90                     | 0.54              |
| 14:B:820:CLA:C4C  | 14:B:825:CLA:H141 | 2.31                     | 0.54              |
| 14:B:822:CLA:HBA1 | 17:B:843:BCR:H282 | 1.90                     | 0.54              |
| 7:E:43:VAL:HG12   | 7:E:49:ASN:HB3    | 1.88                     | 0.54              |
| 14:a:829:CLA:HMC1 | 14:a:837:CLA:HAB  | 1.90                     | 0.54              |
| 12:l:106:THR:HG21 | 12:l:147:LEU:HD12 | 1.89                     | 0.54              |
| 5:P:29:VAL:HG22   | 6:Q:110:ARG:HB3   | 1.89                     | 0.54              |
| 2:g:15:VAL:HG11   | 14:g:808:CLA:HAA2 | 1.88                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:430:VAL:HA    | 2:A:433:HIS:CE1   | 2.43                     | 0.54              |
| 2:A:465:LEU:HD22  | 4:B:96:PHE:HA     | 1.89                     | 0.54              |
| 14:B:838:CLA:H93  | 14:B:839:CLA:HBC1 | 1.89                     | 0.54              |
| 4:b:393:HIS:CE1   | 14:b:830:CLA:NA   | 2.76                     | 0.54              |
| 14:b:808:CLA:HHB  | 14:b:809:CLA:HMB3 | 1.90                     | 0.54              |
| 2:G:320:HIS:NE2   | 14:G:821:CLA:ND   | 2.56                     | 0.53              |
| 14:n:840:CLA:H42  | 15:n:841:PQN:H271 | 1.90                     | 0.53              |
| 2:A:197:MET:HE3   | 14:A:824:CLA:H143 | 1.89                     | 0.53              |
| 2:A:511:GLY:HA2   | 2:A:525:PRO:HG3   | 1.91                     | 0.53              |
| 17:I:101:BCR:H382 | 17:I:101:BCR:H23C | 1.89                     | 0.53              |
| 14:a:819:CLA:HAA2 | 14:a:823:CLA:HAB  | 1.90                     | 0.53              |
| 2:G:462:MET:HE1   | 2:G:467:ARG:HE    | 1.72                     | 0.53              |
| 2:G:734:LEU:HD11  | 17:G:848:BCR:HC8  | 1.90                     | 0.53              |
| 4:N:528:HIS:NE2   | 14:N:839:CLA:NB   | 2.56                     | 0.53              |
| 14:g:828:CLA:H18  | 14:g:839:CLA:H3A  | 1.91                     | 0.53              |
| 2:A:393:HIS:CE1   | 14:A:827:CLA:ND   | 2.75                     | 0.53              |
| 2:A:705:HIS:CE1   | 14:A:854:CLA:NA   | 2.76                     | 0.53              |
| 2:a:116:GLN:OE1   | 14:a:806:CLA:NB   | 2.41                     | 0.53              |
| 2:a:363:LEU:HD11  | 14:a:817:CLA:H71  | 1.89                     | 0.53              |
| 14:G:823:CLA:HHB  | 14:G:840:CLA:HBB1 | 1.90                     | 0.53              |
| 14:G:853:CLA:HBC2 | 17:N:852:BCR:H21C | 1.89                     | 0.53              |
| 4:n:379:HIS:NE2   | 14:n:828:CLA:ND   | 2.56                     | 0.53              |
| 2:A:204:VAL:HG13  | 17:A:846:BCR:H341 | 1.90                     | 0.53              |
| 14:A:807:CLA:H193 | 14:A:853:CLA:H191 | 1.90                     | 0.53              |
| 4:b:442:VAL:HG13  | 14:b:803:CLA:H62  | 1.91                     | 0.53              |
| 4:N:442:VAL:HG12  | 14:N:834:CLA:HAC1 | 1.91                     | 0.53              |
| 14:g:810:CLA:HBB1 | 14:g:818:CLA:HBC2 | 1.90                     | 0.53              |
| 8:s:132:ILE:HA    | 8:s:135:THR:HG22  | 1.90                     | 0.53              |
| 2:a:408:HIS:CE1   | 14:a:828:CLA:NA   | 2.76                     | 0.53              |
| 4:b:426:LEU:HD21  | 4:b:538:THR:HG22  | 1.88                     | 0.53              |
| 19:G:851:CL0:H14  | 14:N:804:CLA:C1A  | 2.38                     | 0.53              |
| 2:g:561:ARG:HD3   | 5:p:80:ALA:HB3    | 1.90                     | 0.53              |
| 14:g:853:CLA:H192 | 14:n:809:CLA:H51  | 1.90                     | 0.53              |
| 4:n:11:ASP:HB3    | 5:p:71:ALA:HB2    | 1.89                     | 0.53              |
| 2:a:333:PHE:HE2   | 12:l:36:PRO:HG2   | 1.74                     | 0.53              |
| 6:d:8:LYS:HB2     | 6:d:52:HIS:CE1    | 2.44                     | 0.53              |
| 2:G:57:HIS:CD2    | 14:G:804:CLA:HBB2 | 2.44                     | 0.53              |
| 2:G:300:ALA:HA    | 14:G:816:CLA:HMC2 | 1.91                     | 0.53              |
| 4:N:415:VAL:HA    | 4:N:418:HIS:CE1   | 2.44                     | 0.53              |
| 4:N:531:ALA:HB2   | 14:N:839:CLA:HMA1 | 1.91                     | 0.53              |
| 17:g:844:BCR:H372 | 17:g:845:BCR:H312 | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:559:SER:HB2   | 2:A:564:PRO:HA    | 1.90                     | 0.53              |
| 2:a:197:MET:HG2   | 14:a:823:CLA:HMD1 | 1.91                     | 0.53              |
| 4:b:528:HIS:CD2   | 17:b:852:BCR:HC21 | 2.44                     | 0.53              |
| 17:b:850:BCR:H10C | 14:f:202:CLA:HAB  | 1.90                     | 0.53              |
| 7:e:14:GLU:HA     | 8:f:163:PRO:HG3   | 1.90                     | 0.53              |
| 8:S:76:VAL:HG12   | 8:S:86:PHE:HB2    | 1.89                     | 0.53              |
| 2:g:429:ARG:HG2   | 2:g:432:ARG:NH2   | 2.24                     | 0.53              |
| 7:r:37:ILE:HG22   | 7:r:37:ILE:O      | 2.09                     | 0.53              |
| 7:r:39:ARG:HG2    | 7:r:50:THR:HG22   | 1.89                     | 0.53              |
| 14:A:825:CLA:HAA2 | 14:A:826:CLA:OBD  | 2.07                     | 0.53              |
| 4:B:415:VAL:HA    | 4:B:418:HIS:CE1   | 2.44                     | 0.53              |
| 2:a:412:PHE:CE2   | 17:a:846:BCR:HC32 | 2.44                     | 0.53              |
| 14:b:822:CLA:HBA1 | 17:b:843:BCR:H282 | 1.90                     | 0.53              |
| 14:b:826:CLA:H102 | 14:b:837:CLA:H121 | 1.91                     | 0.53              |
| 2:g:731:HIS:NE2   | 14:g:839:CLA:NB   | 2.57                     | 0.53              |
| 4:n:534:LEU:HD23  | 4:n:593:THR:HG21  | 1.91                     | 0.53              |
| 2:A:57:HIS:CD2    | 14:A:804:CLA:HBB2 | 2.44                     | 0.53              |
| 4:B:555:PRO:HB3   | 8:F:163:PRO:HG2   | 1.89                     | 0.53              |
| 2:a:458:HIS:O     | 2:a:462:MET:HG2   | 2.09                     | 0.53              |
| 2:G:370:HIS:NE2   | 14:G:826:CLA:NB   | 2.56                     | 0.53              |
| 14:G:852:CLA:HED2 | 17:N:852:BCR:H401 | 0.58                     | 0.53              |
| 4:n:174:ARG:HH11  | 14:n:805:CLA:H151 | 1.73                     | 0.53              |
| 4:n:341:HIS:CG    | 14:n:824:CLA:HAA1 | 2.44                     | 0.53              |
| 2:a:610:PHE:CE1   | 2:a:614:MET:HE2   | 2.44                     | 0.53              |
| 4:b:433:LEU:HB3   | 4:b:532:LEU:HB2   | 1.91                     | 0.53              |
| 4:n:319:PHE:HB2   | 14:n:823:CLA:HMA3 | 1.90                     | 0.53              |
| 14:B:816:CLA:H42  | 17:B:843:BCR:HC31 | 1.90                     | 0.53              |
| 14:a:852:CLA:HED3 | 4:b:539:LEU:HD23  | 1.86                     | 0.53              |
| 14:W:202:CLA:HBC1 | 20:w:202:SQD:H45  | 1.91                     | 0.52              |
| 2:g:486:TRP:CE2   | 2:g:490:LEU:HD11  | 2.43                     | 0.52              |
| 14:g:822:CLA:NC   | 17:g:846:BCR:H352 | 2.25                     | 0.52              |
| 17:w:201:BCR:C20  | 14:w:204:CLA:HAB  | 2.39                     | 0.52              |
| 2:A:203:GLN:HG2   | 2:A:309:GLY:HA3   | 1.90                     | 0.52              |
| 14:A:811:CLA:HAC2 | 14:A:811:CLA:H143 | 1.91                     | 0.52              |
| 2:a:413:MET:HG2   | 2:a:554:VAL:O     | 2.09                     | 0.52              |
| 4:b:341:HIS:CD2   | 14:b:825:CLA:HAA1 | 2.44                     | 0.52              |
| 4:n:608:ILE:HA    | 4:n:613:VAL:HG12  | 1.90                     | 0.52              |
| 8:f:161:VAL:HB    | 8:f:164:ARG:HH12  | 1.74                     | 0.52              |
| 10:k:48:LEU:HD12  | 10:k:48:LEU:H     | 1.74                     | 0.52              |
| 14:N:803:CLA:HHB  | 14:N:804:CLA:H18  | 1.90                     | 0.52              |
| 2:g:574:PRO:HB3   | 2:g:721:ILE:HB    | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:g:803:CLA:HBA1 | 14:g:811:CLA:HBA1 | 1.90                     | 0.52              |
| 14:g:854:CLA:H8   | 14:n:839:CLA:H93  | 1.92                     | 0.52              |
| 14:n:803:CLA:H62  | 14:n:803:CLA:H143 | 1.91                     | 0.52              |
| 14:b:826:CLA:HAA2 | 14:b:827:CLA:OBD  | 2.08                     | 0.52              |
| 14:g:831:CLA:HBB1 | 14:g:832:CLA:H2   | 1.90                     | 0.52              |
| 14:g:831:CLA:H101 | 14:n:840:CLA:H112 | 1.92                     | 0.52              |
| 2:A:121:ILE:HB    | 17:A:856:BCR:H322 | 1.90                     | 0.52              |
| 17:A:856:BCR:HC22 | 9:J:38:ARG:HD3    | 1.91                     | 0.52              |
| 4:B:659:PHE:O     | 4:B:663:VAL:HG23  | 2.10                     | 0.52              |
| 14:B:820:CLA:HAA2 | 14:B:825:CLA:HAB  | 1.92                     | 0.52              |
| 2:a:375:PRO:HG2   | 2:a:381:ALA:HB2   | 1.91                     | 0.52              |
| 14:a:826:CLA:H162 | 14:b:803:CLA:H121 | 1.90                     | 0.52              |
| 4:b:661:HIS:NE2   | 14:b:804:CLA:NB   | 2.57                     | 0.52              |
| 2:G:447:PHE:HE2   | 14:G:837:CLA:HAB  | 1.74                     | 0.52              |
| 2:g:197:MET:HE1   | 14:g:823:CLA:H142 | 1.92                     | 0.52              |
| 14:n:813:CLA:H43  | 17:n:843:BCR:H19C | 1.90                     | 0.52              |
| 2:A:523:MET:HE3   | 2:A:524:MET:N     | 2.23                     | 0.52              |
| 4:b:340:TRP:HE1   | 14:b:825:CLA:C2B  | 2.23                     | 0.52              |
| 4:b:514:SER:HA    | 4:b:517:LEU:HD21  | 1.91                     | 0.52              |
| 4:b:719:HIS:HE1   | 14:b:841:CLA:ND   | 2.07                     | 0.52              |
| 8:f:57:ARG:HD3    | 9:j:42:ASP:OD1    | 2.10                     | 0.52              |
| 8:f:117:THR:O     | 8:f:121:GLU:HG2   | 2.10                     | 0.52              |
| 3:H:21:ARG:HD2    | 18:S:202:LHG:H312 | 1.91                     | 0.52              |
| 14:N:828:CLA:H13  | 17:N:848:BCR:H351 | 1.91                     | 0.52              |
| 14:N:841:CLA:HAA1 | 17:W:205:BCR:H362 | 1.92                     | 0.52              |
| 2:g:77:HIS:NE2    | 14:g:803:CLA:ND   | 2.58                     | 0.52              |
| 14:g:804:CLA:H151 | 14:g:827:CLA:HBB2 | 1.90                     | 0.52              |
| 2:A:121:ILE:HG13  | 17:A:856:BCR:H313 | 1.92                     | 0.52              |
| 2:A:202:LEU:HA    | 2:A:206:LEU:HD12  | 1.91                     | 0.52              |
| 2:A:234:VAL:HA    | 2:A:237:ILE:HD12  | 1.90                     | 0.52              |
| 17:I:103:BCR:H383 | 12:L:109:LEU:HD21 | 1.91                     | 0.52              |
| 4:b:527:HIS:NE2   | 14:b:837:CLA:NC   | 2.58                     | 0.52              |
| 14:b:810:CLA:H13  | 14:b:841:CLA:H11  | 1.91                     | 0.52              |
| 4:N:661:HIS:NE2   | 14:N:804:CLA:NB   | 2.57                     | 0.52              |
| 14:B:840:CLA:H111 | 14:B:841:CLA:H141 | 1.90                     | 0.52              |
| 2:G:216:HIS:HE1   | 14:G:813:CLA:NA   | 2.07                     | 0.52              |
| 2:g:318:ILE:HD12  | 10:u:64:ALA:HB2   | 1.90                     | 0.52              |
| 2:g:320:HIS:NE2   | 14:g:820:CLA:ND   | 2.57                     | 0.52              |
| 2:g:652:TRP:HD1   | 14:n:803:CLA:HBC1 | 1.74                     | 0.52              |
| 4:B:426:LEU:HG    | 4:B:539:LEU:HB2   | 1.92                     | 0.52              |
| 9:J:17:THR:HG22   | 9:J:19:PRO:HD2    | 1.91                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:a:521:VAL:HG11  | 2:a:524:MET:HG2   | 1.92                     | 0.52              |
| 4:b:268:LEU:HB2   | 4:b:273:MET:HE2   | 1.92                     | 0.52              |
| 2:G:227:LEU:HB3   | 2:G:237:ILE:HD12  | 1.92                     | 0.52              |
| 2:G:430:VAL:HA    | 2:G:433:HIS:CE1   | 2.45                     | 0.52              |
| 14:G:829:CLA:H121 | 18:G:849:LHG:H361 | 1.91                     | 0.52              |
| 2:g:234:VAL:HA    | 2:g:237:ILE:HD12  | 1.90                     | 0.52              |
| 14:g:831:CLA:CAD  | 17:w:201:BCR:H21C | 2.39                     | 0.52              |
| 2:a:198:LEU:HD21  | 14:a:819:CLA:HMA2 | 1.92                     | 0.52              |
| 2:a:462:MET:HE1   | 14:a:832:CLA:C3D  | 2.40                     | 0.52              |
| 14:b:830:CLA:H111 | 14:b:841:CLA:HED1 | 1.92                     | 0.52              |
| 2:G:216:HIS:CE1   | 14:G:813:CLA:NA   | 2.78                     | 0.52              |
| 14:G:833:CLA:HED2 | 14:G:833:CLA:H2A  | 1.92                     | 0.52              |
| 10:U:36:ARG:HA    | 10:U:36:ARG:NE    | 2.24                     | 0.52              |
| 2:g:650:PHE:HA    | 2:g:654:GLN:HG3   | 1.91                     | 0.52              |
| 9:t:19:PRO:HB2    | 17:t:104:BCR:H391 | 1.91                     | 0.52              |
| 2:A:393:HIS:HE1   | 14:A:827:CLA:ND   | 2.08                     | 0.52              |
| 2:A:433:HIS:HA    | 6:D:16:THR:OG1    | 2.10                     | 0.52              |
| 14:A:840:CLA:HBB2 | 17:I:103:BCR:H372 | 1.92                     | 0.52              |
| 4:B:476:TYR:HA    | 8:F:25:GLY:HA2    | 1.92                     | 0.52              |
| 2:a:297:HIS:HD2   | 14:a:816:CLA:NA   | 2.07                     | 0.52              |
| 2:a:363:LEU:HD21  | 14:a:817:CLA:H93  | 1.92                     | 0.52              |
| 2:a:705:HIS:HE1   | 14:a:838:CLA:ND   | 2.08                     | 0.52              |
| 2:g:470:ASP:HB3   | 14:g:832:CLA:HED2 | 1.93                     | 0.51              |
| 4:n:381:TYR:O     | 4:n:384:ILE:HG13  | 2.10                     | 0.51              |
| 2:A:205:LEU:HD13  | 14:A:812:CLA:HHB  | 1.92                     | 0.51              |
| 4:B:26:ALA:HA     | 14:B:830:CLA:H43  | 1.91                     | 0.51              |
| 2:a:262:THR:HG22  | 2:a:263:PRO:HD3   | 1.92                     | 0.51              |
| 2:G:212:GLY:HA2   | 14:G:814:CLA:HBB2 | 1.92                     | 0.51              |
| 4:N:174:ARG:HB3   | 14:N:826:CLA:HMD1 | 1.91                     | 0.51              |
| 2:g:531:ALA:HA    | 2:g:534:LEU:HD12  | 1.92                     | 0.51              |
| 4:B:193:HIS:HB2   | 14:B:815:CLA:C1C  | 2.41                     | 0.51              |
| 2:a:121:ILE:HG23  | 2:a:122:VAL:HG22  | 1.91                     | 0.51              |
| 14:b:828:CLA:H3A  | 14:b:828:CLA:CGA  | 2.40                     | 0.51              |
| 14:b:841:CLA:H193 | 17:i:101:BCR:H271 | 1.92                     | 0.51              |
| 9:j:35:GLU:HG3    | 14:j:101:CLA:CHB  | 2.41                     | 0.51              |
| 5:P:28:MET:HE3    | 5:P:38:GLN:HB2    | 1.92                     | 0.51              |
| 6:Q:32:THR:HG22   | 6:Q:57:LEU:HG     | 1.91                     | 0.51              |
| 14:g:829:CLA:HMC3 | 14:g:837:CLA:HAB  | 1.93                     | 0.51              |
| 14:n:830:CLA:HMC2 | 17:n:845:BCR:H272 | 1.90                     | 0.51              |
| 4:B:459:ILE:HB    | 4:B:524:PHE:CE2   | 2.44                     | 0.51              |
| 10:K:35:GLY:O     | 10:K:39:ILE:HG13  | 2.10                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:K:70:HIS:NE2   | 14:K:101:CLA:NC   | 2.58                     | 0.51              |
| 2:G:433:HIS:CE1   | 2:G:437:ILE:HD11  | 2.46                     | 0.51              |
| 2:G:605:ILE:HD12  | 19:G:851:CL0:H53  | 1.92                     | 0.51              |
| 14:G:853:CLA:HED2 | 4:N:424:SER:HB2   | 1.93                     | 0.51              |
| 4:N:343:ALA:HB2   | 17:N:848:BCR:H372 | 1.93                     | 0.51              |
| 2:g:267:LEU:HD11  | 10:u:74:VAL:HG13  | 1.93                     | 0.51              |
| 2:g:305:PHE:HZ    | 14:g:817:CLA:H122 | 1.76                     | 0.51              |
| 2:g:399:GLY:HA3   | 2:g:603:LEU:HD11  | 1.92                     | 0.51              |
| 2:g:401:LEU:HD21  | 14:g:804:CLA:H142 | 1.91                     | 0.51              |
| 14:g:816:CLA:HBC1 | 14:g:819:CLA:H18  | 1.92                     | 0.51              |
| 14:g:831:CLA:H51  | 14:g:854:CLA:HBC2 | 1.91                     | 0.51              |
| 12:w:144:SER:O    | 12:w:148:ILE:HG13 | 2.10                     | 0.51              |
| 4:B:433:LEU:HB3   | 4:B:532:LEU:HB2   | 1.92                     | 0.51              |
| 6:D:63:LYS:HE3    | 6:D:95:ILE:HD12   | 1.92                     | 0.51              |
| 11:I:26:TRP:CZ2   | 17:I:102:BCR:H323 | 2.46                     | 0.51              |
| 14:b:811:CLA:ND   | 17:i:102:BCR:H332 | 2.25                     | 0.51              |
| 2:G:43:PRO:HG3    | 8:S:122:ILE:HD13  | 1.93                     | 0.51              |
| 4:N:276:HIS:HB2   | 14:N:819:CLA:CHB  | 2.41                     | 0.51              |
| 14:N:821:CLA:C4C  | 14:N:826:CLA:H141 | 2.38                     | 0.51              |
| 14:N:833:CLA:HAC1 | 14:N:840:CLA:HBC3 | 1.92                     | 0.51              |
| 10:U:73:GLY:HA2   | 10:U:76:LEU:HD12  | 1.92                     | 0.51              |
| 12:W:73:PHE:CZ    | 14:W:203:CLA:HBB1 | 2.40                     | 0.51              |
| 2:g:305:PHE:HE1   | 14:g:819:CLA:HHC  | 1.75                     | 0.51              |
| 14:n:802:CLA:HBB  | 14:n:803:CLA:H192 | 1.92                     | 0.51              |
| 14:n:808:CLA:H121 | 14:n:808:CLA:H2   | 1.92                     | 0.51              |
| 2:A:363:LEU:HD11  | 14:A:818:CLA:H102 | 1.92                     | 0.51              |
| 2:a:451:HIS:HE1   | 14:a:831:CLA:NA   | 2.08                     | 0.51              |
| 12:l:105:PHE:HB3  | 17:l:205:BCR:H401 | 1.93                     | 0.51              |
| 12:W:167:ILE:HG13 | 12:w:96:LEU:HD21  | 1.92                     | 0.51              |
| 2:g:297:HIS:HB2   | 14:g:816:CLA:CHB  | 2.40                     | 0.51              |
| 14:g:854:CLA:HMD3 | 17:n:847:BCR:H383 | 1.92                     | 0.51              |
| 4:n:80:ASP:HB3    | 4:n:84:VAL:HG23   | 1.92                     | 0.51              |
| 4:n:565:PRO:HB3   | 4:n:709:ILE:HB    | 1.93                     | 0.51              |
| 2:A:194:VAL:HG11  | 14:A:824:CLA:HAC2 | 1.92                     | 0.51              |
| 4:B:182:LEU:HD13  | 14:B:814:CLA:HBB  | 1.92                     | 0.51              |
| 2:a:657:GLN:HG2   | 2:a:750:SER:HB2   | 1.92                     | 0.51              |
| 4:b:638:LEU:HD22  | 4:b:731:PHE:HA    | 1.93                     | 0.51              |
| 14:G:801:CLA:HBB2 | 14:N:805:CLA:HAA1 | 1.93                     | 0.51              |
| 4:N:62:SER:HB2    | 4:N:142:LEU:HB3   | 1.93                     | 0.51              |
| 2:g:57:HIS:CD2    | 14:g:803:CLA:HBB2 | 2.46                     | 0.51              |
| 2:g:363:LEU:HD21  | 14:g:817:CLA:H102 | 1.93                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:A:481:PRO:HG3   | 2:A:533:PHE:HB2   | 1.93                     | 0.51              |
| 2:A:659:ILE:HD12  | 4:B:628:ARG:HG3   | 1.93                     | 0.51              |
| 4:B:528:HIS:HE1   | 14:B:838:CLA:ND   | 2.08                     | 0.51              |
| 2:a:87:TRP:HA     | 14:a:805:CLA:HBB2 | 1.93                     | 0.51              |
| 2:a:146:GLN:HB3   | 2:a:377:TYR:HB3   | 1.92                     | 0.51              |
| 4:b:436:HIS:HB3   | 17:b:852:BCR:H312 | 1.92                     | 0.51              |
| 2:G:93:PHE:CG     | 14:G:806:CLA:HBC3 | 2.45                     | 0.51              |
| 4:N:154:TRP:CD1   | 13:Y:29:GLU:HG3   | 2.46                     | 0.51              |
| 4:n:669:MET:HB2   | 14:n:804:CLA:C1C  | 2.41                     | 0.51              |
| 2:A:305:PHE:HE1   | 14:A:820:CLA:HHC  | 1.75                     | 0.51              |
| 14:A:832:CLA:HBB1 | 14:A:833:CLA:H2   | 1.93                     | 0.51              |
| 2:a:544:HIS:NE2   | 14:a:837:CLA:NA   | 2.59                     | 0.51              |
| 4:b:592:ASN:HB2   | 14:b:803:CLA:HBC2 | 1.91                     | 0.51              |
| 5:c:19:ARG:HG2    | 6:d:104:GLU:HG2   | 1.93                     | 0.51              |
| 5:c:58:CYS:HB3    | 5:c:63:LEU:HD22   | 1.91                     | 0.51              |
| 14:G:825:CLA:HAB  | 17:G:847:BCR:H311 | 1.92                     | 0.51              |
| 4:N:652:VAL:HG11  | 14:N:810:CLA:HAC1 | 1.92                     | 0.51              |
| 14:g:836:CLA:H191 | 14:w:204:CLA:H102 | 1.92                     | 0.51              |
| 4:n:89:HIS:CE1    | 4:n:114:ASN:HD22  | 2.29                     | 0.51              |
| 4:B:495:ASN:HD21  | 14:B:835:CLA:HED2 | 1.75                     | 0.51              |
| 17:B:843:BCR:HC41 | 17:B:845:BCR:H322 | 1.93                     | 0.51              |
| 11:I:24:ILE:HD11  | 17:I:101:BCR:HC42 | 1.93                     | 0.51              |
| 2:a:459:ASN:HB3   | 2:a:642:THR:HG22  | 1.93                     | 0.51              |
| 14:g:803:CLA:H42  | 14:g:804:CLA:HBB1 | 1.92                     | 0.51              |
| 17:A:849:BCR:H21C | 14:A:853:CLA:H13  | 1.93                     | 0.51              |
| 2:a:50:TRP:HE1    | 14:f:201:CLA:HBB1 | 1.76                     | 0.51              |
| 14:b:802:CLA:H141 | 17:l:205:BCR:H17C | 1.91                     | 0.51              |
| 2:G:685:MET:HE3   | 15:G:841:PQN:H2M1 | 1.93                     | 0.50              |
| 4:N:299:HIS:CE1   | 14:N:823:CLA:NA   | 2.79                     | 0.50              |
| 4:N:565:PRO:HB3   | 4:N:709:ILE:HB    | 1.92                     | 0.50              |
| 8:S:116:ASP:HB2   | 8:S:119:GLN:HB3   | 1.93                     | 0.50              |
| 2:g:95:GLY:HA3    | 2:g:148:TRP:CH2   | 2.46                     | 0.50              |
| 14:g:816:CLA:H13  | 14:g:833:CLA:H43  | 1.92                     | 0.50              |
| 14:n:804:CLA:H61  | 14:n:840:CLA:HBB2 | 1.92                     | 0.50              |
| 17:n:845:BCR:H392 | 17:n:846:BCR:H23C | 1.93                     | 0.50              |
| 9:t:31:GLY:HA3    | 14:t:101:CLA:HAB  | 1.93                     | 0.50              |
| 4:B:196:HIS:CE1   | 14:B:816:CLA:NA   | 2.79                     | 0.50              |
| 2:a:215:GLY:HA3   | 14:a:813:CLA:HAB  | 1.92                     | 0.50              |
| 2:a:247:LYS:O     | 2:a:251:ILE:HG12  | 2.11                     | 0.50              |
| 4:b:56:ILE:HD11   | 17:m:102:BCR:HC7  | 1.94                     | 0.50              |
| 14:f:201:CLA:H41  | 14:f:202:CLA:HBC1 | 1.93                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 14:N:831:CLA:O1D   | 14:N:831:CLA:H2A  | 2.11                     | 0.50              |
| 14:N:835:CLA:H2    | 14:N:836:CLA:HMB1 | 1.94                     | 0.50              |
| 14:g:821:CLA:H93   | 14:g:821:CLA:HBC3 | 1.93                     | 0.50              |
| 14:g:830:CLA:HBC2  | 14:g:837:CLA:HMC2 | 1.94                     | 0.50              |
| 4:n:106:GLN:HG3    | 4:n:115:ILE:HD11  | 1.93                     | 0.50              |
| 4:n:343:ALA:HB2    | 17:n:846:BCR:H372 | 1.93                     | 0.50              |
| 4:n:394:GLY:HA3    | 17:n:846:BCR:H382 | 1.93                     | 0.50              |
| 4:B:104:PHE:CZ     | 4:B:652:VAL:HG23  | 2.47                     | 0.50              |
| 12:L:57:LEU:HD22   | 12:L:61:ARG:HG2   | 1.93                     | 0.50              |
| 2:a:533:PHE:HA     | 14:a:836:CLA:HED1 | 1.92                     | 0.50              |
| 4:b:432:PHE:CZ     | 17:b:852:BCR:HC41 | 2.46                     | 0.50              |
| 4:N:193:HIS:CE1    | 14:N:816:CLA:NA   | 2.79                     | 0.50              |
| 4:N:439:GLY:HA3    | 14:N:834:CLA:HAB  | 1.93                     | 0.50              |
| 4:N:526:VAL:HG11   | 4:N:600:TYR:HB2   | 1.94                     | 0.50              |
| 14:N:810:CLA:O1A   | 14:N:829:CLA:HBD  | 2.11                     | 0.50              |
| 2:g:657:GLN:O      | 2:g:661:SER:HB3   | 2.12                     | 0.50              |
| 2:g:695:GLN:O      | 2:g:699:GLU:HG3   | 2.12                     | 0.50              |
| 2:A:296:HIS:CE1    | 14:A:816:CLA:NA   | 2.79                     | 0.50              |
| 14:b:808:CLA:H62   | 17:i:101:BCR:HC32 | 1.93                     | 0.50              |
| 14:b:809:CLA:O1A   | 14:b:828:CLA:HBD  | 2.11                     | 0.50              |
| 14:G:853:CLA:H71   | 14:N:851:CLA:H11  | 1.92                     | 0.50              |
| 5:P:59:PRO:HA      | 7:R:48:ILE:HD13   | 1.94                     | 0.50              |
| 14:g:811:CLA:H122  | 17:g:845:BCR:H353 | 1.92                     | 0.50              |
| 15:g:841:PQN:H172  | 17:n:849:BCR:H382 | 1.94                     | 0.50              |
| 14:n:839:CLA:H142  | 17:w:201:BCR:H10C | 1.93                     | 0.50              |
| 14:A:811:CLA:HBC1  | 14:A:812:CLA:H143 | 1.93                     | 0.50              |
| 3:X:21:ARG:HB3     | 20:B:801:SQD:H45  | 1.93                     | 0.50              |
| 4:B:193:HIS:CE1    | 14:B:815:CLA:NA   | 2.79                     | 0.50              |
| 4:B:434:GLY:HA2    | 4:B:532:LEU:HD22  | 1.92                     | 0.50              |
| 14:B:828:CLA:O1D   | 14:B:829:CLA:HHB  | 2.11                     | 0.50              |
| 14:L:1501:CLA:HBC1 | 20:l:201:SQD:H45  | 1.93                     | 0.50              |
| 5:c:55:GLU:O       | 5:c:63:LEU:HD13   | 2.10                     | 0.50              |
| 2:G:678:PHE:CG     | 17:G:848:BCR:H363 | 2.46                     | 0.50              |
| 3:H:18:TYR:CZ      | 18:S:202:LHG:H271 | 2.47                     | 0.50              |
| 18:g:850:LHG:H351  | 18:g:850:LHG:H122 | 1.94                     | 0.50              |
| 2:A:523:MET:HE3    | 2:A:524:MET:H     | 1.76                     | 0.50              |
| 4:b:276:HIS:HB2    | 14:b:818:CLA:C1B  | 2.41                     | 0.50              |
| 11:i:35:PHE:HD1    | 20:l:201:SQD:H92  | 1.75                     | 0.50              |
| 4:N:65:LEU:HD11    | 17:N:846:BCR:H281 | 1.93                     | 0.50              |
| 17:g:843:BCR:H23C  | 10:u:68:PHE:HB2   | 1.94                     | 0.50              |
| 10:u:24:MET:HE1    | 10:u:70:HIS:HA    | 1.94                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 4:B:597:VAL:HG21   | 14:B:837:CLA:HAB  | 1.94                     | 0.50              |
| 2:a:57:HIS:CD2     | 14:a:803:CLA:HBB2 | 2.47                     | 0.50              |
| 14:a:811:CLA:H41   | 17:a:845:BCR:H19C | 1.92                     | 0.50              |
| 4:b:123:TRP:CH2    | 14:b:829:CLA:H2   | 2.47                     | 0.50              |
| 4:b:426:LEU:HD13   | 14:b:839:CLA:HBB1 | 1.93                     | 0.50              |
| 14:N:820:CLA:HAB   | 14:N:820:CLA:H8   | 1.94                     | 0.50              |
| 2:g:305:PHE:CE1    | 14:g:819:CLA:HAB  | 2.46                     | 0.50              |
| 2:A:737:ILE:HG23   | 14:A:827:CLA:HAB  | 1.94                     | 0.50              |
| 4:B:142:LEU:HG     | 17:B:845:BCR:H382 | 1.93                     | 0.50              |
| 4:B:167:TRP:CZ2    | 14:B:814:CLA:HAC2 | 2.47                     | 0.50              |
| 14:B:826:CLA:HMB1  | 14:B:839:CLA:HBA1 | 1.93                     | 0.50              |
| 4:n:275:HIS:CE1    | 14:n:816:CLA:NA   | 2.79                     | 0.50              |
| 2:A:200:HIS:CE1    | 14:A:811:CLA:NA   | 2.80                     | 0.50              |
| 14:A:831:CLA:OBD   | 12:L:35:THR:HG21  | 2.11                     | 0.50              |
| 14:A:853:CLA:CGA   | 14:A:853:CLA:H3A  | 2.42                     | 0.50              |
| 4:b:462:VAL:HG21   | 8:f:77:ASP:HB3    | 1.93                     | 0.50              |
| 6:d:7:GLY:HA2      | 6:d:55:GLU:HG2    | 1.93                     | 0.50              |
| 2:G:92:ILE:HD13    | 2:G:162:THR:HG22  | 1.94                     | 0.50              |
| 2:G:672:MET:SD     | 14:G:827:CLA:H141 | 2.51                     | 0.50              |
| 8:S:140:PRO:O      | 8:S:144:VAL:HG22  | 2.12                     | 0.50              |
| 2:A:92:ILE:HG21    | 2:A:162:THR:HB    | 1.93                     | 0.50              |
| 14:B:814:CLA:H111  | 14:B:819:CLA:H92  | 1.93                     | 0.50              |
| 14:G:833:CLA:H72   | 17:W:201:BCR:H353 | 1.94                     | 0.49              |
| 4:N:299:HIS:NE2    | 14:N:823:CLA:ND   | 2.59                     | 0.49              |
| 4:N:436:HIS:HB2    | 17:N:853:BCR:HC42 | 1.93                     | 0.49              |
| 4:N:440:LEU:HD22   | 17:N:853:BCR:H311 | 1.94                     | 0.49              |
| 14:N:815:CLA:H43   | 17:N:845:BCR:H19C | 1.94                     | 0.49              |
| 4:n:275:HIS:HB3    | 14:n:817:CLA:HMB2 | 1.94                     | 0.49              |
| 7:r:32:ILE:HG22    | 7:r:34:TYR:H      | 1.77                     | 0.49              |
| 3:X:20:PHE:HD2     | 20:B:801:SQD:H441 | 1.76                     | 0.49              |
| 4:B:526:VAL:HG11   | 4:B:600:TYR:HB2   | 1.94                     | 0.49              |
| 17:L:1504:BCR:H321 | 12:l:148:ILE:HG23 | 1.94                     | 0.49              |
| 4:b:191:ALA:O      | 4:b:195:ILE:HG22  | 2.11                     | 0.49              |
| 2:G:119:TRP:HB3    | 17:T:104:BCR:H323 | 1.94                     | 0.49              |
| 10:U:80:LEU:HB3    | 10:U:85:ARG:HB2   | 1.93                     | 0.49              |
| 2:g:180:HIS:CE1    | 14:g:808:CLA:NA   | 2.80                     | 0.49              |
| 2:g:506:VAL:HG23   | 14:g:816:CLA:HBA2 | 1.94                     | 0.49              |
| 2:g:584:CYS:HB2    | 4:n:674:TRP:HB3   | 1.93                     | 0.49              |
| 8:F:144:VAL:O      | 8:F:148:LEU:HD22  | 2.12                     | 0.49              |
| 14:a:838:CLA:HBC2  | 17:b:850:BCR:H21C | 1.94                     | 0.49              |
| 14:a:839:CLA:HAC1  | 15:a:841:PQN:H172 | 1.94                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:T:28:ILE:HA      | 14:T:101:CLA:HBB2 | 1.94                     | 0.49              |
| 2:g:451:HIS:CE1    | 14:g:831:CLA:NA   | 2.80                     | 0.49              |
| 2:g:740:THR:HG23   | 14:g:826:CLA:HBB2 | 1.93                     | 0.49              |
| 4:n:522:GLY:O      | 4:n:526:VAL:HG23  | 2.11                     | 0.49              |
| 2:A:313:ARG:HH12   | 2:A:321:SER:HB3   | 1.76                     | 0.49              |
| 14:A:831:CLA:H52   | 14:L:1502:CLA:H62 | 1.92                     | 0.49              |
| 14:a:801:CLA:HBB2  | 14:a:809:CLA:H122 | 1.94                     | 0.49              |
| 14:a:829:CLA:HAB   | 14:a:837:CLA:HBB2 | 1.93                     | 0.49              |
| 14:b:820:CLA:H11   | 14:b:824:CLA:H12  | 1.95                     | 0.49              |
| 14:b:827:CLA:H143  | 17:b:846:BCR:H17C | 1.93                     | 0.49              |
| 14:G:805:CLA:H202  | 14:G:827:CLA:HMD1 | 1.94                     | 0.49              |
| 14:G:824:CLA:H42   | 14:G:828:CLA:H193 | 1.93                     | 0.49              |
| 4:N:15:ASP:HB3     | 4:N:20:ARG:HB2    | 1.94                     | 0.49              |
| 2:g:43:PRO:HG3     | 8:s:122:ILE:HD13  | 1.92                     | 0.49              |
| 2:g:322:ILE:HG23   | 14:g:819:CLA:HED2 | 1.94                     | 0.49              |
| 2:g:585:GLN:HG3    | 4:n:674:TRP:HB2   | 1.94                     | 0.49              |
| 14:g:805:CLA:H72   | 14:g:807:CLA:H92  | 1.94                     | 0.49              |
| 14:g:853:CLA:HBB1  | 14:g:853:CLA:HMB3 | 1.95                     | 0.49              |
| 20:h:1702:SQD:H262 | 14:n:830:CLA:H71  | 1.94                     | 0.49              |
| 4:n:231:GLY:HA2    | 14:n:816:CLA:HAA2 | 1.93                     | 0.49              |
| 4:n:514:SER:HA     | 4:n:517:LEU:HD21  | 1.93                     | 0.49              |
| 4:n:669:MET:HB2    | 14:n:804:CLA:C4C  | 2.43                     | 0.49              |
| 7:r:9:ARG:HB3      | 7:r:59:ILE:HG23   | 1.94                     | 0.49              |
| 2:A:652:TRP:CD1    | 14:B:804:CLA:HBC1 | 2.42                     | 0.49              |
| 2:A:678:PHE:CG     | 17:A:849:BCR:H363 | 2.46                     | 0.49              |
| 4:B:255:LEU:HD23   | 4:B:275:HIS:HA    | 1.93                     | 0.49              |
| 17:I:103:BCR:H23C  | 12:L:109:LEU:HG   | 1.95                     | 0.49              |
| 2:a:396:TRP:CD1    | 14:a:826:CLA:HAB  | 2.47                     | 0.49              |
| 4:b:532:LEU:HD21   | 14:b:803:CLA:HBB1 | 1.93                     | 0.49              |
| 2:G:121:ILE:O      | 2:G:124:GLN:HG2   | 2.13                     | 0.49              |
| 14:N:818:CLA:C1D   | 14:N:819:CLA:HBB2 | 2.42                     | 0.49              |
| 2:g:322:ILE:HG21   | 14:g:823:CLA:HAC1 | 1.95                     | 0.49              |
| 14:g:853:CLA:C1B   | 14:n:804:CLA:HBB1 | 2.39                     | 0.49              |
| 8:s:31:CYS:SG      | 8:s:66:CYS:HB2    | 2.52                     | 0.49              |
| 7:E:12:ARG:HG2     | 7:E:14:GLU:HG2    | 1.94                     | 0.49              |
| 2:a:307:ILE:HD13   | 17:a:843:BCR:H17C | 1.94                     | 0.49              |
| 14:a:819:CLA:H171  | 14:a:819:CLA:H101 | 1.94                     | 0.49              |
| 14:a:831:CLA:H3A   | 17:i:101:BCR:H272 | 1.95                     | 0.49              |
| 15:a:841:PQN:H111  | 17:b:850:BCR:H393 | 1.94                     | 0.49              |
| 14:a:852:CLA:O2A   | 14:b:803:CLA:HBB2 | 2.13                     | 0.49              |
| 4:b:92:TRP:HB2     | 14:b:808:CLA:HED1 | 1.94                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:G:843:BCR:H19C | 10:U:71:ILE:HD11   | 1.94                     | 0.49              |
| 14:G:852:CLA:H3A  | 14:G:852:CLA:CGA   | 2.42                     | 0.49              |
| 14:G:852:CLA:CBA  | 4:N:431:LEU:HD23   | 2.40                     | 0.49              |
| 14:N:803:CLA:HMA3 | 14:N:804:CLA:H71   | 1.94                     | 0.49              |
| 5:P:15:THR:HG22   | 5:P:28:MET:HG3     | 1.94                     | 0.49              |
| 5:P:43:PRO:HA     | 6:Q:113:VAL:HG11   | 1.94                     | 0.49              |
| 2:g:204:VAL:CB    | 14:g:811:CLA:HAB   | 2.41                     | 0.49              |
| 3:h:28:LEU:HD21   | 20:h:1702:SQD:H311 | 1.94                     | 0.49              |
| 8:s:100:ILE:HD13  | 14:s:202:CLA:C1D   | 2.40                     | 0.49              |
| 2:A:53:HIS:CE1    | 14:A:802:CLA:NA    | 2.81                     | 0.49              |
| 14:B:837:CLA:HMB1 | 14:B:837:CLA:HBB1  | 1.95                     | 0.49              |
| 14:a:836:CLA:H201 | 14:l:203:CLA:H71   | 1.94                     | 0.49              |
| 4:b:156:HIS:CE1   | 14:b:812:CLA:NA    | 2.80                     | 0.49              |
| 4:b:193:HIS:CE1   | 14:b:815:CLA:NA    | 2.81                     | 0.49              |
| 10:k:18:PRO:O     | 10:k:22:ILE:HG12   | 2.12                     | 0.49              |
| 10:U:45:GLU:HG2   | 10:U:46:PRO:HD2    | 1.95                     | 0.49              |
| 4:n:176:ASN:ND2   | 4:n:291:TYR:HB2    | 2.27                     | 0.49              |
| 14:n:808:CLA:O1A  | 14:n:827:CLA:HBD   | 2.13                     | 0.49              |
| 11:v:37:PHE:HD2   | 12:w:111:LEU:HD22  | 1.78                     | 0.49              |
| 12:w:20:VAL:HG12  | 12:w:36:PRO:HD3    | 1.94                     | 0.49              |
| 12:w:105:PHE:HB3  | 17:w:206:BCR:H401  | 1.95                     | 0.49              |
| 4:b:436:HIS:NE2   | 14:b:833:CLA:NC    | 2.61                     | 0.49              |
| 4:b:554:MET:SD    | 4:b:557:LYS:HG3    | 2.52                     | 0.49              |
| 2:G:320:HIS:CE1   | 14:G:821:CLA:NA    | 2.80                     | 0.49              |
| 14:N:835:CLA:HBA2 | 14:N:836:CLA:HMB2  | 1.95                     | 0.49              |
| 17:W:201:BCR:H332 | 14:W:203:CLA:H2    | 1.94                     | 0.49              |
| 2:g:26:PHE:O      | 9:t:10:TYR:HB3     | 2.13                     | 0.49              |
| 14:n:819:CLA:ND   | 14:n:824:CLA:H141  | 2.27                     | 0.49              |
| 14:n:837:CLA:H121 | 14:n:837:CLA:HMC2  | 1.95                     | 0.49              |
| 8:s:38:GLN:O      | 8:s:42:LYS:HG2     | 2.12                     | 0.49              |
| 4:B:432:PHE:CZ    | 17:B:852:BCR:HC41  | 2.48                     | 0.49              |
| 5:C:39:VAL:HG22   | 5:C:40:ALA:H       | 1.78                     | 0.49              |
| 4:N:183:PHE:HB3   | 4:N:284:PHE:CD2    | 2.47                     | 0.49              |
| 4:N:393:HIS:HE1   | 14:N:831:CLA:NA    | 2.11                     | 0.49              |
| 4:N:528:HIS:HE1   | 14:N:839:CLA:ND    | 2.10                     | 0.49              |
| 14:N:811:CLA:H13  | 14:N:842:CLA:H43   | 1.95                     | 0.49              |
| 14:N:817:CLA:H42  | 17:N:844:BCR:HC31  | 1.95                     | 0.49              |
| 2:g:451:HIS:HE1   | 14:g:831:CLA:NA    | 2.10                     | 0.49              |
| 14:g:807:CLA:HAB  | 14:n:850:CLA:HMD2  | 1.94                     | 0.49              |
| 4:n:180:ALA:HB1   | 14:n:820:CLA:HAC2  | 1.94                     | 0.49              |
| 4:n:434:GLY:HA2   | 4:n:532:LEU:HD22   | 1.95                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:w:50:LEU:HD13   | 14:w:204:CLA:HBD   | 1.95                     | 0.49              |
| 2:A:667:SER:HB2    | 4:B:449:ALA:HB1    | 1.93                     | 0.49              |
| 14:A:853:CLA:HMD3  | 4:B:540:ILE:HG12   | 1.94                     | 0.49              |
| 4:B:57:ILE:HG23    | 14:B:807:CLA:HMC2  | 1.94                     | 0.49              |
| 14:B:832:CLA:HBA2  | 14:B:832:CLA:H3A   | 1.57                     | 0.49              |
| 14:a:819:CLA:H203  | 14:a:825:CLA:H152  | 1.95                     | 0.49              |
| 11:i:35:PHE:CE2    | 18:m:101:LHG:H272  | 2.48                     | 0.49              |
| 2:G:75:ALA:HB2     | 2:G:181:TYR:HB2    | 1.94                     | 0.49              |
| 2:G:360:LEU:HD12   | 14:G:804:CLA:HED3  | 1.95                     | 0.49              |
| 4:N:435:PHE:CZ     | 17:N:852:BCR:H20C  | 2.47                     | 0.49              |
| 4:N:523:ASP:OD2    | 4:N:604:LYS:HE2    | 2.13                     | 0.49              |
| 7:R:12:ARG:HB3     | 7:R:15:SER:HB2     | 1.93                     | 0.49              |
| 8:S:57:ARG:HD3     | 9:T:42:ASP:OD1     | 2.13                     | 0.49              |
| 14:n:837:CLA:H141  | 14:n:837:CLA:H162  | 1.65                     | 0.49              |
| 4:B:156:HIS:CE1    | 14:B:812:CLA:NA    | 2.80                     | 0.49              |
| 10:K:77:VAL:HG13   | 10:K:78:LEU:HD22   | 1.94                     | 0.49              |
| 12:L:64:LEU:O      | 12:L:68:MET:HG3    | 2.13                     | 0.49              |
| 1:1:229:ASN:O      | 1:1:233:ILE:HG13   | 2.12                     | 0.48              |
| 2:G:305:PHE:CE2    | 14:G:820:CLA:HAB   | 2.48                     | 0.48              |
| 4:N:310:PHE:HD1    | 14:N:824:CLA:HBA2  | 1.78                     | 0.48              |
| 4:n:193:HIS:CE1    | 14:n:814:CLA:NA    | 2.81                     | 0.48              |
| 4:n:299:HIS:NE2    | 14:n:821:CLA:ND    | 2.61                     | 0.48              |
| 2:A:582:GLY:HA3    | 4:B:675:ARG:HD3    | 1.94                     | 0.48              |
| 4:B:419:LYS:HE3    | 4:B:546:LEU:HB3    | 1.95                     | 0.48              |
| 12:L:78:PHE:HB3    | 12:L:94:GLY:HA2    | 1.95                     | 0.48              |
| 4:b:269:TRP:HB2    | 4:b:272:ASP:HB2    | 1.94                     | 0.48              |
| 12:l:64:LEU:O      | 12:l:68:MET:HG3    | 2.13                     | 0.48              |
| 2:G:738:ALA:HB2    | 17:G:848:BCR:H322  | 1.95                     | 0.48              |
| 3:H:20:PHE:HD2     | 20:H:1702:SQD:H441 | 1.78                     | 0.48              |
| 4:N:393:HIS:CE1    | 14:N:831:CLA:NA    | 2.81                     | 0.48              |
| 4:N:443:HIS:ND1    | 14:N:834:CLA:ND    | 2.60                     | 0.48              |
| 4:N:659:PHE:O      | 4:N:663:VAL:HG23   | 2.13                     | 0.48              |
| 2:g:112:ARG:HD2    | 2:g:139:GLN:HE22   | 1.78                     | 0.48              |
| 4:n:425:HIS:O      | 4:n:429:VAL:HG23   | 2.13                     | 0.48              |
| 4:n:555:PRO:HD2    | 5:p:62:PHE:CZ      | 2.49                     | 0.48              |
| 7:r:10:ILE:HG22    | 7:r:12:ARG:H       | 1.77                     | 0.48              |
| 14:A:853:CLA:H92   | 4:B:438:LEU:HD23   | 1.95                     | 0.48              |
| 14:X:1701:CLA:HBA2 | 17:F:203:BCR:H393  | 1.95                     | 0.48              |
| 4:B:652:VAL:HG22   | 14:B:810:CLA:HHH   | 1.95                     | 0.48              |
| 2:a:458:HIS:CE1    | 2:a:462:MET:HE3    | 2.48                     | 0.48              |
| 14:a:828:CLA:H102  | 14:a:839:CLA:HAA2  | 1.95                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:a:846:BCR:H372  | 18:a:850:LHG:H142  | 1.95                     | 0.48              |
| 14:h:1701:CLA:HBC1 | 20:h:1702:SQD:H212 | 1.96                     | 0.48              |
| 4:n:340:TRP:HE1    | 14:n:824:CLA:C2B   | 2.26                     | 0.48              |
| 2:a:289:LEU:HD21   | 2:a:374:MET:HB3    | 1.94                     | 0.48              |
| 5:P:17:CYS:HB3     | 16:P:102:SF4:S4    | 2.53                     | 0.48              |
| 12:W:80:LYS:HG2    | 14:W:204:CLA:HMA1  | 1.95                     | 0.48              |
| 2:g:407:ALA:HB2    | 2:g:592:VAL:HG11   | 1.95                     | 0.48              |
| 2:A:731:HIS:NE2    | 14:A:839:CLA:NB    | 2.62                     | 0.48              |
| 4:B:461:PRO:HB3    | 4:B:524:PHE:HB2    | 1.96                     | 0.48              |
| 4:B:661:HIS:NE2    | 14:B:804:CLA:NB    | 2.61                     | 0.48              |
| 4:b:91:ILE:HB      | 4:b:112:PRO:HB2    | 1.95                     | 0.48              |
| 4:b:476:TYR:HD1    | 8:f:26:ALA:H       | 1.61                     | 0.48              |
| 4:b:624:MET:HA     | 4:b:624:MET:HE2    | 1.95                     | 0.48              |
| 4:b:700:TRP:CD1    | 4:b:704:PRO:HD3    | 2.48                     | 0.48              |
| 14:b:823:CLA:H93   | 14:b:823:CLA:HBB1  | 1.95                     | 0.48              |
| 12:l:109:LEU:HG    | 17:l:205:BCR:H24C  | 1.95                     | 0.48              |
| 2:G:333:PHE:HE2    | 12:W:36:PRO:HG2    | 1.77                     | 0.48              |
| 14:G:852:CLA:HBB1  | 14:N:803:CLA:NB    | 2.28                     | 0.48              |
| 11:v:40:ILE:HG13   | 11:v:41:GLU:OE1    | 2.13                     | 0.48              |
| 4:B:435:PHE:HZ     | 17:B:851:BCR:H372  | 1.78                     | 0.48              |
| 2:a:180:HIS:CE1    | 14:a:808:CLA:NA    | 2.81                     | 0.48              |
| 2:a:451:HIS:CE1    | 14:a:831:CLA:NA    | 2.82                     | 0.48              |
| 18:a:850:LHG:H141  | 18:a:850:LHG:H362  | 1.96                     | 0.48              |
| 14:b:810:CLA:H112  | 14:b:828:CLA:H192  | 1.96                     | 0.48              |
| 2:G:501:ASN:HB2    | 14:G:835:CLA:HED2  | 1.95                     | 0.48              |
| 4:N:195:ILE:HD13   | 14:N:817:CLA:HAC1  | 1.96                     | 0.48              |
| 4:N:638:LEU:HD22   | 4:N:731:PHE:HA     | 1.96                     | 0.48              |
| 2:g:214:ALA:O      | 2:g:218:ILE:HG13   | 2.14                     | 0.48              |
| 4:n:173:SER:HA     | 4:n:293:THR:HG22   | 1.96                     | 0.48              |
| 4:n:391:PHE:HB2    | 4:n:541:LEU:HD22   | 1.94                     | 0.48              |
| 14:n:836:CLA:HBB1  | 14:n:836:CLA:HMB1  | 1.96                     | 0.48              |
| 2:A:215:GLY:HA3    | 14:A:814:CLA:HAB   | 1.96                     | 0.48              |
| 2:A:537:HIS:CE1    | 14:A:837:CLA:ND    | 2.80                     | 0.48              |
| 14:B:830:CLA:H102  | 21:B:849:LMG:H401  | 1.94                     | 0.48              |
| 2:a:297:HIS:C      | 2:a:297:HIS:HD1    | 2.21                     | 0.48              |
| 14:a:831:CLA:H102  | 14:b:840:CLA:H52   | 1.95                     | 0.48              |
| 2:G:320:HIS:NE2    | 14:G:821:CLA:NA    | 2.62                     | 0.48              |
| 14:N:805:CLA:H143  | 14:N:805:CLA:H111  | 1.70                     | 0.48              |
| 4:n:375:LEU:HD11   | 14:n:828:CLA:HED3  | 1.94                     | 0.48              |
| 4:n:669:MET:HE2    | 14:n:804:CLA:C4B   | 2.38                     | 0.48              |
| 10:u:32:ILE:HA     | 10:u:65:THR:HG21   | 1.95                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:B:287:ALA:HB2    | 14:B:820:CLA:HBC2  | 1.95                     | 0.48              |
| 2:a:95:GLY:HA3     | 2:a:148:TRP:CH2    | 2.49                     | 0.48              |
| 18:a:850:LHG:H102  | 18:a:850:LHG:H131  | 1.65                     | 0.48              |
| 20:x:1702:SQD:H331 | 20:x:1702:SQD:H362 | 1.55                     | 0.48              |
| 11:V:34:SER:HB2    | 12:W:111:LEU:HD21  | 1.96                     | 0.48              |
| 2:g:127:LEU:HD11   | 14:g:807:CLA:HBC3  | 1.95                     | 0.48              |
| 14:g:824:CLA:H2    | 14:g:824:CLA:H62   | 1.67                     | 0.48              |
| 4:n:174:ARG:HB2    | 14:n:813:CLA:HBC2  | 1.96                     | 0.48              |
| 4:n:471:HIS:NE2    | 14:n:833:CLA:NA    | 2.61                     | 0.48              |
| 8:s:30:PRO:HB2     | 8:s:33:GLU:HG2     | 1.96                     | 0.48              |
| 14:A:831:CLA:H51   | 12:L:47:ILE:HD11   | 1.95                     | 0.48              |
| 4:B:167:TRP:CZ2    | 14:B:812:CLA:HHB   | 2.49                     | 0.48              |
| 4:B:446:VAL:HG21   | 14:B:833:CLA:HAC2  | 1.96                     | 0.48              |
| 4:B:565:PRO:HB3    | 4:B:709:ILE:HD12   | 1.94                     | 0.48              |
| 2:a:201:HIS:O      | 2:a:205:LEU:HB3    | 2.14                     | 0.48              |
| 2:a:679:VAL:HG11   | 2:a:734:LEU:HD23   | 1.95                     | 0.48              |
| 14:b:825:CLA:H71   | 14:b:827:CLA:H42   | 1.96                     | 0.48              |
| 14:l:204:CLA:H3A   | 14:l:204:CLA:HBA1  | 1.57                     | 0.48              |
| 2:G:220:VAL:HG13   | 2:G:240:PRO:HB3    | 1.95                     | 0.48              |
| 14:G:822:CLA:H3A   | 14:G:822:CLA:HBA2  | 1.64                     | 0.48              |
| 4:N:136:TYR:HE1    | 13:Y:12:ALA:HB2    | 1.78                     | 0.48              |
| 4:N:446:VAL:HG21   | 14:N:834:CLA:HAC2  | 1.96                     | 0.48              |
| 14:N:830:CLA:H3A   | 14:N:830:CLA:HBA2  | 1.52                     | 0.48              |
| 2:g:458:HIS:CE1    | 14:g:832:CLA:NA    | 2.82                     | 0.48              |
| 14:g:833:CLA:H2    | 17:g:847:BCR:H381  | 1.95                     | 0.48              |
| 4:n:436:HIS:HB2    | 17:n:851:BCR:HC42  | 1.96                     | 0.48              |
| 2:A:142:SER:HA     | 14:A:827:CLA:HMA2  | 1.95                     | 0.48              |
| 2:A:410:ALA:O      | 2:A:414:VAL:HG22   | 2.14                     | 0.48              |
| 14:A:838:CLA:H52   | 17:A:848:BCR:H14C  | 1.95                     | 0.48              |
| 4:B:276:HIS:O      | 4:B:280:ILE:HG12   | 2.14                     | 0.48              |
| 20:B:801:SQD:H131  | 20:B:801:SQD:H161  | 1.58                     | 0.48              |
| 10:K:29:VAL:HA     | 10:K:32:ILE:HG22   | 1.95                     | 0.48              |
| 14:a:826:CLA:H92   | 14:a:826:CLA:H41   | 1.96                     | 0.48              |
| 2:g:36:ASP:HB3     | 2:g:39:LEU:HD12    | 1.95                     | 0.48              |
| 2:g:442:ASN:O      | 2:g:446:ILE:HG13   | 2.14                     | 0.48              |
| 4:n:12:LEU:HD22    | 4:n:20:ARG:HA      | 1.96                     | 0.48              |
| 11:v:37:PHE:HB2    | 17:w:206:BCR:H12C  | 1.96                     | 0.48              |
| 2:A:438:ILE:HG13   | 2:A:556:PHE:HE2    | 1.78                     | 0.48              |
| 4:B:599:PHE:HB3    | 4:B:626:TRP:HZ3    | 1.78                     | 0.48              |
| 2:a:53:HIS:CE1     | 14:a:801:CLA:ND    | 2.81                     | 0.48              |
| 2:a:739:THR:HG21   | 19:a:851:CL0:H6    | 1.95                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 14:a:836:CLA:H111  | 14:a:836:CLA:H152 | 1.46                     | 0.48              |
| 4:b:694:ILE:HD11   | 12:l:47:ILE:HD12  | 1.96                     | 0.48              |
| 1:l:228:LEU:HD11   | 13:m:11:ILE:HD11  | 1.96                     | 0.47              |
| 2:G:658:VAL:HG22   | 2:G:670:GLY:HA2   | 1.95                     | 0.47              |
| 14:N:831:CLA:H142  | 21:N:850:LMG:H221 | 1.96                     | 0.47              |
| 14:g:826:CLA:H41   | 14:g:826:CLA:H61  | 1.65                     | 0.47              |
| 4:B:319:PHE:CD2    | 14:B:823:CLA:HAB  | 2.49                     | 0.47              |
| 5:C:62:PHE:CG      | 5:C:62:PHE:O      | 2.66                     | 0.47              |
| 4:b:156:HIS:HE1    | 14:b:812:CLA:NA   | 2.11                     | 0.47              |
| 14:b:802:CLA:HAC2  | 17:b:848:BCR:H381 | 1.95                     | 0.47              |
| 14:N:826:CLA:H71   | 14:N:828:CLA:H42  | 1.97                     | 0.47              |
| 14:N:839:CLA:H93   | 14:N:840:CLA:HBC1 | 1.95                     | 0.47              |
| 4:n:711:GLN:HB2    | 21:n:848:LMG:H111 | 1.95                     | 0.47              |
| 14:n:804:CLA:H143  | 14:n:840:CLA:H18  | 1.95                     | 0.47              |
| 10:u:34:PHE:O      | 10:u:38:THR:HG23  | 2.13                     | 0.47              |
| 2:A:86:ILE:HG12    | 2:A:170:ALA:HB1   | 1.96                     | 0.47              |
| 2:A:180:HIS:CE1    | 14:A:809:CLA:NA   | 2.82                     | 0.47              |
| 2:A:622:VAL:HG22   | 2:A:628:VAL:HG22  | 1.95                     | 0.47              |
| 4:B:29:ASN:HD21    | 14:B:805:CLA:C1C  | 2.27                     | 0.47              |
| 4:B:698:VAL:HG11   | 17:I:103:BCR:H371 | 1.96                     | 0.47              |
| 14:B:827:CLA:H72   | 14:B:827:CLA:H111 | 1.46                     | 0.47              |
| 2:a:216:HIS:HB2    | 14:a:812:CLA:CHC  | 2.44                     | 0.47              |
| 2:a:267:LEU:HD21   | 10:k:74:VAL:HG22  | 1.95                     | 0.47              |
| 2:a:393:HIS:HE2    | 14:a:827:CLA:C1B  | 2.27                     | 0.47              |
| 20:x:1702:SQD:H121 | 14:b:831:CLA:H43  | 1.96                     | 0.47              |
| 14:b:833:CLA:HBB2  | 17:b:850:BCR:HC31 | 1.94                     | 0.47              |
| 17:b:852:BCR:H383  | 14:j:102:CLA:C2D  | 2.44                     | 0.47              |
| 2:G:149:ARG:HH22   | 2:G:379:TYR:HE2   | 1.63                     | 0.47              |
| 4:N:334:LEU:HD21   | 14:N:807:CLA:H192 | 1.96                     | 0.47              |
| 4:N:656:MET:HE2    | 17:N:849:BCR:H333 | 1.95                     | 0.47              |
| 2:g:622:VAL:HG22   | 2:g:628:VAL:HG22  | 1.95                     | 0.47              |
| 2:A:705:HIS:NE2    | 14:A:854:CLA:NB   | 2.62                     | 0.47              |
| 2:A:738:ALA:HB2    | 17:A:849:BCR:H322 | 1.96                     | 0.47              |
| 14:B:809:CLA:H202  | 14:B:828:CLA:H192 | 1.96                     | 0.47              |
| 14:b:808:CLA:HMB2  | 17:i:101:BCR:H313 | 1.96                     | 0.47              |
| 20:l:201:SQD:H131  | 20:l:201:SQD:H162 | 1.60                     | 0.47              |
| 2:G:374:MET:SD     | 14:G:817:CLA:HBD  | 2.54                     | 0.47              |
| 2:G:410:ALA:O      | 2:G:414:VAL:HG23  | 2.15                     | 0.47              |
| 14:G:803:CLA:HBA1  | 14:G:803:CLA:H3A  | 1.61                     | 0.47              |
| 17:G:845:BCR:H341  | 17:G:845:BCR:H11C | 1.79                     | 0.47              |
| 19:G:851:CL0:H2    | 19:G:851:CL0:H15  | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:g:430:VAL:HA    | 2:g:433:HIS:CE1   | 2.49                     | 0.47              |
| 14:g:804:CLA:H41  | 14:g:828:CLA:H92  | 1.95                     | 0.47              |
| 8:s:31:CYS:HB2    | 8:s:62:SER:HA     | 1.96                     | 0.47              |
| 4:B:80:ASP:HB3    | 4:B:84:VAL:HG23   | 1.97                     | 0.47              |
| 2:a:624:ALA:HB3   | 2:a:627:ASN:HD21  | 1.78                     | 0.47              |
| 14:a:807:CLA:H112 | 14:a:807:CLA:H152 | 1.67                     | 0.47              |
| 14:b:814:CLA:H172 | 17:b:844:BCR:H271 | 1.96                     | 0.47              |
| 14:b:827:CLA:H161 | 17:b:847:BCR:H17C | 1.97                     | 0.47              |
| 5:c:77:MET:HE3    | 5:c:77:MET:HB3    | 1.81                     | 0.47              |
| 2:G:463:ARG:HD2   | 4:N:642:TYR:HD2   | 1.79                     | 0.47              |
| 2:G:535:ILE:HG13  | 2:G:539:HIS:CE1   | 2.50                     | 0.47              |
| 14:N:807:CLA:HBA1 | 14:N:807:CLA:H3A  | 1.39                     | 0.47              |
| 2:g:648:ARG:O     | 2:g:652:TRP:HB3   | 2.14                     | 0.47              |
| 14:g:830:CLA:H111 | 14:g:830:CLA:H151 | 1.54                     | 0.47              |
| 14:g:852:CLA:H91  | 14:g:852:CLA:H111 | 1.71                     | 0.47              |
| 2:A:394:HIS:NE2   | 14:A:828:CLA:ND   | 2.62                     | 0.47              |
| 4:B:305:MET:HE2   | 4:B:323:HIS:HB3   | 1.95                     | 0.47              |
| 4:B:355:HIS:CE1   | 14:B:827:CLA:NB   | 2.83                     | 0.47              |
| 4:b:652:VAL:HG21  | 14:b:809:CLA:HAC1 | 1.97                     | 0.47              |
| 4:b:669:MET:CG    | 14:b:805:CLA:NC   | 2.69                     | 0.47              |
| 2:G:310:HIS:CE1   | 17:G:843:BCR:H363 | 2.49                     | 0.47              |
| 2:G:453:PHE:CE1   | 14:G:801:CLA:HHB  | 2.49                     | 0.47              |
| 14:G:820:CLA:HBB1 | 14:G:820:CLA:HMB3 | 1.97                     | 0.47              |
| 17:G:844:BCR:H372 | 17:G:845:BCR:H312 | 1.95                     | 0.47              |
| 4:N:693:PRO:C     | 4:N:695:ALA:H     | 2.22                     | 0.47              |
| 2:g:334:THR:HA    | 14:g:829:CLA:OBD  | 2.14                     | 0.47              |
| 17:g:846:BCR:H351 | 17:g:846:BCR:H15C | 1.58                     | 0.47              |
| 4:n:663:VAL:HG22  | 14:n:840:CLA:HMB3 | 1.97                     | 0.47              |
| 4:n:717:LEU:O     | 4:n:721:THR:HG23  | 2.13                     | 0.47              |
| 2:A:408:HIS:HE1   | 14:A:829:CLA:C4A  | 2.28                     | 0.47              |
| 14:A:820:CLA:NB   | 14:A:826:CLA:H122 | 2.29                     | 0.47              |
| 2:a:216:HIS:CE1   | 14:a:812:CLA:NA   | 2.82                     | 0.47              |
| 14:a:816:CLA:HBC1 | 14:a:819:CLA:H18  | 1.96                     | 0.47              |
| 14:a:826:CLA:H192 | 17:j:103:BCR:H14C | 1.97                     | 0.47              |
| 17:a:844:BCR:H15C | 17:a:844:BCR:H351 | 1.78                     | 0.47              |
| 4:b:434:GLY:HA2   | 4:b:532:LEU:HD22  | 1.97                     | 0.47              |
| 2:G:539:HIS:HE1   | 2:G:609:HIS:ND1   | 2.12                     | 0.47              |
| 2:G:677:HIS:NE2   | 19:G:851:CL0:NA   | 2.62                     | 0.47              |
| 14:G:834:CLA:H62  | 14:U:102:CLA:H43  | 1.96                     | 0.47              |
| 4:N:426:LEU:HD11  | 4:N:538:THR:HG22  | 1.95                     | 0.47              |
| 14:N:814:CLA:H3A  | 14:N:814:CLA:HBA2 | 1.57                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:V:101:BCR:H341 | 17:V:101:BCR:H11C | 1.70                     | 0.47              |
| 12:W:50:LEU:HD13  | 14:W:203:CLA:HBD  | 1.96                     | 0.47              |
| 2:g:94:HIS:CE1    | 14:g:805:CLA:NA   | 2.82                     | 0.47              |
| 2:g:119:TRP:CD2   | 14:g:807:CLA:HED2 | 2.49                     | 0.47              |
| 2:g:263:PRO:HB3   | 2:g:268:ASN:HB3   | 1.96                     | 0.47              |
| 2:g:363:LEU:HD11  | 14:g:817:CLA:H72  | 1.95                     | 0.47              |
| 14:g:806:CLA:HBB1 | 17:t:103:BCR:H363 | 1.96                     | 0.47              |
| 14:n:815:CLA:H42  | 17:n:842:BCR:HC31 | 1.95                     | 0.47              |
| 14:n:818:CLA:H3A  | 14:n:818:CLA:HBA2 | 1.45                     | 0.47              |
| 2:A:75:ALA:HB2    | 2:A:181:TYR:HB2   | 1.97                     | 0.47              |
| 2:A:374:MET:HE2   | 2:A:506:VAL:HG22  | 1.97                     | 0.47              |
| 2:A:441:LEU:HD21  | 2:A:547:VAL:HG12  | 1.96                     | 0.47              |
| 14:A:854:CLA:H193 | 8:F:103:VAL:HG12  | 1.95                     | 0.47              |
| 4:B:436:HIS:HB2   | 17:B:852:BCR:HC42 | 1.96                     | 0.47              |
| 4:B:476:TYR:HD1   | 8:F:26:ALA:H      | 1.63                     | 0.47              |
| 4:B:488:VAL:HG23  | 4:B:493:TYR:HB3   | 1.97                     | 0.47              |
| 14:B:805:CLA:H91  | 17:M:101:BCR:H12C | 1.96                     | 0.47              |
| 14:B:809:CLA:O1A  | 14:B:828:CLA:HBD  | 2.15                     | 0.47              |
| 13:M:27:ALA:HB2   | 17:M:101:BCR:H332 | 1.96                     | 0.47              |
| 2:a:506:VAL:HG13  | 14:a:816:CLA:HBA2 | 1.97                     | 0.47              |
| 14:a:831:CLA:H93  | 14:b:841:CLA:H171 | 1.96                     | 0.47              |
| 3:x:18:TYR:HB3    | 3:x:21:ARG:HD2    | 1.97                     | 0.47              |
| 4:b:663:VAL:HG13  | 4:b:719:HIS:HD2   | 1.78                     | 0.47              |
| 4:b:669:MET:HB2   | 14:b:805:CLA:CHC  | 2.44                     | 0.47              |
| 17:b:852:BCR:H21C | 9:j:43:LEU:HD22   | 1.97                     | 0.47              |
| 2:G:202:LEU:HA    | 2:G:206:LEU:HD12  | 1.96                     | 0.47              |
| 2:G:408:HIS:HA    | 2:G:411:ILE:HD12  | 1.95                     | 0.47              |
| 14:G:804:CLA:H143 | 17:G:844:BCR:HC41 | 1.96                     | 0.47              |
| 14:G:831:CLA:H62  | 14:G:831:CLA:H41  | 1.81                     | 0.47              |
| 4:n:26:ALA:HA     | 14:n:829:CLA:H43  | 1.97                     | 0.47              |
| 4:n:719:HIS:CE1   | 14:n:840:CLA:ND   | 2.82                     | 0.47              |
| 14:A:825:CLA:CHB  | 14:A:838:CLA:HAA2 | 2.45                     | 0.47              |
| 14:A:835:CLA:H3A  | 14:A:835:CLA:HBA2 | 1.58                     | 0.47              |
| 14:B:833:CLA:H2   | 17:B:851:BCR:H333 | 1.97                     | 0.47              |
| 14:B:833:CLA:H93  | 14:B:833:CLA:H62  | 1.78                     | 0.47              |
| 8:F:76:VAL:HG12   | 8:F:86:PHE:HB2    | 1.96                     | 0.47              |
| 10:K:51:ALA:HA    | 10:K:54:PHE:HD2   | 1.80                     | 0.47              |
| 14:a:802:CLA:H62  | 14:a:807:CLA:H201 | 1.97                     | 0.47              |
| 14:a:805:CLA:H42  | 14:j:101:CLA:HAC1 | 1.97                     | 0.47              |
| 14:a:854:CLA:HHC  | 10:k:76:LEU:HD23  | 1.97                     | 0.47              |
| 4:b:193:HIS:HB2   | 14:b:815:CLA:C1C  | 2.45                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:b:355:HIS:HE1   | 14:b:827:CLA:C1B  | 2.28                     | 0.47              |
| 8:f:88:ILE:HD12   | 14:j:102:CLA:HMB3 | 1.97                     | 0.47              |
| 2:G:393:HIS:CE1   | 14:G:827:CLA:ND   | 2.83                     | 0.47              |
| 2:G:719:LEU:HB3   | 2:G:723:GLN:HG2   | 1.97                     | 0.47              |
| 4:n:322:PRO:HB2   | 4:n:410:ASN:HA    | 1.97                     | 0.47              |
| 14:n:804:CLA:H143 | 14:n:804:CLA:H111 | 1.71                     | 0.47              |
| 14:n:808:CLA:HAB  | 14:n:809:CLA:HBA1 | 1.96                     | 0.47              |
| 14:n:810:CLA:H91  | 14:n:810:CLA:H112 | 1.77                     | 0.47              |
| 2:A:330:LYS:HA    | 2:A:337:GLY:HA3   | 1.96                     | 0.47              |
| 4:B:195:ILE:HA    | 4:B:199:ILE:HD12  | 1.97                     | 0.47              |
| 4:B:584:TYR:HD1   | 4:B:717:LEU:HD22  | 1.80                     | 0.47              |
| 4:B:594:VAL:HA    | 4:B:597:VAL:HG12  | 1.96                     | 0.47              |
| 17:B:847:BCR:H11C | 17:B:847:BCR:H341 | 1.75                     | 0.47              |
| 5:C:15:THR:HG22   | 5:C:28:MET:HE3    | 1.97                     | 0.47              |
| 6:D:119:SER:HB3   | 6:D:122:GLU:HG3   | 1.96                     | 0.47              |
| 7:E:8:VAL:HG11    | 7:E:58:LEU:HD23   | 1.95                     | 0.47              |
| 2:a:552:LYS:HE3   | 4:b:677:TYR:CE1   | 2.50                     | 0.47              |
| 14:a:853:CLA:H91  | 14:b:805:CLA:H121 | 1.97                     | 0.47              |
| 4:b:436:HIS:CE1   | 14:b:833:CLA:ND   | 2.83                     | 0.47              |
| 2:G:486:TRP:CE2   | 2:G:490:LEU:HD11  | 2.50                     | 0.47              |
| 4:N:596:TRP:CD1   | 14:N:804:CLA:H122 | 2.50                     | 0.47              |
| 4:N:694:ILE:HD12  | 14:W:203:CLA:H42  | 1.96                     | 0.47              |
| 4:n:5:PHE:CD2     | 11:v:40:ILE:HG22  | 2.50                     | 0.47              |
| 4:n:276:HIS:CE1   | 14:n:817:CLA:ND   | 2.82                     | 0.47              |
| 2:A:28:LYS:HB3    | 14:A:810:CLA:HAA2 | 1.95                     | 0.47              |
| 2:A:458:HIS:CE1   | 14:A:833:CLA:NA   | 2.83                     | 0.47              |
| 14:A:830:CLA:H12  | 12:L:37:VAL:HG23  | 1.95                     | 0.47              |
| 18:A:851:LHG:H302 | 18:A:851:LHG:H271 | 1.78                     | 0.47              |
| 2:a:329:HIS:HE1   | 14:a:821:CLA:C4D  | 2.28                     | 0.47              |
| 14:a:821:CLA:HBA2 | 14:a:821:CLA:H3A  | 1.44                     | 0.47              |
| 14:b:811:CLA:HBA1 | 12:l:83:PRO:HG2   | 1.97                     | 0.47              |
| 2:G:393:HIS:HE2   | 14:G:828:CLA:C1B  | 2.28                     | 0.46              |
| 4:N:50:HIS:HE1    | 14:N:807:CLA:H161 | 1.80                     | 0.46              |
| 8:S:111:ILE:HG22  | 8:S:128:ILE:HD11  | 1.96                     | 0.46              |
| 2:g:264:PHE:HZ    | 17:g:843:BCR:H343 | 1.78                     | 0.46              |
| 2:g:267:LEU:HG    | 10:u:77:VAL:HG21  | 1.96                     | 0.46              |
| 2:g:521:VAL:HG22  | 2:g:622:VAL:HG23  | 1.98                     | 0.46              |
| 4:n:284:PHE:CE1   | 14:n:819:CLA:HAB  | 2.50                     | 0.46              |
| 14:n:808:CLA:H112 | 14:n:827:CLA:H93  | 1.96                     | 0.46              |
| 7:r:27:VAL:HG12   | 7:r:29:GLN:OE1    | 2.15                     | 0.46              |
| 2:A:77:HIS:NE2    | 14:A:804:CLA:ND   | 2.63                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:A:108:PRO:HG3    | 2:A:149:ARG:HH12  | 1.80                     | 0.46              |
| 14:B:806:CLA:H202  | 14:B:806:CLA:H161 | 1.77                     | 0.46              |
| 2:a:374:MET:SD     | 14:a:816:CLA:HBD  | 2.56                     | 0.46              |
| 2:a:408:HIS:HA     | 2:a:411:ILE:HD12  | 1.97                     | 0.46              |
| 14:a:803:CLA:HBA1  | 14:a:811:CLA:HBA1 | 1.98                     | 0.46              |
| 4:b:275:HIS:HB3    | 14:b:818:CLA:HMB2 | 1.96                     | 0.46              |
| 4:b:417:GLN:HA     | 8:f:164:ARG:HE    | 1.79                     | 0.46              |
| 2:G:94:HIS:CE1     | 14:G:806:CLA:NA   | 2.83                     | 0.46              |
| 2:G:694:TRP:O      | 2:G:698:ILE:HG12  | 2.15                     | 0.46              |
| 14:N:812:CLA:H8    | 17:W:201:BCR:H281 | 1.98                     | 0.46              |
| 14:N:820:CLA:H3A   | 14:N:820:CLA:HBA2 | 1.43                     | 0.46              |
| 2:g:224:ILE:O      | 2:g:228:MET:HG3   | 2.14                     | 0.46              |
| 14:g:801:CLA:H2    | 14:g:801:CLA:HED2 | 1.96                     | 0.46              |
| 14:g:807:CLA:H122  | 17:t:103:BCR:H272 | 1.97                     | 0.46              |
| 4:n:432:PHE:CZ     | 17:n:851:BCR:HC41 | 2.50                     | 0.46              |
| 17:n:846:BCR:H11C  | 17:n:846:BCR:H341 | 1.74                     | 0.46              |
| 2:A:282:LEU:HD21   | 2:A:375:PRO:HD2   | 1.96                     | 0.46              |
| 2:A:297:HIS:HB2    | 14:A:817:CLA:C1B  | 2.45                     | 0.46              |
| 2:A:372:TYR:CZ     | 14:A:836:CLA:HBC3 | 2.50                     | 0.46              |
| 14:A:811:CLA:H91   | 14:A:811:CLA:H112 | 1.66                     | 0.46              |
| 14:X:1701:CLA:HBA1 | 14:X:1701:CLA:H3A | 1.50                     | 0.46              |
| 14:B:807:CLA:H111  | 14:B:807:CLA:H151 | 1.78                     | 0.46              |
| 14:B:807:CLA:HBA1  | 14:B:807:CLA:H11  | 1.38                     | 0.46              |
| 17:I:102:BCR:H393  | 14:L:1502:CLA:H51 | 1.98                     | 0.46              |
| 2:a:388:LEU:HD23   | 2:a:748:ILE:HG21  | 1.97                     | 0.46              |
| 14:b:806:CLA:H62   | 14:b:814:CLA:H62  | 1.96                     | 0.46              |
| 2:G:53:HIS:CE1     | 14:G:802:CLA:ND   | 2.82                     | 0.46              |
| 4:n:276:HIS:HB2    | 14:n:817:CLA:C1B  | 2.45                     | 0.46              |
| 2:A:121:ILE:O      | 2:A:124:GLN:HG2   | 2.15                     | 0.46              |
| 2:A:318:ILE:HD12   | 10:K:64:ALA:HB2   | 1.98                     | 0.46              |
| 14:A:830:CLA:HAB   | 14:A:838:CLA:HBB2 | 1.98                     | 0.46              |
| 4:B:257:PHE:CE2    | 14:B:818:CLA:HBB1 | 2.50                     | 0.46              |
| 4:B:638:LEU:HD22   | 4:B:731:PHE:HA    | 1.96                     | 0.46              |
| 14:B:821:CLA:HBA2  | 14:B:821:CLA:H3A  | 1.44                     | 0.46              |
| 17:B:844:BCR:H11C  | 17:B:844:BCR:H341 | 1.84                     | 0.46              |
| 14:a:839:CLA:H192  | 14:f:202:CLA:HBB1 | 1.97                     | 0.46              |
| 18:a:850:LHG:H342  | 18:a:850:LHG:H132 | 1.97                     | 0.46              |
| 10:k:14:LEU:HB2    | 10:k:81:HIS:CD2   | 2.50                     | 0.46              |
| 18:m:101:LHG:H192  | 18:m:101:LHG:H311 | 1.96                     | 0.46              |
| 2:G:239:LEU:HB2    | 2:G:242:GLU:HG3   | 1.97                     | 0.46              |
| 2:G:442:ASN:ND2    | 4:N:685:LEU:HD21  | 2.30                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:N:814:CLA:H93  | 17:N:845:BCR:H311  | 1.97                     | 0.46              |
| 2:g:204:VAL:HG12  | 17:g:845:BCR:H352  | 1.96                     | 0.46              |
| 14:g:827:CLA:H2   | 17:g:845:BCR:H24C  | 1.96                     | 0.46              |
| 8:s:76:VAL:HG12   | 8:s:86:PHE:HB2     | 1.98                     | 0.46              |
| 9:t:17:THR:HG22   | 9:t:19:PRO:HD2     | 1.97                     | 0.46              |
| 17:w:201:BCR:H15C | 17:w:201:BCR:H351  | 1.79                     | 0.46              |
| 2:A:458:HIS:HE1   | 14:A:833:CLA:C1A   | 2.28                     | 0.46              |
| 14:A:827:CLA:H162 | 14:A:827:CLA:H141  | 1.67                     | 0.46              |
| 14:A:841:CLA:NB   | 18:A:851:LHG:O4    | 2.48                     | 0.46              |
| 17:A:856:BCR:H403 | 9:J:23:THR:HG21    | 1.97                     | 0.46              |
| 12:L:49:ASN:HB3   | 14:L:1501:CLA:HAC1 | 1.96                     | 0.46              |
| 2:a:393:HIS:CE1   | 14:a:826:CLA:ND    | 2.84                     | 0.46              |
| 2:a:535:ILE:HG12  | 2:a:609:HIS:CG     | 2.50                     | 0.46              |
| 2:a:731:HIS:NE2   | 14:a:839:CLA:NB    | 2.64                     | 0.46              |
| 14:a:821:CLA:HBC1 | 14:a:825:CLA:H141  | 1.96                     | 0.46              |
| 14:a:838:CLA:C1B  | 14:b:833:CLA:H41   | 2.45                     | 0.46              |
| 17:a:843:BCR:H11C | 17:a:843:BCR:H341  | 1.70                     | 0.46              |
| 4:b:62:SER:HB2    | 4:b:142:LEU:HB3    | 1.97                     | 0.46              |
| 4:b:275:HIS:CE1   | 14:b:817:CLA:NA    | 2.84                     | 0.46              |
| 4:b:343:ALA:HB2   | 17:b:847:BCR:H372  | 1.98                     | 0.46              |
| 14:b:832:CLA:HMB1 | 14:b:832:CLA:HBB1  | 1.98                     | 0.46              |
| 1:1:207:ASP:HB3   | 14:b:812:CLA:OBD   | 2.15                     | 0.46              |
| 2:G:218:ILE:HD11  | 2:G:276:LEU:HD21   | 1.96                     | 0.46              |
| 2:G:719:LEU:HD21  | 15:G:841:PQN:H152  | 1.98                     | 0.46              |
| 14:G:852:CLA:HMA2 | 17:N:852:BCR:H403  | 1.98                     | 0.46              |
| 4:N:453:PRO:O     | 4:N:456:GLN:HB2    | 2.15                     | 0.46              |
| 4:N:534:LEU:HD12  | 14:N:827:CLA:C4C   | 2.45                     | 0.46              |
| 13:Y:16:ALA:C     | 13:Y:19:PRO:HD2    | 2.41                     | 0.46              |
| 2:g:408:HIS:HA    | 2:g:411:ILE:HD12   | 1.97                     | 0.46              |
| 14:g:837:CLA:H102 | 14:g:837:CLA:H61   | 1.52                     | 0.46              |
| 14:n:813:CLA:HBB1 | 14:n:813:CLA:HMB3  | 1.98                     | 0.46              |
| 17:n:846:BCR:H15C | 17:n:846:BCR:H351  | 1.70                     | 0.46              |
| 17:w:207:BCR:H351 | 17:w:207:BCR:H15C  | 1.78                     | 0.46              |
| 14:A:801:CLA:HBB1 | 14:A:801:CLA:HMB3  | 1.98                     | 0.46              |
| 4:B:276:HIS:HB2   | 14:B:818:CLA:CHB   | 2.46                     | 0.46              |
| 11:I:34:SER:HB3   | 12:L:111:LEU:HD21  | 1.97                     | 0.46              |
| 2:a:204:VAL:CB    | 14:a:811:CLA:HAB   | 2.45                     | 0.46              |
| 2:a:305:PHE:HZ    | 14:a:817:CLA:H121  | 1.80                     | 0.46              |
| 2:a:373:ALA:HB1   | 14:a:825:CLA:HMC2  | 1.96                     | 0.46              |
| 4:N:319:PHE:HB2   | 14:N:825:CLA:HMA3  | 1.98                     | 0.46              |
| 14:N:819:CLA:H161 | 14:N:819:CLA:H121  | 1.65                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:g:217:LEU:HA    | 2:g:221:SER:HB2   | 1.98                     | 0.46              |
| 4:n:355:HIS:CE1   | 14:n:826:CLA:NB   | 2.83                     | 0.46              |
| 14:n:813:CLA:H51  | 14:n:818:CLA:HBC3 | 1.98                     | 0.46              |
| 14:n:850:CLA:H41  | 14:n:850:CLA:H62  | 1.67                     | 0.46              |
| 17:A:847:BCR:H15C | 17:A:847:BCR:H351 | 1.67                     | 0.46              |
| 14:A:855:CLA:CBB  | 4:B:665:ALA:CB    | 2.81                     | 0.46              |
| 4:B:191:ALA:O     | 4:B:195:ILE:HG13  | 2.15                     | 0.46              |
| 2:a:202:LEU:HD23  | 2:a:206:LEU:HD12  | 1.98                     | 0.46              |
| 4:b:584:TYR:HD1   | 4:b:717:LEU:HD22  | 1.81                     | 0.46              |
| 4:b:710:VAL:O     | 4:b:714:VAL:HG23  | 2.16                     | 0.46              |
| 14:b:826:CLA:HBA2 | 14:b:826:CLA:H3A  | 1.55                     | 0.46              |
| 17:b:852:BCR:H24C | 14:j:102:CLA:HBC3 | 1.97                     | 0.46              |
| 17:j:103:BCR:H11C | 17:j:103:BCR:H341 | 1.74                     | 0.46              |
| 3:H:27:LEU:HD22   | 21:N:802:LMG:H181 | 1.97                     | 0.46              |
| 4:N:44:GLN:NE2    | 4:N:162:ARG:HB3   | 2.31                     | 0.46              |
| 4:N:410:ASN:O     | 4:N:414:ARG:HG3   | 2.16                     | 0.46              |
| 4:N:442:VAL:HB    | 14:N:834:CLA:HMC2 | 1.97                     | 0.46              |
| 14:g:817:CLA:HAB  | 14:g:817:CLA:H8   | 1.97                     | 0.46              |
| 14:g:837:CLA:H101 | 17:g:846:BCR:H353 | 1.98                     | 0.46              |
| 4:n:268:LEU:HD22  | 14:n:817:CLA:HBA1 | 1.97                     | 0.46              |
| 4:n:384:ILE:HG21  | 4:n:594:VAL:HB    | 1.97                     | 0.46              |
| 14:n:812:CLA:HBA2 | 14:n:812:CLA:H3A  | 1.46                     | 0.46              |
| 17:s:203:BCR:H11C | 17:s:203:BCR:H341 | 1.76                     | 0.46              |
| 14:A:804:CLA:H62  | 14:A:804:CLA:H102 | 1.75                     | 0.46              |
| 14:A:823:CLA:H3A  | 14:A:823:CLA:HBA1 | 1.65                     | 0.46              |
| 4:B:398:LEU:HA    | 4:B:398:LEU:HD23  | 1.80                     | 0.46              |
| 4:B:433:LEU:HD13  | 4:B:532:LEU:HA    | 1.97                     | 0.46              |
| 4:B:602:HIS:CE1   | 4:B:732:LEU:HD12  | 2.51                     | 0.46              |
| 14:B:817:CLA:C1D  | 14:B:818:CLA:HBB2 | 2.45                     | 0.46              |
| 14:b:803:CLA:H112 | 14:b:803:CLA:H152 | 1.73                     | 0.46              |
| 18:m:101:LHG:H112 | 18:m:101:LHG:H141 | 1.83                     | 0.46              |
| 2:G:197:MET:HE3   | 2:G:197:MET:HB2   | 1.78                     | 0.46              |
| 3:H:42:ILE:HG22   | 3:H:43:ILE:HD12   | 1.98                     | 0.46              |
| 14:N:821:CLA:HAA2 | 14:N:826:CLA:HAB  | 1.97                     | 0.46              |
| 2:g:715:GLN:OE1   | 7:r:42:LYS:HD2    | 2.16                     | 0.46              |
| 14:n:805:CLA:HBA1 | 14:n:805:CLA:H3A  | 1.48                     | 0.46              |
| 14:B:813:CLA:H62  | 14:B:813:CLA:H2   | 1.66                     | 0.46              |
| 2:a:53:HIS:HE1    | 14:a:801:CLA:C4D  | 2.28                     | 0.46              |
| 17:a:844:BCR:H372 | 17:a:845:BCR:H312 | 1.96                     | 0.46              |
| 4:b:39:GLU:HB3    | 4:b:165:LEU:HD11  | 1.98                     | 0.46              |
| 4:b:440:LEU:HD22  | 4:b:457:ILE:HD12  | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:b:659:PHE:O     | 4:b:663:VAL:HG23  | 2.15                     | 0.46              |
| 17:b:843:BCR:H351 | 17:b:843:BCR:H15C | 1.77                     | 0.46              |
| 2:G:109:LEU:HD22  | 2:G:518:GLY:HA3   | 1.97                     | 0.46              |
| 2:G:296:HIS:HE1   | 14:G:816:CLA:C4D  | 2.29                     | 0.46              |
| 14:N:806:CLA:HMA2 | 13:Y:30:LEU:HD22  | 1.97                     | 0.46              |
| 14:N:808:CLA:H11  | 14:N:808:CLA:HBA1 | 1.71                     | 0.46              |
| 14:g:830:CLA:HBB1 | 14:g:854:CLA:HAA2 | 1.98                     | 0.46              |
| 2:A:216:HIS:HB2   | 14:A:813:CLA:CHC  | 2.46                     | 0.46              |
| 14:A:854:CLA:H92  | 14:A:854:CLA:H61  | 1.76                     | 0.46              |
| 4:B:445:ASP:OD2   | 14:B:803:CLA:H2   | 2.16                     | 0.46              |
| 14:a:802:CLA:HMA2 | 14:a:809:CLA:HMD1 | 1.97                     | 0.46              |
| 14:a:803:CLA:H172 | 14:a:811:CLA:H62  | 1.97                     | 0.46              |
| 14:a:838:CLA:HBC1 | 15:a:841:PQN:H212 | 1.98                     | 0.46              |
| 3:x:28:LEU:HD22   | 14:b:837:CLA:H141 | 1.98                     | 0.46              |
| 2:G:215:GLY:HA3   | 14:G:814:CLA:HAB  | 1.97                     | 0.46              |
| 2:G:389:CYS:HB3   | 14:G:827:CLA:HMA1 | 1.98                     | 0.46              |
| 14:G:804:CLA:H71  | 17:G:845:BCR:H23C | 1.98                     | 0.46              |
| 11:V:26:TRP:CZ2   | 17:W:201:BCR:H292 | 2.51                     | 0.46              |
| 14:W:203:CLA:HAC2 | 17:W:205:BCR:C25  | 2.46                     | 0.46              |
| 2:g:375:PRO:HG2   | 2:g:381:ALA:HB2   | 1.98                     | 0.46              |
| 17:n:851:BCR:H383 | 14:t:102:CLA:C2D  | 2.46                     | 0.46              |
| 17:t:104:BCR:H11C | 17:t:104:BCR:H341 | 1.84                     | 0.46              |
| 4:B:534:LEU:HD23  | 4:B:593:THR:HG21  | 1.98                     | 0.46              |
| 4:B:600:TYR:HA    | 4:B:626:TRP:HH2   | 1.80                     | 0.46              |
| 4:N:122:HIS:HB2   | 4:N:365:ILE:HD12  | 1.97                     | 0.45              |
| 4:N:443:HIS:CD2   | 4:N:457:ILE:HG13  | 2.51                     | 0.45              |
| 4:N:551:SER:HA    | 8:S:162:SER:HB2   | 1.97                     | 0.45              |
| 14:N:804:CLA:O2D  | 14:N:804:CLA:H2A  | 2.15                     | 0.45              |
| 17:N:844:BCR:H351 | 17:N:844:BCR:H15C | 1.75                     | 0.45              |
| 8:S:164:ARG:HD3   | 8:S:164:ARG:HA    | 1.59                     | 0.45              |
| 9:T:48:LEU:HD13   | 9:T:49:PRO:HD2    | 1.97                     | 0.45              |
| 14:g:820:CLA:HMD1 | 17:g:843:BCR:H371 | 1.98                     | 0.45              |
| 4:n:129:MET:HE3   | 4:n:135:LEU:HD23  | 1.98                     | 0.45              |
| 4:n:657:PHE:CE1   | 4:n:731:PHE:HB2   | 2.50                     | 0.45              |
| 2:A:87:TRP:O      | 2:A:91:MET:HG2    | 2.16                     | 0.45              |
| 2:A:176:ALA:HB2   | 14:A:809:CLA:HBC2 | 1.97                     | 0.45              |
| 4:B:601:TRP:CD1   | 14:B:837:CLA:HBC2 | 2.51                     | 0.45              |
| 4:b:470:ALA:O     | 4:b:482:LEU:HB2   | 2.16                     | 0.45              |
| 14:b:831:CLA:H41  | 14:b:831:CLA:H93  | 1.98                     | 0.45              |
| 17:b:846:BCR:H24C | 17:b:847:BCR:H21C | 1.97                     | 0.45              |
| 2:G:77:HIS:CD2    | 14:G:804:CLA:NA   | 2.84                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:N:434:GLY:HA2   | 4:N:532:LEU:HD22   | 1.99                     | 0.45              |
| 14:N:842:CLA:H11  | 15:N:843:PQN:H271  | 1.98                     | 0.45              |
| 6:Q:70:GLY:O      | 6:Q:74:ARG:HG2     | 2.16                     | 0.45              |
| 2:A:358:ALA:HB1   | 17:A:848:BCR:H343  | 1.98                     | 0.45              |
| 2:A:408:HIS:CE1   | 14:A:829:CLA:NA    | 2.84                     | 0.45              |
| 21:B:802:LMG:H302 | 14:B:823:CLA:HBB1  | 1.97                     | 0.45              |
| 14:B:825:CLA:H71  | 14:B:827:CLA:H42   | 1.98                     | 0.45              |
| 2:a:296:HIS:HE1   | 14:a:815:CLA:C4D   | 2.29                     | 0.45              |
| 2:a:329:HIS:CE1   | 14:a:821:CLA:ND    | 2.85                     | 0.45              |
| 2:a:641:ILE:HG13  | 2:a:642:THR:HG23   | 1.98                     | 0.45              |
| 14:a:831:CLA:H51  | 14:b:802:CLA:HBC2  | 1.98                     | 0.45              |
| 14:a:831:CLA:HAA1 | 17:i:102:BCR:H363  | 1.97                     | 0.45              |
| 3:x:34:LEU:HG     | 3:x:38:TYR:HE2     | 1.81                     | 0.45              |
| 4:b:26:ALA:HA     | 14:b:830:CLA:H43   | 1.99                     | 0.45              |
| 4:b:435:PHE:HZ    | 17:b:850:BCR:H372  | 1.81                     | 0.45              |
| 14:b:820:CLA:HAA2 | 14:b:825:CLA:HAB   | 1.98                     | 0.45              |
| 14:G:819:CLA:HBA2 | 14:G:819:CLA:H3A   | 1.51                     | 0.45              |
| 14:G:820:CLA:H112 | 14:G:820:CLA:H91   | 1.67                     | 0.45              |
| 4:N:534:LEU:CD1   | 14:N:827:CLA:C4C   | 2.87                     | 0.45              |
| 14:g:807:CLA:CBB  | 17:t:103:BCR:HC8   | 2.38                     | 0.45              |
| 4:n:619:ASN:O     | 4:n:625:GLY:HA3    | 2.16                     | 0.45              |
| 14:A:832:CLA:HBB2 | 12:L:81:LEU:HD13   | 1.99                     | 0.45              |
| 4:B:340:TRP:HE1   | 14:B:825:CLA:HMB2  | 1.81                     | 0.45              |
| 2:a:32:PRO:HB2    | 2:a:48:TRP:HH2     | 1.81                     | 0.45              |
| 2:a:310:HIS:CE1   | 17:a:843:BCR:H363  | 2.52                     | 0.45              |
| 4:b:334:LEU:HD13  | 14:b:806:CLA:HAC1  | 1.97                     | 0.45              |
| 4:b:355:HIS:HE1   | 14:b:827:CLA:NB    | 2.11                     | 0.45              |
| 2:G:338:HIS:NE2   | 14:G:823:CLA:ND    | 2.64                     | 0.45              |
| 14:G:808:CLA:HHB  | 9:T:34:ILE:HD11    | 1.97                     | 0.45              |
| 4:N:29:ASN:HD21   | 14:N:806:CLA:C4B   | 2.29                     | 0.45              |
| 14:N:829:CLA:O1D  | 14:N:830:CLA:HHB   | 2.17                     | 0.45              |
| 14:N:851:CLA:HBB1 | 17:N:852:BCR:H323  | 1.97                     | 0.45              |
| 14:n:816:CLA:C1D  | 14:n:817:CLA:HBB2  | 2.46                     | 0.45              |
| 14:n:826:CLA:H13  | 17:n:846:BCR:H351  | 1.98                     | 0.45              |
| 14:A:806:CLA:H61  | 14:A:808:CLA:H93   | 1.97                     | 0.45              |
| 14:A:832:CLA:H2   | 14:A:832:CLA:H62   | 1.74                     | 0.45              |
| 14:B:805:CLA:HBA2 | 13:M:31:TYR:HB2    | 1.98                     | 0.45              |
| 5:C:18:VAL:HG22   | 5:C:26:LEU:HB2     | 1.99                     | 0.45              |
| 12:L:73:PHE:HZ    | 14:L:1502:CLA:HBB1 | 1.82                     | 0.45              |
| 2:a:430:VAL:HA    | 2:a:433:HIS:CE1    | 2.51                     | 0.45              |
| 2:a:685:MET:CB    | 14:a:852:CLA:C1C   | 2.94                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 14:x:1701:CLA:HBA2 | 17:f:203:BCR:H393 | 1.97                     | 0.45              |
| 4:b:152:ALA:HB2    | 14:b:812:CLA:HBC2 | 1.98                     | 0.45              |
| 4:b:533:GLY:HA2    | 4:b:589:TRP:CZ3   | 2.51                     | 0.45              |
| 4:b:675:ARG:HG3    | 15:b:842:PQN:H7   | 1.97                     | 0.45              |
| 14:G:808:CLA:H102  | 14:G:808:CLA:H13  | 1.54                     | 0.45              |
| 14:G:820:CLA:H61   | 14:G:820:CLA:H92  | 1.74                     | 0.45              |
| 14:N:809:CLA:H92   | 14:N:809:CLA:HMC1 | 1.98                     | 0.45              |
| 17:U:103:BCR:H351  | 17:U:103:BCR:H15C | 1.77                     | 0.45              |
| 2:g:544:HIS:NE2    | 14:g:837:CLA:NA   | 2.65                     | 0.45              |
| 4:n:647:VAL:HG13   | 4:n:651:SER:HB2   | 1.99                     | 0.45              |
| 4:n:664:TRP:CZ3    | 14:n:803:CLA:HHB  | 2.52                     | 0.45              |
| 14:n:802:CLA:H61   | 14:n:802:CLA:H41  | 1.69                     | 0.45              |
| 14:n:807:CLA:H91   | 14:n:807:CLA:H111 | 1.75                     | 0.45              |
| 14:n:840:CLA:H161  | 17:v:101:BCR:H382 | 1.98                     | 0.45              |
| 10:u:80:LEU:HB3    | 10:u:85:ARG:HB2   | 1.98                     | 0.45              |
| 17:A:844:BCR:H11C  | 17:A:844:BCR:H341 | 1.67                     | 0.45              |
| 4:B:29:ASN:HD21    | 14:B:805:CLA:CHC  | 2.30                     | 0.45              |
| 2:a:119:TRP:CD2    | 14:a:807:CLA:HED3 | 2.52                     | 0.45              |
| 4:b:148:LEU:HD11   | 20:b:801:SQD:H162 | 1.97                     | 0.45              |
| 14:b:823:CLA:H2A   | 14:b:823:CLA:O1D  | 2.17                     | 0.45              |
| 14:b:838:CLA:H2    | 14:b:838:CLA:H62  | 1.64                     | 0.45              |
| 2:G:356:ASN:O      | 2:G:360:LEU:HB2   | 2.17                     | 0.45              |
| 2:G:659:ILE:HA     | 4:N:624:MET:CE    | 2.47                     | 0.45              |
| 14:G:838:CLA:H43   | 18:G:850:LHG:H161 | 1.99                     | 0.45              |
| 4:N:195:ILE:HA     | 4:N:199:ILE:HD12  | 1.98                     | 0.45              |
| 4:N:537:THR:HA     | 4:N:540:ILE:HD12  | 1.98                     | 0.45              |
| 8:S:139:TRP:CD1    | 8:S:140:PRO:HD3   | 2.52                     | 0.45              |
| 12:W:161:THR:HG23  | 14:W:204:CLA:HED2 | 1.97                     | 0.45              |
| 2:g:216:HIS:HB2    | 14:g:812:CLA:CHC  | 2.47                     | 0.45              |
| 2:g:427:LEU:HD23   | 14:g:837:CLA:H201 | 1.98                     | 0.45              |
| 2:g:721:ILE:O      | 2:g:725:ARG:HG3   | 2.16                     | 0.45              |
| 14:g:826:CLA:HBB1  | 14:g:826:CLA:HMB1 | 1.99                     | 0.45              |
| 4:n:669:MET:HB2    | 14:n:804:CLA:C2C  | 2.46                     | 0.45              |
| 14:n:829:CLA:H141  | 14:n:829:CLA:H161 | 1.65                     | 0.45              |
| 14:n:832:CLA:H2    | 14:n:832:CLA:H62  | 1.71                     | 0.45              |
| 10:u:54:PHE:N      | 10:u:54:PHE:CD1   | 2.84                     | 0.45              |
| 2:A:45:THR:HB      | 2:A:717:ARG:HG3   | 1.97                     | 0.45              |
| 2:A:305:PHE:CE1    | 14:A:820:CLA:HAB  | 2.51                     | 0.45              |
| 17:A:845:BCR:H20C  | 17:A:845:BCR:H361 | 1.84                     | 0.45              |
| 2:a:176:ALA:HB2    | 14:a:808:CLA:HBC2 | 1.98                     | 0.45              |
| 2:a:305:PHE:HE1    | 14:a:819:CLA:HHC  | 1.81                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 14:a:815:CLA:H12   | 10:k:78:LEU:HD12  | 1.99                     | 0.45              |
| 4:b:381:TYR:O      | 4:b:384:ILE:HG13  | 2.15                     | 0.45              |
| 4:b:548:ALA:O      | 4:b:557:LYS:HB3   | 2.16                     | 0.45              |
| 14:b:809:CLA:H202  | 14:b:828:CLA:H202 | 1.98                     | 0.45              |
| 8:f:31:CYS:HB2     | 8:f:62:SER:HA     | 1.99                     | 0.45              |
| 2:G:17:VAL:HG12    | 2:G:186:PRO:HA    | 1.99                     | 0.45              |
| 2:G:353:LEU:O      | 2:G:357:LEU:HB2   | 2.17                     | 0.45              |
| 2:G:524:MET:HE3    | 2:G:524:MET:HB2   | 1.78                     | 0.45              |
| 2:G:675:GLY:O      | 2:G:679:VAL:HG23  | 2.17                     | 0.45              |
| 14:G:812:CLA:H43   | 17:G:845:BCR:H19C | 1.99                     | 0.45              |
| 14:N:832:CLA:HAB   | 14:N:840:CLA:CBB  | 2.46                     | 0.45              |
| 14:N:841:CLA:H112  | 14:N:842:CLA:H141 | 1.99                     | 0.45              |
| 14:W:203:CLA:HAC2  | 17:W:205:BCR:C26  | 2.47                     | 0.45              |
| 14:g:840:CLA:C3C   | 18:g:850:LHG:HC42 | 2.47                     | 0.45              |
| 14:g:840:CLA:HMC3  | 17:g:846:BCR:H281 | 1.99                     | 0.45              |
| 12:w:70:HIS:CE1    | 14:w:204:CLA:ND   | 2.84                     | 0.45              |
| 12:w:95:LEU:HG     | 12:w:99:ILE:HD12  | 1.98                     | 0.45              |
| 17:w:206:BCR:H15C  | 17:w:206:BCR:H351 | 1.74                     | 0.45              |
| 2:A:119:TRP:CD2    | 14:A:808:CLA:HED3 | 2.52                     | 0.45              |
| 2:A:322:ILE:HG21   | 14:A:824:CLA:HAC1 | 1.99                     | 0.45              |
| 2:A:695:GLN:O      | 2:A:699:GLU:HG3   | 2.16                     | 0.45              |
| 14:A:855:CLA:HMA2  | 17:B:848:BCR:H371 | 1.98                     | 0.45              |
| 10:K:20:VAL:HG13   | 10:K:77:VAL:HG21  | 1.98                     | 0.45              |
| 10:K:71:ILE:HG13   | 10:K:72:LEU:N     | 2.31                     | 0.45              |
| 2:a:566:LYS:HD3    | 2:a:586:VAL:HG12  | 1.99                     | 0.45              |
| 14:b:825:CLA:H141  | 14:b:825:CLA:H161 | 1.75                     | 0.45              |
| 17:j:104:BCR:H11C  | 17:j:104:BCR:H341 | 1.64                     | 0.45              |
| 2:G:216:HIS:ND1    | 14:G:813:CLA:NB   | 2.65                     | 0.45              |
| 4:N:7:LYS:HE2      | 4:N:7:LYS:HB2     | 1.79                     | 0.45              |
| 8:S:144:VAL:O      | 8:S:148:LEU:HD22  | 2.17                     | 0.45              |
| 12:W:58:THR:HG21   | 12:w:141:ASN:HD21 | 1.81                     | 0.45              |
| 2:g:731:HIS:CE1    | 14:g:839:CLA:NA   | 2.84                     | 0.45              |
| 14:h:1701:CLA:HBA1 | 17:s:203:BCR:H382 | 1.97                     | 0.45              |
| 14:n:817:CLA:HBA2  | 14:n:817:CLA:H3A  | 1.50                     | 0.45              |
| 17:n:844:BCR:H371  | 17:n:844:BCR:H24C | 1.71                     | 0.45              |
| 17:n:849:BCR:H24C  | 17:n:849:BCR:H371 | 1.80                     | 0.45              |
| 12:w:57:LEU:HD22   | 12:w:61:ARG:HG2   | 1.99                     | 0.45              |
| 14:A:804:CLA:H193  | 17:A:845:BCR:H10C | 1.98                     | 0.45              |
| 14:A:830:CLA:H3A   | 14:A:831:CLA:OBD  | 2.17                     | 0.45              |
| 15:A:842:PQN:H172  | 17:B:851:BCR:H382 | 1.98                     | 0.45              |
| 2:a:219:HIS:NE2    | 14:a:813:CLA:NA   | 2.65                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 17:a:845:BCR:H15C  | 17:a:845:BCR:H351 | 1.75                     | 0.45              |
| 4:b:176:ASN:ND2    | 4:b:291:TYR:HB2   | 2.28                     | 0.45              |
| 14:b:853:CLA:H52   | 18:m:101:LHG:H262 | 1.99                     | 0.45              |
| 2:G:247:LYS:O      | 2:G:251:ILE:HG12  | 2.16                     | 0.45              |
| 14:G:832:CLA:H11   | 14:N:801:CLA:H43  | 1.99                     | 0.45              |
| 4:N:66:PHE:HZ      | 13:Y:9:VAL:HG13   | 1.81                     | 0.45              |
| 4:N:276:HIS:HB2    | 14:N:819:CLA:C1B  | 2.47                     | 0.45              |
| 4:N:593:THR:O      | 4:N:597:VAL:HG12  | 2.17                     | 0.45              |
| 2:g:442:ASN:HD22   | 4:n:685:LEU:HD21  | 1.82                     | 0.45              |
| 14:g:827:CLA:H92   | 14:g:827:CLA:HMD1 | 1.99                     | 0.45              |
| 4:n:446:VAL:HG21   | 14:n:850:CLA:HAC2 | 1.99                     | 0.45              |
| 6:q:8:LYS:HB2      | 6:q:52:HIS:ND1    | 2.31                     | 0.45              |
| 17:v:101:BCR:H11C  | 17:v:101:BCR:H341 | 1.87                     | 0.45              |
| 12:w:95:LEU:HD22   | 12:w:158:TYR:CD1  | 2.52                     | 0.45              |
| 12:w:137:GLU:N     | 12:w:137:GLU:OE1  | 2.49                     | 0.45              |
| 17:y:101:BCR:H15C  | 17:y:101:BCR:H351 | 1.81                     | 0.45              |
| 2:A:197:MET:HG2    | 14:A:824:CLA:HMD3 | 1.97                     | 0.45              |
| 14:A:807:CLA:HBA2  | 14:A:807:CLA:H3A  | 1.55                     | 0.45              |
| 14:X:1701:CLA:HBC3 | 14:B:839:CLA:HBC2 | 1.98                     | 0.45              |
| 4:B:95:HIS:CE1     | 14:B:811:CLA:NB   | 2.85                     | 0.45              |
| 4:B:199:ILE:CG2    | 4:B:203:ARG:HE    | 2.30                     | 0.45              |
| 14:B:814:CLA:H62   | 14:B:814:CLA:H2   | 1.73                     | 0.45              |
| 5:C:59:PRO:O       | 7:E:48:ILE:HD13   | 2.16                     | 0.45              |
| 10:K:14:LEU:HD21   | 10:K:77:VAL:HG22  | 1.99                     | 0.45              |
| 2:a:394:HIS:NE2    | 14:a:827:CLA:ND   | 2.64                     | 0.45              |
| 2:a:408:HIS:HE1    | 14:a:828:CLA:NA   | 2.14                     | 0.45              |
| 14:a:801:CLA:H13   | 9:j:26:LEU:HB3    | 1.99                     | 0.45              |
| 14:a:803:CLA:H143  | 17:a:844:BCR:HC41 | 1.99                     | 0.45              |
| 14:a:804:CLA:H62   | 14:a:804:CLA:H41  | 1.70                     | 0.45              |
| 14:a:826:CLA:H41   | 14:a:826:CLA:H61  | 1.51                     | 0.45              |
| 14:a:826:CLA:H71   | 14:a:826:CLA:H112 | 1.71                     | 0.45              |
| 4:b:374:ALA:HB2    | 4:b:733:ILE:HD11  | 1.98                     | 0.45              |
| 4:b:443:HIS:CD2    | 4:b:457:ILE:HG13  | 2.52                     | 0.45              |
| 14:b:809:CLA:H92   | 17:b:848:BCR:H331 | 1.99                     | 0.45              |
| 14:b:819:CLA:H8    | 14:b:819:CLA:HAB  | 1.97                     | 0.45              |
| 1:l:214:VAL:HG13   | 20:b:801:SQD:C15  | 2.47                     | 0.45              |
| 14:G:818:CLA:H8    | 14:G:818:CLA:HAB  | 1.99                     | 0.45              |
| 4:N:58:PHE:HZ      | 17:N:845:BCR:H361 | 1.82                     | 0.45              |
| 4:N:156:HIS:HE1    | 14:N:813:CLA:NA   | 2.13                     | 0.45              |
| 4:N:534:LEU:HG     | 14:N:840:CLA:HMA3 | 1.99                     | 0.45              |
| 17:N:845:BCR:H15C  | 17:N:845:BCR:H351 | 1.77                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:g:81:LEU:HD12   | 14:g:811:CLA:HED2 | 1.98                     | 0.45              |
| 2:g:738:ALA:HB2   | 17:g:848:BCR:H322 | 1.98                     | 0.45              |
| 4:n:91:ILE:HB     | 4:n:112:PRO:HB2   | 1.99                     | 0.45              |
| 4:n:394:GLY:HA2   | 17:n:846:BCR:H393 | 1.99                     | 0.45              |
| 14:n:822:CLA:H62  | 14:n:822:CLA:H41  | 1.63                     | 0.45              |
| 5:p:15:THR:HG22   | 5:p:28:MET:HE3    | 1.99                     | 0.45              |
| 14:A:830:CLA:HMC1 | 14:A:838:CLA:HAB  | 1.98                     | 0.45              |
| 2:a:57:HIS:HB3    | 14:a:803:CLA:HAB  | 1.98                     | 0.45              |
| 14:a:852:CLA:HED2 | 14:a:852:CLA:HBD  | 1.64                     | 0.45              |
| 4:b:692:THR:HG23  | 4:b:695:ALA:HB3   | 1.99                     | 0.45              |
| 8:f:130:LEU:HA    | 8:f:133:ILE:HG22  | 1.99                     | 0.45              |
| 14:G:804:CLA:HBA1 | 14:G:812:CLA:HBA1 | 1.99                     | 0.44              |
| 14:G:807:CLA:H71  | 14:G:829:CLA:H172 | 1.98                     | 0.44              |
| 14:G:832:CLA:H93  | 14:N:842:CLA:H171 | 1.97                     | 0.44              |
| 14:G:853:CLA:H202 | 14:G:853:CLA:H162 | 1.79                     | 0.44              |
| 4:N:177:HIS:CE1   | 14:N:814:CLA:NA   | 2.85                     | 0.44              |
| 4:N:423:ILE:HG21  | 4:N:543:LYS:HG3   | 1.98                     | 0.44              |
| 14:N:831:CLA:H102 | 21:N:850:LMG:H392 | 1.99                     | 0.44              |
| 8:S:133:ILE:HB    | 14:S:203:CLA:OBD  | 2.17                     | 0.44              |
| 12:W:78:PHE:HB3   | 12:W:94:GLY:HA2   | 1.99                     | 0.44              |
| 2:g:457:ILE:HG22  | 14:g:832:CLA:HBC2 | 1.98                     | 0.44              |
| 2:g:459:ASN:HD21  | 2:g:472:PHE:HB2   | 1.82                     | 0.44              |
| 14:g:815:CLA:H92  | 14:g:815:CLA:H61  | 1.80                     | 0.44              |
| 14:n:804:CLA:HHD  | 14:n:804:CLA:HBC2 | 1.98                     | 0.44              |
| 14:n:807:CLA:H102 | 17:v:101:BCR:HC31 | 1.99                     | 0.44              |
| 2:A:345:LEU:HD21  | 17:A:847:BCR:H312 | 1.97                     | 0.44              |
| 2:A:572:ARG:HG2   | 2:A:722:THR:HG21  | 1.99                     | 0.44              |
| 14:A:827:CLA:H11  | 17:A:849:BCR:HC42 | 1.99                     | 0.44              |
| 4:B:106:GLN:HG3   | 4:B:115:ILE:HD11  | 1.98                     | 0.44              |
| 4:B:341:HIS:CD2   | 14:B:825:CLA:HAA1 | 2.52                     | 0.44              |
| 4:B:464:ALA:O     | 4:B:468:GLN:HG3   | 2.17                     | 0.44              |
| 17:I:103:BCR:H11C | 17:I:103:BCR:H341 | 1.85                     | 0.44              |
| 14:a:837:CLA:H62  | 14:a:837:CLA:H2   | 1.75                     | 0.44              |
| 14:b:833:CLA:H142 | 17:f:203:BCR:HC42 | 1.99                     | 0.44              |
| 14:b:833:CLA:H161 | 14:b:833:CLA:H122 | 1.92                     | 0.44              |
| 17:b:847:BCR:H351 | 17:b:847:BCR:H15C | 1.72                     | 0.44              |
| 17:l:206:BCR:H11C | 17:l:206:BCR:H341 | 1.81                     | 0.44              |
| 2:G:456:TYR:HE2   | 2:G:538:ILE:HG13  | 1.82                     | 0.44              |
| 14:H:1701:CLA:CGA | 14:H:1701:CLA:H3A | 2.40                     | 0.44              |
| 4:N:377:THR:HG23  | 4:N:598:THR:HG21  | 1.99                     | 0.44              |
| 4:N:652:VAL:HG22  | 14:N:811:CLA:HHD  | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:g:183:LYS:HD3   | 2:g:183:LYS:HA    | 1.83                     | 0.44              |
| 2:g:393:HIS:CE1   | 14:g:826:CLA:ND   | 2.86                     | 0.44              |
| 4:n:669:MET:HB2   | 14:n:804:CLA:C3C  | 2.47                     | 0.44              |
| 14:n:827:CLA:H13  | 14:n:829:CLA:H151 | 1.99                     | 0.44              |
| 11:v:13:ALA:HB1   | 11:v:16:LEU:HD12  | 1.99                     | 0.44              |
| 2:A:734:LEU:HD22  | 14:A:839:CLA:HMA3 | 1.99                     | 0.44              |
| 14:A:804:CLA:H142 | 17:A:846:BCR:H372 | 1.98                     | 0.44              |
| 14:A:806:CLA:H13  | 17:A:856:BCR:H383 | 1.98                     | 0.44              |
| 2:a:59:PHE:HD2    | 2:a:73:ILE:HG13   | 1.82                     | 0.44              |
| 14:a:801:CLA:H162 | 14:a:801:CLA:H203 | 1.67                     | 0.44              |
| 14:a:826:CLA:C4C  | 17:a:848:BCR:HC41 | 2.46                     | 0.44              |
| 14:a:837:CLA:H42  | 18:a:850:LHG:H162 | 1.99                     | 0.44              |
| 4:b:101:ILE:HG23  | 4:b:112:PRO:HG3   | 1.98                     | 0.44              |
| 4:b:719:HIS:NE2   | 14:b:841:CLA:C4A  | 2.80                     | 0.44              |
| 14:b:809:CLA:H72  | 14:b:809:CLA:H112 | 1.66                     | 0.44              |
| 4:N:663:VAL:HG13  | 4:N:719:HIS:HD2   | 1.81                     | 0.44              |
| 14:N:810:CLA:H51  | 14:N:810:CLA:H8   | 1.62                     | 0.44              |
| 6:Q:22:LYS:HG3    | 6:Q:26:GLU:HB3    | 2.00                     | 0.44              |
| 2:g:441:LEU:HD21  | 2:g:547:VAL:HG12  | 1.99                     | 0.44              |
| 2:g:491:HIS:NE2   | 14:g:833:CLA:NA   | 2.65                     | 0.44              |
| 2:g:623:ASP:HB2   | 2:g:627:ASN:HB2   | 1.99                     | 0.44              |
| 2:g:682:PHE:HZ    | 14:g:839:CLA:HBC2 | 1.81                     | 0.44              |
| 14:g:806:CLA:H3A  | 14:g:806:CLA:HBA2 | 1.44                     | 0.44              |
| 14:g:837:CLA:H161 | 14:g:837:CLA:H141 | 1.79                     | 0.44              |
| 14:g:839:CLA:HAC1 | 15:g:841:PQN:H171 | 1.98                     | 0.44              |
| 14:n:808:CLA:H51  | 14:n:808:CLA:H8   | 1.84                     | 0.44              |
| 17:n:849:BCR:H11C | 17:n:849:BCR:H341 | 1.87                     | 0.44              |
| 17:n:849:BCR:HC41 | 17:t:103:BCR:HC31 | 1.99                     | 0.44              |
| 11:v:36:LEU:O     | 11:v:40:ILE:HG12  | 2.18                     | 0.44              |
| 17:w:201:BCR:H11C | 17:w:201:BCR:H341 | 1.88                     | 0.44              |
| 2:A:659:ILE:HG13  | 2:A:660:ASN:N     | 2.31                     | 0.44              |
| 14:A:804:CLA:HBA2 | 14:A:804:CLA:H11  | 1.69                     | 0.44              |
| 4:B:387:MET:HB2   | 14:B:826:CLA:HBC3 | 1.98                     | 0.44              |
| 14:B:812:CLA:H72  | 17:B:844:BCR:H401 | 1.98                     | 0.44              |
| 14:B:829:CLA:H3A  | 14:B:829:CLA:HBA2 | 1.67                     | 0.44              |
| 14:a:821:CLA:H41  | 14:a:821:CLA:H61  | 1.63                     | 0.44              |
| 4:b:225:PHE:HZ    | 17:b:843:BCR:H343 | 1.81                     | 0.44              |
| 4:b:436:HIS:HB2   | 17:b:852:BCR:HC42 | 1.99                     | 0.44              |
| 14:b:837:CLA:HMB1 | 14:b:837:CLA:HBB1 | 1.98                     | 0.44              |
| 17:b:846:BCR:H15C | 17:b:846:BCR:H351 | 1.61                     | 0.44              |
| 17:j:103:BCR:H15C | 17:j:103:BCR:H351 | 1.77                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:G:802:CLA:H3A   | 14:G:802:CLA:HBA1  | 1.77                     | 0.44              |
| 14:G:803:CLA:H52   | 14:G:810:CLA:H8    | 1.99                     | 0.44              |
| 17:G:844:BCR:H351  | 17:G:844:BCR:H15C  | 1.79                     | 0.44              |
| 20:H:1702:SQD:H161 | 20:H:1702:SQD:H132 | 1.63                     | 0.44              |
| 4:N:499:VAL:HG11   | 14:N:818:CLA:HED1  | 1.99                     | 0.44              |
| 17:N:849:BCR:H351  | 17:N:849:BCR:H15C  | 1.76                     | 0.44              |
| 2:g:675:GLY:CA     | 17:g:848:BCR:H17C  | 2.48                     | 0.44              |
| 4:n:304:MET:HG2    | 14:n:822:CLA:CGD   | 2.48                     | 0.44              |
| 4:n:433:LEU:HD11   | 14:n:837:CLA:HMB2  | 1.99                     | 0.44              |
| 14:n:803:CLA:H111  | 14:n:803:CLA:H151  | 1.61                     | 0.44              |
| 5:p:66:ARG:HG2     | 6:q:120:ILE:HD11   | 2.00                     | 0.44              |
| 13:y:16:ALA:C      | 13:y:19:PRO:HD2    | 2.42                     | 0.44              |
| 2:A:174:LEU:HD21   | 14:A:808:CLA:H191  | 1.98                     | 0.44              |
| 14:A:832:CLA:H51   | 14:A:840:CLA:HBC2  | 1.99                     | 0.44              |
| 4:B:158:GLN:O      | 4:B:162:ARG:HG3    | 2.17                     | 0.44              |
| 14:B:837:CLA:H91   | 14:B:837:CLA:H111  | 1.77                     | 0.44              |
| 8:F:139:TRP:CD1    | 8:F:140:PRO:HD3    | 2.53                     | 0.44              |
| 12:L:73:PHE:CZ     | 14:L:1502:CLA:HBB1 | 2.53                     | 0.44              |
| 2:a:534:LEU:O      | 2:a:538:ILE:HG13   | 2.18                     | 0.44              |
| 14:a:831:CLA:H112  | 14:a:831:CLA:H152  | 1.69                     | 0.44              |
| 4:b:527:HIS:HE1    | 14:b:837:CLA:C4D   | 2.29                     | 0.44              |
| 14:b:805:CLA:H92   | 14:b:805:CLA:H62   | 1.85                     | 0.44              |
| 17:f:203:BCR:H341  | 17:f:203:BCR:H11C  | 1.72                     | 0.44              |
| 17:i:102:BCR:H10C  | 17:i:102:BCR:HC7   | 1.78                     | 0.44              |
| 2:G:107:ASP:HB3    | 2:G:111:VAL:HG23   | 2.00                     | 0.44              |
| 2:G:282:LEU:HD12   | 2:G:515:LEU:HD13   | 2.00                     | 0.44              |
| 2:G:394:HIS:NE2    | 14:G:828:CLA:ND    | 2.66                     | 0.44              |
| 14:G:838:CLA:HBA1  | 18:G:850:LHG:H362  | 2.00                     | 0.44              |
| 17:G:843:BCR:H15C  | 17:G:843:BCR:H351  | 1.74                     | 0.44              |
| 4:N:50:HIS:CE1     | 14:N:807:CLA:H161  | 2.53                     | 0.44              |
| 18:g:850:LHG:H312  | 18:g:850:LHG:H342  | 1.91                     | 0.44              |
| 4:n:62:SER:HB2     | 4:n:142:LEU:HB2    | 1.98                     | 0.44              |
| 11:v:26:TRP:C      | 11:v:29:PRO:HD2    | 2.42                     | 0.44              |
| 12:w:26:ARG:HD3    | 12:w:26:ARG:HA     | 1.76                     | 0.44              |
| 2:A:216:HIS:CE1    | 14:A:813:CLA:NA    | 2.86                     | 0.44              |
| 14:A:807:CLA:HBB1  | 14:A:808:CLA:C2D   | 2.48                     | 0.44              |
| 14:B:809:CLA:H51   | 14:B:809:CLA:H8    | 1.62                     | 0.44              |
| 17:B:852:BCR:H15C  | 17:B:852:BCR:H351  | 1.75                     | 0.44              |
| 17:I:103:BCR:H15C  | 17:I:103:BCR:H351  | 1.84                     | 0.44              |
| 2:a:43:PRO:HB3     | 2:a:48:TRP:CD2     | 2.53                     | 0.44              |
| 2:a:94:HIS:CE1     | 14:a:805:CLA:NA    | 2.85                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:a:322:ILE:HG23  | 14:a:819:CLA:HED2 | 1.98                     | 0.44              |
| 14:b:841:CLA:H13  | 17:i:101:BCR:H21C | 2.00                     | 0.44              |
| 15:b:842:PQN:H211 | 15:b:842:PQN:H252 | 1.65                     | 0.44              |
| 17:b:848:BCR:H24C | 17:b:848:BCR:H371 | 1.82                     | 0.44              |
| 6:d:105:LYS:HE3   | 6:d:105:LYS:HB2   | 1.84                     | 0.44              |
| 14:f:201:CLA:H62  | 14:f:201:CLA:H2   | 1.64                     | 0.44              |
| 2:G:679:VAL:HG11  | 2:G:734:LEU:HD23  | 1.98                     | 0.44              |
| 14:G:804:CLA:HBA2 | 14:G:804:CLA:H11  | 1.73                     | 0.44              |
| 15:G:841:PQN:H211 | 15:G:841:PQN:H191 | 1.69                     | 0.44              |
| 21:N:850:LMG:H352 | 21:N:850:LMG:H381 | 1.71                     | 0.44              |
| 2:g:149:ARG:HD3   | 2:g:378:PRO:HB2   | 1.97                     | 0.44              |
| 2:g:351:ALA:HB2   | 2:g:412:PHE:CD1   | 2.53                     | 0.44              |
| 14:g:807:CLA:HBC2 | 4:n:450:PHE:CE1   | 2.53                     | 0.44              |
| 14:g:830:CLA:H61  | 14:g:830:CLA:H41  | 1.40                     | 0.44              |
| 3:h:15:LYS:HG3    | 3:h:18:TYR:H      | 1.82                     | 0.44              |
| 4:n:668:PHE:HB3   | 14:n:804:CLA:HMC2 | 1.99                     | 0.44              |
| 4:n:678:TRP:O     | 4:n:682:ILE:HG13  | 2.17                     | 0.44              |
| 14:n:827:CLA:HBA2 | 14:n:827:CLA:H3A  | 1.59                     | 0.44              |
| 14:n:840:CLA:H13  | 17:v:101:BCR:H21C | 1.99                     | 0.44              |
| 17:u:103:BCR:H371 | 17:u:103:BCR:H24C | 1.81                     | 0.44              |
| 14:w:204:CLA:HAC2 | 17:w:206:BCR:C26  | 2.48                     | 0.44              |
| 2:A:94:HIS:CE1    | 14:A:806:CLA:NA   | 2.85                     | 0.44              |
| 2:A:672:MET:HE1   | 14:A:827:CLA:H121 | 1.99                     | 0.44              |
| 14:A:802:CLA:H71  | 14:A:802:CLA:H112 | 1.60                     | 0.44              |
| 14:A:853:CLA:HMB1 | 14:A:853:CLA:H41  | 1.99                     | 0.44              |
| 14:B:813:CLA:H3A  | 14:B:813:CLA:HBA2 | 1.59                     | 0.44              |
| 5:C:16:GLN:HB3    | 5:C:57:ALA:HB1    | 2.00                     | 0.44              |
| 2:a:59:PHE:HA     | 2:a:62:HIS:CD2    | 2.53                     | 0.44              |
| 18:a:850:LHG:H302 | 18:a:850:LHG:H272 | 1.77                     | 0.44              |
| 4:b:68:VAL:HG11   | 4:b:124:TRP:HZ3   | 1.83                     | 0.44              |
| 4:b:177:HIS:CE1   | 14:b:813:CLA:NA   | 2.86                     | 0.44              |
| 4:b:191:ALA:HA    | 4:b:194:LEU:HD12  | 1.99                     | 0.44              |
| 4:b:658:LEU:HD23  | 4:b:658:LEU:HA    | 1.82                     | 0.44              |
| 14:b:825:CLA:HBB2 | 17:b:846:BCR:H363 | 2.00                     | 0.44              |
| 14:b:837:CLA:H62  | 14:b:837:CLA:H2   | 1.61                     | 0.44              |
| 17:b:850:BCR:H15C | 17:b:850:BCR:H351 | 1.78                     | 0.44              |
| 2:G:367:ILE:HD12  | 14:G:828:CLA:HAC2 | 1.99                     | 0.44              |
| 2:G:668:ALA:O     | 2:G:672:MET:HG2   | 2.17                     | 0.44              |
| 17:G:846:BCR:H15C | 17:G:846:BCR:H351 | 1.72                     | 0.44              |
| 10:U:85:ARG:HH12  | 4:n:214:SER:HA    | 1.83                     | 0.44              |
| 2:g:708:LEU:HD11  | 17:s:203:BCR:H342 | 2.00                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:g:804:CLA:H191 | 18:g:849:LHG:H211 | 1.98                     | 0.44              |
| 14:g:854:CLA:H93  | 14:g:854:CLA:H111 | 1.75                     | 0.44              |
| 4:n:551:SER:HA    | 8:s:162:SER:HB2   | 1.98                     | 0.44              |
| 15:n:841:PQN:H252 | 15:n:841:PQN:H211 | 1.72                     | 0.44              |
| 5:p:31:TRP:HB2    | 5:p:39:VAL:HG22   | 1.99                     | 0.44              |
| 8:s:133:ILE:HD11  | 14:s:201:CLA:H92  | 1.98                     | 0.44              |
| 8:s:139:TRP:CD1   | 8:s:140:PRO:HD3   | 2.52                     | 0.44              |
| 2:A:219:HIS:HB3   | 2:A:244:ILE:HD11  | 1.98                     | 0.44              |
| 2:A:276:LEU:HD21  | 2:A:299:LEU:HD23  | 1.99                     | 0.44              |
| 4:B:276:HIS:HE2   | 14:B:819:CLA:C2B  | 2.31                     | 0.44              |
| 4:B:341:HIS:CG    | 14:B:825:CLA:HAA1 | 2.53                     | 0.44              |
| 4:B:642:TYR:CD2   | 4:B:642:TYR:O     | 2.71                     | 0.44              |
| 14:a:831:CLA:CBB  | 14:a:832:CLA:H3A  | 2.48                     | 0.44              |
| 17:b:847:BCR:H341 | 17:b:847:BCR:H11C | 1.72                     | 0.44              |
| 9:j:48:LEU:HD23   | 9:j:48:LEU:HA     | 1.82                     | 0.44              |
| 12:l:74:LEU:HD22  | 12:l:101:LEU:HD23 | 1.98                     | 0.44              |
| 20:l:201:SQD:H142 | 20:l:201:SQD:H111 | 1.45                     | 0.44              |
| 14:G:838:CLA:H161 | 14:G:838:CLA:H141 | 1.77                     | 0.44              |
| 14:N:811:CLA:H142 | 21:N:850:LMG:H222 | 1.99                     | 0.44              |
| 14:N:819:CLA:HBA2 | 14:N:819:CLA:H3A  | 1.52                     | 0.44              |
| 6:Q:73:LEU:HB3    | 6:Q:78:ILE:HB     | 1.99                     | 0.44              |
| 2:g:200:HIS:CE1   | 14:g:810:CLA:NA   | 2.85                     | 0.44              |
| 17:g:845:BCR:H11C | 17:g:845:BCR:H341 | 1.80                     | 0.44              |
| 12:w:95:LEU:HD22  | 12:w:158:TYR:HD1  | 1.83                     | 0.44              |
| 2:A:119:TRP:HB3   | 17:A:856:BCR:H323 | 2.00                     | 0.44              |
| 17:A:856:BCR:H15C | 17:A:856:BCR:H351 | 1.75                     | 0.44              |
| 14:B:832:CLA:HBC2 | 14:B:839:CLA:HMC2 | 1.99                     | 0.44              |
| 15:B:842:PQN:H302 | 17:I:103:BCR:H343 | 1.99                     | 0.44              |
| 2:a:297:HIS:C     | 2:a:297:HIS:ND1   | 2.76                     | 0.44              |
| 14:a:828:CLA:H62  | 14:a:828:CLA:H41  | 1.72                     | 0.44              |
| 1:1:230:TRP:CE3   | 1:1:231:LEU:HD23  | 2.53                     | 0.44              |
| 2:G:264:PHE:CZ    | 17:G:843:BCR:H343 | 2.53                     | 0.44              |
| 2:G:275:PHE:HE2   | 14:G:814:CLA:HAC2 | 1.83                     | 0.44              |
| 14:G:805:CLA:H42  | 18:G:849:LHG:H261 | 2.00                     | 0.44              |
| 14:G:831:CLA:H62  | 14:G:831:CLA:H102 | 1.72                     | 0.44              |
| 14:N:825:CLA:H141 | 14:N:825:CLA:H162 | 1.79                     | 0.44              |
| 14:N:827:CLA:H102 | 14:N:838:CLA:H122 | 2.00                     | 0.44              |
| 14:N:838:CLA:H92  | 14:N:838:CLA:H61  | 1.84                     | 0.44              |
| 5:P:66:ARG:HA     | 5:P:66:ARG:HD2    | 1.72                     | 0.44              |
| 7:R:9:ARG:HH12    | 7:R:61:VAL:HG21   | 1.83                     | 0.44              |
| 9:T:19:PRO:HB2    | 17:T:104:BCR:H292 | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:W:206:BCR:H11C | 17:W:206:BCR:H341 | 1.89                     | 0.44              |
| 2:g:86:ILE:HG13   | 2:g:170:ALA:HB1   | 2.00                     | 0.44              |
| 2:g:584:CYS:HB3   | 4:n:674:TRP:HE3   | 1.82                     | 0.44              |
| 14:g:821:CLA:H3A  | 14:g:821:CLA:HBA2 | 1.65                     | 0.44              |
| 4:n:181:GLY:HA2   | 4:n:185:VAL:HB    | 2.00                     | 0.44              |
| 4:n:195:ILE:HA    | 4:n:199:ILE:HD12  | 2.00                     | 0.44              |
| 4:n:533:GLY:HA2   | 4:n:589:TRP:CZ3   | 2.53                     | 0.44              |
| 14:n:803:CLA:H192 | 14:n:803:CLA:H162 | 1.87                     | 0.44              |
| 14:n:834:CLA:H3A  | 14:n:834:CLA:HBA1 | 1.67                     | 0.44              |
| 14:n:839:CLA:HBB2 | 15:n:841:PQN:H141 | 1.99                     | 0.44              |
| 10:u:40:LYS:C     | 10:u:41:TYR:HD1   | 2.26                     | 0.44              |
| 2:A:320:HIS:HE1   | 14:A:821:CLA:C4A  | 2.31                     | 0.44              |
| 2:A:352:GLN:HG3   | 14:A:824:CLA:H13  | 2.00                     | 0.44              |
| 14:A:803:CLA:H3A  | 14:A:803:CLA:HBA1 | 1.77                     | 0.44              |
| 14:A:839:CLA:HAB  | 14:A:853:CLA:H151 | 2.00                     | 0.44              |
| 17:A:849:BCR:H20C | 17:A:849:BCR:H361 | 1.73                     | 0.44              |
| 17:A:856:BCR:H11C | 17:A:856:BCR:H341 | 1.89                     | 0.44              |
| 2:a:414:VAL:HG11  | 2:a:571:PHE:N     | 2.32                     | 0.44              |
| 14:b:805:CLA:HBA2 | 14:b:805:CLA:HED2 | 2.00                     | 0.44              |
| 2:G:374:MET:SD    | 14:G:817:CLA:HAA1 | 2.58                     | 0.43              |
| 14:G:801:CLA:H122 | 17:N:849:BCR:H12C | 1.99                     | 0.43              |
| 14:G:803:CLA:HHC  | 14:G:805:CLA:OBD  | 2.18                     | 0.43              |
| 14:G:824:CLA:H143 | 14:G:824:CLA:H111 | 1.84                     | 0.43              |
| 4:N:351:TRP:HZ3   | 14:N:820:CLA:H102 | 1.82                     | 0.43              |
| 14:N:831:CLA:H161 | 14:N:842:CLA:HBA2 | 2.00                     | 0.43              |
| 17:N:848:BCR:H11C | 17:N:848:BCR:H341 | 1.73                     | 0.43              |
| 6:Q:31:ILE:HG12   | 6:Q:33:TRP:CE3    | 2.53                     | 0.43              |
| 17:T:103:BCR:H15C | 17:T:103:BCR:H351 | 1.76                     | 0.43              |
| 2:g:278:PHE:HE1   | 14:g:816:CLA:H11  | 1.82                     | 0.43              |
| 2:g:671:LEU:HD21  | 4:n:446:VAL:HA    | 1.99                     | 0.43              |
| 17:g:843:BCR:H15C | 17:g:843:BCR:H351 | 1.82                     | 0.43              |
| 14:g:854:CLA:H62  | 14:g:854:CLA:H41  | 1.83                     | 0.43              |
| 17:n:845:BCR:H15C | 17:n:845:BCR:H351 | 1.69                     | 0.43              |
| 5:p:43:PRO:HG2    | 5:p:44:ARG:HE     | 1.83                     | 0.43              |
| 8:s:63:GLN:HE22   | 9:t:48:LEU:HG     | 1.82                     | 0.43              |
| 17:v:101:BCR:H15C | 17:v:101:BCR:H351 | 1.86                     | 0.43              |
| 18:v:102:LHG:H122 | 17:w:206:BCR:HC31 | 1.99                     | 0.43              |
| 2:A:413:MET:HG3   | 2:A:558:ARG:HG3   | 1.99                     | 0.43              |
| 2:A:714:ILE:HD11  | 8:F:121:GLU:HB2   | 1.98                     | 0.43              |
| 14:A:827:CLA:H192 | 17:J:103:BCR:H14C | 2.00                     | 0.43              |
| 4:B:66:PHE:HZ     | 13:M:9:VAL:HG13   | 1.83                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:B:377:THR:HG23   | 4:B:598:THR:HG21   | 2.00                     | 0.43              |
| 14:B:803:CLA:H13   | 14:B:803:CLA:H171  | 1.78                     | 0.43              |
| 17:L:1504:BCR:H351 | 17:L:1504:BCR:H15C | 1.75                     | 0.43              |
| 2:a:608:PHE:HB3    | 2:a:646:TRP:CZ3    | 2.53                     | 0.43              |
| 14:a:806:CLA:H3A   | 14:a:806:CLA:HBA2  | 1.34                     | 0.43              |
| 14:a:819:CLA:HMB3  | 14:a:819:CLA:HBB1  | 1.99                     | 0.43              |
| 14:a:828:CLA:H41   | 18:a:849:LHG:H102  | 2.00                     | 0.43              |
| 5:c:6:LYS:HD2      | 6:d:114:ARG:HB3    | 2.00                     | 0.43              |
| 10:k:86:ILE:H      | 10:k:86:ILE:CD1    | 2.27                     | 0.43              |
| 2:G:59:PHE:HD2     | 2:G:73:ILE:HD13    | 1.83                     | 0.43              |
| 14:G:802:CLA:H11   | 14:G:839:CLA:H72   | 2.00                     | 0.43              |
| 17:G:848:BCR:H361  | 17:G:848:BCR:H20C  | 1.74                     | 0.43              |
| 4:N:193:HIS:HB2    | 14:N:816:CLA:C1C   | 2.49                     | 0.43              |
| 4:N:629:ASP:O      | 4:N:633:ALA:HB3    | 2.19                     | 0.43              |
| 14:N:805:CLA:HHD   | 14:N:805:CLA:HBC2  | 2.00                     | 0.43              |
| 9:T:43:LEU:HD23    | 9:T:43:LEU:HA      | 1.90                     | 0.43              |
| 14:W:202:CLA:C1B   | 14:W:203:CLA:HED1  | 2.47                     | 0.43              |
| 2:g:100:ASN:HB3    | 2:g:135:PHE:HB2    | 2.00                     | 0.43              |
| 2:g:297:HIS:HB2    | 14:g:816:CLA:C1B   | 2.48                     | 0.43              |
| 2:g:552:LYS:HZ1    | 4:n:680:GLU:HB2    | 1.83                     | 0.43              |
| 2:g:719:LEU:HD21   | 15:g:841:PQN:H151  | 1.99                     | 0.43              |
| 2:g:737:ILE:HG23   | 14:g:826:CLA:HAB   | 1.99                     | 0.43              |
| 14:A:807:CLA:HBB1  | 14:A:808:CLA:C3D   | 2.48                     | 0.43              |
| 14:A:812:CLA:HBB1  | 14:A:812:CLA:HHC   | 2.00                     | 0.43              |
| 17:A:845:BCR:H351  | 17:A:845:BCR:H15C  | 1.76                     | 0.43              |
| 4:B:592:ASN:HB2    | 14:B:803:CLA:HBC2  | 2.00                     | 0.43              |
| 14:B:808:CLA:H91   | 14:B:808:CLA:H111  | 1.78                     | 0.43              |
| 17:B:848:BCR:H11C  | 17:B:848:BCR:H341  | 1.89                     | 0.43              |
| 6:D:12:PHE:CZ      | 12:L:28:PRO:HB2    | 2.53                     | 0.43              |
| 12:L:21:VAL:HG12   | 12:L:35:THR:HA     | 2.00                     | 0.43              |
| 20:x:1702:SQD:H102 | 20:x:1702:SQD:H132 | 1.65                     | 0.43              |
| 4:b:200:PRO:HB3    | 4:b:205:GLN:HG3    | 2.00                     | 0.43              |
| 4:b:276:HIS:CE1    | 14:b:818:CLA:ND    | 2.86                     | 0.43              |
| 14:b:817:CLA:C1D   | 14:b:818:CLA:HBB2  | 2.49                     | 0.43              |
| 2:G:462:MET:CE     | 2:G:467:ARG:HE     | 2.31                     | 0.43              |
| 14:G:803:CLA:HBD   | 14:G:810:CLA:H2    | 2.00                     | 0.43              |
| 14:G:820:CLA:H162  | 14:G:820:CLA:H122  | 1.47                     | 0.43              |
| 14:N:821:CLA:H172  | 14:N:821:CLA:H13   | 1.58                     | 0.43              |
| 14:N:851:CLA:H61   | 17:S:204:BCR:HC32  | 2.00                     | 0.43              |
| 17:N:852:BCR:H15C  | 17:N:852:BCR:H351  | 1.81                     | 0.43              |
| 2:g:599:MET:HE3    | 2:g:599:MET:HB3    | 1.85                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:n:810:CLA:H52  | 12:w:96:LEU:HB3   | 1.99                     | 0.43              |
| 7:r:39:ARG:HD3    | 7:r:49:ASN:HD22   | 1.84                     | 0.43              |
| 14:A:854:CLA:H142 | 14:A:854:CLA:H112 | 1.72                     | 0.43              |
| 4:B:552:LYS:HD2   | 4:B:552:LYS:HA    | 1.66                     | 0.43              |
| 2:a:422:ASN:ND2   | 2:a:427:LEU:HD23  | 2.34                     | 0.43              |
| 2:a:442:ASN:O     | 2:a:446:ILE:HG13  | 2.18                     | 0.43              |
| 4:b:580:TRP:CZ2   | 4:b:714:VAL:HG22  | 2.53                     | 0.43              |
| 14:b:813:CLA:H3A  | 14:b:813:CLA:HBA2 | 1.51                     | 0.43              |
| 17:b:843:BCR:H11C | 17:b:843:BCR:H341 | 1.76                     | 0.43              |
| 2:G:282:LEU:H     | 2:G:508:TYR:HE2   | 1.65                     | 0.43              |
| 2:G:351:ALA:O     | 2:G:355:THR:HG23  | 2.18                     | 0.43              |
| 14:G:837:CLA:H111 | 14:G:837:CLA:H152 | 1.50                     | 0.43              |
| 17:G:847:BCR:H11C | 17:G:847:BCR:H341 | 1.84                     | 0.43              |
| 4:N:224:PRO:HA    | 4:N:227:THR:HG22  | 2.00                     | 0.43              |
| 4:N:433:LEU:HD13  | 4:N:532:LEU:HA    | 2.00                     | 0.43              |
| 4:N:600:TYR:HA    | 4:N:626:TRP:HH2   | 1.83                     | 0.43              |
| 2:g:39:LEU:HD23   | 2:g:48:TRP:CD1    | 2.53                     | 0.43              |
| 2:g:375:PRO:HA    | 2:g:376:PRO:HD3   | 1.88                     | 0.43              |
| 2:g:710:VAL:HG12  | 8:s:105:ARG:HG3   | 1.99                     | 0.43              |
| 14:g:810:CLA:H61  | 14:g:810:CLA:H41  | 1.83                     | 0.43              |
| 17:g:847:BCR:H24C | 17:g:847:BCR:H371 | 1.84                     | 0.43              |
| 17:g:847:BCR:H361 | 17:g:847:BCR:H20C | 1.87                     | 0.43              |
| 4:n:330:TYR:OH    | 4:n:341:HIS:HE1   | 2.00                     | 0.43              |
| 4:n:340:TRP:HE1   | 14:n:824:CLA:HMB2 | 1.84                     | 0.43              |
| 4:n:426:LEU:HD21  | 4:n:538:THR:HG22  | 2.00                     | 0.43              |
| 14:n:804:CLA:H193 | 14:n:840:CLA:H2   | 2.01                     | 0.43              |
| 14:n:806:CLA:H162 | 14:n:806:CLA:H143 | 1.76                     | 0.43              |
| 17:n:845:BCR:H11C | 17:n:845:BCR:H341 | 1.68                     | 0.43              |
| 14:A:834:CLA:CBB  | 14:A:836:CLA:HBA1 | 2.48                     | 0.43              |
| 14:A:840:CLA:HBC1 | 15:B:842:PQN:H191 | 2.01                     | 0.43              |
| 4:B:77:TRP:CZ2    | 4:B:81:PRO:HB3    | 2.53                     | 0.43              |
| 4:B:657:PHE:HZ    | 14:B:804:CLA:C1D  | 2.31                     | 0.43              |
| 14:B:830:CLA:H2A  | 14:B:830:CLA:O1D  | 2.18                     | 0.43              |
| 14:B:840:CLA:HED3 | 11:I:37:PHE:HZ    | 1.83                     | 0.43              |
| 17:B:843:BCR:H351 | 17:B:843:BCR:H15C | 1.77                     | 0.43              |
| 2:a:386:THR:O     | 2:a:390:ILE:HG12  | 2.18                     | 0.43              |
| 14:a:802:CLA:H11  | 14:a:809:CLA:H92  | 2.00                     | 0.43              |
| 14:a:817:CLA:HBA2 | 14:a:817:CLA:H3A  | 1.49                     | 0.43              |
| 14:b:819:CLA:HBA2 | 14:b:819:CLA:H3A  | 1.44                     | 0.43              |
| 14:b:819:CLA:H121 | 14:b:825:CLA:H72  | 2.00                     | 0.43              |
| 2:G:53:HIS:NE2    | 14:G:802:CLA:NB   | 2.67                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:G:180:HIS:CE1   | 14:G:809:CLA:NA   | 2.86                     | 0.43              |
| 2:G:297:HIS:HB2   | 14:G:817:CLA:CHB  | 2.49                     | 0.43              |
| 2:G:462:MET:HE2   | 2:G:470:ASP:HB2   | 2.00                     | 0.43              |
| 14:G:823:CLA:HHB  | 14:G:840:CLA:CBB  | 2.47                     | 0.43              |
| 15:G:841:PQN:H212 | 15:G:841:PQN:H251 | 1.69                     | 0.43              |
| 14:g:832:CLA:H2A  | 14:g:832:CLA:O2D  | 2.18                     | 0.43              |
| 14:n:828:CLA:H203 | 17:n:844:BCR:H15C | 2.01                     | 0.43              |
| 7:r:39:ARG:HH11   | 7:r:49:ASN:ND2    | 2.17                     | 0.43              |
| 11:v:26:TRP:CH2   | 17:w:201:BCR:HC31 | 2.53                     | 0.43              |
| 2:A:323:LYS:O     | 2:A:327:GLU:HG2   | 2.19                     | 0.43              |
| 2:A:414:VAL:HG13  | 2:A:557:ALA:HB1   | 2.00                     | 0.43              |
| 14:A:804:CLA:H143 | 17:A:845:BCR:HC41 | 2.00                     | 0.43              |
| 14:A:820:CLA:H92  | 14:A:820:CLA:H61  | 1.73                     | 0.43              |
| 17:A:845:BCR:H11C | 17:A:845:BCR:H341 | 1.82                     | 0.43              |
| 14:A:855:CLA:HAB  | 4:B:665:ALA:C     | 2.44                     | 0.43              |
| 4:B:707:LEU:HD22  | 4:B:711:GLN:NE2   | 2.34                     | 0.43              |
| 20:B:801:SQD:H102 | 20:B:801:SQD:H132 | 1.37                     | 0.43              |
| 17:K:102:BCR:H24C | 17:K:102:BCR:H371 | 1.83                     | 0.43              |
| 17:I:101:BCR:H11C | 17:I:101:BCR:H341 | 1.79                     | 0.43              |
| 12:L:42:LEU:HD12  | 12:L:42:LEU:HA    | 1.87                     | 0.43              |
| 2:a:479:LEU:H     | 2:a:530:THR:HG23  | 1.83                     | 0.43              |
| 2:a:688:PHE:HE1   | 4:b:672:ILE:HG13  | 1.83                     | 0.43              |
| 14:a:832:CLA:H62  | 14:a:832:CLA:H2   | 1.80                     | 0.43              |
| 3:x:18:TYR:HD1    | 3:x:21:ARG:HH11   | 1.65                     | 0.43              |
| 8:f:42:LYS:HE2    | 8:f:42:LYS:HB2    | 1.82                     | 0.43              |
| 17:k:102:BCR:H20C | 17:k:102:BCR:H361 | 1.79                     | 0.43              |
| 2:G:144:LEU:HD12  | 2:G:144:LEU:HA    | 1.88                     | 0.43              |
| 14:G:833:CLA:H2   | 14:G:833:CLA:H62  | 1.72                     | 0.43              |
| 17:G:847:BCR:H15C | 17:G:847:BCR:H351 | 1.78                     | 0.43              |
| 4:N:435:PHE:HZ    | 17:N:852:BCR:H372 | 1.83                     | 0.43              |
| 14:N:827:CLA:H142 | 14:N:827:CLA:H112 | 1.79                     | 0.43              |
| 17:T:104:BCR:HC8  | 17:T:104:BCR:H321 | 2.01                     | 0.43              |
| 2:g:142:SER:HA    | 14:g:826:CLA:HMA2 | 2.00                     | 0.43              |
| 2:g:393:HIS:HE2   | 14:g:827:CLA:C2B  | 2.32                     | 0.43              |
| 4:n:378:HIS:HB2   | 14:n:827:CLA:CHB  | 2.48                     | 0.43              |
| 4:n:698:VAL:HG12  | 12:w:112:TYR:CE2  | 2.54                     | 0.43              |
| 14:n:840:CLA:HBC1 | 15:n:841:PQN:H2M2 | 2.00                     | 0.43              |
| 10:u:18:PRO:O     | 10:u:22:ILE:HG12  | 2.18                     | 0.43              |
| 2:A:705:HIS:HE1   | 14:A:854:CLA:ND   | 2.16                     | 0.43              |
| 4:B:65:LEU:HD11   | 17:B:845:BCR:H281 | 2.00                     | 0.43              |
| 4:B:597:VAL:CG2   | 14:B:837:CLA:HAB  | 2.49                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:B:805:CLA:HMB1 | 17:M:101:BCR:HC42 | 2.00                     | 0.43              |
| 17:B:852:BCR:H383 | 14:J:102:CLA:C2D  | 2.48                     | 0.43              |
| 2:a:91:MET:HE2    | 14:a:806:CLA:H2A  | 2.00                     | 0.43              |
| 2:a:524:MET:HE3   | 2:a:524:MET:HB2   | 1.79                     | 0.43              |
| 14:a:826:CLA:H13  | 14:a:826:CLA:H172 | 1.78                     | 0.43              |
| 17:a:846:BCR:H15C | 17:a:846:BCR:H351 | 1.92                     | 0.43              |
| 4:b:306:ASN:ND2   | 4:b:324:GLN:HA    | 2.33                     | 0.43              |
| 14:b:804:CLA:H102 | 14:b:804:CLA:H62  | 1.37                     | 0.43              |
| 6:d:12:PHE:HB3    | 6:d:49:ALA:HA     | 2.01                     | 0.43              |
| 6:d:19:LEU:HD12   | 6:d:19:LEU:H      | 1.83                     | 0.43              |
| 8:f:139:TRP:CD1   | 8:f:140:PRO:HD3   | 2.54                     | 0.43              |
| 1:1:228:LEU:HD11  | 13:m:11:ILE:CD1   | 2.48                     | 0.43              |
| 2:G:487:VAL:HA    | 2:G:490:LEU:HD12  | 2.01                     | 0.43              |
| 2:G:648:ARG:O     | 2:G:652:TRP:HB3   | 2.17                     | 0.43              |
| 14:G:823:CLA:H3A  | 14:G:823:CLA:HBA1 | 1.66                     | 0.43              |
| 14:G:831:CLA:HBC3 | 18:G:850:LHG:H291 | 2.01                     | 0.43              |
| 14:N:828:CLA:H93  | 14:N:828:CLA:H112 | 1.81                     | 0.43              |
| 14:N:829:CLA:HBA2 | 14:N:829:CLA:H3A  | 1.45                     | 0.43              |
| 14:N:833:CLA:H3A  | 14:N:833:CLA:HBA2 | 1.68                     | 0.43              |
| 17:N:852:BCR:H11C | 17:N:852:BCR:H341 | 1.88                     | 0.43              |
| 4:n:710:VAL:O     | 4:n:714:VAL:HG23  | 2.18                     | 0.43              |
| 14:n:819:CLA:CED  | 14:n:819:CLA:H2A  | 2.49                     | 0.43              |
| 14:n:827:CLA:O1D  | 14:n:828:CLA:HHB  | 2.18                     | 0.43              |
| 17:n:842:BCR:H20C | 17:n:842:BCR:H361 | 1.80                     | 0.43              |
| 17:t:103:BCR:H341 | 17:t:103:BCR:H11C | 1.79                     | 0.43              |
| 2:A:32:PRO:HB2    | 2:A:48:TRP:HH2    | 1.82                     | 0.43              |
| 2:A:264:PHE:CZ    | 17:A:844:BCR:H343 | 2.54                     | 0.43              |
| 2:A:334:THR:HA    | 14:A:830:CLA:OBD  | 2.18                     | 0.43              |
| 14:A:802:CLA:H162 | 14:A:802:CLA:H141 | 1.66                     | 0.43              |
| 14:A:818:CLA:HBA2 | 14:A:818:CLA:H3A  | 1.44                     | 0.43              |
| 17:A:848:BCR:H351 | 17:A:848:BCR:H15C | 1.80                     | 0.43              |
| 4:B:203:ARG:HH11  | 4:B:251:GLY:H     | 1.67                     | 0.43              |
| 14:B:850:CLA:H143 | 8:F:94:LEU:HD22   | 2.01                     | 0.43              |
| 5:C:8:TYR:HE2     | 6:D:123:ASN:HD21  | 1.66                     | 0.43              |
| 7:E:59:ILE:N      | 7:E:59:ILE:HD12   | 2.34                     | 0.43              |
| 4:b:581:ASP:HA    | 4:b:584:TYR:HB3   | 2.00                     | 0.43              |
| 4:b:719:HIS:CE1   | 14:b:841:CLA:ND   | 2.86                     | 0.43              |
| 17:b:850:BCR:H343 | 8:f:93:PHE:CD2    | 2.53                     | 0.43              |
| 7:e:8:VAL:HG21    | 7:e:58:LEU:HD22   | 2.01                     | 0.43              |
| 2:G:261:LEU:HD21  | 17:G:843:BCR:HC21 | 2.01                     | 0.43              |
| 2:G:588:GLY:O     | 2:G:592:VAL:HG23  | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:G:802:CLA:C4B  | 17:T:104:BCR:H291 | 2.49                     | 0.43              |
| 14:G:807:CLA:CHC  | 14:G:808:CLA:HMD2 | 2.49                     | 0.43              |
| 4:N:163:PRO:HB2   | 4:N:168:PHE:CE2   | 2.53                     | 0.43              |
| 4:N:341:HIS:ND1   | 14:N:826:CLA:HAA1 | 2.34                     | 0.43              |
| 17:T:104:BCR:H15C | 17:T:104:BCR:H351 | 1.77                     | 0.43              |
| 10:U:34:PHE:O     | 10:U:38:THR:HB    | 2.18                     | 0.43              |
| 14:W:203:CLA:HMB3 | 14:W:204:CLA:HBC2 | 2.00                     | 0.43              |
| 17:W:206:BCR:H15C | 17:W:206:BCR:H351 | 1.86                     | 0.43              |
| 14:g:830:CLA:H2   | 14:w:204:CLA:H43  | 2.00                     | 0.43              |
| 4:n:150:LEU:HD22  | 13:y:23:ALA:HA    | 2.00                     | 0.43              |
| 4:n:701:LYS:HE3   | 4:n:701:LYS:HB3   | 1.71                     | 0.43              |
| 2:A:297:HIS:HB2   | 14:A:817:CLA:CHB  | 2.49                     | 0.43              |
| 2:A:334:THR:HB    | 2:A:426:VAL:HG22  | 2.01                     | 0.43              |
| 14:A:828:CLA:H61  | 14:A:828:CLA:H41  | 1.72                     | 0.43              |
| 15:A:842:PQN:H12  | 15:A:842:PQN:H162 | 1.81                     | 0.43              |
| 4:B:67:HIS:NE2    | 14:B:808:CLA:NA   | 2.67                     | 0.43              |
| 14:B:828:CLA:H202 | 21:B:849:LMG:H252 | 2.01                     | 0.43              |
| 12:L:33:LEU:HD23  | 12:L:33:LEU:HA    | 1.81                     | 0.43              |
| 12:L:70:HIS:HE1   | 14:L:1502:CLA:C4D | 2.32                     | 0.43              |
| 2:a:321:SER:OG    | 2:a:324:GLU:HB2   | 2.19                     | 0.43              |
| 4:b:66:PHE:HB2    | 4:b:139:SER:OG    | 2.19                     | 0.43              |
| 4:b:276:HIS:HB2   | 14:b:818:CLA:CHB  | 2.49                     | 0.43              |
| 2:G:197:MET:HE2   | 14:G:812:CLA:CHD  | 2.49                     | 0.43              |
| 2:G:598:TRP:CZ2   | 14:G:801:CLA:HAB  | 2.54                     | 0.43              |
| 14:G:821:CLA:CHD  | 17:G:843:BCR:H382 | 2.49                     | 0.43              |
| 4:N:485:PRO:HA    | 4:N:490:TYR:CG    | 2.54                     | 0.43              |
| 10:U:48:LEU:HD13  | 10:U:54:PHE:CD2   | 2.53                     | 0.43              |
| 2:g:675:GLY:HA2   | 17:g:848:BCR:H17C | 2.00                     | 0.43              |
| 14:g:819:CLA:NC   | 14:g:825:CLA:H152 | 2.34                     | 0.43              |
| 14:g:838:CLA:H202 | 14:g:838:CLA:H162 | 1.86                     | 0.43              |
| 4:n:722:VAL:HG22  | 21:n:848:LMG:H441 | 2.01                     | 0.43              |
| 14:n:808:CLA:H141 | 14:n:808:CLA:H161 | 1.73                     | 0.43              |
| 2:A:211:LEU:HD11  | 17:A:844:BCR:H331 | 2.00                     | 0.43              |
| 2:A:715:GLN:H     | 2:A:715:GLN:HG3   | 1.57                     | 0.43              |
| 14:A:803:CLA:HAB  | 14:A:810:CLA:H121 | 1.99                     | 0.43              |
| 14:A:824:CLA:HBB1 | 14:A:824:CLA:HMB3 | 2.01                     | 0.43              |
| 14:A:830:CLA:HBA1 | 18:A:851:LHG:H241 | 2.01                     | 0.43              |
| 19:A:852:CL0:H15  | 4:B:631:LEU:HD13  | 2.00                     | 0.43              |
| 6:D:31:ILE:HG12   | 6:D:33:TRP:CE3    | 2.54                     | 0.43              |
| 17:K:102:BCR:H20C | 17:K:102:BCR:H361 | 1.85                     | 0.43              |
| 17:I:101:BCR:H361 | 17:I:101:BCR:H20C | 1.84                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:a:367:ILE:O     | 2:a:371:MET:HB2   | 2.18                     | 0.43              |
| 17:a:848:BCR:H361 | 17:a:848:BCR:H20C | 1.75                     | 0.43              |
| 4:b:54:LEU:HD23   | 4:b:54:LEU:HA     | 1.87                     | 0.43              |
| 7:e:4:ARG:HH11    | 7:e:25:ALA:HA     | 1.83                     | 0.43              |
| 11:i:26:TRP:HZ2   | 17:i:102:BCR:H333 | 1.84                     | 0.43              |
| 17:i:101:BCR:H11C | 17:i:101:BCR:H341 | 1.82                     | 0.43              |
| 14:l:203:CLA:H102 | 14:l:203:CLA:H62  | 1.67                     | 0.43              |
| 2:G:55:LEU:HD11   | 18:G:849:LHG:HC12 | 2.01                     | 0.43              |
| 2:G:680:TRP:HZ3   | 14:N:803:CLA:HMD3 | 1.84                     | 0.43              |
| 14:G:806:CLA:H93  | 14:G:806:CLA:H111 | 1.67                     | 0.43              |
| 14:G:838:CLA:H2   | 17:G:847:BCR:H14C | 2.01                     | 0.43              |
| 5:P:26:LEU:HA     | 5:P:41:SER:O      | 2.19                     | 0.43              |
| 12:W:79:ALA:HB2   | 12:W:94:GLY:HA3   | 2.00                     | 0.43              |
| 2:g:316:TRP:CD1   | 10:u:60:PRO:HG3   | 2.54                     | 0.43              |
| 14:g:830:CLA:H101 | 14:g:830:CLA:H62  | 1.76                     | 0.43              |
| 4:n:597:VAL:HG21  | 14:n:836:CLA:HBB2 | 2.00                     | 0.43              |
| 4:n:724:TYR:OH    | 14:n:803:CLA:H12  | 2.19                     | 0.43              |
| 14:n:808:CLA:H151 | 14:n:827:CLA:H91  | 2.00                     | 0.43              |
| 14:n:837:CLA:H92  | 14:n:837:CLA:H61  | 1.86                     | 0.43              |
| 17:n:844:BCR:H20C | 17:n:844:BCR:H361 | 1.91                     | 0.43              |
| 10:u:85:ARG:HD3   | 10:u:85:ARG:HA    | 1.85                     | 0.43              |
| 2:A:87:TRP:HA     | 14:A:806:CLA:HBB2 | 1.99                     | 0.43              |
| 2:A:318:ILE:HD11  | 14:A:819:CLA:H2A  | 2.00                     | 0.43              |
| 2:A:719:LEU:HD21  | 15:A:842:PQN:H152 | 2.01                     | 0.43              |
| 17:A:845:BCR:H372 | 17:A:846:BCR:H312 | 2.01                     | 0.43              |
| 4:B:528:HIS:CE1   | 14:B:838:CLA:ND   | 2.86                     | 0.43              |
| 17:B:845:BCR:H15C | 17:B:845:BCR:H351 | 1.75                     | 0.43              |
| 2:a:506:VAL:HG23  | 14:a:833:CLA:HED3 | 2.01                     | 0.43              |
| 14:a:840:CLA:HBA2 | 14:a:840:CLA:H3A  | 1.33                     | 0.43              |
| 4:b:384:ILE:HG21  | 4:b:594:VAL:HB    | 2.00                     | 0.43              |
| 4:N:22:TRP:CG     | 4:N:711:GLN:HE22  | 2.37                     | 0.42              |
| 4:N:726:LEU:HD23  | 14:N:829:CLA:H51  | 2.01                     | 0.42              |
| 14:N:824:CLA:H2   | 14:N:824:CLA:ND   | 2.34                     | 0.42              |
| 2:g:385:ALA:HA    | 2:g:748:ILE:HD12  | 2.01                     | 0.42              |
| 2:g:397:ILE:O     | 2:g:401:LEU:HG    | 2.19                     | 0.42              |
| 2:g:734:LEU:HD22  | 14:g:839:CLA:HMA3 | 2.01                     | 0.42              |
| 14:g:825:CLA:H112 | 14:g:825:CLA:H143 | 1.68                     | 0.42              |
| 4:n:330:TYR:CZ    | 14:n:824:CLA:NC   | 2.86                     | 0.42              |
| 14:n:818:CLA:H162 | 14:n:818:CLA:H122 | 1.76                     | 0.42              |
| 17:n:845:BCR:H371 | 17:n:845:BCR:H24C | 1.68                     | 0.42              |
| 14:A:811:CLA:HBA2 | 14:A:811:CLA:H3A  | 1.66                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:A:846:BCR:H341 | 17:A:846:BCR:H11C | 1.83                     | 0.42              |
| 4:B:203:ARG:HG2   | 4:B:250:ALA:HB1   | 2.00                     | 0.42              |
| 4:B:642:TYR:O     | 4:B:642:TYR:HD2   | 2.01                     | 0.42              |
| 4:B:697:LEU:HD11  | 12:L:52:ALA:HB1   | 2.01                     | 0.42              |
| 14:B:812:CLA:H12  | 14:B:813:CLA:C3D  | 2.49                     | 0.42              |
| 14:B:823:CLA:H62  | 14:B:823:CLA:H41  | 1.70                     | 0.42              |
| 17:J:103:BCR:H20C | 17:J:103:BCR:H361 | 1.91                     | 0.42              |
| 17:I:102:BCR:H11C | 17:I:102:BCR:H341 | 1.88                     | 0.42              |
| 2:a:75:ALA:HB2    | 2:a:181:TYR:HB2   | 2.01                     | 0.42              |
| 14:a:806:CLA:HMC2 | 14:a:807:CLA:HMD1 | 2.01                     | 0.42              |
| 18:a:850:LHG:HC82 | 18:a:850:LHG:H111 | 1.78                     | 0.42              |
| 14:b:828:CLA:O1D  | 14:b:829:CLA:HHB  | 2.19                     | 0.42              |
| 17:b:850:BCR:H24C | 17:b:850:BCR:H371 | 1.80                     | 0.42              |
| 7:e:4:ARG:NH1     | 7:e:25:ALA:HA     | 2.34                     | 0.42              |
| 17:f:203:BCR:H20C | 17:f:203:BCR:H361 | 1.85                     | 0.42              |
| 1:l:214:VAL:HA    | 20:b:801:SQD:H132 | 1.99                     | 0.42              |
| 4:N:181:GLY:HA3   | 14:N:815:CLA:HBB1 | 2.00                     | 0.42              |
| 4:N:351:TRP:CE2   | 14:N:828:CLA:HAA1 | 2.54                     | 0.42              |
| 4:N:669:MET:HB2   | 14:N:805:CLA:CHC  | 2.49                     | 0.42              |
| 14:N:830:CLA:H142 | 17:N:846:BCR:H21C | 2.01                     | 0.42              |
| 17:N:846:BCR:H24C | 17:N:846:BCR:H371 | 1.73                     | 0.42              |
| 4:n:31:PHE:HB3    | 4:n:37:MET:HE3    | 2.00                     | 0.42              |
| 4:n:193:HIS:HB2   | 14:n:814:CLA:C1C  | 2.49                     | 0.42              |
| 14:n:806:CLA:H62  | 14:n:829:CLA:HBC3 | 2.01                     | 0.42              |
| 14:n:830:CLA:H3A  | 14:n:830:CLA:HBA1 | 1.83                     | 0.42              |
| 17:n:851:BCR:H20C | 17:n:851:BCR:H361 | 1.82                     | 0.42              |
| 14:A:825:CLA:HBA2 | 14:A:838:CLA:HAA1 | 2.00                     | 0.42              |
| 4:B:369:TYR:HB3   | 4:B:609:TRP:CZ3   | 2.54                     | 0.42              |
| 14:B:830:CLA:H193 | 14:B:841:CLA:HBA2 | 2.00                     | 0.42              |
| 17:B:846:BCR:H15C | 17:B:846:BCR:H351 | 1.78                     | 0.42              |
| 17:K:102:BCR:H11C | 17:K:102:BCR:H341 | 1.86                     | 0.42              |
| 4:b:179:LEU:HG    | 14:b:825:CLA:HED1 | 2.02                     | 0.42              |
| 4:b:322:PRO:O     | 4:b:411:VAL:HG23  | 2.19                     | 0.42              |
| 21:b:849:LMG:H242 | 18:m:101:LHG:H221 | 2.01                     | 0.42              |
| 17:b:850:BCR:HC32 | 17:b:852:BCR:H16C | 2.01                     | 0.42              |
| 17:i:101:BCR:H15C | 17:i:101:BCR:H351 | 1.77                     | 0.42              |
| 14:l:203:CLA:HAC2 | 17:l:205:BCR:C26  | 2.49                     | 0.42              |
| 2:G:12:LYS:HB3    | 2:G:13:ALA:H      | 1.75                     | 0.42              |
| 2:G:297:HIS:HE2   | 14:G:818:CLA:C2B  | 2.32                     | 0.42              |
| 14:G:831:CLA:HBC2 | 14:G:838:CLA:HMC2 | 2.01                     | 0.42              |
| 14:G:832:CLA:H102 | 14:G:832:CLA:H62  | 1.71                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:G:849:LHG:H132 | 18:G:849:LHG:H101 | 1.84                     | 0.42              |
| 4:N:136:TYR:CE1   | 13:Y:12:ALA:HB2   | 2.53                     | 0.42              |
| 4:N:461:PRO:HB3   | 4:N:524:PHE:HB2   | 2.01                     | 0.42              |
| 4:N:555:PRO:HB3   | 8:S:163:PRO:HG2   | 2.02                     | 0.42              |
| 17:N:853:BCR:H271 | 9:T:47:PRO:HG2    | 2.00                     | 0.42              |
| 6:Q:69:LEU:O      | 6:Q:73:LEU:HG     | 2.19                     | 0.42              |
| 2:g:149:ARG:HG3   | 2:g:228:MET:HE1   | 2.00                     | 0.42              |
| 14:g:817:CLA:H3A  | 14:g:817:CLA:HBA2 | 1.45                     | 0.42              |
| 14:g:832:CLA:H92  | 14:g:832:CLA:H61  | 1.87                     | 0.42              |
| 17:g:844:BCR:H15C | 17:g:844:BCR:H351 | 1.77                     | 0.42              |
| 4:n:701:LYS:HD3   | 11:v:41:GLU:HG2   | 2.01                     | 0.42              |
| 14:n:826:CLA:H112 | 14:n:826:CLA:H72  | 1.75                     | 0.42              |
| 17:n:851:BCR:H15C | 17:n:851:BCR:H351 | 1.77                     | 0.42              |
| 14:A:837:CLA:H152 | 14:A:837:CLA:H112 | 1.79                     | 0.42              |
| 3:X:21:ARG:HB2    | 14:B:831:CLA:H42  | 2.01                     | 0.42              |
| 4:B:207:VAL:HA    | 4:B:211:ASN:HD21  | 1.84                     | 0.42              |
| 4:B:681:LEU:HD12  | 4:B:681:LEU:HA    | 1.84                     | 0.42              |
| 2:a:334:THR:HA    | 14:a:829:CLA:OBD  | 2.19                     | 0.42              |
| 2:a:685:MET:HG3   | 14:a:852:CLA:C1C  | 2.41                     | 0.42              |
| 4:b:44:GLN:NE2    | 4:b:162:ARG:HB3   | 2.33                     | 0.42              |
| 4:b:138:GLY:HA2   | 14:b:815:CLA:O1A  | 2.19                     | 0.42              |
| 4:b:326:ILE:HD12  | 14:b:824:CLA:HBC3 | 2.00                     | 0.42              |
| 4:b:533:GLY:HA2   | 4:b:589:TRP:HZ3   | 1.83                     | 0.42              |
| 4:b:701:LYS:HB3   | 4:b:701:LYS:HE3   | 1.58                     | 0.42              |
| 2:G:205:LEU:HD13  | 14:G:812:CLA:HHB  | 2.01                     | 0.42              |
| 2:G:458:HIS:CE1   | 14:G:833:CLA:NA   | 2.87                     | 0.42              |
| 14:G:829:CLA:H142 | 14:G:829:CLA:H111 | 1.80                     | 0.42              |
| 14:G:830:CLA:HMC1 | 14:G:838:CLA:HAB  | 2.00                     | 0.42              |
| 4:N:326:ILE:HD11  | 4:N:410:ASN:OD1   | 2.19                     | 0.42              |
| 14:N:820:CLA:HBB2 | 14:N:820:CLA:H111 | 2.00                     | 0.42              |
| 14:N:839:CLA:H121 | 14:N:839:CLA:HMC2 | 2.01                     | 0.42              |
| 17:W:205:BCR:H15C | 17:W:205:BCR:H351 | 1.92                     | 0.42              |
| 14:g:819:CLA:H111 | 14:g:825:CLA:HMA3 | 2.02                     | 0.42              |
| 14:g:829:CLA:HAB  | 14:g:837:CLA:HBB2 | 2.00                     | 0.42              |
| 14:A:803:CLA:HHC  | 14:A:805:CLA:OBD  | 2.19                     | 0.42              |
| 14:A:805:CLA:H52  | 18:A:850:LHG:H281 | 2.00                     | 0.42              |
| 4:B:26:ALA:HB2    | 21:B:849:LMG:H132 | 2.01                     | 0.42              |
| 4:B:399:VAL:HG23  | 4:B:548:ALA:HB1   | 2.01                     | 0.42              |
| 4:B:462:VAL:HG21  | 8:F:77:ASP:HB3    | 2.02                     | 0.42              |
| 14:B:824:CLA:H62  | 14:B:825:CLA:H162 | 2.01                     | 0.42              |
| 17:B:845:BCR:H24C | 17:B:845:BCR:H371 | 1.69                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:D:19:LEU:HD21   | 6:D:59:TYR:HB3    | 2.01                     | 0.42              |
| 6:D:29:TYR:HB2    | 6:D:60:ILE:HG13   | 2.01                     | 0.42              |
| 2:a:166:GLY:HA2   | 17:a:844:BCR:HC22 | 2.02                     | 0.42              |
| 4:b:273:MET:HE1   | 4:b:361:SER:O     | 2.18                     | 0.42              |
| 4:b:341:HIS:CG    | 14:b:825:CLA:HAA1 | 2.54                     | 0.42              |
| 4:b:555:PRO:HB2   | 5:c:62:PHE:CE1    | 2.55                     | 0.42              |
| 4:b:653:TRP:CH2   | 4:b:733:ILE:HG21  | 2.55                     | 0.42              |
| 14:b:802:CLA:HHD  | 17:b:848:BCR:H383 | 2.02                     | 0.42              |
| 11:i:34:SER:HB3   | 12:l:111:LEU:HD21 | 2.01                     | 0.42              |
| 12:l:51:PRO:HG3   | 14:l:203:CLA:HED2 | 2.01                     | 0.42              |
| 2:G:226:LYS:HD3   | 2:G:253:LEU:HB3   | 2.01                     | 0.42              |
| 2:G:643:ILE:HG21  | 14:G:801:CLA:CGA  | 2.50                     | 0.42              |
| 4:N:686:VAL:O     | 4:N:690:GLU:HG2   | 2.20                     | 0.42              |
| 14:N:804:CLA:H142 | 14:N:804:CLA:H111 | 1.79                     | 0.42              |
| 4:n:12:LEU:HD11   | 4:n:23:TYR:HB3    | 2.02                     | 0.42              |
| 14:n:823:CLA:H161 | 14:n:823:CLA:H143 | 1.72                     | 0.42              |
| 17:t:103:BCR:H15C | 17:t:103:BCR:H351 | 1.75                     | 0.42              |
| 2:A:179:PHE:CE2   | 2:A:184:ARG:HB2   | 2.55                     | 0.42              |
| 2:A:445:CYS:HB3   | 2:A:545:VAL:HG22  | 2.01                     | 0.42              |
| 2:A:453:PHE:CE1   | 14:A:801:CLA:HHB  | 2.54                     | 0.42              |
| 2:A:685:MET:HB2   | 14:A:853:CLA:NC   | 2.33                     | 0.42              |
| 14:A:803:CLA:H11  | 14:A:803:CLA:H52  | 1.80                     | 0.42              |
| 4:B:86:PRO:HB2    | 4:B:116:ALA:HB3   | 2.01                     | 0.42              |
| 4:B:435:PHE:CZ    | 17:B:851:BCR:H372 | 2.53                     | 0.42              |
| 14:B:819:CLA:H8   | 14:B:819:CLA:HAB  | 2.00                     | 0.42              |
| 10:K:39:ILE:HD12  | 10:K:39:ILE:O     | 2.18                     | 0.42              |
| 10:K:47:ALA:HA    | 10:K:58:GLY:HA2   | 2.00                     | 0.42              |
| 14:a:804:CLA:H192 | 14:a:804:CLA:H161 | 1.71                     | 0.42              |
| 4:b:465:GLN:HG2   | 4:b:476:TYR:CZ    | 2.54                     | 0.42              |
| 4:b:630:TYR:O     | 4:b:634:ASN:HB2   | 2.18                     | 0.42              |
| 14:b:811:CLA:H92  | 14:b:811:CLA:H61  | 1.68                     | 0.42              |
| 17:b:850:BCR:H11C | 17:b:850:BCR:H341 | 1.77                     | 0.42              |
| 7:e:12:ARG:HD3    | 7:e:14:GLU:OE1    | 2.19                     | 0.42              |
| 12:l:167:ILE:HD13 | 12:l:167:ILE:HA   | 1.87                     | 0.42              |
| 14:G:814:CLA:C1C  | 17:G:843:BCR:H312 | 2.50                     | 0.42              |
| 18:G:850:LHG:H322 | 18:G:850:LHG:H351 | 1.90                     | 0.42              |
| 4:N:701:LYS:HB3   | 4:N:701:LYS:HE3   | 1.71                     | 0.42              |
| 17:S:204:BCR:H341 | 17:S:204:BCR:H11C | 1.71                     | 0.42              |
| 12:W:64:LEU:O     | 12:W:68:MET:HG3   | 2.19                     | 0.42              |
| 2:g:598:TRP:HE1   | 14:n:804:CLA:C1D  | 2.33                     | 0.42              |
| 4:n:415:VAL:HA    | 4:n:418:HIS:CE1   | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:n:719:HIS:HE1   | 14:n:840:CLA:ND   | 2.17                     | 0.42              |
| 2:A:53:HIS:NE2    | 14:A:802:CLA:NA   | 2.67                     | 0.42              |
| 4:B:652:VAL:HG11  | 14:B:809:CLA:HAC1 | 2.01                     | 0.42              |
| 17:B:852:BCR:H361 | 17:B:852:BCR:H20C | 1.82                     | 0.42              |
| 2:a:538:ILE:HD12  | 19:a:851:CL0:H55  | 2.00                     | 0.42              |
| 4:b:378:HIS:HB2   | 14:b:828:CLA:CHB  | 2.49                     | 0.42              |
| 14:b:804:CLA:HBA2 | 14:b:804:CLA:H3A  | 1.92                     | 0.42              |
| 14:b:806:CLA:H3A  | 14:b:806:CLA:HBA1 | 1.49                     | 0.42              |
| 14:b:831:CLA:HAB  | 14:b:839:CLA:HBB2 | 2.00                     | 0.42              |
| 14:l:202:CLA:C2B  | 14:l:203:CLA:HED1 | 2.50                     | 0.42              |
| 2:G:53:HIS:CD2    | 18:G:849:LHG:H141 | 2.55                     | 0.42              |
| 2:G:408:HIS:HE1   | 14:G:829:CLA:C4A  | 2.32                     | 0.42              |
| 2:G:685:MET:HE3   | 15:G:841:PQN:C2M  | 2.49                     | 0.42              |
| 14:G:801:CLA:C1B  | 14:N:805:CLA:HBB1 | 2.45                     | 0.42              |
| 14:G:807:CLA:HBA2 | 14:G:807:CLA:H3A  | 1.35                     | 0.42              |
| 14:G:823:CLA:HAC2 | 14:G:838:CLA:H172 | 2.02                     | 0.42              |
| 14:G:827:CLA:H52  | 14:G:827:CLA:H8   | 1.89                     | 0.42              |
| 14:N:851:CLA:H143 | 14:N:851:CLA:H112 | 1.81                     | 0.42              |
| 7:R:56:ASP:OD2    | 7:R:56:ASP:C      | 2.62                     | 0.42              |
| 12:W:71:GLY:HA3   | 12:W:150:GLY:HA2  | 2.02                     | 0.42              |
| 2:g:658:VAL:HB    | 2:g:746:ALA:HB3   | 2.02                     | 0.42              |
| 8:s:98:GLY:HA3    | 8:s:139:TRP:CE2   | 2.55                     | 0.42              |
| 12:w:152:GLY:HA2  | 17:w:207:BCR:HC42 | 2.01                     | 0.42              |
| 14:A:802:CLA:H161 | 14:A:802:CLA:H192 | 1.72                     | 0.42              |
| 2:a:361:GLY:HA2   | 2:a:398:GLY:HA2   | 2.01                     | 0.42              |
| 2:a:544:HIS:CE1   | 14:a:837:CLA:NA   | 2.88                     | 0.42              |
| 8:f:45:ARG:H      | 8:f:57:ARG:HH22   | 1.66                     | 0.42              |
| 2:G:351:ALA:HB1   | 17:G:846:BCR:HC22 | 2.00                     | 0.42              |
| 2:G:412:PHE:CD1   | 2:G:416:ASP:HB2   | 2.54                     | 0.42              |
| 2:G:650:PHE:HA    | 2:G:654:GLN:HG3   | 2.01                     | 0.42              |
| 4:N:34:HIS:HB2    | 4:N:37:MET:HE3    | 2.01                     | 0.42              |
| 4:N:54:LEU:HD12   | 4:N:54:LEU:HA     | 1.90                     | 0.42              |
| 4:N:56:ILE:HD11   | 17:Y:101:BCR:HC7  | 2.02                     | 0.42              |
| 4:N:182:LEU:HD11  | 14:N:815:CLA:H12  | 2.01                     | 0.42              |
| 14:n:802:CLA:HBA1 | 14:n:802:CLA:H3A  | 1.41                     | 0.42              |
| 14:n:808:CLA:CGA  | 14:n:808:CLA:C1A  | 2.98                     | 0.42              |
| 10:u:48:LEU:HD13  | 10:u:54:PHE:HD2   | 1.85                     | 0.42              |
| 10:u:52:LYS:HE3   | 10:u:52:LYS:HB3   | 1.62                     | 0.42              |
| 12:w:53:TYR:HD1   | 12:w:130:PRO:HD3  | 1.85                     | 0.42              |
| 2:A:89:SER:HB3    | 2:A:166:GLY:HA3   | 2.01                     | 0.42              |
| 2:A:104:TRP:HZ3   | 2:A:149:ARG:HB2   | 1.85                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:A:433:HIS:CE1   | 14:A:830:CLA:ND    | 2.88                     | 0.42              |
| 17:A:846:BCR:H20C | 17:A:846:BCR:H361  | 1.90                     | 0.42              |
| 4:B:89:HIS:CE1    | 4:B:114:ASN:HD22   | 2.37                     | 0.42              |
| 4:B:127:ILE:HG22  | 14:B:819:CLA:HED2  | 2.02                     | 0.42              |
| 4:B:351:TRP:CZ2   | 14:B:827:CLA:H3A   | 2.55                     | 0.42              |
| 14:B:810:CLA:H8   | 14:B:810:CLA:H51   | 1.66                     | 0.42              |
| 14:B:838:CLA:H3A  | 14:B:838:CLA:HBA2  | 1.87                     | 0.42              |
| 3:x:34:LEU:HG     | 3:x:38:TYR:CE2     | 2.54                     | 0.42              |
| 14:x:1701:CLA:H3A | 14:x:1701:CLA:HBA1 | 1.61                     | 0.42              |
| 4:b:74:PHE:O      | 4:b:78:ILE:HG12    | 2.20                     | 0.42              |
| 4:b:174:ARG:O     | 4:b:178:HIS:HB2    | 2.20                     | 0.42              |
| 14:b:802:CLA:HMD3 | 17:b:848:BCR:H383  | 2.02                     | 0.42              |
| 14:b:805:CLA:HED3 | 14:b:805:CLA:HBD   | 1.74                     | 0.42              |
| 12:l:53:TYR:HE1   | 12:l:126:VAL:HG21  | 1.85                     | 0.42              |
| 2:G:197:MET:HB2   | 14:G:812:CLA:HBC2  | 2.01                     | 0.42              |
| 14:G:827:CLA:H11  | 17:G:848:BCR:HC42  | 2.02                     | 0.42              |
| 4:N:104:PHE:CZ    | 4:N:652:VAL:HG23   | 2.55                     | 0.42              |
| 4:N:216:ALA:HB2   | 14:N:817:CLA:HED2  | 2.02                     | 0.42              |
| 14:N:810:CLA:H143 | 14:N:810:CLA:H161  | 1.87                     | 0.42              |
| 15:N:843:PQN:H261 | 15:N:843:PQN:H222  | 1.80                     | 0.42              |
| 17:N:853:BCR:H383 | 14:T:102:CLA:C2D   | 2.50                     | 0.42              |
| 17:U:103:BCR:H24C | 17:U:103:BCR:H371  | 1.84                     | 0.42              |
| 2:g:394:HIS:NE2   | 14:g:827:CLA:ND    | 2.68                     | 0.42              |
| 2:g:432:ARG:HH12  | 6:q:13:ALA:HB3     | 1.84                     | 0.42              |
| 2:g:572:ARG:HG2   | 2:g:722:THR:HG21   | 2.02                     | 0.42              |
| 2:g:588:GLY:O     | 2:g:592:VAL:HG23   | 2.20                     | 0.42              |
| 14:g:834:CLA:H3A  | 14:g:834:CLA:HBA2  | 1.73                     | 0.42              |
| 4:n:145:PHE:HD1   | 4:n:145:PHE:HA     | 1.75                     | 0.42              |
| 4:n:222:LEU:HG    | 14:n:815:CLA:C3D   | 2.50                     | 0.42              |
| 14:n:806:CLA:H111 | 14:n:806:CLA:H72   | 1.59                     | 0.42              |
| 14:n:808:CLA:H112 | 14:n:808:CLA:H72   | 1.72                     | 0.42              |
| 14:n:825:CLA:HBA2 | 14:n:825:CLA:H3A   | 1.68                     | 0.42              |
| 12:w:113:ALA:O    | 12:w:136:LYS:HG3   | 2.20                     | 0.42              |
| 12:w:113:ALA:HB2  | 12:w:139:TRP:HB3   | 2.02                     | 0.42              |
| 14:A:820:CLA:C4C  | 14:A:826:CLA:H152  | 2.49                     | 0.42              |
| 14:A:821:CLA:HBA1 | 10:K:38:THR:HG21   | 2.02                     | 0.42              |
| 4:B:378:HIS:HB2   | 14:B:828:CLA:CHB   | 2.50                     | 0.42              |
| 2:a:263:PRO:HB3   | 2:a:268:ASN:HB3    | 2.00                     | 0.42              |
| 2:a:297:HIS:CE1   | 2:a:301:ILE:HG13   | 2.55                     | 0.42              |
| 14:a:801:CLA:HBB1 | 14:a:801:CLA:HMB3  | 2.02                     | 0.42              |
| 4:b:330:TYR:CZ    | 14:b:825:CLA:NC    | 2.87                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:b:523:ASP:HA    | 4:b:526:VAL:HG22  | 2.00                     | 0.42              |
| 6:d:85:ARG:HB3    | 6:d:93:THR:OG1    | 2.20                     | 0.42              |
| 2:G:200:HIS:CE1   | 14:G:811:CLA:NA   | 2.88                     | 0.42              |
| 2:G:532:ASP:HA    | 2:G:535:ILE:HG22  | 2.00                     | 0.42              |
| 2:G:657:GLN:HG2   | 2:G:750:SER:HB2   | 2.01                     | 0.42              |
| 14:G:812:CLA:H41  | 17:G:845:BCR:H17C | 2.02                     | 0.42              |
| 14:G:818:CLA:H203 | 14:G:826:CLA:H3A  | 2.02                     | 0.42              |
| 4:N:367:LYS:HD3   | 4:N:367:LYS:HA    | 1.67                     | 0.42              |
| 17:N:848:BCR:H361 | 17:N:848:BCR:H20C | 1.86                     | 0.42              |
| 14:N:851:CLA:H93  | 14:N:851:CLA:CAD  | 2.50                     | 0.42              |
| 17:S:204:BCR:H15C | 17:S:204:BCR:H12C | 1.85                     | 0.42              |
| 2:g:67:GLU:O      | 2:g:71:ARG:HG2    | 2.20                     | 0.42              |
| 2:g:600:TYR:OH    | 19:g:851:CL0:H9   | 2.20                     | 0.42              |
| 14:g:803:CLA:H143 | 17:g:844:BCR:HC41 | 2.01                     | 0.42              |
| 14:g:833:CLA:O1A  | 14:g:834:CLA:HHB  | 2.20                     | 0.42              |
| 14:g:837:CLA:H92  | 18:g:850:LHG:H383 | 2.02                     | 0.42              |
| 19:g:851:CL0:H56  | 19:g:851:CL0:H51  | 1.93                     | 0.42              |
| 4:n:101:ILE:O     | 4:n:105:THR:HG23  | 2.20                     | 0.42              |
| 4:n:426:LEU:HG    | 4:n:539:LEU:HB2   | 2.01                     | 0.42              |
| 4:n:610:GLN:HG2   | 4:n:740:PHE:HZ    | 1.84                     | 0.42              |
| 8:s:38:GLN:H      | 8:s:38:GLN:HG3    | 1.67                     | 0.42              |
| 11:v:35:PHE:CE2   | 18:v:102:LHG:H241 | 2.54                     | 0.42              |
| 14:A:821:CLA:CHD  | 17:A:844:BCR:H382 | 2.50                     | 0.42              |
| 14:A:826:CLA:HAB  | 14:A:834:CLA:HMA2 | 2.02                     | 0.42              |
| 14:A:831:CLA:H192 | 14:A:831:CLA:H161 | 1.74                     | 0.42              |
| 4:B:419:LYS:HD3   | 8:F:164:ARG:NH1   | 2.35                     | 0.42              |
| 14:B:814:CLA:H42  | 17:B:844:BCR:H12C | 2.01                     | 0.42              |
| 14:B:833:CLA:HED2 | 14:B:833:CLA:H2A  | 2.02                     | 0.42              |
| 5:C:15:THR:O      | 5:C:19:ARG:HB2    | 2.20                     | 0.42              |
| 2:a:264:PHE:CZ    | 17:a:843:BCR:H343 | 2.54                     | 0.42              |
| 2:a:606:VAL:HG21  | 14:a:835:CLA:HBB2 | 2.01                     | 0.42              |
| 2:a:731:HIS:CE1   | 14:a:839:CLA:NA   | 2.87                     | 0.42              |
| 14:a:819:CLA:H61  | 14:a:819:CLA:H41  | 1.80                     | 0.42              |
| 14:a:852:CLA:HBA2 | 4:b:431:LEU:HD23  | 2.02                     | 0.42              |
| 14:b:803:CLA:H61  | 14:b:803:CLA:H41  | 1.71                     | 0.42              |
| 17:b:845:BCR:H371 | 17:b:845:BCR:H24C | 1.69                     | 0.42              |
| 8:f:86:PHE:C      | 8:f:89:PRO:HD2    | 2.43                     | 0.42              |
| 2:G:15:VAL:HG11   | 14:G:809:CLA:HAA2 | 2.02                     | 0.41              |
| 2:G:264:PHE:HB2   | 2:G:272:TYR:HE2   | 1.84                     | 0.41              |
| 2:G:537:HIS:HE1   | 14:G:837:CLA:ND   | 2.17                     | 0.41              |
| 2:G:578:PRO:HD3   | 4:N:568:GLY:HA2   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:G:817:CLA:H93  | 14:G:817:CLA:H111 | 1.84                     | 0.41              |
| 15:G:841:PQN:H12  | 15:G:841:PQN:H162 | 1.77                     | 0.41              |
| 4:N:104:PHE:HZ    | 4:N:652:VAL:HG23  | 1.85                     | 0.41              |
| 4:N:522:GLY:O     | 4:N:526:VAL:HG23  | 2.20                     | 0.41              |
| 14:N:809:CLA:HMA1 | 14:N:810:CLA:CHB  | 2.49                     | 0.41              |
| 17:N:853:BCR:H371 | 17:N:853:BCR:H24C | 1.84                     | 0.41              |
| 2:g:282:LEU:HD11  | 2:g:375:PRO:HD2   | 2.01                     | 0.41              |
| 14:g:805:CLA:H2   | 14:g:807:CLA:H2   | 2.02                     | 0.41              |
| 14:g:822:CLA:HMD3 | 17:g:846:BCR:H321 | 2.01                     | 0.41              |
| 14:g:827:CLA:C2   | 17:g:845:BCR:H24C | 2.49                     | 0.41              |
| 14:g:832:CLA:HHD  | 14:n:809:CLA:HBB2 | 2.02                     | 0.41              |
| 14:g:837:CLA:NC   | 18:g:850:LHG:H332 | 2.35                     | 0.41              |
| 4:n:216:ALA:HA    | 14:n:815:CLA:HED2 | 2.02                     | 0.41              |
| 4:n:443:HIS:CD2   | 4:n:457:ILE:HG13  | 2.54                     | 0.41              |
| 4:n:653:TRP:CZ2   | 4:n:733:ILE:HG21  | 2.54                     | 0.41              |
| 14:n:829:CLA:H202 | 14:n:829:CLA:H162 | 1.84                     | 0.41              |
| 2:A:310:HIS:NE2   | 14:A:819:CLA:NA   | 2.68                     | 0.41              |
| 14:A:805:CLA:H62  | 14:A:805:CLA:H41  | 1.62                     | 0.41              |
| 14:A:818:CLA:HAB  | 14:A:818:CLA:H8   | 2.02                     | 0.41              |
| 14:A:827:CLA:H61  | 14:A:827:CLA:H41  | 1.81                     | 0.41              |
| 4:B:378:HIS:HE2   | 14:B:829:CLA:C1B  | 2.33                     | 0.41              |
| 4:B:651:SER:OG    | 14:B:810:CLA:HBC1 | 2.21                     | 0.41              |
| 14:B:806:CLA:H92  | 14:B:814:CLA:H2   | 2.02                     | 0.41              |
| 17:B:848:BCR:H20C | 17:B:848:BCR:H361 | 1.78                     | 0.41              |
| 8:F:83:ALA:HB3    | 9:J:48:LEU:HD11   | 2.01                     | 0.41              |
| 17:J:103:BCR:H11C | 17:J:103:BCR:H341 | 1.79                     | 0.41              |
| 2:a:117:VAL:O     | 14:a:807:CLA:HED2 | 2.20                     | 0.41              |
| 2:a:149:ARG:HD3   | 2:a:378:PRO:HB2   | 2.02                     | 0.41              |
| 2:a:397:ILE:HD12  | 14:a:804:CLA:H143 | 2.01                     | 0.41              |
| 14:a:828:CLA:H122 | 14:a:828:CLA:H162 | 1.80                     | 0.41              |
| 4:b:150:LEU:HD22  | 13:m:23:ALA:HA    | 2.02                     | 0.41              |
| 4:b:223:GLN:HB3   | 4:b:224:PRO:HD3   | 2.02                     | 0.41              |
| 4:b:619:ASN:O     | 4:b:625:GLY:HA3   | 2.19                     | 0.41              |
| 14:b:826:CLA:H111 | 14:b:826:CLA:H72  | 1.69                     | 0.41              |
| 14:b:832:CLA:H62  | 8:f:147:LEU:HD22  | 2.02                     | 0.41              |
| 17:b:846:BCR:H24C | 17:b:846:BCR:H371 | 1.90                     | 0.41              |
| 17:l:205:BCR:H351 | 17:l:205:BCR:H15C | 1.76                     | 0.41              |
| 2:G:361:GLY:O     | 2:G:365:ILE:HG13  | 2.20                     | 0.41              |
| 2:G:495:PRO:HB3   | 2:G:502:ALA:O     | 2.20                     | 0.41              |
| 14:G:808:CLA:H162 | 14:G:808:CLA:H141 | 1.82                     | 0.41              |
| 14:G:835:CLA:H3A  | 14:G:835:CLA:HBA2 | 1.87                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:N:820:CLA:HBB2 | 14:N:820:CLA:H151 | 2.01                     | 0.41              |
| 6:Q:58:LEU:HD12   | 12:W:29:GLN:HG2   | 2.02                     | 0.41              |
| 9:T:38:ARG:HD3    | 17:T:104:BCR:HC22 | 2.02                     | 0.41              |
| 2:g:373:ALA:HA    | 2:g:523:MET:HE3   | 2.02                     | 0.41              |
| 2:g:731:HIS:HE1   | 14:g:839:CLA:ND   | 2.17                     | 0.41              |
| 4:n:276:HIS:HB2   | 14:n:817:CLA:CHB  | 2.50                     | 0.41              |
| 4:n:528:HIS:NE2   | 14:n:837:CLA:NB   | 2.68                     | 0.41              |
| 4:n:531:ALA:HB2   | 14:n:837:CLA:HMA3 | 2.02                     | 0.41              |
| 14:n:832:CLA:HMB1 | 17:n:849:BCR:H12C | 2.02                     | 0.41              |
| 2:A:43:PRO:HB3    | 2:A:48:TRP:CD2    | 2.55                     | 0.41              |
| 2:A:442:ASN:O     | 2:A:446:ILE:HG13  | 2.20                     | 0.41              |
| 18:A:850:LHG:H111 | 18:A:850:LHG:H142 | 1.73                     | 0.41              |
| 14:A:855:CLA:HMA2 | 17:B:848:BCR:C37  | 2.50                     | 0.41              |
| 4:B:650:LEU:HD12  | 4:B:650:LEU:O     | 2.20                     | 0.41              |
| 7:E:56:ASP:OD2    | 7:E:56:ASP:C      | 2.63                     | 0.41              |
| 14:K:101:CLA:HBA2 | 14:K:101:CLA:H3A  | 1.47                     | 0.41              |
| 2:a:81:LEU:HD21   | 14:a:811:CLA:H12  | 2.03                     | 0.41              |
| 2:a:554:VAL:HG21  | 17:a:847:BCR:HC31 | 2.02                     | 0.41              |
| 2:a:674:LEU:HD23  | 2:a:674:LEU:HA    | 1.84                     | 0.41              |
| 14:a:839:CLA:H203 | 14:f:202:CLA:HBB2 | 2.01                     | 0.41              |
| 18:a:849:LHG:H291 | 18:a:849:LHG:H262 | 1.68                     | 0.41              |
| 17:l:206:BCR:H15C | 17:l:206:BCR:H351 | 1.78                     | 0.41              |
| 2:G:320:HIS:HB3   | 2:G:325:ILE:HD11  | 2.02                     | 0.41              |
| 14:G:806:CLA:H92  | 14:G:808:CLA:H71  | 2.02                     | 0.41              |
| 14:G:812:CLA:H93  | 14:G:812:CLA:H61  | 1.91                     | 0.41              |
| 14:G:837:CLA:CBB  | 14:G:838:CLA:HBC3 | 2.49                     | 0.41              |
| 3:H:21:ARG:HB2    | 14:N:832:CLA:H42  | 2.03                     | 0.41              |
| 14:N:822:CLA:H3A  | 14:N:822:CLA:HBA2 | 1.36                     | 0.41              |
| 17:N:844:BCR:H341 | 17:N:844:BCR:H11C | 1.78                     | 0.41              |
| 10:U:15:GLU:OE2   | 10:U:15:GLU:N     | 2.48                     | 0.41              |
| 2:g:538:ILE:HG21  | 19:g:851:CL0:H60  | 2.01                     | 0.41              |
| 14:g:804:CLA:H193 | 14:g:804:CLA:H161 | 1.81                     | 0.41              |
| 4:n:22:TRP:CG     | 4:n:711:GLN:HE22  | 2.38                     | 0.41              |
| 4:n:680:GLU:O     | 4:n:684:THR:HG23  | 2.19                     | 0.41              |
| 14:n:840:CLA:H61  | 14:n:840:CLA:H41  | 1.73                     | 0.41              |
| 8:s:25:GLY:O      | 8:s:28:LEU:HG     | 2.20                     | 0.41              |
| 14:A:801:CLA:O2A  | 4:B:658:LEU:HB3   | 2.21                     | 0.41              |
| 4:B:664:TRP:CZ3   | 14:B:804:CLA:HHB  | 2.55                     | 0.41              |
| 17:B:843:BCR:H11C | 17:B:843:BCR:H341 | 1.84                     | 0.41              |
| 5:C:66:ARG:HD3    | 5:C:66:ARG:HA     | 1.77                     | 0.41              |
| 5:C:73:THR:H      | 5:C:76:SER:HB2    | 1.85                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:a:116:GLN:HG2   | 2:a:138:ILE:HD12  | 2.02                     | 0.41              |
| 2:a:747:HIS:O     | 2:a:751:VAL:HG22  | 2.21                     | 0.41              |
| 12:l:70:HIS:HE1   | 14:l:203:CLA:C4D  | 2.33                     | 0.41              |
| 4:N:196:HIS:CE1   | 14:N:817:CLA:NA   | 2.89                     | 0.41              |
| 4:N:552:LYS:HD2   | 4:N:552:LYS:HA    | 1.74                     | 0.41              |
| 6:Q:65:TYR:CD2    | 6:Q:65:TYR:N      | 2.89                     | 0.41              |
| 11:V:21:VAL:HA    | 11:V:24:ILE:HG22  | 2.02                     | 0.41              |
| 12:W:85:ARG:HG3   | 12:W:86:ASP:OD2   | 2.21                     | 0.41              |
| 2:g:213:TRP:O     | 2:g:217:LEU:HG    | 2.20                     | 0.41              |
| 2:g:393:HIS:HE2   | 14:g:827:CLA:C1B  | 2.33                     | 0.41              |
| 4:n:158:GLN:O     | 4:n:162:ARG:HG3   | 2.19                     | 0.41              |
| 4:n:318:PRO:HD2   | 4:n:323:HIS:HB2   | 2.02                     | 0.41              |
| 4:n:369:TYR:HB3   | 4:n:609:TRP:CZ3   | 2.55                     | 0.41              |
| 14:n:807:CLA:HBB  | 14:n:808:CLA:HMB3 | 2.01                     | 0.41              |
| 12:w:17:ASN:OD1   | 12:w:18:ARG:HG3   | 2.20                     | 0.41              |
| 2:A:599:MET:SD    | 2:A:599:MET:C     | 3.04                     | 0.41              |
| 14:A:817:CLA:H111 | 14:A:817:CLA:H91  | 1.83                     | 0.41              |
| 4:B:32:GLU:H      | 4:B:32:GLU:HG3    | 1.67                     | 0.41              |
| 7:E:32:ILE:HD11   | 7:E:35:PRO:HA     | 2.02                     | 0.41              |
| 2:a:547:VAL:HG21  | 14:a:837:CLA:HMA1 | 2.02                     | 0.41              |
| 14:a:802:CLA:H11  | 14:a:802:CLA:H52  | 1.77                     | 0.41              |
| 4:b:178:HIS:O     | 4:b:182:LEU:HB3   | 2.20                     | 0.41              |
| 4:b:305:MET:HE3   | 4:b:305:MET:HB3   | 1.90                     | 0.41              |
| 4:b:427:SER:HA    | 4:b:539:LEU:HD22  | 2.02                     | 0.41              |
| 14:b:807:CLA:HBA1 | 14:b:807:CLA:H11  | 1.72                     | 0.41              |
| 17:b:852:BCR:H15C | 17:b:852:BCR:H351 | 1.75                     | 0.41              |
| 5:c:43:PRO:HG2    | 5:c:44:ARG:HE     | 1.85                     | 0.41              |
| 8:f:88:ILE:HB     | 8:f:89:PRO:HD3    | 2.01                     | 0.41              |
| 14:l:202:CLA:C1B  | 14:l:203:CLA:HED1 | 2.50                     | 0.41              |
| 2:G:408:HIS:CE1   | 14:G:829:CLA:NA   | 2.88                     | 0.41              |
| 14:G:813:CLA:H61  | 14:G:813:CLA:H2   | 1.79                     | 0.41              |
| 14:G:831:CLA:H192 | 14:G:831:CLA:H161 | 1.82                     | 0.41              |
| 4:N:304:MET:HE2   | 4:N:304:MET:HB3   | 1.82                     | 0.41              |
| 15:N:843:PQN:H192 | 15:N:843:PQN:H162 | 1.82                     | 0.41              |
| 12:W:70:HIS:HE1   | 14:W:203:CLA:C4D  | 2.34                     | 0.41              |
| 19:g:851:CL0:H66  | 14:g:853:CLA:C2B  | 2.50                     | 0.41              |
| 4:n:592:ASN:HB2   | 14:n:802:CLA:HBC2 | 2.02                     | 0.41              |
| 4:n:603:TRP:CZ2   | 4:n:629:ASP:HB2   | 2.55                     | 0.41              |
| 4:n:679:GLN:HE21  | 4:n:683:GLU:HG3   | 1.85                     | 0.41              |
| 14:n:809:CLA:H142 | 21:n:848:LMG:H211 | 2.03                     | 0.41              |
| 17:n:847:BCR:H11C | 17:n:847:BCR:H341 | 1.90                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:n:850:CLA:H43  | 9:t:36:PHE:CD1     | 2.56                     | 0.41              |
| 8:s:64:ALA:HA     | 8:s:82:ARG:HH21    | 1.84                     | 0.41              |
| 11:v:25:GLY:O     | 11:v:29:PRO:HG2    | 2.21                     | 0.41              |
| 2:A:351:ALA:HB1   | 17:A:847:BCR:HC22  | 2.03                     | 0.41              |
| 2:A:539:HIS:HE1   | 2:A:605:ILE:HG22   | 1.86                     | 0.41              |
| 17:A:847:BCR:H381 | 18:A:851:LHG:H222  | 2.02                     | 0.41              |
| 3:X:18:TYR:CD1    | 18:X:1702:LHG:H282 | 2.56                     | 0.41              |
| 4:B:275:HIS:HE1   | 14:B:817:CLA:C4D   | 2.33                     | 0.41              |
| 14:B:803:CLA:H3A  | 14:B:803:CLA:HBA1  | 1.36                     | 0.41              |
| 14:B:831:CLA:H3A  | 14:B:832:CLA:OBD   | 2.20                     | 0.41              |
| 17:J:103:BCR:H24C | 17:J:103:BCR:H371  | 1.87                     | 0.41              |
| 12:L:18:ARG:HD2   | 12:L:18:ARG:H      | 1.86                     | 0.41              |
| 12:L:26:ARG:HB2   | 12:L:26:ARG:CZ     | 2.51                     | 0.41              |
| 14:a:807:CLA:HMA1 | 9:j:34:ILE:HD12    | 2.01                     | 0.41              |
| 14:a:831:CLA:HBB1 | 14:a:831:CLA:HMB3  | 2.01                     | 0.41              |
| 14:a:832:CLA:H122 | 17:i:102:BCR:H372  | 2.02                     | 0.41              |
| 15:b:842:PQN:H192 | 17:b:848:BCR:H23C  | 2.01                     | 0.41              |
| 2:G:386:THR:O     | 2:G:390:ILE:HG12   | 2.21                     | 0.41              |
| 2:G:662:TYR:HD2   | 4:N:448:VAL:HG12   | 1.85                     | 0.41              |
| 14:G:804:CLA:H12  | 14:G:805:CLA:CBB   | 2.50                     | 0.41              |
| 4:N:24:ALA:O      | 14:N:806:CLA:HMD2  | 2.20                     | 0.41              |
| 4:N:100:ALA:O     | 4:N:104:PHE:HD1    | 2.04                     | 0.41              |
| 4:N:597:VAL:HG21  | 14:N:838:CLA:CBB   | 2.50                     | 0.41              |
| 14:N:820:CLA:H8   | 14:N:820:CLA:CAB   | 2.50                     | 0.41              |
| 6:Q:111:GLU:HG2   | 6:Q:113:VAL:HG23   | 2.02                     | 0.41              |
| 2:g:216:HIS:CE1   | 14:g:812:CLA:NA    | 2.88                     | 0.41              |
| 14:g:828:CLA:H92  | 14:g:828:CLA:H61   | 1.76                     | 0.41              |
| 14:g:830:CLA:H93  | 14:g:830:CLA:H112  | 1.84                     | 0.41              |
| 17:n:842:BCR:H24C | 17:n:842:BCR:H371  | 1.86                     | 0.41              |
| 5:p:58:CYS:HA     | 16:p:102:SF4:S4    | 2.60                     | 0.41              |
| 14:s:201:CLA:H93  | 14:s:201:CLA:H62   | 1.72                     | 0.41              |
| 12:w:70:HIS:HE1   | 14:w:204:CLA:C4D   | 2.32                     | 0.41              |
| 12:w:80:LYS:HD3   | 12:w:80:LYS:HA     | 1.82                     | 0.41              |
| 17:w:207:BCR:H24C | 17:w:207:BCR:H371  | 1.89                     | 0.41              |
| 2:A:235:LYS:HE2   | 2:A:235:LYS:HB3    | 1.96                     | 0.41              |
| 2:A:553:GLY:O     | 2:A:557:ALA:HB2    | 2.20                     | 0.41              |
| 4:B:409:GLY:H     | 4:B:413:GLU:CD     | 2.29                     | 0.41              |
| 14:a:820:CLA:HBA2 | 14:a:820:CLA:H3A   | 1.14                     | 0.41              |
| 14:a:823:CLA:H143 | 14:a:823:CLA:H111  | 1.77                     | 0.41              |
| 4:b:600:TYR:HA    | 4:b:626:TRP:HH2    | 1.86                     | 0.41              |
| 4:b:664:TRP:CZ3   | 14:b:804:CLA:HHB   | 2.55                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 14:b:821:CLA:H3A  | 14:b:821:CLA:HBA2  | 1.56                     | 0.41              |
| 14:b:824:CLA:H142 | 14:b:824:CLA:H112  | 1.86                     | 0.41              |
| 14:b:824:CLA:HBB1 | 14:b:831:CLA:HBC2  | 2.02                     | 0.41              |
| 6:d:77:LYS:HB2    | 6:d:77:LYS:HE2     | 1.90                     | 0.41              |
| 2:G:461:THR:HG23  | 14:N:811:CLA:HMC3  | 2.03                     | 0.41              |
| 14:G:802:CLA:C2B  | 17:T:104:BCR:H393  | 2.51                     | 0.41              |
| 19:G:851:CL0:H18  | 14:N:804:CLA:HBC2  | 2.02                     | 0.41              |
| 4:N:86:PRO:HB2    | 4:N:116:ALA:HB3    | 2.02                     | 0.41              |
| 14:N:817:CLA:C3B  | 17:N:844:BCR:H333  | 2.51                     | 0.41              |
| 2:g:425:ASN:O     | 2:g:429:ARG:HG3    | 2.21                     | 0.41              |
| 2:g:668:ALA:HA    | 2:g:671:LEU:HD12   | 2.02                     | 0.41              |
| 17:g:845:BCR:H20C | 17:g:845:BCR:H361  | 1.88                     | 0.41              |
| 4:n:581:ASP:HA    | 4:n:584:TYR:HB3    | 2.02                     | 0.41              |
| 14:n:826:CLA:H152 | 17:n:846:BCR:H17C  | 2.03                     | 0.41              |
| 14:n:831:CLA:HAB  | 14:n:832:CLA:H202  | 2.03                     | 0.41              |
| 14:n:839:CLA:H41  | 14:n:839:CLA:H62   | 1.87                     | 0.41              |
| 2:A:249:LEU:HD22  | 2:A:249:LEU:H      | 1.86                     | 0.41              |
| 2:A:486:TRP:CZ2   | 2:A:490:LEU:HD11   | 2.55                     | 0.41              |
| 14:A:808:CLA:H141 | 14:A:808:CLA:H162  | 1.81                     | 0.41              |
| 14:A:819:CLA:H92  | 14:A:819:CLA:H61   | 1.91                     | 0.41              |
| 14:A:853:CLA:O1A  | 4:B:434:GLY:HA3    | 2.21                     | 0.41              |
| 4:B:18:THR:HG22   | 4:B:702:ASP:HB2    | 2.03                     | 0.41              |
| 14:B:818:CLA:H71  | 14:B:818:CLA:H111  | 1.57                     | 0.41              |
| 17:B:847:BCR:H20C | 17:B:847:BCR:H361  | 1.94                     | 0.41              |
| 2:a:456:TYR:HE1   | 2:a:534:LEU:HB3    | 1.84                     | 0.41              |
| 14:b:818:CLA:H202 | 14:b:818:CLA:H162  | 1.84                     | 0.41              |
| 14:b:838:CLA:H112 | 14:b:838:CLA:H142  | 1.74                     | 0.41              |
| 2:G:264:PHE:HZ    | 17:G:843:BCR:H343  | 1.86                     | 0.41              |
| 2:G:342:TYR:O     | 2:G:346:THR:HB     | 2.21                     | 0.41              |
| 2:G:412:PHE:CD2   | 17:G:846:BCR:HC32  | 2.56                     | 0.41              |
| 14:G:831:CLA:HBB1 | 14:N:801:CLA:HAA2  | 2.02                     | 0.41              |
| 19:G:851:CL0:H15  | 4:N:631:LEU:HD13   | 2.02                     | 0.41              |
| 3:H:20:PHE:CD2    | 20:H:1702:SQD:H441 | 2.56                     | 0.41              |
| 17:N:847:BCR:H351 | 17:N:847:BCR:H15C  | 1.68                     | 0.41              |
| 17:N:848:BCR:H351 | 17:N:848:BCR:H15C  | 1.71                     | 0.41              |
| 2:g:300:ALA:HB1   | 14:g:815:CLA:HBC2  | 2.03                     | 0.41              |
| 2:g:639:SER:O     | 2:g:645:GLY:HA3    | 2.21                     | 0.41              |
| 14:g:839:CLA:HAB  | 14:g:852:CLA:H151  | 2.02                     | 0.41              |
| 14:g:840:CLA:NA   | 14:g:840:CLA:H12   | 2.36                     | 0.41              |
| 4:n:532:LEU:HD21  | 14:n:802:CLA:HBB1  | 2.03                     | 0.41              |
| 14:n:840:CLA:HBA1 | 14:n:840:CLA:H3A   | 1.81                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 17:n:847:BCR:H15C  | 17:n:847:BCR:H351 | 1.83                     | 0.41              |
| 12:w:70:HIS:HE1    | 14:w:204:CLA:ND   | 2.19                     | 0.41              |
| 20:w:202:SQD:H131  | 20:w:202:SQD:H102 | 1.61                     | 0.41              |
| 17:A:844:BCR:H15C  | 17:A:844:BCR:H351 | 1.82                     | 0.41              |
| 4:B:330:TYR:CZ     | 14:B:825:CLA:NC   | 2.88                     | 0.41              |
| 4:B:445:ASP:OD1    | 4:B:622:TYR:HB2   | 2.21                     | 0.41              |
| 4:B:597:VAL:HG23   | 14:B:837:CLA:HHC  | 2.03                     | 0.41              |
| 14:B:828:CLA:HBC3  | 21:B:849:LMG:H421 | 2.03                     | 0.41              |
| 14:B:838:CLA:H2    | 14:B:838:CLA:H62  | 1.74                     | 0.41              |
| 14:B:838:CLA:H151  | 14:B:850:CLA:HBC1 | 2.02                     | 0.41              |
| 13:M:18:ILE:HB     | 13:M:19:PRO:HD3   | 2.03                     | 0.41              |
| 14:a:801:CLA:H3A   | 14:a:801:CLA:HBA1 | 1.87                     | 0.41              |
| 14:a:804:CLA:H41   | 14:a:828:CLA:H92  | 2.03                     | 0.41              |
| 14:a:810:CLA:H91   | 14:a:810:CLA:H112 | 1.80                     | 0.41              |
| 14:a:818:CLA:H41   | 14:a:818:CLA:H61  | 1.87                     | 0.41              |
| 14:a:818:CLA:HBA1  | 14:a:818:CLA:H3A  | 1.96                     | 0.41              |
| 4:b:275:HIS:HE1    | 14:b:817:CLA:C4D  | 2.34                     | 0.41              |
| 14:b:807:CLA:H162  | 14:b:807:CLA:H143 | 1.81                     | 0.41              |
| 14:b:820:CLA:C1C   | 14:b:825:CLA:H141 | 2.42                     | 0.41              |
| 2:G:77:HIS:CE1     | 14:G:804:CLA:C4D  | 3.04                     | 0.41              |
| 2:G:221:SER:O      | 2:G:225:ASN:HB2   | 2.20                     | 0.41              |
| 2:G:300:ALA:HB1    | 14:G:816:CLA:HBC2 | 2.02                     | 0.41              |
| 2:G:357:LEU:HD12   | 2:G:357:LEU:HA    | 1.90                     | 0.41              |
| 14:G:814:CLA:CAB   | 17:G:843:BCR:H333 | 2.51                     | 0.41              |
| 4:N:426:LEU:HG     | 14:N:840:CLA:CBB  | 2.51                     | 0.41              |
| 14:N:813:CLA:H43   | 14:N:814:CLA:ND   | 2.36                     | 0.41              |
| 17:N:844:BCR:H361  | 17:N:844:BCR:H20C | 1.83                     | 0.41              |
| 12:W:36:PRO:O      | 12:W:40:SER:HB2   | 2.20                     | 0.41              |
| 12:W:57:LEU:HD22   | 12:W:61:ARG:HG2   | 2.03                     | 0.41              |
| 2:g:220:VAL:C      | 2:g:223:PRO:HD2   | 2.46                     | 0.41              |
| 2:g:290:TRP:O      | 2:g:294:ILE:HG13  | 2.21                     | 0.41              |
| 2:g:572:ARG:HG3    | 2:g:589:TRP:CG    | 2.56                     | 0.41              |
| 2:g:590:ASP:HA     | 2:g:593:PHE:HB3   | 2.03                     | 0.41              |
| 14:g:826:CLA:O1D   | 14:g:827:CLA:HHB  | 2.21                     | 0.41              |
| 14:g:836:CLA:H93   | 14:g:836:CLA:H111 | 1.92                     | 0.41              |
| 17:g:844:BCR:H361  | 17:g:844:BCR:H20C | 1.81                     | 0.41              |
| 17:g:846:BCR:H24C  | 17:g:846:BCR:H371 | 1.82                     | 0.41              |
| 14:h:1701:CLA:HBA1 | 14:h:1701:CLA:H3A | 1.45                     | 0.41              |
| 4:n:12:LEU:HD23    | 4:n:12:LEU:HA     | 1.86                     | 0.41              |
| 4:n:29:ASN:HB3     | 14:n:805:CLA:HAB  | 2.01                     | 0.41              |
| 4:n:341:HIS:HD2    | 14:n:805:CLA:OBD  | 2.03                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:n:614:ALA:O     | 4:n:618:GLU:HG2    | 2.21                     | 0.41              |
| 4:n:658:LEU:HD23  | 4:n:658:LEU:HA     | 1.95                     | 0.41              |
| 14:n:825:CLA:H141 | 14:n:825:CLA:H162  | 1.92                     | 0.41              |
| 17:n:847:BCR:H361 | 17:n:847:BCR:H20C  | 1.83                     | 0.41              |
| 5:p:6:LYS:HD2     | 6:q:114:ARG:HB3    | 2.02                     | 0.41              |
| 5:p:16:GLN:HB3    | 5:p:57:ALA:HB1     | 2.02                     | 0.41              |
| 5:p:66:ARG:HD2    | 5:p:66:ARG:HA      | 1.86                     | 0.41              |
| 17:t:104:BCR:H15C | 17:t:104:BCR:H351  | 1.83                     | 0.41              |
| 17:u:103:BCR:H361 | 17:u:103:BCR:H20C  | 1.81                     | 0.41              |
| 12:w:36:PRO:O     | 12:w:40:SER:HB2    | 2.20                     | 0.41              |
| 17:w:201:BCR:H24C | 17:w:201:BCR:H371  | 1.81                     | 0.41              |
| 17:w:201:BCR:H402 | 14:w:204:CLA:H52   | 2.02                     | 0.41              |
| 2:A:21:PRO:HG3    | 2:A:185:ALA:HB2    | 2.03                     | 0.41              |
| 2:A:392:THR:HG22  | 2:A:607:ILE:HB     | 2.02                     | 0.41              |
| 2:A:539:HIS:CE1   | 2:A:605:ILE:HG22   | 2.56                     | 0.41              |
| 2:A:561:ARG:CZ    | 6:D:17:GLY:HA2     | 2.51                     | 0.41              |
| 14:A:808:CLA:H92  | 14:A:808:CLA:H61   | 1.86                     | 0.41              |
| 14:A:808:CLA:HHB  | 9:J:34:ILE:HD13    | 2.02                     | 0.41              |
| 14:A:821:CLA:H3A  | 14:A:821:CLA:HBA2  | 1.25                     | 0.41              |
| 14:A:831:CLA:H92  | 14:A:831:CLA:H61   | 1.83                     | 0.41              |
| 4:B:86:PRO:HB3    | 4:B:121:TYR:CG     | 2.56                     | 0.41              |
| 4:B:142:LEU:HD23  | 4:B:142:LEU:HA     | 1.92                     | 0.41              |
| 4:B:393:HIS:CE1   | 14:B:830:CLA:NA    | 2.88                     | 0.41              |
| 4:B:552:LYS:HD3   | 8:F:162:SER:HA     | 2.02                     | 0.41              |
| 14:B:806:CLA:HBA1 | 14:B:806:CLA:H3A   | 1.43                     | 0.41              |
| 14:B:834:CLA:H11  | 14:B:834:CLA:HBA2  | 1.75                     | 0.41              |
| 14:B:838:CLA:HBC2 | 17:B:852:BCR:HC7   | 2.03                     | 0.41              |
| 17:B:851:BCR:H15C | 17:B:851:BCR:H351  | 1.83                     | 0.41              |
| 8:F:88:ILE:HG21   | 9:J:46:HIS:CD2     | 2.56                     | 0.41              |
| 17:I:103:BCR:C26  | 14:L:1502:CLA:HAC2 | 2.51                     | 0.41              |
| 2:a:153:ILE:HG21  | 2:a:159:LEU:HG     | 2.03                     | 0.41              |
| 2:a:247:LYS:HB2   | 2:a:247:LYS:HE2    | 1.86                     | 0.41              |
| 2:a:585:GLN:HG2   | 2:a:590:ASP:HB3    | 2.03                     | 0.41              |
| 14:a:826:CLA:H152 | 14:b:803:CLA:H162  | 2.03                     | 0.41              |
| 4:b:196:HIS:CE1   | 14:b:816:CLA:NA    | 2.89                     | 0.41              |
| 4:b:378:HIS:HB2   | 14:b:828:CLA:C1B   | 2.51                     | 0.41              |
| 4:b:689:HIS:HE1   | 4:b:698:VAL:O      | 2.03                     | 0.41              |
| 14:b:809:CLA:C1A  | 14:b:809:CLA:CGA   | 2.99                     | 0.41              |
| 14:b:813:CLA:HBA2 | 14:b:813:CLA:H12   | 1.86                     | 0.41              |
| 9:j:43:LEU:HD23   | 9:j:43:LEU:HA      | 1.86                     | 0.41              |
| 17:k:102:BCR:H371 | 17:k:102:BCR:H24C  | 1.79                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:i:26:TRP:CZ2   | 17:i:102:BCR:H333 | 2.55                     | 0.41              |
| 12:l:46:PHE:HZ    | 14:l:202:CLA:HBB2 | 1.86                     | 0.41              |
| 17:l:206:BCR:H371 | 17:l:206:BCR:H24C | 1.82                     | 0.41              |
| 3:H:16:PRO:N      | 3:H:17:PRO:HD2    | 2.36                     | 0.41              |
| 14:N:803:CLA:H3A  | 14:N:803:CLA:HBA1 | 1.39                     | 0.41              |
| 10:U:74:VAL:HA    | 10:U:77:VAL:HG12  | 2.03                     | 0.41              |
| 17:Y:101:BCR:H11C | 17:Y:101:BCR:H341 | 1.89                     | 0.41              |
| 2:g:105:LEU:HB3   | 2:g:234:VAL:HG21  | 2.03                     | 0.41              |
| 2:g:276:LEU:HB2   | 14:g:815:CLA:HMA2 | 2.03                     | 0.41              |
| 2:g:462:MET:HG3   | 2:g:470:ASP:O     | 2.21                     | 0.41              |
| 2:g:547:VAL:HG21  | 14:g:837:CLA:HMA1 | 2.02                     | 0.41              |
| 2:g:723:GLN:O     | 2:g:727:VAL:HG12  | 2.21                     | 0.41              |
| 4:n:275:HIS:HE1   | 14:n:816:CLA:C4D  | 2.34                     | 0.41              |
| 4:B:431:LEU:HD21  | 17:B:851:BCR:H402 | 2.02                     | 0.41              |
| 4:B:436:HIS:HB3   | 17:B:852:BCR:H312 | 2.02                     | 0.41              |
| 4:B:721:THR:HG23  | 21:B:849:LMG:H411 | 2.02                     | 0.41              |
| 14:B:841:CLA:CBC  | 15:B:842:PQN:H2M2 | 2.51                     | 0.41              |
| 13:M:11:ILE:HA    | 13:M:14:VAL:HG12  | 2.02                     | 0.41              |
| 13:M:16:ALA:C     | 13:M:19:PRO:HD2   | 2.46                     | 0.41              |
| 2:a:15:VAL:HA     | 2:a:190:TRP:HD1   | 1.86                     | 0.41              |
| 2:a:370:HIS:NE2   | 14:a:825:CLA:NB   | 2.69                     | 0.41              |
| 2:a:723:GLN:HA    | 18:a:849:LHG:HC5  | 2.02                     | 0.41              |
| 14:a:806:CLA:H162 | 14:a:806:CLA:H193 | 1.85                     | 0.41              |
| 14:a:824:CLA:HBA2 | 14:a:824:CLA:H3A  | 1.78                     | 0.41              |
| 4:b:525:LEU:HD23  | 4:b:525:LEU:HA    | 1.95                     | 0.41              |
| 14:G:805:CLA:H112 | 14:G:805:CLA:H152 | 1.93                     | 0.40              |
| 17:G:843:BCR:H11C | 17:G:843:BCR:H341 | 1.66                     | 0.40              |
| 2:g:91:MET:SD     | 14:g:806:CLA:HAA2 | 2.61                     | 0.40              |
| 2:g:357:LEU:HD23  | 2:g:357:LEU:HA    | 1.95                     | 0.40              |
| 2:g:578:PRO:HD3   | 4:n:568:GLY:HA2   | 2.02                     | 0.40              |
| 2:g:599:MET:HG3   | 14:g:824:CLA:HBC1 | 2.02                     | 0.40              |
| 14:g:830:CLA:H12  | 4:n:693:PRO:HG2   | 2.02                     | 0.40              |
| 17:g:843:BCR:H341 | 17:g:843:BCR:H11C | 1.64                     | 0.40              |
| 14:g:852:CLA:H3A  | 14:g:852:CLA:CGA  | 2.50                     | 0.40              |
| 4:n:301:ILE:HG21  | 14:n:824:CLA:HAC1 | 2.03                     | 0.40              |
| 14:n:820:CLA:H3A  | 14:n:820:CLA:HBA2 | 1.41                     | 0.40              |
| 17:n:843:BCR:H351 | 17:n:843:BCR:H15C | 1.77                     | 0.40              |
| 17:t:104:BCR:H361 | 17:t:104:BCR:H20C | 1.81                     | 0.40              |
| 17:w:207:BCR:H11C | 17:w:207:BCR:H341 | 1.83                     | 0.40              |
| 2:A:296:HIS:HE1   | 14:A:816:CLA:C4D  | 2.34                     | 0.40              |
| 14:A:810:CLA:H112 | 14:A:810:CLA:H72  | 1.92                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:A:826:CLA:H62  | 14:A:826:CLA:H93  | 1.67                     | 0.40              |
| 14:A:838:CLA:CED  | 14:A:838:CLA:H2A  | 2.51                     | 0.40              |
| 4:B:181:GLY:HA3   | 14:B:814:CLA:CBB  | 2.48                     | 0.40              |
| 14:B:809:CLA:H141 | 14:B:809:CLA:HBA2 | 2.03                     | 0.40              |
| 14:B:811:CLA:H2A  | 14:B:811:CLA:O1D  | 2.21                     | 0.40              |
| 2:a:107:ASP:HB3   | 2:a:111:VAL:HG23  | 2.02                     | 0.40              |
| 4:b:167:TRP:CZ2   | 14:b:812:CLA:HHB  | 2.56                     | 0.40              |
| 4:b:665:ALA:O     | 4:b:668:PHE:HB2   | 2.21                     | 0.40              |
| 17:b:844:BCR:H24C | 17:b:844:BCR:H371 | 1.89                     | 0.40              |
| 2:G:43:PRO:HB3    | 2:G:48:TRP:CD2    | 2.56                     | 0.40              |
| 2:G:434:ARG:HB2   | 2:G:555:LEU:HD13  | 2.03                     | 0.40              |
| 2:G:741:TRP:HD1   | 14:G:827:CLA:HMB2 | 1.86                     | 0.40              |
| 14:G:825:CLA:H42  | 14:G:836:CLA:H12  | 2.03                     | 0.40              |
| 17:G:847:BCR:H24C | 17:G:847:BCR:H371 | 1.87                     | 0.40              |
| 3:H:44:GLN:NE2    | 4:N:488:VAL:HG12  | 2.35                     | 0.40              |
| 3:H:44:GLN:HE22   | 4:N:488:VAL:HG12  | 1.86                     | 0.40              |
| 4:N:432:PHE:CZ    | 17:N:853:BCR:HC41 | 2.56                     | 0.40              |
| 4:N:534:LEU:HD13  | 14:N:827:CLA:C4C  | 2.51                     | 0.40              |
| 14:N:811:CLA:H51  | 14:N:811:CLA:H8   | 1.71                     | 0.40              |
| 6:Q:105:LYS:HE3   | 6:Q:105:LYS:HB3   | 1.81                     | 0.40              |
| 17:W:205:BCR:H11C | 17:W:205:BCR:H341 | 1.89                     | 0.40              |
| 2:g:705:HIS:NE2   | 14:g:838:CLA:NA   | 2.69                     | 0.40              |
| 14:g:807:CLA:HBA1 | 17:t:104:BCR:H12C | 2.04                     | 0.40              |
| 14:g:837:CLA:H2   | 14:g:837:CLA:H62  | 1.76                     | 0.40              |
| 4:n:48:ALA:HB3    | 13:y:30:LEU:HD21  | 2.03                     | 0.40              |
| 4:n:433:LEU:HB3   | 4:n:532:LEU:HB2   | 2.02                     | 0.40              |
| 4:n:593:THR:O     | 4:n:597:VAL:HG23  | 2.20                     | 0.40              |
| 2:A:539:HIS:HB3   | 14:A:836:CLA:HAB  | 2.02                     | 0.40              |
| 17:A:849:BCR:H15C | 17:A:849:BCR:H351 | 1.86                     | 0.40              |
| 18:A:851:LHG:HC91 | 18:A:851:LHG:H122 | 1.98                     | 0.40              |
| 4:B:381:TYR:O     | 4:B:384:ILE:HG13  | 2.21                     | 0.40              |
| 17:B:851:BCR:H11C | 17:B:851:BCR:H341 | 1.81                     | 0.40              |
| 10:K:67:ALA:O     | 10:K:71:ILE:HG23  | 2.20                     | 0.40              |
| 2:a:202:LEU:HA    | 2:a:206:LEU:HD12  | 2.03                     | 0.40              |
| 14:a:823:CLA:H202 | 14:a:823:CLA:H161 | 1.85                     | 0.40              |
| 14:a:830:CLA:CHA  | 14:a:830:CLA:HBA1 | 2.51                     | 0.40              |
| 17:a:848:BCR:H15C | 17:a:848:BCR:H351 | 1.88                     | 0.40              |
| 4:b:56:ILE:HG12   | 17:m:102:BCR:H343 | 2.03                     | 0.40              |
| 14:b:808:CLA:HAA1 | 11:i:21:VAL:HG22  | 2.03                     | 0.40              |
| 14:b:812:CLA:H61  | 14:b:812:CLA:H2   | 1.81                     | 0.40              |
| 7:e:55:VAL:HA     | 7:e:58:LEU:HD12   | 2.04                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:G:147:VAL:HG22   | 2:G:377:TYR:CZ    | 2.57                     | 0.40              |
| 14:G:803:CLA:HED1  | 14:G:810:CLA:HED2 | 2.02                     | 0.40              |
| 14:G:814:CLA:C3B   | 17:G:843:BCR:H333 | 2.51                     | 0.40              |
| 4:N:91:ILE:HB      | 4:N:112:PRO:HB2   | 2.03                     | 0.40              |
| 14:N:815:CLA:H143  | 14:N:815:CLA:H112 | 1.71                     | 0.40              |
| 14:N:826:CLA:H141  | 14:N:826:CLA:H161 | 1.89                     | 0.40              |
| 14:N:829:CLA:H93   | 14:N:829:CLA:H111 | 1.82                     | 0.40              |
| 5:P:36:ALA:O       | 5:P:38:GLN:HG2    | 2.21                     | 0.40              |
| 2:g:278:PHE:CZ     | 14:g:834:CLA:HED1 | 2.56                     | 0.40              |
| 2:g:597:PHE:HE1    | 2:g:732:TYR:CG    | 2.39                     | 0.40              |
| 14:g:804:CLA:HBA2  | 14:g:804:CLA:HED3 | 2.03                     | 0.40              |
| 4:n:177:HIS:CE1    | 14:n:812:CLA:NA   | 2.89                     | 0.40              |
| 6:q:23:ALA:HA      | 6:q:27:GLU:O      | 2.22                     | 0.40              |
| 7:r:36:VAL:O       | 7:r:52:ASN:HA     | 2.22                     | 0.40              |
| 2:A:239:LEU:HB2    | 2:A:242:GLU:HG3   | 2.03                     | 0.40              |
| 2:A:491:HIS:NE2    | 14:A:834:CLA:NA   | 2.70                     | 0.40              |
| 4:B:433:LEU:HD11   | 14:B:838:CLA:HMB1 | 2.03                     | 0.40              |
| 4:B:531:ALA:HB2    | 14:B:838:CLA:HMA3 | 2.04                     | 0.40              |
| 14:B:814:CLA:H152  | 17:B:844:BCR:H322 | 2.03                     | 0.40              |
| 2:a:55:LEU:HD11    | 18:a:849:LHG:HC11 | 2.03                     | 0.40              |
| 2:a:396:TRP:HB3    | 14:a:826:CLA:HMC2 | 2.03                     | 0.40              |
| 2:a:605:ILE:HD12   | 19:a:851:CL0:H53  | 2.02                     | 0.40              |
| 14:a:826:CLA:H11   | 17:a:848:BCR:HC42 | 2.02                     | 0.40              |
| 4:b:287:ALA:HB2    | 14:b:820:CLA:HBC2 | 2.03                     | 0.40              |
| 14:b:807:CLA:H151  | 14:b:807:CLA:H111 | 1.71                     | 0.40              |
| 14:b:830:CLA:H112  | 14:b:830:CLA:H143 | 1.82                     | 0.40              |
| 17:b:844:BCR:H351  | 17:b:844:BCR:H15C | 1.77                     | 0.40              |
| 10:k:24:MET:CE     | 10:k:70:HIS:HA    | 2.51                     | 0.40              |
| 1:l:215:LEU:HD13   | 1:l:215:LEU:HA    | 1.93                     | 0.40              |
| 2:G:73:ILE:HD12    | 14:G:804:CLA:C2C  | 2.52                     | 0.40              |
| 2:G:294:ILE:HG23   | 14:G:818:CLA:HMA3 | 2.04                     | 0.40              |
| 2:G:462:MET:HA     | 2:G:462:MET:HE3   | 2.02                     | 0.40              |
| 14:G:804:CLA:H203  | 14:G:812:CLA:H71  | 2.04                     | 0.40              |
| 14:G:825:CLA:HBA2  | 14:G:825:CLA:H3A  | 1.79                     | 0.40              |
| 14:G:832:CLA:HAA1  | 17:W:201:BCR:C35  | 2.52                     | 0.40              |
| 19:G:851:CL0:H57   | 19:G:851:CL0:H60  | 1.94                     | 0.40              |
| 3:H:20:PHE:HD1     | 21:N:802:LMG:H112 | 1.86                     | 0.40              |
| 14:H:1701:CLA:HBA2 | 17:S:204:BCR:H393 | 2.04                     | 0.40              |
| 4:N:29:ASN:HD21    | 14:N:806:CLA:CHC  | 2.34                     | 0.40              |
| 4:N:351:TRP:HE1    | 4:N:355:HIS:CE1   | 2.39                     | 0.40              |
| 14:N:801:CLA:HBB1  | 14:N:841:CLA:C3D  | 2.51                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:N:813:CLA:H11  | 12:l:42:LEU:HD21  | 2.02                     | 0.40              |
| 14:N:819:CLA:H93  | 14:N:819:CLA:H61  | 1.87                     | 0.40              |
| 14:N:834:CLA:H2   | 17:N:852:BCR:H333 | 2.03                     | 0.40              |
| 12:W:56:GLY:HA3   | 12:w:136:LYS:HD2  | 2.04                     | 0.40              |
| 17:Y:101:BCR:H20C | 17:Y:101:BCR:H361 | 1.88                     | 0.40              |
| 2:g:216:HIS:HB2   | 14:g:812:CLA:C1C  | 2.52                     | 0.40              |
| 2:g:458:HIS:HE1   | 14:g:832:CLA:C1A  | 2.34                     | 0.40              |
| 14:g:806:CLA:H111 | 14:g:828:CLA:H203 | 2.02                     | 0.40              |
| 14:g:812:CLA:HBA1 | 14:g:812:CLA:H3A  | 1.92                     | 0.40              |
| 17:g:846:BCR:H20C | 18:g:850:LHG:HC91 | 2.03                     | 0.40              |
| 4:n:179:LEU:HD21  | 14:n:819:CLA:C3B  | 2.51                     | 0.40              |
| 4:n:278:LEU:HD11  | 14:n:816:CLA:HAB  | 2.03                     | 0.40              |
| 4:n:326:ILE:HD12  | 14:n:823:CLA:HBC3 | 2.04                     | 0.40              |
| 4:n:408:LYS:HB2   | 4:n:408:LYS:HE3   | 1.63                     | 0.40              |
| 4:n:691:ARG:HH21  | 6:q:20:LEU:HD23   | 1.86                     | 0.40              |
| 14:n:806:CLA:H2   | 14:n:806:CLA:H61  | 1.67                     | 0.40              |
| 10:u:78:LEU:HD23  | 10:u:78:LEU:HA    | 1.88                     | 0.40              |
| 12:w:70:HIS:CE1   | 14:w:204:CLA:NA   | 2.89                     | 0.40              |
| 2:A:224:ILE:HG13  | 2:A:243:PHE:HE2   | 1.85                     | 0.40              |
| 2:A:533:PHE:HA    | 14:A:837:CLA:HED1 | 2.02                     | 0.40              |
| 2:A:683:SER:HB2   | 2:A:728:GLY:O     | 2.22                     | 0.40              |
| 17:A:847:BCR:H20C | 17:A:847:BCR:H361 | 1.87                     | 0.40              |
| 17:A:856:BCR:H20C | 17:A:856:BCR:H361 | 1.88                     | 0.40              |
| 14:B:827:CLA:H121 | 17:B:846:BCR:H20C | 2.03                     | 0.40              |
| 14:B:840:CLA:HAA1 | 17:I:103:BCR:H362 | 2.02                     | 0.40              |
| 14:a:852:CLA:O1A  | 4:b:434:GLY:HA3   | 2.20                     | 0.40              |
| 4:b:530:ILE:HG12  | 4:b:597:VAL:HG22  | 2.03                     | 0.40              |
| 14:b:805:CLA:H143 | 14:b:805:CLA:H111 | 1.73                     | 0.40              |
| 14:b:841:CLA:H42  | 15:b:842:PQN:H271 | 2.03                     | 0.40              |
| 17:b:850:BCR:H332 | 17:j:103:BCR:HC22 | 2.03                     | 0.40              |
| 9:j:41:PRO:HB2    | 9:j:42:ASP:OD2    | 2.20                     | 0.40              |
| 17:i:101:BCR:H24C | 17:i:101:BCR:H371 | 1.82                     | 0.40              |
| 13:m:15:VAL:O     | 13:m:19:PRO:HD2   | 2.22                     | 0.40              |
| 14:G:802:CLA:H192 | 14:G:802:CLA:H161 | 1.76                     | 0.40              |
| 14:G:806:CLA:H41  | 14:G:806:CLA:H61  | 1.58                     | 0.40              |
| 4:N:330:TYR:CZ    | 14:N:826:CLA:NC   | 2.90                     | 0.40              |
| 14:N:842:CLA:H142 | 14:N:842:CLA:H112 | 1.87                     | 0.40              |
| 6:Q:43:LEU:HD12   | 6:Q:47:GLY:HA3    | 2.04                     | 0.40              |
| 17:T:103:BCR:H11C | 17:T:103:BCR:H341 | 1.82                     | 0.40              |
| 2:g:264:PHE:CZ    | 17:g:843:BCR:H343 | 2.55                     | 0.40              |
| 2:g:299:LEU:HD21  | 14:g:815:CLA:HAB  | 2.03                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:g:506:VAL:HG11   | 14:g:833:CLA:HMA3 | 2.03                     | 0.40              |
| 14:g:807:CLA:H13   | 14:g:807:CLA:H102 | 1.88                     | 0.40              |
| 17:g:845:BCR:H15C  | 17:g:845:BCR:H351 | 1.75                     | 0.40              |
| 14:n:805:CLA:H152  | 14:n:813:CLA:CAD  | 2.52                     | 0.40              |
| 14:n:807:CLA:H61   | 17:v:101:BCR:HC32 | 2.04                     | 0.40              |
| 14:n:840:CLA:H92   | 14:n:840:CLA:H62  | 1.77                     | 0.40              |
| 17:n:849:BCR:H15C  | 17:n:849:BCR:H351 | 1.78                     | 0.40              |
| 2:A:53:HIS:HE1     | 14:A:802:CLA:C4D  | 2.34                     | 0.40              |
| 2:A:311:GLN:O      | 2:A:320:HIS:HD2   | 2.05                     | 0.40              |
| 2:A:407:ALA:HB2    | 2:A:592:VAL:HG11  | 2.04                     | 0.40              |
| 2:A:694:TRP:O      | 2:A:698:ILE:HG12  | 2.21                     | 0.40              |
| 14:A:825:CLA:O1D   | 14:A:825:CLA:H2A  | 2.20                     | 0.40              |
| 17:A:844:BCR:H371  | 17:A:844:BCR:H24C | 1.81                     | 0.40              |
| 4:B:551:SER:HA     | 8:F:162:SER:HB2   | 2.04                     | 0.40              |
| 14:B:826:CLA:H52   | 14:B:837:CLA:H2   | 2.04                     | 0.40              |
| 17:J:103:BCR:H15C  | 17:J:103:BCR:H351 | 1.75                     | 0.40              |
| 10:K:29:VAL:O      | 10:K:32:ILE:HG22  | 2.22                     | 0.40              |
| 2:a:294:ILE:HG23   | 14:a:817:CLA:HMA3 | 2.04                     | 0.40              |
| 14:a:830:CLA:H151  | 14:a:830:CLA:H111 | 1.84                     | 0.40              |
| 20:x:1702:SQD:H251 | 14:b:831:CLA:H71  | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | 1     | 31/237 (13%)  | 30 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 2   | A     | 740/752 (98%) | 707 (96%) | 32 (4%) | 1 (0%)   | 48          | 78  |
| 2   | G     | 739/752 (98%) | 707 (96%) | 31 (4%) | 1 (0%)   | 48          | 78  |
| 2   | a     | 740/752 (98%) | 701 (95%) | 39 (5%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|---------|----------|-------------|-----|
| 2   | g     | 740/752 (98%)  | 711 (96%) | 29 (4%) | 0        | 100         | 100 |
| 3   | H     | 29/44 (66%)    | 28 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 3   | X     | 29/44 (66%)    | 29 (100%) | 0       | 0        | 100         | 100 |
| 3   | h     | 28/44 (64%)    | 27 (96%)  | 1 (4%)  | 0        | 100         | 100 |
| 3   | x     | 29/44 (66%)    | 28 (97%)  | 1 (3%)  | 0        | 100         | 100 |
| 4   | B     | 738/741 (100%) | 702 (95%) | 36 (5%) | 0        | 100         | 100 |
| 4   | N     | 737/741 (100%) | 718 (97%) | 18 (2%) | 1 (0%)   | 48          | 78  |
| 4   | b     | 738/741 (100%) | 705 (96%) | 32 (4%) | 1 (0%)   | 48          | 78  |
| 4   | n     | 736/741 (99%)  | 706 (96%) | 29 (4%) | 1 (0%)   | 48          | 78  |
| 5   | C     | 78/81 (96%)    | 71 (91%)  | 7 (9%)  | 0        | 100         | 100 |
| 5   | P     | 78/81 (96%)    | 71 (91%)  | 7 (9%)  | 0        | 100         | 100 |
| 5   | c     | 78/81 (96%)    | 72 (92%)  | 6 (8%)  | 0        | 100         | 100 |
| 5   | p     | 78/81 (96%)    | 75 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 6   | D     | 133/139 (96%)  | 127 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 6   | Q     | 133/139 (96%)  | 127 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 6   | d     | 134/139 (96%)  | 123 (92%) | 11 (8%) | 0        | 100         | 100 |
| 6   | q     | 134/139 (96%)  | 130 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 7   | E     | 59/70 (84%)    | 57 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 7   | R     | 59/70 (84%)    | 55 (93%)  | 4 (7%)  | 0        | 100         | 100 |
| 7   | e     | 59/70 (84%)    | 55 (93%)  | 4 (7%)  | 0        | 100         | 100 |
| 7   | r     | 58/70 (83%)    | 54 (93%)  | 4 (7%)  | 0        | 100         | 100 |
| 8   | F     | 139/164 (85%)  | 133 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 8   | S     | 139/164 (85%)  | 130 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 8   | f     | 139/164 (85%)  | 133 (96%) | 6 (4%)  | 0        | 100         | 100 |
| 8   | s     | 139/164 (85%)  | 136 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 9   | J     | 43/49 (88%)    | 42 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 9   | T     | 42/49 (86%)    | 42 (100%) | 0       | 0        | 100         | 100 |
| 9   | j     | 43/49 (88%)    | 43 (100%) | 0       | 0        | 100         | 100 |
| 9   | t     | 43/49 (88%)    | 43 (100%) | 0       | 0        | 100         | 100 |
| 10  | K     | 71/86 (83%)    | 68 (96%)  | 3 (4%)  | 0        | 100         | 100 |
| 10  | U     | 71/86 (83%)    | 67 (94%)  | 4 (6%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 10  | k     | 76/86 (88%)     | 72 (95%)   | 4 (5%)   | 0        | 100         | 100 |
| 10  | u     | 76/86 (88%)     | 74 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 11  | I     | 32/46 (70%)     | 31 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 11  | V     | 31/46 (67%)     | 30 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 11  | i     | 32/46 (70%)     | 32 (100%)  | 0        | 0        | 100         | 100 |
| 11  | v     | 32/46 (70%)     | 31 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 12  | L     | 153/172 (89%)   | 149 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 12  | W     | 153/172 (89%)   | 148 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 12  | l     | 153/172 (89%)   | 146 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 12  | w     | 153/172 (89%)   | 148 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 13  | M     | 29/32 (91%)     | 29 (100%)  | 0        | 0        | 100         | 100 |
| 13  | Y     | 29/32 (91%)     | 29 (100%)  | 0        | 0        | 100         | 100 |
| 13  | m     | 29/32 (91%)     | 29 (100%)  | 0        | 0        | 100         | 100 |
| 13  | y     | 29/32 (91%)     | 29 (100%)  | 0        | 0        | 100         | 100 |
| All | All   | 9011/9741 (92%) | 8630 (96%) | 376 (4%) | 5 (0%)   | 49          | 78  |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | G     | 122 | VAL  |
| 4   | N     | 694 | ILE  |
| 2   | A     | 122 | VAL  |
| 4   | b     | 694 | ILE  |
| 4   | n     | 694 | ILE  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |    |
|-----|-------|--------------|-----------|----------|-------------|----|
| 1   | 1     | 26/206 (13%) | 23 (88%)  | 3 (12%)  | 5           | 22 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 2   | A     | 595/605 (98%)  | 587 (99%)  | 8 (1%)   | 61          | 81  |
| 2   | G     | 594/605 (98%)  | 591 (100%) | 3 (0%)   | 81          | 89  |
| 2   | a     | 595/605 (98%)  | 592 (100%) | 3 (0%)   | 81          | 89  |
| 2   | g     | 595/605 (98%)  | 586 (98%)  | 9 (2%)   | 57          | 79  |
| 3   | H     | 25/34 (74%)    | 25 (100%)  | 0        | 100         | 100 |
| 3   | X     | 25/34 (74%)    | 25 (100%)  | 0        | 100         | 100 |
| 3   | h     | 24/34 (71%)    | 23 (96%)   | 1 (4%)   | 26          | 59  |
| 3   | x     | 25/34 (74%)    | 25 (100%)  | 0        | 100         | 100 |
| 4   | B     | 600/602 (100%) | 595 (99%)  | 5 (1%)   | 73          | 86  |
| 4   | N     | 600/602 (100%) | 595 (99%)  | 5 (1%)   | 73          | 86  |
| 4   | b     | 600/602 (100%) | 594 (99%)  | 6 (1%)   | 68          | 83  |
| 4   | n     | 599/602 (100%) | 595 (99%)  | 4 (1%)   | 76          | 87  |
| 5   | C     | 67/69 (97%)    | 63 (94%)   | 4 (6%)   | 17          | 48  |
| 5   | P     | 67/69 (97%)    | 67 (100%)  | 0        | 100         | 100 |
| 5   | c     | 67/69 (97%)    | 65 (97%)   | 2 (3%)   | 36          | 67  |
| 5   | p     | 67/69 (97%)    | 66 (98%)   | 1 (2%)   | 57          | 79  |
| 6   | D     | 107/110 (97%)  | 106 (99%)  | 1 (1%)   | 70          | 85  |
| 6   | Q     | 107/110 (97%)  | 104 (97%)  | 3 (3%)   | 38          | 69  |
| 6   | d     | 108/110 (98%)  | 106 (98%)  | 2 (2%)   | 50          | 75  |
| 6   | q     | 108/110 (98%)  | 108 (100%) | 0        | 100         | 100 |
| 7   | E     | 54/60 (90%)    | 54 (100%)  | 0        | 100         | 100 |
| 7   | R     | 54/60 (90%)    | 52 (96%)   | 2 (4%)   | 30          | 62  |
| 7   | e     | 54/60 (90%)    | 53 (98%)   | 1 (2%)   | 50          | 75  |
| 7   | r     | 53/60 (88%)    | 53 (100%)  | 0        | 100         | 100 |
| 8   | F     | 110/129 (85%)  | 108 (98%)  | 2 (2%)   | 51          | 76  |
| 8   | S     | 110/129 (85%)  | 107 (97%)  | 3 (3%)   | 39          | 70  |
| 8   | f     | 110/129 (85%)  | 110 (100%) | 0        | 100         | 100 |
| 8   | s     | 110/129 (85%)  | 110 (100%) | 0        | 100         | 100 |
| 9   | J     | 39/42 (93%)    | 39 (100%)  | 0        | 100         | 100 |
| 9   | T     | 39/42 (93%)    | 37 (95%)   | 2 (5%)   | 21          | 53  |
| 9   | j     | 39/42 (93%)    | 39 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 9   | t     | 39/42 (93%)     | 37 (95%)   | 2 (5%)   | 21          | 53  |
| 10  | K     | 54/64 (84%)     | 53 (98%)   | 1 (2%)   | 50          | 75  |
| 10  | U     | 54/64 (84%)     | 54 (100%)  | 0        | 100         | 100 |
| 10  | k     | 57/64 (89%)     | 55 (96%)   | 2 (4%)   | 32          | 63  |
| 10  | u     | 57/64 (89%)     | 56 (98%)   | 1 (2%)   | 51          | 76  |
| 11  | I     | 31/39 (80%)     | 30 (97%)   | 1 (3%)   | 34          | 65  |
| 11  | V     | 30/39 (77%)     | 30 (100%)  | 0        | 100         | 100 |
| 11  | i     | 31/39 (80%)     | 31 (100%)  | 0        | 100         | 100 |
| 11  | v     | 31/39 (80%)     | 30 (97%)   | 1 (3%)   | 34          | 65  |
| 12  | L     | 118/131 (90%)   | 115 (98%)  | 3 (2%)   | 42          | 71  |
| 12  | W     | 118/131 (90%)   | 116 (98%)  | 2 (2%)   | 53          | 77  |
| 12  | l     | 118/131 (90%)   | 116 (98%)  | 2 (2%)   | 53          | 77  |
| 12  | w     | 118/131 (90%)   | 116 (98%)  | 2 (2%)   | 53          | 77  |
| 13  | M     | 26/27 (96%)     | 26 (100%)  | 0        | 100         | 100 |
| 13  | Y     | 26/27 (96%)     | 26 (100%)  | 0        | 100         | 100 |
| 13  | m     | 26/27 (96%)     | 26 (100%)  | 0        | 100         | 100 |
| 13  | y     | 26/27 (96%)     | 26 (100%)  | 0        | 100         | 100 |
| All | All   | 7333/7854 (93%) | 7246 (99%) | 87 (1%)  | 61          | 82  |

All (87) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 214 | VAL  |
| 1   | 1     | 215 | LEU  |
| 1   | 1     | 218 | ILE  |
| 2   | G     | 121 | ILE  |
| 2   | G     | 174 | LEU  |
| 2   | G     | 395 | ILE  |
| 4   | N     | 195 | ILE  |
| 4   | N     | 207 | VAL  |
| 4   | N     | 303 | GLU  |
| 4   | N     | 399 | VAL  |
| 4   | N     | 456 | GLN  |
| 6   | Q     | 40  | VAL  |
| 6   | Q     | 95  | ILE  |
| 6   | Q     | 129 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | R     | 29  | GLN  |
| 7   | R     | 57  | GLU  |
| 8   | S     | 31  | CYS  |
| 8   | S     | 80  | LEU  |
| 8   | S     | 148 | LEU  |
| 9   | T     | 11  | LEU  |
| 9   | T     | 37  | ASN  |
| 12  | W     | 73  | PHE  |
| 12  | W     | 164 | LEU  |
| 2   | g     | 11  | LYS  |
| 2   | g     | 16  | ILE  |
| 2   | g     | 98  | PHE  |
| 2   | g     | 112 | ARG  |
| 2   | g     | 121 | ILE  |
| 2   | g     | 203 | GLN  |
| 2   | g     | 584 | CYS  |
| 2   | g     | 604 | SER  |
| 2   | g     | 737 | ILE  |
| 3   | h     | 26  | LEU  |
| 4   | n     | 145 | PHE  |
| 4   | n     | 319 | PHE  |
| 4   | n     | 371 | THR  |
| 4   | n     | 669 | MET  |
| 5   | p     | 35  | LYS  |
| 9   | t     | 28  | ILE  |
| 9   | t     | 40  | PHE  |
| 10  | u     | 57  | PHE  |
| 11  | v     | 17  | SER  |
| 12  | w     | 73  | PHE  |
| 12  | w     | 92  | LEU  |
| 2   | A     | 67  | GLU  |
| 2   | A     | 121 | ILE  |
| 2   | A     | 122 | VAL  |
| 2   | A     | 372 | TYR  |
| 2   | A     | 374 | MET  |
| 2   | A     | 395 | ILE  |
| 2   | A     | 444 | VAL  |
| 2   | A     | 524 | MET  |
| 4   | B     | 129 | MET  |
| 4   | B     | 426 | LEU  |
| 4   | B     | 527 | HIS  |
| 4   | B     | 658 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | B     | 732 | LEU  |
| 5   | C     | 10  | THR  |
| 5   | C     | 19  | ARG  |
| 5   | C     | 63  | LEU  |
| 5   | C     | 77  | MET  |
| 6   | D     | 111 | GLU  |
| 8   | F     | 87  | LEU  |
| 8   | F     | 146 | GLU  |
| 10  | K     | 70  | HIS  |
| 11  | I     | 16  | LEU  |
| 12  | L     | 21  | VAL  |
| 12  | L     | 73  | PHE  |
| 12  | L     | 162 | SER  |
| 2   | a     | 47  | THR  |
| 2   | a     | 275 | PHE  |
| 2   | a     | 710 | VAL  |
| 4   | b     | 195 | ILE  |
| 4   | b     | 235 | GLN  |
| 4   | b     | 356 | MET  |
| 4   | b     | 426 | LEU  |
| 4   | b     | 692 | THR  |
| 4   | b     | 702 | ASP  |
| 5   | c     | 12  | ILE  |
| 5   | c     | 21  | CYS  |
| 6   | d     | 52  | HIS  |
| 6   | d     | 57  | LEU  |
| 7   | e     | 37  | ILE  |
| 10  | k     | 24  | MET  |
| 10  | k     | 57  | PHE  |
| 12  | l     | 73  | PHE  |
| 12  | l     | 125 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | G     | 192 | GLN  |
| 2   | G     | 193 | ASN  |
| 2   | G     | 296 | HIS  |
| 2   | G     | 458 | HIS  |
| 2   | G     | 501 | ASN  |
| 2   | G     | 539 | HIS  |
| 3   | H     | 32  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | N     | 156 | HIS  |
| 4   | N     | 158 | GLN  |
| 4   | N     | 406 | GLN  |
| 4   | N     | 407 | ASN  |
| 4   | N     | 468 | GLN  |
| 4   | N     | 528 | HIS  |
| 4   | N     | 610 | GLN  |
| 4   | N     | 619 | ASN  |
| 4   | N     | 640 | ASN  |
| 4   | N     | 711 | GLN  |
| 8   | S     | 119 | GLN  |
| 12  | W     | 48  | ASN  |
| 12  | W     | 70  | HIS  |
| 2   | g     | 203 | GLN  |
| 2   | g     | 328 | ASN  |
| 2   | g     | 422 | ASN  |
| 2   | g     | 423 | GLN  |
| 2   | g     | 451 | HIS  |
| 2   | g     | 458 | HIS  |
| 3   | h     | 41  | HIS  |
| 4   | n     | 14  | GLN  |
| 4   | n     | 275 | HIS  |
| 4   | n     | 341 | HIS  |
| 4   | n     | 605 | HIS  |
| 4   | n     | 637 | GLN  |
| 5   | p     | 16  | GLN  |
| 6   | q     | 116 | ASN  |
| 7   | r     | 19  | GLN  |
| 7   | r     | 49  | ASN  |
| 8   | s     | 52  | GLN  |
| 8   | s     | 63  | GLN  |
| 8   | s     | 109 | GLN  |
| 8   | s     | 123 | GLN  |
| 9   | t     | 37  | ASN  |
| 12  | w     | 70  | HIS  |
| 12  | w     | 114 | ASN  |
| 12  | w     | 140 | ASN  |
| 2   | A     | 193 | ASN  |
| 2   | A     | 296 | HIS  |
| 2   | A     | 408 | HIS  |
| 2   | A     | 458 | HIS  |
| 2   | A     | 568 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | A     | 706 | ASN  |
| 2   | A     | 715 | GLN  |
| 3   | X     | 32  | ASN  |
| 4   | B     | 156 | HIS  |
| 4   | B     | 196 | HIS  |
| 4   | B     | 275 | HIS  |
| 4   | B     | 484 | ASN  |
| 4   | B     | 528 | HIS  |
| 5   | C     | 16  | GLN  |
| 6   | D     | 52  | HIS  |
| 9   | J     | 37  | ASN  |
| 12  | L     | 17  | ASN  |
| 12  | L     | 38  | ASN  |
| 2   | a     | 53  | HIS  |
| 2   | a     | 62  | HIS  |
| 2   | a     | 155 | ASN  |
| 2   | a     | 180 | HIS  |
| 2   | a     | 350 | HIS  |
| 2   | a     | 488 | GLN  |
| 2   | a     | 644 | ASN  |
| 4   | b     | 193 | HIS  |
| 4   | b     | 275 | HIS  |
| 4   | b     | 335 | HIS  |
| 4   | b     | 341 | HIS  |
| 4   | b     | 354 | GLN  |
| 4   | b     | 355 | HIS  |
| 4   | b     | 425 | HIS  |
| 4   | b     | 465 | GLN  |
| 4   | b     | 696 | ASN  |
| 4   | b     | 711 | GLN  |
| 7   | e     | 49  | ASN  |
| 8   | f     | 123 | GLN  |
| 9   | j     | 37  | ASN  |
| 12  | l     | 140 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

518 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | # $ Z  > 2$ | Counts      | RMSZ | # $ Z  > 2$ |
| 14  | CLA  | N     | 851 | 4    | 69,73,73     | 1.17 | 7 (10%)     | 82,113,113  | 1.27 | 6 (7%)      |
| 14  | CLA  | b     | 809 | 4    | 69,73,73     | 1.16 | 9 (13%)     | 82,113,113  | 1.28 | 7 (8%)      |
| 14  | CLA  | B     | 836 | -    | 49,53,73     | 1.39 | 8 (16%)     | 58,89,113   | 1.39 | 5 (8%)      |
| 14  | CLA  | G     | 811 | 2    | 63,67,73     | 1.24 | 7 (11%)     | 74,105,113  | 1.30 | 5 (6%)      |
| 14  | CLA  | G     | 803 | 2    | 58,62,73     | 1.28 | 9 (15%)     | 68,99,113   | 1.33 | 5 (7%)      |
| 14  | CLA  | g     | 835 | 2    | 55,59,73     | 1.30 | 8 (14%)     | 64,96,113   | 1.41 | 6 (9%)      |
| 14  | CLA  | g     | 836 | 2    | 69,73,73     | 1.17 | 8 (11%)     | 82,113,113  | 1.28 | 7 (8%)      |
| 17  | BCR  | G     | 845 | -    | 41,41,41     | 0.72 | 0           | 56,56,56    | 2.12 | 17 (30%)    |
| 14  | CLA  | G     | 835 | 2    | 49,53,73     | 1.39 | 8 (16%)     | 58,89,113   | 1.41 | 4 (6%)      |
| 14  | CLA  | G     | 836 | 2    | 55,59,73     | 1.31 | 8 (14%)     | 64,96,113   | 1.41 | 7 (10%)     |
| 17  | BCR  | A     | 856 | -    | 41,41,41     | 0.64 | 0           | 56,56,56    | 2.20 | 17 (30%)    |
| 14  | CLA  | G     | 833 | 2    | 69,73,73     | 1.17 | 9 (13%)     | 82,113,113  | 1.25 | 4 (4%)      |
| 14  | CLA  | G     | 826 | 2    | 69,73,73     | 1.17 | 9 (13%)     | 82,113,113  | 1.28 | 7 (8%)      |
| 18  | LHG  | a     | 850 | 14   | 48,48,48     | 1.15 | 6 (12%)     | 51,54,54    | 0.96 | 2 (3%)      |
| 14  | CLA  | b     | 817 | 4    | 49,53,73     | 1.38 | 8 (16%)     | 58,89,113   | 1.44 | 4 (6%)      |
| 14  | CLA  | N     | 835 | 4    | 58,62,73     | 1.27 | 8 (13%)     | 68,99,113   | 1.33 | 5 (7%)      |
| 18  | LHG  | A     | 851 | 14   | 48,48,48     | 1.15 | 6 (12%)     | 51,54,54    | 0.93 | 2 (3%)      |
| 14  | CLA  | A     | 832 | 2    | 69,73,73     | 1.17 | 8 (11%)     | 82,113,113  | 1.25 | 6 (7%)      |
| 19  | CL0  | A     | 852 | -    | 38,53,73     | 3.68 | 17 (44%)    | 36,89,113   | 1.93 | 10 (27%)    |
| 14  | CLA  | w     | 203 | 12   | 49,53,73     | 1.39 | 8 (16%)     | 58,89,113   | 1.44 | 4 (6%)      |
| 14  | CLA  | B     | 829 | 4    | 69,73,73     | 1.16 | 9 (13%)     | 82,113,113  | 1.23 | 7 (8%)      |
| 21  | LMG  | B     | 849 | -    | 55,55,55     | 0.48 | 0           | 63,63,63    | 0.55 | 0           |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | N     | 837  | -    | 49,53,73     | 1.40 | 8 (16%)  | 58,89,113   | 1.40 | 4 (6%)   |
| 14  | CLA  | a     | 840  | 18   | 49,53,73     | 1.40 | 8 (16%)  | 58,89,113   | 1.41 | 4 (6%)   |
| 14  | CLA  | g     | 852  | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.35 | 9 (10%)  |
| 14  | CLA  | G     | 829  | 2    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.28 | 7 (8%)   |
| 14  | CLA  | N     | 842  | 4    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 14  | CLA  | N     | 812  | 4    | 64,68,73     | 1.21 | 9 (14%)  | 76,107,113  | 1.28 | 5 (6%)   |
| 16  | SF4  | c     | 101  | 5    | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CLA  | a     | 822  | 2    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.44 | 4 (6%)   |
| 14  | CLA  | a     | 839  | 2    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.28 | 5 (6%)   |
| 14  | CLA  | g     | 805  | 2    | 64,68,73     | 1.23 | 7 (10%)  | 76,107,113  | 1.28 | 6 (7%)   |
| 14  | CLA  | b     | 808  | 4    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 17  | BCR  | G     | 843  | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 2.09 | 13 (23%) |
| 14  | CLA  | b     | 837  | 4    | 64,68,73     | 1.22 | 7 (10%)  | 76,107,113  | 1.31 | 8 (10%)  |
| 14  | CLA  | g     | 823  | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.29 | 7 (8%)   |
| 14  | CLA  | b     | 802  | -    | 69,73,73     | 1.19 | 8 (11%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 14  | CLA  | L     | 1502 | 12   | 64,68,73     | 1.20 | 8 (12%)  | 76,107,113  | 1.29 | 6 (7%)   |
| 17  | BCR  | B     | 843  | -    | 41,41,41     | 0.67 | 0        | 56,56,56    | 2.07 | 16 (28%) |
| 15  | PQN  | A     | 842  | -    | 34,34,34     | 1.61 | 2 (5%)   | 43,45,45    | 1.19 | 4 (9%)   |
| 17  | BCR  | i     | 102  | -    | 41,41,41     | 0.74 | 1 (2%)   | 56,56,56    | 2.05 | 17 (30%) |
| 14  | CLA  | b     | 821  | 4    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.41 | 4 (6%)   |
| 17  | BCR  | b     | 848  | -    | 41,41,41     | 0.73 | 1 (2%)   | 56,56,56    | 1.89 | 16 (28%) |
| 14  | CLA  | n     | 852  | 4    | 59,63,73     | 1.27 | 9 (15%)  | 70,101,113  | 1.30 | 6 (8%)   |
| 16  | SF4  | C     | 102  | 5    | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CLA  | N     | 810  | 4    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.30 | 7 (8%)   |
| 14  | CLA  | K     | 101  | 10   | 45,49,73     | 1.44 | 10 (22%) | 54,83,113   | 1.37 | 3 (5%)   |
| 14  | CLA  | b     | 805  | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.27 | 7 (8%)   |
| 18  | LHG  | S     | 202  | -    | 42,42,48     | 1.22 | 6 (14%)  | 45,48,54    | 0.98 | 2 (4%)   |
| 17  | BCR  | B     | 847  | -    | 41,41,41     | 0.68 | 0        | 56,56,56    | 2.08 | 15 (26%) |
| 14  | CLA  | n     | 820  | 4    | 49,53,73     | 1.39 | 7 (14%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 14  | CLA  | G     | 837  | 2    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 14  | CLA  | b     | 853  | 4    | 59,63,73     | 1.27 | 8 (13%)  | 70,101,113  | 1.31 | 6 (8%)   |
| 14  | CLA  | N     | 824  | -    | 59,63,73     | 1.26 | 8 (13%)  | 70,101,113  | 1.32 | 5 (7%)   |
| 15  | PQN  | a     | 841  | -    | 34,34,34     | 1.61 | 2 (5%)   | 43,45,45    | 1.17 | 5 (11%)  |
| 14  | CLA  | G     | 812  | 2    | 64,68,73     | 1.23 | 9 (14%)  | 76,107,113  | 1.29 | 6 (7%)   |
| 17  | BCR  | N     | 853  | -    | 41,41,41     | 0.73 | 1 (2%)   | 56,56,56    | 2.09 | 15 (26%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | A     | 811  | 2    | 63,67,73     | 1.23 | 8 (12%)  | 74,105,113  | 1.31 | 6 (8%)   |
| 14  | CLA  | g     | 854  | -    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 17  | BCR  | a     | 848  | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 2.26 | 19 (33%) |
| 14  | CLA  | A     | 855  | -    | 49,53,73     | 1.35 | 9 (18%)  | 58,89,113   | 1.39 | 5 (8%)   |
| 14  | CLA  | n     | 836  | 4    | 64,68,73     | 1.21 | 8 (12%)  | 76,107,113  | 1.35 | 8 (10%)  |
| 14  | CLA  | B     | 839  | 4    | 51,55,73     | 1.36 | 8 (15%)  | 60,91,113   | 1.35 | 4 (6%)   |
| 14  | CLA  | g     | 831  | 2    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 14  | CLA  | U     | 102  | -    | 53,57,73     | 1.33 | 8 (15%)  | 61,93,113   | 1.41 | 5 (8%)   |
| 14  | CLA  | a     | 820  | 2    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.46 | 4 (6%)   |
| 14  | CLA  | w     | 205  | -    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.40 | 4 (6%)   |
| 18  | LHG  | a     | 849  | -    | 48,48,48     | 1.15 | 6 (12%)  | 51,54,54    | 0.89 | 2 (3%)   |
| 20  | SQD  | l     | 201  | -    | 52,54,54     | 1.57 | 7 (13%)  | 62,65,65    | 1.34 | 7 (11%)  |
| 21  | LMG  | n     | 848  | -    | 55,55,55     | 0.50 | 0        | 63,63,63    | 0.58 | 0        |
| 14  | CLA  | B     | 850  | 4    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.24 | 6 (7%)   |
| 14  | CLA  | B     | 817  | 4    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.43 | 4 (6%)   |
| 15  | PQN  | g     | 841  | -    | 34,34,34     | 1.60 | 2 (5%)   | 43,45,45    | 1.22 | 5 (11%)  |
| 14  | CLA  | g     | 832  | 2    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.27 | 7 (8%)   |
| 14  | CLA  | g     | 839  | 2    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 14  | CLA  | A     | 820  | -    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 14  | CLA  | b     | 838  | 4    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.28 | 8 (9%)   |
| 14  | CLA  | g     | 811  | 2    | 64,68,73     | 1.22 | 9 (14%)  | 76,107,113  | 1.27 | 6 (7%)   |
| 14  | CLA  | n     | 806  | 4    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 17  | BCR  | j     | 104  | -    | 41,41,41     | 0.69 | 0        | 56,56,56    | 2.42 | 19 (33%) |
| 14  | CLA  | t     | 102  | 9    | 41,45,73     | 1.48 | 9 (21%)  | 50,78,113   | 1.41 | 4 (8%)   |
| 17  | BCR  | w     | 206  | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 2.13 | 13 (23%) |
| 16  | SF4  | c     | 102  | 5    | 0,12,12      | -    | -        | -           | -    | -        |
| 17  | BCR  | N     | 848  | -    | 41,41,41     | 0.73 | 1 (2%)   | 56,56,56    | 2.10 | 15 (26%) |
| 17  | BCR  | n     | 844  | -    | 41,41,41     | 0.69 | 0        | 56,56,56    | 2.06 | 13 (23%) |
| 14  | CLA  | L     | 1501 | 12   | 55,59,73     | 1.31 | 8 (14%)  | 64,96,113   | 1.42 | 6 (9%)   |
| 14  | CLA  | g     | 834  | 2    | 49,53,73     | 1.38 | 7 (14%)  | 58,89,113   | 1.43 | 5 (8%)   |
| 14  | CLA  | N     | 801  | -    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.24 | 6 (7%)   |
| 14  | CLA  | g     | 826  | 2    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.25 | 7 (8%)   |
| 14  | CLA  | n     | 823  | 4    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 14  | CLA  | B     | 815  | 4    | 54,58,73     | 1.31 | 9 (16%)  | 64,95,113   | 1.40 | 6 (9%)   |
| 17  | BCR  | A     | 848  | -    | 41,41,41     | 0.73 | 1 (2%)   | 56,56,56    | 1.94 | 18 (32%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 16  | SF4  | P     | 102 | 5    | 0,12,12      | -    | -        | -           |      |          |
| 14  | CLA  | A     | 804 | 2    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.30 | 6 (7%)   |
| 17  | BCR  | B     | 851 | -    | 41,41,41     | 0.73 | 1 (2%)   | 56,56,56    | 2.30 | 17 (30%) |
| 14  | CLA  | A     | 805 | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.21 | 6 (7%)   |
| 14  | CLA  | g     | 802 | 2    | 58,62,73     | 1.28 | 9 (15%)  | 68,99,113   | 1.35 | 6 (8%)   |
| 14  | CLA  | n     | 807 | 4    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 14  | CLA  | A     | 819 | 2    | 58,62,73     | 1.28 | 9 (15%)  | 68,99,113   | 1.37 | 5 (7%)   |
| 17  | BCR  | T     | 104 | -    | 41,41,41     | 0.69 | 0        | 56,56,56    | 2.10 | 14 (25%) |
| 14  | CLA  | A     | 801 | -    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.17 | 3 (3%)   |
| 14  | CLA  | B     | 826 | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 14  | CLA  | n     | 824 | 4    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 14  | CLA  | G     | 817 | 2    | 64,68,73     | 1.22 | 9 (14%)  | 76,107,113  | 1.28 | 5 (6%)   |
| 14  | CLA  | a     | 838 | 2    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.29 | 6 (7%)   |
| 17  | BCR  | W     | 201 | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 2.62 | 21 (37%) |
| 17  | BCR  | w     | 201 | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 2.04 | 17 (30%) |
| 17  | BCR  | W     | 206 | -    | 41,41,41     | 0.68 | 0        | 56,56,56    | 2.11 | 17 (30%) |
| 14  | CLA  | G     | 822 | 2    | 58,62,73     | 1.27 | 7 (12%)  | 68,99,113   | 1.37 | 7 (10%)  |
| 14  | CLA  | n     | 804 | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 17  | BCR  | A     | 844 | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 2.04 | 15 (26%) |
| 14  | CLA  | B     | 805 | 4    | 59,63,73     | 1.27 | 8 (13%)  | 70,101,113  | 1.35 | 5 (7%)   |
| 14  | CLA  | g     | 814 | -    | 49,53,73     | 1.39 | 7 (14%)  | 58,89,113   | 1.43 | 4 (6%)   |
| 15  | PQN  | b     | 842 | -    | 34,34,34     | 1.60 | 2 (5%)   | 43,45,45    | 1.22 | 4 (9%)   |
| 14  | CLA  | n     | 832 | 4    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.28 | 7 (8%)   |
| 14  | CLA  | a     | 832 | 2    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 14  | CLA  | B     | 808 | 4    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.24 | 8 (9%)   |
| 14  | CLA  | a     | 827 | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.24 | 6 (7%)   |
| 17  | BCR  | Y     | 101 | -    | 41,41,41     | 0.66 | 0        | 56,56,56    | 2.02 | 15 (26%) |
| 19  | CL0  | g     | 851 | 2    | 58,73,73     | 3.01 | 18 (31%) | 60,113,113  | 1.52 | 12 (20%) |
| 14  | CLA  | G     | 808 | 2    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.29 | 6 (7%)   |
| 14  | CLA  | B     | 804 | 4    | 49,53,73     | 1.39 | 7 (14%)  | 58,89,113   | 1.33 | 4 (6%)   |
| 14  | CLA  | s     | 201 | -    | 63,67,73     | 1.23 | 8 (12%)  | 74,105,113  | 1.31 | 6 (8%)   |
| 14  | CLA  | A     | 807 | 2    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.31 | 7 (8%)   |
| 17  | BCR  | g     | 847 | -    | 41,41,41     | 0.78 | 2 (4%)   | 56,56,56    | 2.08 | 17 (30%) |
| 14  | CLA  | N     | 825 | 4    | 69,73,73     | 1.18 | 9 (13%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 14  | CLA  | g     | 821 | 2    | 58,62,73     | 1.28 | 8 (13%)  | 68,99,113   | 1.31 | 6 (8%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | N     | 808 | 4    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 14  | CLA  | G     | 821 | 2    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.49 | 6 (10%)  |
| 17  | BCR  | A     | 845 | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 2.11 | 17 (30%) |
| 17  | BCR  | v     | 101 | -    | 41,41,41     | 0.69 | 0        | 56,56,56    | 2.27 | 17 (30%) |
| 17  | BCR  | J     | 103 | -    | 41,41,41     | 0.68 | 0        | 56,56,56    | 2.00 | 17 (30%) |
| 14  | CLA  | b     | 827 | 4    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.29 | 7 (8%)   |
| 18  | LHG  | g     | 849 | -    | 48,48,48     | 1.15 | 6 (12%)  | 51,54,54    | 0.91 | 2 (3%)   |
| 14  | CLA  | N     | 840 | 4    | 51,55,73     | 1.35 | 8 (15%)  | 60,91,113   | 1.38 | 5 (8%)   |
| 14  | CLA  | N     | 809 | 4    | 69,73,73     | 1.16 | 7 (10%)  | 82,113,113  | 1.28 | 9 (10%)  |
| 18  | LHG  | G     | 849 | -    | 48,48,48     | 1.15 | 6 (12%)  | 51,54,54    | 0.94 | 2 (3%)   |
| 14  | CLA  | N     | 821 | -    | 69,73,73     | 1.18 | 9 (13%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 14  | CLA  | b     | 803 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 14  | CLA  | g     | 812 | 2    | 58,62,73     | 1.28 | 7 (12%)  | 68,99,113   | 1.36 | 6 (8%)   |
| 14  | CLA  | S     | 201 | -    | 63,67,73     | 1.22 | 9 (14%)  | 74,105,113  | 1.31 | 6 (8%)   |
| 14  | CLA  | g     | 853 | -    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.21 | 6 (7%)   |
| 14  | CLA  | T     | 102 | 9    | 41,45,73     | 1.47 | 9 (21%)  | 50,78,113   | 1.41 | 4 (8%)   |
| 14  | CLA  | N     | 841 | -    | 69,73,73     | 1.18 | 9 (13%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 17  | BCR  | a     | 846 | -    | 41,41,41     | 0.68 | 0        | 56,56,56    | 2.79 | 22 (39%) |
| 14  | CLA  | J     | 101 | 9    | 49,53,73     | 1.40 | 8 (16%)  | 58,89,113   | 1.43 | 4 (6%)   |
| 14  | CLA  | S     | 203 | -    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.42 | 5 (8%)   |
| 14  | CLA  | n     | 819 | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 17  | BCR  | n     | 851 | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 2.05 | 17 (30%) |
| 14  | CLA  | n     | 808 | 4    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.28 | 7 (8%)   |
| 14  | CLA  | a     | 801 | 2    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.30 | 8 (9%)   |
| 14  | CLA  | G     | 809 | 2    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 14  | CLA  | G     | 825 | -    | 58,62,73     | 1.28 | 9 (15%)  | 68,99,113   | 1.33 | 5 (7%)   |
| 14  | CLA  | b     | 828 | 4    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.22 | 6 (7%)   |
| 14  | CLA  | N     | 831 | 4    | 69,73,73     | 1.16 | 7 (10%)  | 82,113,113  | 1.31 | 6 (7%)   |
| 14  | CLA  | B     | 833 | 4    | 62,66,73     | 1.24 | 9 (14%)  | 73,104,113  | 1.32 | 5 (6%)   |
| 18  | LHG  | G     | 850 | 14   | 48,48,48     | 1.15 | 6 (12%)  | 51,54,54    | 0.93 | 2 (3%)   |
| 17  | BCR  | j     | 103 | -    | 41,41,41     | 0.73 | 1 (2%)   | 56,56,56    | 2.02 | 16 (28%) |
| 14  | CLA  | g     | 833 | 2    | 58,62,73     | 1.27 | 8 (13%)  | 68,99,113   | 1.34 | 5 (7%)   |
| 14  | CLA  | G     | 838 | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.24 | 6 (7%)   |
| 14  | CLA  | G     | 840 | 18   | 49,53,73     | 1.39 | 9 (18%)  | 58,89,113   | 1.37 | 4 (6%)   |
| 14  | CLA  | b     | 810 | 4    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.26 | 6 (7%)   |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | A     | 837  | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 14  | CLA  | T     | 101  | 9    | 49,53,73     | 1.40 | 8 (16%)  | 58,89,113   | 1.43 | 4 (6%)   |
| 17  | BCR  | b     | 846  | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 2.30 | 18 (32%) |
| 14  | CLA  | b     | 811  | 4    | 64,68,73     | 1.22 | 8 (12%)  | 76,107,113  | 1.27 | 5 (6%)   |
| 14  | CLA  | B     | 838  | 4    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.29 | 6 (7%)   |
| 14  | CLA  | G     | 805  | 2    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.26 | 8 (9%)   |
| 14  | CLA  | a     | 813  | 2    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 17  | BCR  | n     | 843  | -    | 41,41,41     | 0.71 | 1 (2%)   | 56,56,56    | 1.96 | 17 (30%) |
| 17  | BCR  | b     | 845  | -    | 41,41,41     | 0.68 | 0        | 56,56,56    | 2.03 | 12 (21%) |
| 14  | CLA  | n     | 818  | 4    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 14  | CLA  | A     | 833  | 2    | 69,73,73     | 1.18 | 7 (10%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 20  | SQD  | h     | 1702 | -    | 52,54,54     | 1.57 | 7 (13%)  | 62,65,65    | 1.27 | 6 (9%)   |
| 14  | CLA  | n     | 814  | 4    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.42 | 7 (10%)  |
| 14  | CLA  | b     | 804  | 4    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.19 | 5 (6%)   |
| 14  | CLA  | a     | 811  | 2    | 64,68,73     | 1.21 | 8 (12%)  | 76,107,113  | 1.31 | 5 (6%)   |
| 20  | SQD  | x     | 1702 | -    | 52,54,54     | 1.55 | 7 (13%)  | 62,65,65    | 1.31 | 6 (9%)   |
| 14  | CLA  | a     | 828  | 2    | 69,73,73     | 1.15 | 6 (8%)   | 82,113,113  | 1.26 | 5 (6%)   |
| 14  | CLA  | g     | 817  | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 14  | CLA  | j     | 101  | 9    | 49,53,73     | 1.40 | 8 (16%)  | 58,89,113   | 1.38 | 4 (6%)   |
| 14  | CLA  | B     | 831  | 4    | 58,62,73     | 1.28 | 8 (13%)  | 68,99,113   | 1.33 | 5 (7%)   |
| 17  | BCR  | g     | 845  | -    | 41,41,41     | 0.73 | 0        | 56,56,56    | 2.15 | 16 (28%) |
| 14  | CLA  | b     | 841  | 4    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 14  | CLA  | x     | 1701 | 3    | 53,57,73     | 1.33 | 8 (15%)  | 61,93,113   | 1.39 | 5 (8%)   |
| 14  | CLA  | a     | 825  | 2    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 14  | CLA  | n     | 809  | 4    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 14  | CLA  | B     | 822  | 4    | 49,53,73     | 1.39 | 9 (18%)  | 58,89,113   | 1.44 | 4 (6%)   |
| 14  | CLA  | G     | 802  | 2    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 14  | CLA  | b     | 807  | 4    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.28 | 7 (8%)   |
| 14  | CLA  | a     | 802  | 14,2 | 58,62,73     | 1.28 | 8 (13%)  | 68,99,113   | 1.38 | 5 (7%)   |
| 14  | CLA  | B     | 835  | -    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.41 | 5 (8%)   |
| 17  | BCR  | s     | 203  | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 2.07 | 16 (28%) |
| 14  | CLA  | A     | 823  | 2    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.43 | 4 (6%)   |
| 14  | CLA  | B     | 830  | 4    | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 17  | BCR  | A     | 849  | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 2.23 | 19 (33%) |
| 14  | CLA  | N     | 804  | 4    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.22 | 6 (7%)   |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | A     | 814  | 2    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.43 | 4 (6%)   |
| 14  | CLA  | F     | 201  | -    | 63,67,73     | 1.23 | 9 (14%)  | 74,105,113  | 1.31 | 5 (6%)   |
| 14  | CLA  | A     | 839  | 2    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 16  | SF4  | G     | 842  | 2,4  | 0,12,12      | -    | -        | -           |      |          |
| 14  | CLA  | n     | 816  | 4    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.44 | 4 (6%)   |
| 14  | CLA  | n     | 817  | 4    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 14  | CLA  | A     | 831  | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 17  | BCR  | G     | 848  | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 2.18 | 18 (32%) |
| 14  | CLA  | n     | 811  | 4    | 58,62,73     | 1.28 | 8 (13%)  | 68,99,113   | 1.33 | 5 (7%)   |
| 14  | CLA  | A     | 802  | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 14  | CLA  | L     | 1503 | -    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.39 | 4 (6%)   |
| 14  | CLA  | h     | 1701 | 3    | 53,57,73     | 1.34 | 8 (15%)  | 61,93,113   | 1.37 | 5 (8%)   |
| 14  | CLA  | a     | 803  | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.24 | 7 (8%)   |
| 14  | CLA  | g     | 813  | 2    | 49,53,73     | 1.38 | 7 (14%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 17  | BCR  | K     | 102  | -    | 41,41,41     | 0.67 | 0        | 56,56,56    | 2.04 | 17 (30%) |
| 14  | CLA  | n     | 839  | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 14  | CLA  | N     | 807  | 4    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 14  | CLA  | B     | 828  | 4    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 17  | BCR  | t     | 104  | -    | 41,41,41     | 0.68 | 0        | 56,56,56    | 2.27 | 17 (30%) |
| 18  | LHG  | X     | 1702 | -    | 42,42,48     | 1.23 | 6 (14%)  | 45,48,54    | 0.97 | 2 (4%)   |
| 14  | CLA  | g     | 824  | -    | 58,62,73     | 1.27 | 8 (13%)  | 68,99,113   | 1.35 | 6 (8%)   |
| 14  | CLA  | N     | 828  | 4    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.30 | 6 (7%)   |
| 17  | BCR  | n     | 845  | -    | 41,41,41     | 0.73 | 0        | 56,56,56    | 2.49 | 17 (30%) |
| 14  | CLA  | a     | 854  | -    | 53,57,73     | 1.33 | 8 (15%)  | 61,93,113   | 1.38 | 5 (8%)   |
| 14  | CLA  | n     | 802  | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.17 | 3 (3%)   |
| 14  | CLA  | g     | 837  | 2    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.25 | 5 (6%)   |
| 17  | BCR  | I     | 102  | -    | 41,41,41     | 0.80 | 1 (2%)   | 56,56,56    | 2.86 | 21 (37%) |
| 14  | CLA  | b     | 812  | 4    | 58,62,73     | 1.29 | 8 (13%)  | 68,99,113   | 1.35 | 6 (8%)   |
| 14  | CLA  | B     | 814  | 4    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.31 | 6 (7%)   |
| 17  | BCR  | B     | 846  | -    | 41,41,41     | 0.70 | 1 (2%)   | 56,56,56    | 2.28 | 17 (30%) |
| 14  | CLA  | n     | 826  | 4    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 14  | CLA  | g     | 804  | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.24 | 6 (7%)   |
| 14  | CLA  | A     | 854  | 2    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 20  | SQD  | B     | 801  | -    | 52,54,54     | 1.55 | 8 (15%)  | 62,65,65    | 1.34 | 6 (9%)   |
| 14  | CLA  | b     | 806  | 4    | 69,73,73     | 1.16 | 7 (10%)  | 82,113,113  | 1.28 | 7 (8%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | f     | 202 | -    | 49,53,73     | 1.40 | 8 (16%)  | 58,89,113   | 1.39 | 4 (6%)   |
| 14  | CLA  | a     | 852 | -    | 49,53,73     | 1.36 | 9 (18%)  | 58,89,113   | 1.39 | 4 (6%)   |
| 14  | CLA  | b     | 820 | -    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.27 | 7 (8%)   |
| 14  | CLA  | B     | 809 | 4    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.32 | 7 (8%)   |
| 14  | CLA  | b     | 824 | 4    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.26 | 7 (8%)   |
| 14  | CLA  | a     | 807 | 2    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.33 | 6 (7%)   |
| 14  | CLA  | g     | 828 | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.31 | 8 (9%)   |
| 14  | CLA  | n     | 805 | 4    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.27 | 7 (8%)   |
| 15  | PQN  | G     | 841 | -    | 34,34,34     | 1.60 | 2 (5%)   | 43,45,45    | 1.22 | 4 (9%)   |
| 14  | CLA  | G     | 828 | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 14  | CLA  | b     | 832 | 4    | 64,68,73     | 1.21 | 7 (10%)  | 76,107,113  | 1.31 | 8 (10%)  |
| 14  | CLA  | g     | 838 | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 14  | CLA  | a     | 834 | 2    | 49,53,73     | 1.38 | 7 (14%)  | 58,89,113   | 1.40 | 4 (6%)   |
| 18  | LHG  | m     | 101 | -    | 42,42,48     | 1.21 | 6 (14%)  | 45,48,54    | 0.95 | 3 (6%)   |
| 14  | CLA  | g     | 810 | 2    | 63,67,73     | 1.23 | 8 (12%)  | 74,105,113  | 1.31 | 5 (6%)   |
| 17  | BCR  | f     | 203 | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 2.11 | 15 (26%) |
| 14  | CLA  | G     | 810 | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 14  | CLA  | A     | 826 | 2    | 69,73,73     | 1.19 | 7 (10%)  | 82,113,113  | 1.37 | 7 (8%)   |
| 14  | CLA  | N     | 814 | 4    | 58,62,73     | 1.28 | 7 (12%)  | 68,99,113   | 1.36 | 6 (8%)   |
| 14  | CLA  | g     | 803 | 2    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 14  | CLA  | a     | 824 | -    | 58,62,73     | 1.27 | 8 (13%)  | 68,99,113   | 1.35 | 6 (8%)   |
| 14  | CLA  | n     | 837 | 4    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 14  | CLA  | A     | 816 | 2    | 63,67,73     | 1.22 | 9 (14%)  | 74,105,113  | 1.32 | 5 (6%)   |
| 17  | BCR  | n     | 847 | -    | 41,41,41     | 0.76 | 1 (2%)   | 56,56,56    | 2.00 | 16 (28%) |
| 14  | CLA  | n     | 821 | 4    | 49,53,73     | 1.40 | 8 (16%)  | 58,89,113   | 1.40 | 4 (6%)   |
| 14  | CLA  | B     | 825 | 4    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 16  | SF4  | P     | 101 | 5    | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CLA  | b     | 813 | 4    | 58,62,73     | 1.27 | 8 (13%)  | 68,99,113   | 1.37 | 7 (10%)  |
| 14  | CLA  | F     | 202 | -    | 49,53,73     | 1.40 | 8 (16%)  | 58,89,113   | 1.41 | 4 (6%)   |
| 14  | CLA  | A     | 829 | 2    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.31 | 7 (8%)   |
| 17  | BCR  | W     | 205 | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 1.70 | 14 (25%) |
| 14  | CLA  | B     | 840 | -    | 69,73,73     | 1.18 | 9 (13%)  | 82,113,113  | 1.27 | 5 (6%)   |
| 17  | BCR  | N     | 852 | -    | 41,41,41     | 0.72 | 1 (2%)   | 56,56,56    | 2.05 | 16 (28%) |
| 14  | CLA  | n     | 812 | 4    | 58,62,73     | 1.29 | 9 (15%)  | 68,99,113   | 1.35 | 6 (8%)   |
| 14  | CLA  | A     | 825 | -    | 58,62,73     | 1.27 | 7 (12%)  | 68,99,113   | 1.39 | 6 (8%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | a     | 809 | 14,2 | 69,73,73     | 1.18 | 9 (13%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 14  | CLA  | g     | 829 | 2    | 58,62,73     | 1.27 | 8 (13%)  | 68,99,113   | 1.33 | 5 (7%)   |
| 14  | CLA  | b     | 818 | 4    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.22 | 4 (4%)   |
| 14  | CLA  | a     | 821 | 2    | 58,62,73     | 1.29 | 8 (13%)  | 68,99,113   | 1.31 | 5 (7%)   |
| 17  | BCR  | g     | 848 | -    | 41,41,41     | 0.75 | 1 (2%)   | 56,56,56    | 2.14 | 16 (28%) |
| 14  | CLA  | g     | 822 | 2    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 14  | CLA  | B     | 834 | 4    | 58,62,73     | 1.28 | 8 (13%)  | 68,99,113   | 1.37 | 7 (10%)  |
| 14  | CLA  | g     | 830 | 2    | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 14  | CLA  | A     | 840 | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 14  | CLA  | G     | 814 | 2    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.44 | 5 (8%)   |
| 14  | CLA  | n     | 835 | -    | 49,53,73     | 1.39 | 6 (12%)  | 58,89,113   | 1.39 | 4 (6%)   |
| 14  | CLA  | g     | 816 | 2    | 64,68,73     | 1.23 | 9 (14%)  | 76,107,113  | 1.30 | 5 (6%)   |
| 14  | CLA  | G     | 830 | 2    | 58,62,73     | 1.28 | 8 (13%)  | 68,99,113   | 1.35 | 6 (8%)   |
| 14  | CLA  | n     | 850 | 4    | 62,66,73     | 1.23 | 9 (14%)  | 73,104,113  | 1.32 | 5 (6%)   |
| 14  | CLA  | g     | 801 | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.29 | 7 (8%)   |
| 14  | CLA  | A     | 821 | 2    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.43 | 5 (8%)   |
| 17  | BCR  | N     | 844 | -    | 41,41,41     | 0.73 | 0        | 56,56,56    | 2.09 | 11 (19%) |
| 14  | CLA  | t     | 101 | 9    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 14  | CLA  | A     | 815 | -    | 49,53,73     | 1.38 | 7 (14%)  | 58,89,113   | 1.43 | 5 (8%)   |
| 17  | BCR  | V     | 101 | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 2.16 | 13 (23%) |
| 17  | BCR  | n     | 849 | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 1.97 | 18 (32%) |
| 14  | CLA  | N     | 823 | 4    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.44 | 4 (6%)   |
| 14  | CLA  | N     | 830 | 4    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.26 | 7 (8%)   |
| 14  | CLA  | N     | 820 | 4    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 14  | CLA  | a     | 836 | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.23 | 4 (4%)   |
| 17  | BCR  | b     | 850 | -    | 41,41,41     | 0.69 | 0        | 56,56,56    | 2.00 | 13 (23%) |
| 14  | CLA  | n     | 838 | 4    | 51,55,73     | 1.35 | 8 (15%)  | 60,91,113   | 1.36 | 5 (8%)   |
| 17  | BCR  | t     | 103 | -    | 41,41,41     | 0.67 | 0        | 56,56,56    | 2.02 | 15 (26%) |
| 17  | BCR  | F     | 203 | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 2.03 | 16 (28%) |
| 14  | CLA  | A     | 812 | 2    | 64,68,73     | 1.23 | 9 (14%)  | 76,107,113  | 1.29 | 6 (7%)   |
| 14  | CLA  | b     | 816 | 4    | 53,57,73     | 1.32 | 8 (15%)  | 61,93,113   | 1.38 | 5 (8%)   |
| 14  | CLA  | b     | 829 | 4    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.26 | 7 (8%)   |
| 19  | CL0  | a     | 851 | 2    | 58,73,73     | 2.99 | 17 (29%) | 60,113,113  | 1.69 | 14 (23%) |
| 14  | CLA  | l     | 204 | -    | 49,53,73     | 1.39 | 9 (18%)  | 58,89,113   | 1.38 | 4 (6%)   |
| 14  | CLA  | W     | 203 | 12   | 64,68,73     | 1.20 | 8 (12%)  | 76,107,113  | 1.34 | 7 (9%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | W     | 204 | -    | 49,53,73     | 1.38 | 9 (18%)  | 58,89,113   | 1.39 | 4 (6%)   |
| 14  | CLA  | w     | 204 | 12   | 64,68,73     | 1.19 | 8 (12%)  | 76,107,113  | 1.30 | 4 (5%)   |
| 14  | CLA  | A     | 827 | 2    | 69,73,73     | 1.16 | 7 (10%)  | 82,113,113  | 1.24 | 7 (8%)   |
| 17  | BCR  | a     | 844 | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 2.16 | 16 (28%) |
| 14  | CLA  | A     | 835 | 2    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.40 | 4 (6%)   |
| 14  | CLA  | a     | 853 | -    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.19 | 5 (6%)   |
| 14  | CLA  | j     | 102 | 9    | 41,45,73     | 1.48 | 9 (21%)  | 50,78,113   | 1.41 | 4 (8%)   |
| 17  | BCR  | w     | 207 | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 2.14 | 18 (32%) |
| 14  | CLA  | g     | 806 | 2    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.29 | 8 (9%)   |
| 14  | CLA  | g     | 807 | 2    | 69,73,73     | 1.18 | 9 (13%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 14  | CLA  | n     | 831 | 4    | 64,68,73     | 1.22 | 9 (14%)  | 76,107,113  | 1.27 | 5 (6%)   |
| 17  | BCR  | b     | 852 | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 2.00 | 14 (25%) |
| 14  | CLA  | G     | 806 | 2    | 63,67,73     | 1.23 | 7 (11%)  | 74,105,113  | 1.30 | 5 (6%)   |
| 17  | BCR  | B     | 848 | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 2.13 | 18 (32%) |
| 14  | CLA  | a     | 829 | 2    | 58,62,73     | 1.28 | 9 (15%)  | 68,99,113   | 1.33 | 6 (8%)   |
| 14  | CLA  | G     | 820 | -    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.26 | 8 (9%)   |
| 14  | CLA  | n     | 822 | -    | 59,63,73     | 1.27 | 8 (13%)  | 70,101,113  | 1.30 | 6 (8%)   |
| 14  | CLA  | n     | 833 | 4    | 58,62,73     | 1.28 | 7 (12%)  | 68,99,113   | 1.35 | 5 (7%)   |
| 14  | CLA  | u     | 102 | -    | 53,57,73     | 1.33 | 8 (15%)  | 61,93,113   | 1.39 | 6 (9%)   |
| 14  | CLA  | G     | 801 | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.20 | 6 (7%)   |
| 18  | LHG  | A     | 850 | -    | 48,48,48     | 1.15 | 6 (12%)  | 51,54,54    | 0.90 | 2 (3%)   |
| 14  | CLA  | N     | 815 | 4    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.31 | 6 (7%)   |
| 14  | CLA  | B     | 832 | 4    | 64,68,73     | 1.21 | 8 (12%)  | 76,107,113  | 1.26 | 4 (5%)   |
| 14  | CLA  | N     | 806 | 4    | 59,63,73     | 1.27 | 9 (15%)  | 70,101,113  | 1.29 | 6 (8%)   |
| 14  | CLA  | a     | 805 | 2    | 64,68,73     | 1.22 | 8 (12%)  | 76,107,113  | 1.29 | 5 (6%)   |
| 14  | CLA  | B     | 813 | 4    | 58,62,73     | 1.28 | 7 (12%)  | 68,99,113   | 1.34 | 5 (7%)   |
| 16  | SF4  | a     | 842 | 2,4  | 0,12,12      | -    | -        | -           | -    | -        |
| 17  | BCR  | T     | 103 | -    | 41,41,41     | 0.67 | 0        | 56,56,56    | 1.97 | 17 (30%) |
| 17  | BCR  | y     | 101 | -    | 41,41,41     | 0.68 | 0        | 56,56,56    | 2.00 | 16 (28%) |
| 14  | CLA  | A     | 857 | -    | 53,57,73     | 1.33 | 9 (16%)  | 61,93,113   | 1.41 | 5 (8%)   |
| 21  | LMG  | b     | 849 | -    | 55,55,55     | 0.51 | 0        | 63,63,63    | 0.60 | 0        |
| 14  | CLA  | f     | 201 | -    | 63,67,73     | 1.22 | 8 (12%)  | 74,105,113  | 1.33 | 6 (8%)   |
| 17  | BCR  | g     | 843 | -    | 41,41,41     | 0.68 | 0        | 56,56,56    | 2.08 | 18 (32%) |
| 14  | CLA  | g     | 809 | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.23 | 5 (6%)   |
| 14  | CLA  | N     | 813 | 4    | 58,62,73     | 1.27 | 8 (13%)  | 68,99,113   | 1.35 | 7 (10%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | B     | 821  | 4    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 17  | BCR  | A     | 846  | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 2.08 | 16 (28%) |
| 14  | CLA  | A     | 822  | 2    | 58,62,73     | 1.26 | 8 (13%)  | 68,99,113   | 1.35 | 5 (7%)   |
| 17  | BCR  | N     | 845  | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 1.99 | 14 (25%) |
| 14  | CLA  | u     | 101  | 10   | 45,49,73     | 1.44 | 9 (20%)  | 54,83,113   | 1.38 | 3 (5%)   |
| 14  | CLA  | k     | 101  | 10   | 45,49,73     | 1.44 | 9 (20%)  | 54,83,113   | 1.38 | 3 (5%)   |
| 14  | CLA  | g     | 815  | 2    | 63,67,73     | 1.22 | 8 (12%)  | 74,105,113  | 1.29 | 5 (6%)   |
| 14  | CLA  | N     | 836  | -    | 49,53,73     | 1.40 | 8 (16%)  | 58,89,113   | 1.42 | 5 (8%)   |
| 14  | CLA  | n     | 828  | 4    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 14  | CLA  | G     | 813  | 2    | 58,62,73     | 1.27 | 9 (15%)  | 68,99,113   | 1.35 | 5 (7%)   |
| 14  | CLA  | n     | 830  | 4    | 58,62,73     | 1.28 | 8 (13%)  | 68,99,113   | 1.35 | 6 (8%)   |
| 14  | CLA  | b     | 839  | 4    | 51,55,73     | 1.35 | 8 (15%)  | 60,91,113   | 1.36 | 4 (6%)   |
| 14  | CLA  | N     | 826  | 4    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 17  | BCR  | u     | 103  | -    | 41,41,41     | 0.67 | 0        | 56,56,56    | 2.10 | 16 (28%) |
| 18  | LHG  | v     | 102  | -    | 42,42,48     | 1.21 | 6 (14%)  | 45,48,54    | 1.00 | 3 (6%)   |
| 17  | BCR  | l     | 206  | -    | 41,41,41     | 0.67 | 0        | 56,56,56    | 2.11 | 18 (32%) |
| 17  | BCR  | n     | 846  | -    | 41,41,41     | 0.68 | 0        | 56,56,56    | 2.16 | 15 (26%) |
| 14  | CLA  | U     | 101  | 10   | 45,49,73     | 1.44 | 9 (20%)  | 54,83,113   | 1.38 | 3 (5%)   |
| 14  | CLA  | G     | 831  | 2    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.26 | 7 (8%)   |
| 14  | CLA  | g     | 818  | 2    | 58,62,73     | 1.29 | 9 (15%)  | 68,99,113   | 1.35 | 4 (5%)   |
| 21  | LMG  | B     | 802  | -    | 35,35,55     | 0.59 | 0        | 43,43,63    | 0.67 | 0        |
| 14  | CLA  | b     | 815  | 4    | 54,58,73     | 1.30 | 8 (14%)  | 64,95,113   | 1.40 | 7 (10%)  |
| 14  | CLA  | B     | 827  | 4    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.30 | 7 (8%)   |
| 14  | CLA  | B     | 811  | 4    | 64,68,73     | 1.22 | 9 (14%)  | 76,107,113  | 1.31 | 6 (7%)   |
| 14  | CLA  | N     | 805  | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.26 | 7 (8%)   |
| 14  | CLA  | g     | 827  | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 14  | CLA  | N     | 829  | 4    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 17  | BCR  | U     | 103  | -    | 41,41,41     | 0.68 | 0        | 56,56,56    | 2.04 | 16 (28%) |
| 17  | BCR  | A     | 847  | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 2.30 | 18 (32%) |
| 14  | CLA  | n     | 825  | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.29 | 5 (6%)   |
| 17  | BCR  | L     | 1504 | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 1.95 | 16 (28%) |
| 16  | SF4  | C     | 101  | 5    | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CLA  | a     | 810  | 2    | 63,67,73     | 1.23 | 8 (12%)  | 74,105,113  | 1.31 | 6 (8%)   |
| 14  | CLA  | A     | 828  | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.23 | 6 (7%)   |
| 17  | BCR  | N     | 846  | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 2.09 | 16 (28%) |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | A     | 830  | 2    | 58,62,73     | 1.28 | 9 (15%)  | 68,99,113   | 1.35 | 6 (8%)   |
| 14  | CLA  | N     | 827  | -    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.29 | 9 (10%)  |
| 14  | CLA  | a     | 808  | 2    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.39 | 4 (6%)   |
| 14  | CLA  | G     | 853  | 2    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.29 | 6 (7%)   |
| 16  | SF4  | p     | 101  | 5    | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CLA  | b     | 826  | -    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.28 | 8 (9%)   |
| 17  | BCR  | S     | 204  | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 2.02 | 16 (28%) |
| 15  | PQN  | B     | 842  | -    | 34,34,34     | 1.61 | 2 (5%)   | 43,45,45    | 1.18 | 4 (9%)   |
| 14  | CLA  | X     | 1701 | 3    | 53,57,73     | 1.33 | 8 (15%)  | 61,93,113   | 1.38 | 5 (8%)   |
| 14  | CLA  | G     | 852  | -    | 49,53,73     | 1.34 | 10 (20%) | 58,89,113   | 1.35 | 4 (6%)   |
| 14  | CLA  | B     | 841  | 4    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 14  | CLA  | n     | 815  | 4    | 53,57,73     | 1.32 | 8 (15%)  | 61,93,113   | 1.38 | 5 (8%)   |
| 14  | CLA  | a     | 815  | 2    | 63,67,73     | 1.23 | 9 (14%)  | 74,105,113  | 1.30 | 5 (6%)   |
| 14  | CLA  | n     | 810  | 4    | 64,68,73     | 1.22 | 8 (12%)  | 76,107,113  | 1.28 | 5 (6%)   |
| 17  | BCR  | N     | 847  | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 2.18 | 17 (30%) |
| 14  | CLA  | b     | 819  | 4    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.23 | 5 (6%)   |
| 17  | BCR  | B     | 852  | -    | 41,41,41     | 0.72 | 1 (2%)   | 56,56,56    | 2.02 | 13 (23%) |
| 14  | CLA  | G     | 804  | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 14  | CLA  | n     | 803  | 4    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.22 | 7 (8%)   |
| 14  | CLA  | A     | 841  | 18   | 49,53,73     | 1.39 | 9 (18%)  | 58,89,113   | 1.44 | 4 (6%)   |
| 14  | CLA  | B     | 810  | 4    | 69,73,73     | 1.18 | 9 (13%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 17  | BCR  | G     | 847  | -    | 41,41,41     | 0.73 | 1 (2%)   | 56,56,56    | 2.02 | 16 (28%) |
| 17  | BCR  | g     | 846  | -    | 41,41,41     | 0.74 | 0        | 56,56,56    | 2.50 | 16 (28%) |
| 17  | BCR  | b     | 844  | -    | 41,41,41     | 0.71 | 1 (2%)   | 56,56,56    | 2.04 | 17 (30%) |
| 14  | CLA  | B     | 803  | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.17 | 3 (3%)   |
| 19  | CL0  | G     | 851  | 2    | 58,73,73     | 2.97 | 18 (31%) | 60,113,113  | 1.62 | 13 (21%) |
| 14  | CLA  | A     | 838  | 2    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 17  | BCR  | a     | 845  | -    | 41,41,41     | 0.72 | 0        | 56,56,56    | 2.13 | 18 (32%) |
| 14  | CLA  | A     | 810  | 14,2 | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 17  | BCR  | G     | 844  | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 2.07 | 18 (32%) |
| 14  | CLA  | b     | 823  | -    | 59,63,73     | 1.27 | 7 (11%)  | 70,101,113  | 1.32 | 5 (7%)   |
| 14  | CLA  | a     | 819  | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.28 | 8 (9%)   |
| 14  | CLA  | J     | 102  | 9    | 41,45,73     | 1.47 | 8 (19%)  | 50,78,113   | 1.44 | 4 (8%)   |
| 17  | BCR  | N     | 849  | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 1.87 | 17 (30%) |
| 14  | CLA  | N     | 832  | 4    | 58,62,73     | 1.29 | 8 (13%)  | 68,99,113   | 1.32 | 5 (7%)   |



| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 16  | SF4  | A     | 843  | 2,4  | 0,12,12      | -    | -        | -           |      |          |
| 14  | CLA  | A     | 803  | 14,2 | 58,62,73     | 1.27 | 9 (15%)  | 68,99,113   | 1.34 | 4 (5%)   |
| 21  | LMG  | N     | 802  | -    | 35,35,55     | 0.59 | 0        | 43,43,63    | 0.68 | 0        |
| 14  | CLA  | N     | 839  | 4    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 21  | LMG  | N     | 850  | -    | 55,55,55     | 0.49 | 0        | 63,63,63    | 0.59 | 0        |
| 14  | CLA  | a     | 806  | 2    | 69,73,73     | 1.15 | 9 (13%)  | 82,113,113  | 1.29 | 7 (8%)   |
| 14  | CLA  | B     | 807  | 4    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.29 | 6 (7%)   |
| 14  | CLA  | G     | 824  | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.31 | 6 (7%)   |
| 16  | SF4  | g     | 842  | 2,4  | 0,12,12      | -    | -        | -           |      |          |
| 15  | PQN  | N     | 843  | -    | 34,34,34     | 1.61 | 2 (5%)   | 43,45,45    | 1.24 | 4 (9%)   |
| 14  | CLA  | N     | 834  | 4    | 62,66,73     | 1.23 | 9 (14%)  | 73,104,113  | 1.35 | 6 (8%)   |
| 14  | CLA  | A     | 808  | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.27 | 8 (9%)   |
| 14  | CLA  | A     | 853  | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 14  | CLA  | N     | 817  | 4    | 53,57,73     | 1.32 | 8 (15%)  | 61,93,113   | 1.38 | 5 (8%)   |
| 14  | CLA  | a     | 814  | -    | 49,53,73     | 1.39 | 7 (14%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 14  | CLA  | n     | 834  | -    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.42 | 5 (8%)   |
| 14  | CLA  | A     | 813  | 2    | 58,62,73     | 1.28 | 9 (15%)  | 68,99,113   | 1.36 | 6 (8%)   |
| 14  | CLA  | N     | 822  | 4    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.40 | 4 (6%)   |
| 14  | CLA  | l     | 203  | 12   | 64,68,73     | 1.21 | 9 (14%)  | 76,107,113  | 1.30 | 4 (5%)   |
| 14  | CLA  | a     | 837  | 2    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.24 | 5 (6%)   |
| 14  | CLA  | a     | 831  | 2    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.25 | 8 (9%)   |
| 14  | CLA  | a     | 812  | 2    | 58,62,73     | 1.28 | 8 (13%)  | 68,99,113   | 1.37 | 6 (8%)   |
| 17  | BCR  | n     | 842  | -    | 41,41,41     | 0.74 | 1 (2%)   | 56,56,56    | 2.13 | 15 (26%) |
| 14  | CLA  | G     | 832  | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 14  | CLA  | b     | 851  | 4    | 62,66,73     | 1.24 | 9 (14%)  | 73,104,113  | 1.33 | 4 (5%)   |
| 14  | CLA  | a     | 826  | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 14  | CLA  | W     | 202  | 12   | 55,59,73     | 1.31 | 8 (14%)  | 64,96,113   | 1.44 | 5 (7%)   |
| 20  | SQD  | w     | 202  | -    | 52,54,54     | 1.56 | 7 (13%)  | 62,65,65    | 1.31 | 6 (9%)   |
| 14  | CLA  | n     | 813  | 4    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.28 | 7 (8%)   |
| 14  | CLA  | a     | 816  | -    | 64,68,73     | 1.22 | 9 (14%)  | 76,107,113  | 1.29 | 5 (6%)   |
| 17  | BCR  | M     | 101  | -    | 41,41,41     | 0.65 | 0        | 56,56,56    | 2.00 | 17 (30%) |
| 14  | CLA  | s     | 202  | -    | 49,53,73     | 1.40 | 8 (16%)  | 58,89,113   | 1.42 | 4 (6%)   |
| 14  | CLA  | a     | 823  | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 20  | SQD  | H     | 1702 | -    | 52,54,54     | 1.56 | 7 (13%)  | 62,65,65    | 1.34 | 6 (9%)   |
| 14  | CLA  | b     | 831  | 4    | 58,62,73     | 1.28 | 8 (13%)  | 68,99,113   | 1.34 | 7 (10%)  |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | a     | 818  | 2    | 58,62,73     | 1.27 | 8 (13%)  | 68,99,113   | 1.36 | 5 (7%)   |
| 14  | CLA  | b     | 835  | -    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.42 | 6 (10%)  |
| 14  | CLA  | b     | 836  | -    | 49,53,73     | 1.39 | 7 (14%)  | 58,89,113   | 1.38 | 4 (6%)   |
| 14  | CLA  | H     | 1701 | 3    | 53,57,73     | 1.33 | 8 (15%)  | 61,93,113   | 1.38 | 4 (6%)   |
| 14  | CLA  | A     | 834  | 2    | 58,62,73     | 1.28 | 8 (13%)  | 68,99,113   | 1.33 | 6 (8%)   |
| 14  | CLA  | G     | 816  | 2    | 63,67,73     | 1.22 | 9 (14%)  | 74,105,113  | 1.29 | 5 (6%)   |
| 14  | CLA  | B     | 837  | 4    | 64,68,73     | 1.22 | 9 (14%)  | 76,107,113  | 1.29 | 7 (9%)   |
| 14  | CLA  | b     | 833  | 4    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 14  | CLA  | n     | 840  | 4    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.30 | 5 (6%)   |
| 17  | BCR  | B     | 845  | -    | 41,41,41     | 0.69 | 0        | 56,56,56    | 2.10 | 13 (23%) |
| 14  | CLA  | b     | 834  | 4    | 58,62,73     | 1.27 | 8 (13%)  | 68,99,113   | 1.36 | 7 (10%)  |
| 17  | BCR  | I     | 101  | -    | 41,41,41     | 0.73 | 1 (2%)   | 56,56,56    | 2.22 | 17 (30%) |
| 14  | CLA  | A     | 809  | 2    | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.41 | 4 (6%)   |
| 17  | BCR  | a     | 843  | -    | 41,41,41     | 0.68 | 0        | 56,56,56    | 2.02 | 15 (26%) |
| 14  | CLA  | g     | 819  | -    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.26 | 5 (6%)   |
| 14  | CLA  | A     | 806  | 2    | 64,68,73     | 1.22 | 8 (12%)  | 76,107,113  | 1.29 | 5 (6%)   |
| 14  | CLA  | N     | 816  | 4    | 54,58,73     | 1.31 | 8 (14%)  | 64,95,113   | 1.41 | 6 (9%)   |
| 14  | CLA  | G     | 819  | 2    | 58,62,73     | 1.28 | 9 (15%)  | 68,99,113   | 1.35 | 5 (7%)   |
| 14  | CLA  | B     | 819  | 4    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.27 | 6 (7%)   |
| 17  | BCR  | k     | 102  | -    | 41,41,41     | 0.68 | 0        | 56,56,56    | 2.09 | 17 (30%) |
| 14  | CLA  | G     | 807  | 2    | 69,73,73     | 1.15 | 8 (11%)  | 82,113,113  | 1.28 | 7 (8%)   |
| 14  | CLA  | n     | 829  | 4    | 69,73,73     | 1.15 | 6 (8%)   | 82,113,113  | 1.26 | 6 (7%)   |
| 14  | CLA  | A     | 817  | 2    | 64,68,73     | 1.21 | 9 (14%)  | 76,107,113  | 1.28 | 4 (5%)   |
| 14  | CLA  | N     | 811  | 4    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.29 | 7 (8%)   |
| 14  | CLA  | N     | 819  | 4    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.28 | 5 (6%)   |
| 14  | CLA  | g     | 820  | 2    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.44 | 5 (8%)   |
| 14  | CLA  | A     | 818  | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.27 | 8 (9%)   |
| 14  | CLA  | g     | 808  | 2    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.41 | 4 (6%)   |
| 17  | BCR  | g     | 844  | -    | 41,41,41     | 0.72 | 0        | 56,56,56    | 2.10 | 17 (30%) |
| 14  | CLA  | G     | 834  | 2    | 58,62,73     | 1.27 | 8 (13%)  | 68,99,113   | 1.33 | 5 (7%)   |
| 14  | CLA  | A     | 836  | 2    | 55,59,73     | 1.33 | 8 (14%)  | 64,96,113   | 1.37 | 5 (7%)   |
| 14  | CLA  | a     | 833  | 2    | 58,62,73     | 1.27 | 9 (15%)  | 68,99,113   | 1.33 | 6 (8%)   |
| 17  | BCR  | b     | 843  | -    | 41,41,41     | 0.73 | 1 (2%)   | 56,56,56    | 2.07 | 16 (28%) |
| 14  | CLA  | a     | 830  | 2    | 69,73,73     | 1.16 | 8 (11%)  | 82,113,113  | 1.29 | 5 (6%)   |
| 14  | CLA  | n     | 827  | 4    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.24 | 6 (7%)   |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | A     | 824 | -    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.30 | 6 (7%)   |
| 17  | BCR  | m     | 102 | -    | 41,41,41     | 0.67 | 0        | 56,56,56    | 2.06 | 15 (26%) |
| 17  | BCR  | B     | 844 | -    | 41,41,41     | 0.72 | 0        | 56,56,56    | 2.11 | 21 (37%) |
| 14  | CLA  | G     | 823 | 2    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.45 | 4 (6%)   |
| 14  | CLA  | b     | 814 | 4    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.27 | 7 (8%)   |
| 14  | CLA  | b     | 822 | 4    | 49,53,73     | 1.39 | 7 (14%)  | 58,89,113   | 1.43 | 4 (6%)   |
| 14  | CLA  | B     | 823 | -    | 59,63,73     | 1.26 | 8 (13%)  | 70,101,113  | 1.31 | 6 (8%)   |
| 17  | BCR  | i     | 101 | -    | 41,41,41     | 0.71 | 0        | 56,56,56    | 2.25 | 15 (26%) |
| 14  | CLA  | N     | 838 | 4    | 64,68,73     | 1.22 | 9 (14%)  | 76,107,113  | 1.28 | 5 (6%)   |
| 14  | CLA  | B     | 820 | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.26 | 8 (9%)   |
| 17  | BCR  | b     | 847 | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 2.07 | 16 (28%) |
| 14  | CLA  | G     | 839 | 2    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.28 | 6 (7%)   |
| 14  | CLA  | B     | 818 | 4    | 69,73,73     | 1.18 | 8 (11%)  | 82,113,113  | 1.21 | 4 (4%)   |
| 14  | CLA  | l     | 202 | 12   | 49,53,73     | 1.38 | 8 (16%)  | 58,89,113   | 1.45 | 6 (10%)  |
| 14  | CLA  | G     | 818 | 2    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.27 | 7 (8%)   |
| 14  | CLA  | N     | 803 | -    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.21 | 6 (7%)   |
| 17  | BCR  | a     | 847 | -    | 41,41,41     | 0.78 | 2 (4%)   | 56,56,56    | 2.07 | 18 (32%) |
| 14  | CLA  | N     | 818 | 4    | 49,53,73     | 1.39 | 8 (16%)  | 58,89,113   | 1.41 | 4 (6%)   |
| 15  | PQN  | n     | 841 | -    | 34,34,34     | 1.58 | 2 (5%)   | 43,45,45    | 1.19 | 4 (9%)   |
| 14  | CLA  | a     | 804 | 2    | 69,73,73     | 1.16 | 9 (13%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 18  | LHG  | g     | 850 | -    | 48,48,48     | 1.15 | 6 (12%)  | 51,54,54    | 0.93 | 2 (3%)   |
| 14  | CLA  | b     | 830 | 4    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.29 | 8 (9%)   |
| 14  | CLA  | g     | 825 | 2    | 69,73,73     | 1.17 | 9 (13%)  | 82,113,113  | 1.27 | 7 (8%)   |
| 14  | CLA  | G     | 815 | -    | 49,53,73     | 1.40 | 6 (12%)  | 58,89,113   | 1.37 | 4 (6%)   |
| 14  | CLA  | N     | 833 | 4    | 64,68,73     | 1.22 | 9 (14%)  | 76,107,113  | 1.27 | 4 (5%)   |
| 20  | SQD  | n     | 801 | -    | 52,54,54     | 1.57 | 8 (15%)  | 62,65,65    | 1.31 | 6 (9%)   |
| 14  | CLA  | B     | 812 | 4    | 58,62,73     | 1.27 | 8 (13%)  | 68,99,113   | 1.36 | 6 (8%)   |
| 17  | BCR  | l     | 205 | -    | 41,41,41     | 0.70 | 0        | 56,56,56    | 1.99 | 13 (23%) |
| 14  | CLA  | g     | 840 | -    | 54,58,73     | 1.31 | 7 (12%)  | 64,95,113   | 1.42 | 8 (12%)  |
| 17  | BCR  | I     | 103 | -    | 41,41,41     | 0.74 | 0        | 56,56,56    | 1.80 | 14 (25%) |
| 14  | CLA  | B     | 806 | 4    | 69,73,73     | 1.16 | 7 (10%)  | 82,113,113  | 1.26 | 7 (8%)   |
| 14  | CLA  | B     | 816 | 4    | 53,57,73     | 1.32 | 8 (15%)  | 61,93,113   | 1.39 | 5 (8%)   |
| 14  | CLA  | B     | 824 | 4    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.25 | 6 (7%)   |
| 14  | CLA  | b     | 825 | 4    | 69,73,73     | 1.17 | 7 (10%)  | 82,113,113  | 1.26 | 6 (7%)   |
| 17  | BCR  | G     | 846 | -    | 41,41,41     | 0.67 | 0        | 56,56,56    | 2.07 | 17 (30%) |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | CLA  | a     | 817 | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.24 | 6 (7%)   |
| 16  | SF4  | p     | 102 | 5    | 0,12,12      | -    | -        | -           | -    | -        |
| 14  | CLA  | a     | 835 | 2    | 55,59,73     | 1.31 | 7 (12%)  | 64,96,113   | 1.39 | 6 (9%)   |
| 14  | CLA  | G     | 827 | 2    | 69,73,73     | 1.17 | 8 (11%)  | 82,113,113  | 1.28 | 5 (6%)   |
| 20  | SQD  | b     | 801 | -    | 52,54,54     | 1.58 | 8 (15%)  | 62,65,65    | 1.27 | 7 (11%)  |
| 14  | CLA  | b     | 840 | -    | 69,73,73     | 1.18 | 9 (13%)  | 82,113,113  | 1.27 | 6 (7%)   |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 14  | CLA  | N     | 851 | 4    | 1/1/15/20 | 16/39/115/115 | -       |
| 14  | CLA  | b     | 809 | 4    | 1/1/15/20 | 11/39/115/115 | -       |
| 14  | CLA  | B     | 836 | -    | 1/1/11/20 | 7/15/91/115   | -       |
| 14  | CLA  | G     | 811 | 2    | 1/1/13/20 | 8/32/108/115  | -       |
| 14  | CLA  | G     | 803 | 2    | 1/1/12/20 | 5/26/102/115  | -       |
| 14  | CLA  | g     | 835 | 2    | 1/1/12/20 | 6/23/99/115   | -       |
| 14  | CLA  | g     | 836 | 2    | 1/1/15/20 | 15/39/115/115 | -       |
| 17  | BCR  | G     | 845 | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 835 | 2    | 1/1/11/20 | 7/15/91/115   | -       |
| 14  | CLA  | G     | 836 | 2    | 1/1/12/20 | 2/23/99/115   | -       |
| 17  | BCR  | A     | 856 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 833 | 2    | 1/1/15/20 | 12/39/115/115 | -       |
| 14  | CLA  | G     | 826 | 2    | 1/1/15/20 | 9/39/115/115  | -       |
| 18  | LHG  | a     | 850 | 14   | -         | 29/53/53/53   | -       |
| 14  | CLA  | b     | 817 | 4    | 1/1/11/20 | 4/15/91/115   | -       |
| 14  | CLA  | N     | 835 | 4    | 1/1/12/20 | 7/26/102/115  | -       |
| 18  | LHG  | A     | 851 | 14   | -         | 25/53/53/53   | -       |
| 14  | CLA  | A     | 832 | 2    | 1/1/15/20 | 9/39/115/115  | -       |
| 19  | CL0  | A     | 852 | -    | 3/3/16/25 | 3/13/111/135  | -       |
| 14  | CLA  | w     | 203 | 12   | 1/1/11/20 | 7/15/91/115   | -       |
| 14  | CLA  | B     | 829 | 4    | 1/1/15/20 | 10/39/115/115 | -       |
| 21  | LMG  | B     | 849 | -    | -         | 20/50/70/70   | 0/1/1/1 |
| 14  | CLA  | N     | 837 | -    | 1/1/11/20 | 8/15/91/115   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | a     | 840  | 18   | 1/1/11/20 | 7/15/91/115   | -       |
| 14  | CLA  | g     | 852  | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 14  | CLA  | G     | 829  | 2    | 1/1/15/20 | 7/39/115/115  | -       |
| 14  | CLA  | N     | 842  | 4    | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CLA  | N     | 812  | 4    | 1/1/14/20 | 10/33/109/115 | -       |
| 16  | SF4  | c     | 101  | 5    | -         | -             | 0/6/5/5 |
| 14  | CLA  | a     | 822  | 2    | 1/1/11/20 | 6/15/91/115   | -       |
| 14  | CLA  | a     | 839  | 2    | 1/1/15/20 | 3/39/115/115  | -       |
| 14  | CLA  | g     | 805  | 2    | 1/1/14/20 | 4/33/109/115  | -       |
| 14  | CLA  | b     | 808  | 4    | 1/1/15/20 | 4/39/115/115  | -       |
| 17  | BCR  | G     | 843  | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | b     | 837  | 4    | 1/1/14/20 | 10/33/109/115 | -       |
| 14  | CLA  | g     | 823  | -    | 1/1/15/20 | 9/39/115/115  | -       |
| 14  | CLA  | b     | 802  | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 14  | CLA  | L     | 1502 | 12   | 1/1/14/20 | 8/33/109/115  | -       |
| 17  | BCR  | B     | 843  | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 15  | PQN  | A     | 842  | -    | -         | 6/23/43/43    | 0/2/2/2 |
| 17  | BCR  | i     | 102  | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 14  | CLA  | b     | 821  | 4    | 1/1/11/20 | 6/15/91/115   | -       |
| 17  | BCR  | b     | 848  | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 14  | CLA  | n     | 852  | 4    | 1/1/13/20 | 6/27/103/115  | -       |
| 16  | SF4  | C     | 102  | 5    | -         | -             | 0/6/5/5 |
| 14  | CLA  | N     | 810  | 4    | 1/1/15/20 | 12/39/115/115 | -       |
| 14  | CLA  | K     | 101  | 10   | 1/1/9/20  | 7/9/81/115    | -       |
| 14  | CLA  | b     | 805  | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 18  | LHG  | S     | 202  | -    | -         | 24/47/47/53   | -       |
| 17  | BCR  | B     | 847  | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | n     | 820  | 4    | 1/1/11/20 | 9/15/91/115   | -       |
| 14  | CLA  | G     | 837  | 2    | 1/1/15/20 | 16/39/115/115 | -       |
| 14  | CLA  | b     | 853  | 4    | 1/1/13/20 | 8/27/103/115  | -       |
| 14  | CLA  | N     | 824  | -    | 1/1/13/20 | 3/27/103/115  | -       |
| 15  | PQN  | a     | 841  | -    | -         | 3/23/43/43    | 0/2/2/2 |
| 14  | CLA  | G     | 812  | 2    | 1/1/14/20 | 8/33/109/115  | -       |
| 17  | BCR  | N     | 853  | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 811  | 2    | 1/1/13/20 | 17/32/108/115 | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | g     | 854  | -    | 1/1/15/20 | 20/39/115/115 | -       |
| 17  | BCR  | a     | 848  | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 14  | CLA  | A     | 855  | -    | 1/1/11/20 | 9/15/91/115   | -       |
| 14  | CLA  | n     | 836  | 4    | 1/1/14/20 | 2/33/109/115  | -       |
| 14  | CLA  | B     | 839  | 4    | 1/1/11/20 | 6/18/94/115   | -       |
| 14  | CLA  | g     | 831  | 2    | 1/1/15/20 | 5/39/115/115  | -       |
| 14  | CLA  | U     | 102  | -    | 1/1/11/20 | 1/20/96/115   | -       |
| 14  | CLA  | a     | 820  | 2    | 1/1/11/20 | 7/15/91/115   | -       |
| 14  | CLA  | w     | 205  | -    | 1/1/11/20 | 5/15/91/115   | -       |
| 18  | LHG  | a     | 849  | -    | -         | 27/53/53/53   | -       |
| 20  | SQD  | l     | 201  | -    | -         | 19/49/69/69   | 0/1/1/1 |
| 21  | LMG  | n     | 848  | -    | -         | 13/50/70/70   | 0/1/1/1 |
| 14  | CLA  | B     | 850  | 4    | 1/1/15/20 | 14/39/115/115 | -       |
| 14  | CLA  | B     | 817  | 4    | 1/1/11/20 | 8/15/91/115   | -       |
| 15  | PQN  | g     | 841  | -    | -         | 2/23/43/43    | 0/2/2/2 |
| 14  | CLA  | g     | 832  | 2    | 1/1/15/20 | 9/39/115/115  | -       |
| 14  | CLA  | g     | 839  | 2    | 1/1/15/20 | 7/39/115/115  | -       |
| 14  | CLA  | A     | 820  | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 14  | CLA  | b     | 838  | 4    | 1/1/15/20 | 6/39/115/115  | -       |
| 14  | CLA  | g     | 811  | 2    | 1/1/14/20 | 3/33/109/115  | -       |
| 14  | CLA  | n     | 806  | 4    | 1/1/15/20 | 15/39/115/115 | -       |
| 17  | BCR  | j     | 104  | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | t     | 102  | 9    | 1/1/8/20  | 0/4/76/115    | -       |
| 17  | BCR  | w     | 206  | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 17  | BCR  | N     | 848  | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 16  | SF4  | c     | 102  | 5    | -         | -             | 0/6/5/5 |
| 17  | BCR  | n     | 844  | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 14  | CLA  | L     | 1501 | 12   | 1/1/12/20 | 7/23/99/115   | -       |
| 14  | CLA  | g     | 834  | 2    | 1/1/11/20 | 5/15/91/115   | -       |
| 14  | CLA  | N     | 801  | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 14  | CLA  | g     | 826  | 2    | 1/1/15/20 | 13/39/115/115 | -       |
| 14  | CLA  | n     | 823  | 4    | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CLA  | B     | 815  | 4    | 1/1/12/20 | 4/21/97/115   | -       |
| 17  | BCR  | A     | 848  | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 16  | SF4  | P     | 102  | 5    | -         | -             | 0/6/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 14  | CLA  | A     | 804 | 2    | 1/1/15/20 | 15/39/115/115 | -       |
| 17  | BCR  | B     | 851 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 805 | 2    | 1/1/15/20 | 18/39/115/115 | -       |
| 14  | CLA  | g     | 802 | 2    | 1/1/12/20 | 7/26/102/115  | -       |
| 14  | CLA  | n     | 807 | 4    | 1/1/15/20 | 6/39/115/115  | -       |
| 14  | CLA  | A     | 819 | 2    | 1/1/12/20 | 14/26/102/115 | -       |
| 17  | BCR  | T     | 104 | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 801 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 14  | CLA  | B     | 826 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 14  | CLA  | n     | 824 | 4    | 1/1/15/20 | 9/39/115/115  | -       |
| 14  | CLA  | G     | 817 | 2    | 1/1/14/20 | 9/33/109/115  | -       |
| 14  | CLA  | a     | 838 | 2    | 1/1/15/20 | 5/39/115/115  | -       |
| 17  | BCR  | W     | 201 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 17  | BCR  | w     | 201 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 17  | BCR  | W     | 206 | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 822 | 2    | 1/1/12/20 | 8/26/102/115  | -       |
| 14  | CLA  | n     | 804 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 17  | BCR  | A     | 844 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | B     | 805 | 4    | 1/1/13/20 | 11/27/103/115 | -       |
| 14  | CLA  | g     | 814 | -    | 1/1/11/20 | 4/15/91/115   | -       |
| 15  | PQN  | b     | 842 | -    | -         | 1/23/43/43    | 0/2/2/2 |
| 14  | CLA  | n     | 832 | 4    | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CLA  | a     | 832 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 14  | CLA  | B     | 808 | 4    | 1/1/15/20 | 9/39/115/115  | -       |
| 14  | CLA  | a     | 827 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 17  | BCR  | Y     | 101 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 19  | CL0  | g     | 851 | 2    | 3/3/20/25 | 4/37/135/135  | -       |
| 14  | CLA  | G     | 808 | 2    | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CLA  | B     | 804 | 4    | 1/1/11/20 | 6/15/91/115   | -       |
| 14  | CLA  | s     | 201 | -    | 1/1/13/20 | 16/32/108/115 | -       |
| 14  | CLA  | A     | 807 | 2    | 1/1/15/20 | 18/39/115/115 | -       |
| 17  | BCR  | g     | 847 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 14  | CLA  | N     | 825 | 4    | 1/1/15/20 | 13/39/115/115 | -       |
| 14  | CLA  | g     | 821 | 2    | 1/1/12/20 | 12/26/102/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 14  | CLA  | N     | 808 | 4    | 1/1/15/20 | 11/39/115/115 | -       |
| 14  | CLA  | G     | 821 | 2    | 1/1/11/20 | 7/15/91/115   | -       |
| 17  | BCR  | A     | 845 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 17  | BCR  | v     | 101 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 17  | BCR  | J     | 103 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | b     | 827 | 4    | 1/1/15/20 | 9/39/115/115  | -       |
| 18  | LHG  | g     | 849 | -    | -         | 30/53/53/53   | -       |
| 14  | CLA  | N     | 840 | 4    | 1/1/11/20 | 5/18/94/115   | -       |
| 14  | CLA  | N     | 809 | 4    | 1/1/15/20 | 7/39/115/115  | -       |
| 18  | LHG  | G     | 849 | -    | -         | 28/53/53/53   | -       |
| 14  | CLA  | N     | 821 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 14  | CLA  | b     | 803 | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 14  | CLA  | g     | 812 | 2    | 1/1/12/20 | 8/26/102/115  | -       |
| 14  | CLA  | S     | 201 | -    | 1/1/13/20 | 8/32/108/115  | -       |
| 14  | CLA  | g     | 853 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 14  | CLA  | T     | 102 | 9    | 1/1/8/20  | 0/4/76/115    | -       |
| 14  | CLA  | N     | 841 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 17  | BCR  | a     | 846 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | J     | 101 | 9    | 1/1/11/20 | 9/15/91/115   | -       |
| 14  | CLA  | S     | 203 | -    | 1/1/11/20 | 4/15/91/115   | -       |
| 14  | CLA  | n     | 819 | -    | 1/1/15/20 | 6/39/115/115  | -       |
| 17  | BCR  | n     | 851 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 14  | CLA  | n     | 808 | 4    | 1/1/15/20 | 12/39/115/115 | -       |
| 14  | CLA  | a     | 801 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 14  | CLA  | G     | 809 | 2    | 1/1/11/20 | 4/15/91/115   | -       |
| 14  | CLA  | G     | 825 | -    | 1/1/12/20 | 3/26/102/115  | -       |
| 14  | CLA  | b     | 828 | 4    | 1/1/15/20 | 11/39/115/115 | -       |
| 14  | CLA  | N     | 831 | 4    | 1/1/15/20 | 11/39/115/115 | -       |
| 14  | CLA  | B     | 833 | 4    | 1/1/13/20 | 10/31/107/115 | -       |
| 18  | LHG  | G     | 850 | 14   | -         | 27/53/53/53   | -       |
| 17  | BCR  | j     | 103 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | g     | 833 | 2    | 1/1/12/20 | 4/26/102/115  | -       |
| 14  | CLA  | G     | 838 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 14  | CLA  | G     | 840 | 18   | 1/1/11/20 | 8/15/91/115   | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | b     | 810  | 4    | 1/1/15/20 | 13/39/115/115 | -       |
| 14  | CLA  | A     | 837  | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 14  | CLA  | T     | 101  | 9    | 1/1/11/20 | 11/15/91/115  | -       |
| 17  | BCR  | b     | 846  | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | b     | 811  | 4    | 1/1/14/20 | 16/33/109/115 | -       |
| 14  | CLA  | B     | 838  | 4    | 1/1/15/20 | 3/39/115/115  | -       |
| 14  | CLA  | G     | 805  | 2    | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CLA  | a     | 813  | 2    | 1/1/11/20 | 7/15/91/115   | -       |
| 17  | BCR  | n     | 843  | -    | -         | 5/29/63/63    | 0/2/2/2 |
| 17  | BCR  | b     | 845  | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 14  | CLA  | n     | 818  | 4    | 1/1/15/20 | 9/39/115/115  | -       |
| 14  | CLA  | A     | 833  | 2    | 1/1/15/20 | 14/39/115/115 | -       |
| 20  | SQD  | h     | 1702 | -    | -         | 28/49/69/69   | 0/1/1/1 |
| 14  | CLA  | n     | 814  | 4    | 1/1/12/20 | 3/21/97/115   | -       |
| 14  | CLA  | b     | 804  | 4    | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CLA  | a     | 811  | 2    | 1/1/14/20 | 12/33/109/115 | -       |
| 20  | SQD  | x     | 1702 | -    | -         | 29/49/69/69   | 0/1/1/1 |
| 14  | CLA  | a     | 828  | 2    | 1/1/15/20 | 9/39/115/115  | -       |
| 14  | CLA  | g     | 817  | 2    | 1/1/15/20 | 7/39/115/115  | -       |
| 14  | CLA  | j     | 101  | 9    | 1/1/11/20 | 10/15/91/115  | -       |
| 14  | CLA  | B     | 831  | 4    | 1/1/12/20 | 7/26/102/115  | -       |
| 17  | BCR  | g     | 845  | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | b     | 841  | 4    | 1/1/15/20 | 16/39/115/115 | -       |
| 14  | CLA  | x     | 1701 | 3    | 1/1/11/20 | 10/20/96/115  | -       |
| 14  | CLA  | a     | 825  | 2    | 1/1/15/20 | 5/39/115/115  | -       |
| 14  | CLA  | n     | 809  | 4    | 1/1/15/20 | 14/39/115/115 | -       |
| 14  | CLA  | B     | 822  | 4    | 1/1/11/20 | 5/15/91/115   | -       |
| 14  | CLA  | G     | 802  | 2    | 1/1/15/20 | 7/39/115/115  | -       |
| 14  | CLA  | b     | 807  | 4    | 1/1/15/20 | 9/39/115/115  | -       |
| 14  | CLA  | a     | 802  | 14,2 | 1/1/12/20 | 6/26/102/115  | -       |
| 14  | CLA  | B     | 835  | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 17  | BCR  | s     | 203  | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 823  | 2    | 1/1/11/20 | 4/15/91/115   | -       |
| 14  | CLA  | B     | 830  | 4    | 1/1/15/20 | 7/39/115/115  | -       |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 17  | BCR  | A     | 849  | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 14  | CLA  | N     | 804  | 4    | 1/1/15/20 | 18/39/115/115 | -       |
| 14  | CLA  | A     | 814  | 2    | 1/1/11/20 | 5/15/91/115   | -       |
| 14  | CLA  | F     | 201  | -    | 1/1/13/20 | 8/32/108/115  | -       |
| 14  | CLA  | A     | 839  | 2    | 1/1/15/20 | 17/39/115/115 | -       |
| 16  | SF4  | G     | 842  | 2,4  | -         | -             | 0/6/5/5 |
| 14  | CLA  | n     | 816  | 4    | 1/1/11/20 | 6/15/91/115   | -       |
| 14  | CLA  | n     | 817  | 4    | 1/1/15/20 | 12/39/115/115 | -       |
| 14  | CLA  | A     | 831  | 2    | 1/1/15/20 | 17/39/115/115 | -       |
| 17  | BCR  | G     | 848  | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 14  | CLA  | n     | 811  | 4    | 1/1/12/20 | 9/26/102/115  | -       |
| 14  | CLA  | A     | 802  | 2    | 1/1/15/20 | 14/39/115/115 | -       |
| 14  | CLA  | L     | 1503 | -    | 1/1/11/20 | 2/15/91/115   | -       |
| 14  | CLA  | h     | 1701 | 3    | 1/1/11/20 | 10/20/96/115  | -       |
| 14  | CLA  | a     | 803  | 2    | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CLA  | g     | 813  | 2    | 1/1/11/20 | 4/15/91/115   | -       |
| 17  | BCR  | K     | 102  | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 14  | CLA  | n     | 839  | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 14  | CLA  | N     | 807  | 4    | 1/1/15/20 | 11/39/115/115 | -       |
| 14  | CLA  | B     | 828  | 4    | 1/1/15/20 | 8/39/115/115  | -       |
| 17  | BCR  | t     | 104  | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 18  | LHG  | X     | 1702 | -    | -         | 25/47/47/53   | -       |
| 14  | CLA  | g     | 824  | -    | 1/1/12/20 | 2/26/102/115  | -       |
| 14  | CLA  | N     | 828  | 4    | 1/1/15/20 | 9/39/115/115  | -       |
| 17  | BCR  | n     | 845  | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 14  | CLA  | a     | 854  | -    | 1/1/11/20 | 5/20/96/115   | -       |
| 14  | CLA  | n     | 802  | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CLA  | g     | 837  | 2    | 1/1/15/20 | 17/39/115/115 | -       |
| 17  | BCR  | I     | 102  | -    | -         | 14/29/63/63   | 0/2/2/2 |
| 14  | CLA  | b     | 812  | 4    | 1/1/12/20 | 11/26/102/115 | -       |
| 14  | CLA  | B     | 814  | 4    | 1/1/15/20 | 14/39/115/115 | -       |
| 17  | BCR  | B     | 846  | -    | -         | 7/29/63/63    | 0/2/2/2 |
| 14  | CLA  | n     | 826  | 4    | 1/1/15/20 | 4/39/115/115  | -       |
| 14  | CLA  | g     | 804  | 2    | 1/1/15/20 | 13/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 14  | CLA  | A     | 854 | 2    | 1/1/15/20 | 13/39/115/115 | -       |
| 20  | SQD  | B     | 801 | -    | -         | 22/49/69/69   | 0/1/1/1 |
| 14  | CLA  | b     | 806 | 4    | 1/1/15/20 | 11/39/115/115 | -       |
| 14  | CLA  | f     | 202 | -    | 1/1/11/20 | 5/15/91/115   | -       |
| 14  | CLA  | a     | 852 | -    | 1/1/11/20 | 7/15/91/115   | -       |
| 14  | CLA  | b     | 820 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 14  | CLA  | B     | 809 | 4    | 1/1/15/20 | 8/39/115/115  | -       |
| 14  | CLA  | b     | 824 | 4    | 1/1/15/20 | 14/39/115/115 | -       |
| 14  | CLA  | a     | 807 | 2    | 1/1/15/20 | 7/39/115/115  | -       |
| 14  | CLA  | g     | 828 | 2    | 1/1/15/20 | 9/39/115/115  | -       |
| 14  | CLA  | n     | 805 | 4    | 1/1/15/20 | 10/39/115/115 | -       |
| 15  | PQN  | G     | 841 | -    | -         | 5/23/43/43    | 0/2/2/2 |
| 14  | CLA  | G     | 828 | 2    | 1/1/15/20 | 9/39/115/115  | -       |
| 14  | CLA  | b     | 832 | 4    | 1/1/14/20 | 4/33/109/115  | -       |
| 14  | CLA  | g     | 838 | 2    | 1/1/15/20 | 11/39/115/115 | -       |
| 14  | CLA  | a     | 834 | 2    | 1/1/11/20 | 7/15/91/115   | -       |
| 18  | LHG  | m     | 101 | -    | -         | 25/47/47/53   | -       |
| 14  | CLA  | g     | 810 | 2    | 1/1/13/20 | 10/32/108/115 | -       |
| 17  | BCR  | f     | 203 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 810 | 2    | 1/1/15/20 | 16/39/115/115 | -       |
| 14  | CLA  | A     | 826 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 14  | CLA  | N     | 814 | 4    | 1/1/12/20 | 9/26/102/115  | -       |
| 14  | CLA  | g     | 803 | 2    | 1/1/15/20 | 17/39/115/115 | -       |
| 14  | CLA  | a     | 824 | -    | 1/1/12/20 | 6/26/102/115  | -       |
| 14  | CLA  | n     | 837 | 4    | 1/1/15/20 | 14/39/115/115 | -       |
| 14  | CLA  | A     | 816 | 2    | 1/1/13/20 | 9/32/108/115  | -       |
| 17  | BCR  | n     | 847 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | n     | 821 | 4    | 1/1/11/20 | 4/15/91/115   | -       |
| 14  | CLA  | B     | 825 | 4    | 1/1/15/20 | 8/39/115/115  | -       |
| 16  | SF4  | P     | 101 | 5    | -         | -             | 0/6/5/5 |
| 14  | CLA  | b     | 813 | 4    | 1/1/12/20 | 7/26/102/115  | -       |
| 14  | CLA  | F     | 202 | -    | 1/1/11/20 | 5/15/91/115   | -       |
| 14  | CLA  | A     | 829 | 2    | 1/1/15/20 | 8/39/115/115  | -       |
| 17  | BCR  | W     | 205 | -    | -         | 4/29/63/63    | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 14  | CLA  | B     | 840 | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 17  | BCR  | N     | 852 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 14  | CLA  | n     | 812 | 4    | 1/1/12/20 | 6/26/102/115  | -       |
| 14  | CLA  | A     | 825 | -    | 1/1/12/20 | 9/26/102/115  | -       |
| 14  | CLA  | a     | 809 | 14,2 | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CLA  | g     | 829 | 2    | 1/1/12/20 | 4/26/102/115  | -       |
| 14  | CLA  | b     | 818 | 4    | 1/1/15/20 | 11/39/115/115 | -       |
| 14  | CLA  | a     | 821 | 2    | 1/1/12/20 | 13/26/102/115 | -       |
| 17  | BCR  | g     | 848 | -    | -         | 12/29/63/63   | 0/2/2/2 |
| 14  | CLA  | g     | 822 | 2    | 1/1/11/20 | 2/15/91/115   | -       |
| 14  | CLA  | B     | 834 | 4    | 1/1/12/20 | 11/26/102/115 | -       |
| 14  | CLA  | g     | 830 | 2    | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CLA  | A     | 840 | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 14  | CLA  | G     | 814 | 2    | 1/1/11/20 | 6/15/91/115   | -       |
| 14  | CLA  | n     | 835 | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 14  | CLA  | g     | 816 | 2    | 1/1/14/20 | 14/33/109/115 | -       |
| 14  | CLA  | G     | 830 | 2    | 1/1/12/20 | 8/26/102/115  | -       |
| 14  | CLA  | n     | 850 | 4    | 1/1/13/20 | 13/31/107/115 | -       |
| 14  | CLA  | g     | 801 | 2    | 1/1/15/20 | 8/39/115/115  | -       |
| 14  | CLA  | A     | 821 | 2    | 1/1/11/20 | 7/15/91/115   | -       |
| 17  | BCR  | N     | 844 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | t     | 101 | 9    | 1/1/11/20 | 5/15/91/115   | -       |
| 14  | CLA  | A     | 815 | -    | 1/1/11/20 | 3/15/91/115   | -       |
| 17  | BCR  | V     | 101 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 17  | BCR  | n     | 849 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 14  | CLA  | N     | 823 | 4    | 1/1/11/20 | 4/15/91/115   | -       |
| 14  | CLA  | N     | 830 | 4    | 1/1/15/20 | 9/39/115/115  | -       |
| 14  | CLA  | N     | 820 | 4    | 1/1/15/20 | 9/39/115/115  | -       |
| 14  | CLA  | a     | 836 | 2    | 1/1/15/20 | 13/39/115/115 | -       |
| 17  | BCR  | b     | 850 | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 14  | CLA  | n     | 838 | 4    | 1/1/11/20 | 4/18/94/115   | -       |
| 17  | BCR  | t     | 103 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 17  | BCR  | F     | 203 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 812 | 2    | 1/1/14/20 | 10/33/109/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 14  | CLA  | b     | 816 | 4    | 1/1/11/20 | 4/20/96/115   | -       |
| 14  | CLA  | b     | 829 | 4    | 1/1/15/20 | 10/39/115/115 | -       |
| 19  | CL0  | a     | 851 | 2    | 3/3/20/25 | 10/37/135/135 | -       |
| 14  | CLA  | l     | 204 | -    | 1/1/11/20 | 8/15/91/115   | -       |
| 14  | CLA  | W     | 203 | 12   | 1/1/14/20 | 7/33/109/115  | -       |
| 14  | CLA  | W     | 204 | -    | 1/1/11/20 | 3/15/91/115   | -       |
| 14  | CLA  | w     | 204 | 12   | 1/1/14/20 | 9/33/109/115  | -       |
| 14  | CLA  | A     | 827 | 2    | 1/1/15/20 | 7/39/115/115  | -       |
| 17  | BCR  | a     | 844 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 835 | 2    | 1/1/11/20 | 7/15/91/115   | -       |
| 14  | CLA  | a     | 853 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 14  | CLA  | j     | 102 | 9    | 1/1/8/20  | 2/4/76/115    | -       |
| 17  | BCR  | w     | 207 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 14  | CLA  | g     | 806 | 2    | 1/1/15/20 | 16/39/115/115 | -       |
| 14  | CLA  | g     | 807 | 2    | 1/1/15/20 | 16/39/115/115 | -       |
| 14  | CLA  | n     | 831 | 4    | 1/1/14/20 | 7/33/109/115  | -       |
| 17  | BCR  | b     | 852 | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 806 | 2    | 1/1/13/20 | 9/32/108/115  | -       |
| 17  | BCR  | B     | 848 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | a     | 829 | 2    | 1/1/12/20 | 5/26/102/115  | -       |
| 14  | CLA  | G     | 820 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 14  | CLA  | n     | 822 | -    | 1/1/13/20 | 9/27/103/115  | -       |
| 14  | CLA  | n     | 833 | 4    | 1/1/12/20 | 13/26/102/115 | -       |
| 14  | CLA  | u     | 102 | -    | 1/1/11/20 | 5/20/96/115   | -       |
| 14  | CLA  | G     | 801 | -    | 1/1/15/20 | 8/39/115/115  | -       |
| 18  | LHG  | A     | 850 | -    | -         | 25/53/53/53   | -       |
| 14  | CLA  | N     | 815 | 4    | 1/1/15/20 | 11/39/115/115 | -       |
| 14  | CLA  | B     | 832 | 4    | 1/1/14/20 | 12/33/109/115 | -       |
| 14  | CLA  | N     | 806 | 4    | 1/1/13/20 | 9/27/103/115  | -       |
| 14  | CLA  | a     | 805 | 2    | 1/1/14/20 | 5/33/109/115  | -       |
| 14  | CLA  | B     | 813 | 4    | 1/1/12/20 | 9/26/102/115  | -       |
| 16  | SF4  | a     | 842 | 2,4  | -         | -             | 0/6/5/5 |
| 17  | BCR  | T     | 103 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 17  | BCR  | y     | 101 | -    | -         | 5/29/63/63    | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 14  | CLA  | A     | 857 | -    | 1/1/11/20 | 3/20/96/115   | -       |
| 21  | LMG  | b     | 849 | -    | -         | 21/50/70/70   | 0/1/1/1 |
| 14  | CLA  | f     | 201 | -    | 1/1/13/20 | 8/32/108/115  | -       |
| 17  | BCR  | g     | 843 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | g     | 809 | 2    | 1/1/15/20 | 12/39/115/115 | -       |
| 14  | CLA  | N     | 813 | 4    | 1/1/12/20 | 6/26/102/115  | -       |
| 14  | CLA  | B     | 821 | 4    | 1/1/11/20 | 9/15/91/115   | -       |
| 17  | BCR  | A     | 846 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 822 | 2    | 1/1/12/20 | 9/26/102/115  | -       |
| 17  | BCR  | N     | 845 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | u     | 101 | 10   | 1/1/9/20  | 5/9/81/115    | -       |
| 14  | CLA  | k     | 101 | 10   | 1/1/9/20  | 5/9/81/115    | -       |
| 14  | CLA  | g     | 815 | 2    | 1/1/13/20 | 5/32/108/115  | -       |
| 14  | CLA  | N     | 836 | -    | 1/1/11/20 | 2/15/91/115   | -       |
| 14  | CLA  | n     | 828 | 4    | 1/1/15/20 | 12/39/115/115 | -       |
| 14  | CLA  | G     | 813 | 2    | 1/1/12/20 | 5/26/102/115  | -       |
| 14  | CLA  | n     | 830 | 4    | 1/1/12/20 | 10/26/102/115 | -       |
| 14  | CLA  | b     | 839 | 4    | 1/1/11/20 | 3/18/94/115   | -       |
| 14  | CLA  | N     | 826 | 4    | 1/1/15/20 | 13/39/115/115 | -       |
| 17  | BCR  | u     | 103 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 18  | LHG  | v     | 102 | -    | -         | 27/47/47/53   | -       |
| 17  | BCR  | l     | 206 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 17  | BCR  | n     | 846 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | U     | 101 | 10   | 1/1/9/20  | 7/9/81/115    | -       |
| 14  | CLA  | G     | 831 | 2    | 1/1/15/20 | 11/39/115/115 | -       |
| 14  | CLA  | g     | 818 | 2    | 1/1/12/20 | 7/26/102/115  | -       |
| 21  | LMG  | B     | 802 | -    | -         | 11/30/50/70   | 0/1/1/1 |
| 14  | CLA  | b     | 815 | 4    | 1/1/12/20 | 9/21/97/115   | -       |
| 14  | CLA  | B     | 827 | 4    | 1/1/15/20 | 7/39/115/115  | -       |
| 14  | CLA  | B     | 811 | 4    | 1/1/14/20 | 12/33/109/115 | -       |
| 14  | CLA  | N     | 805 | -    | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CLA  | g     | 827 | 2    | 1/1/15/20 | 11/39/115/115 | -       |
| 14  | CLA  | N     | 829 | 4    | 1/1/15/20 | 8/39/115/115  | -       |
| 17  | BCR  | U     | 103 | -    | -         | 0/29/63/63    | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 17  | BCR  | A     | 847  | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | n     | 825  | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 17  | BCR  | L     | 1504 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 16  | SF4  | C     | 101  | 5    | -         | -             | 0/6/5/5 |
| 14  | CLA  | a     | 810  | 2    | 1/1/13/20 | 9/32/108/115  | -       |
| 14  | CLA  | A     | 828  | 2    | 1/1/15/20 | 8/39/115/115  | -       |
| 17  | BCR  | N     | 846  | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 830  | 2    | 1/1/12/20 | 9/26/102/115  | -       |
| 14  | CLA  | N     | 827  | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 14  | CLA  | a     | 808  | 2    | 1/1/11/20 | 7/15/91/115   | -       |
| 14  | CLA  | G     | 853  | 2    | 1/1/15/20 | 7/39/115/115  | -       |
| 16  | SF4  | p     | 101  | 5    | -         | -             | 0/6/5/5 |
| 14  | CLA  | b     | 826  | -    | 1/1/15/20 | 16/39/115/115 | -       |
| 17  | BCR  | S     | 204  | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 15  | PQN  | B     | 842  | -    | -         | 4/23/43/43    | 0/2/2/2 |
| 14  | CLA  | X     | 1701 | 3    | 1/1/11/20 | 10/20/96/115  | -       |
| 14  | CLA  | G     | 852  | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 14  | CLA  | B     | 841  | 4    | 1/1/15/20 | 16/39/115/115 | -       |
| 14  | CLA  | n     | 815  | 4    | 1/1/11/20 | 6/20/96/115   | -       |
| 14  | CLA  | a     | 815  | 2    | 1/1/13/20 | 8/32/108/115  | -       |
| 14  | CLA  | n     | 810  | 4    | 1/1/14/20 | 16/33/109/115 | -       |
| 17  | BCR  | N     | 847  | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 14  | CLA  | b     | 819  | 4    | 1/1/15/20 | 8/39/115/115  | -       |
| 17  | BCR  | B     | 852  | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 804  | 2    | 1/1/15/20 | 17/39/115/115 | -       |
| 14  | CLA  | n     | 803  | 4    | 1/1/15/20 | 14/39/115/115 | -       |
| 14  | CLA  | A     | 841  | 18   | 1/1/11/20 | 7/15/91/115   | -       |
| 14  | CLA  | B     | 810  | 4    | 1/1/15/20 | 19/39/115/115 | -       |
| 17  | BCR  | G     | 847  | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 17  | BCR  | g     | 846  | -    | -         | 9/29/63/63    | 0/2/2/2 |
| 17  | BCR  | b     | 844  | -    | -         | 6/29/63/63    | 0/2/2/2 |
| 14  | CLA  | B     | 803  | -    | 1/1/15/20 | 13/39/115/115 | -       |
| 19  | CL0  | G     | 851  | 2    | 3/3/20/25 | 9/37/135/135  | -       |
| 14  | CLA  | A     | 838  | 2    | 1/1/15/20 | 13/39/115/115 | -       |
| 17  | BCR  | a     | 845  | -    | -         | 0/29/63/63    | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 14  | CLA  | A     | 810 | 14,2 | 1/1/15/20 | 11/39/115/115 | -       |
| 17  | BCR  | G     | 844 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | b     | 823 | -    | 1/1/13/20 | 13/27/103/115 | -       |
| 14  | CLA  | a     | 819 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 14  | CLA  | J     | 102 | 9    | 1/1/8/20  | 0/4/76/115    | -       |
| 17  | BCR  | N     | 849 | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 14  | CLA  | N     | 832 | 4    | 1/1/12/20 | 6/26/102/115  | -       |
| 16  | SF4  | A     | 843 | 2,4  | -         | -             | 0/6/5/5 |
| 14  | CLA  | A     | 803 | 14,2 | 1/1/12/20 | 8/26/102/115  | -       |
| 21  | LMG  | N     | 802 | -    | -         | 9/30/50/70    | 0/1/1/1 |
| 14  | CLA  | N     | 839 | 4    | 1/1/15/20 | 5/39/115/115  | -       |
| 21  | LMG  | N     | 850 | -    | -         | 15/50/70/70   | 0/1/1/1 |
| 14  | CLA  | a     | 806 | 2    | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CLA  | B     | 807 | 4    | 1/1/15/20 | 14/39/115/115 | -       |
| 14  | CLA  | G     | 824 | -    | 1/1/15/20 | 12/39/115/115 | -       |
| 16  | SF4  | g     | 842 | 2,4  | -         | -             | 0/6/5/5 |
| 15  | PQN  | N     | 843 | -    | -         | 1/23/43/43    | 0/2/2/2 |
| 14  | CLA  | N     | 834 | 4    | 1/1/13/20 | 11/31/107/115 | -       |
| 14  | CLA  | A     | 808 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 14  | CLA  | A     | 853 | -    | 1/1/15/20 | 11/39/115/115 | -       |
| 14  | CLA  | N     | 817 | 4    | 1/1/11/20 | 6/20/96/115   | -       |
| 14  | CLA  | a     | 814 | -    | 1/1/11/20 | 3/15/91/115   | -       |
| 14  | CLA  | n     | 834 | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 14  | CLA  | A     | 813 | 2    | 1/1/12/20 | 6/26/102/115  | -       |
| 14  | CLA  | N     | 822 | 4    | 1/1/11/20 | 7/15/91/115   | -       |
| 14  | CLA  | l     | 203 | 12   | 1/1/14/20 | 9/33/109/115  | -       |
| 14  | CLA  | a     | 837 | 2    | 1/1/15/20 | 12/39/115/115 | -       |
| 14  | CLA  | a     | 831 | 2    | 1/1/15/20 | 7/39/115/115  | -       |
| 14  | CLA  | a     | 812 | 2    | 1/1/12/20 | 7/26/102/115  | -       |
| 17  | BCR  | n     | 842 | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 832 | 2    | 1/1/15/20 | 14/39/115/115 | -       |
| 14  | CLA  | b     | 851 | 4    | 1/1/13/20 | 7/31/107/115  | -       |
| 14  | CLA  | a     | 826 | 2    | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CLA  | W     | 202 | 12   | 1/1/12/20 | 5/23/99/115   | -       |
| 20  | SQD  | w     | 202 | -    | -         | 27/49/69/69   | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|------|------|-----------|---------------|---------|
| 14  | CLA  | n     | 813  | 4    | 1/1/15/20 | 9/39/115/115  | -       |
| 14  | CLA  | a     | 816  | -    | 1/1/14/20 | 10/33/109/115 | -       |
| 17  | BCR  | M     | 101  | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | s     | 202  | -    | 1/1/11/20 | 4/15/91/115   | -       |
| 14  | CLA  | a     | 823  | -    | 1/1/15/20 | 10/39/115/115 | -       |
| 20  | SQD  | H     | 1702 | -    | -         | 23/49/69/69   | 0/1/1/1 |
| 14  | CLA  | b     | 831  | 4    | 1/1/12/20 | 10/26/102/115 | -       |
| 14  | CLA  | a     | 818  | 2    | 1/1/12/20 | 9/26/102/115  | -       |
| 14  | CLA  | b     | 835  | -    | 1/1/11/20 | 4/15/91/115   | -       |
| 14  | CLA  | b     | 836  | -    | 1/1/11/20 | 6/15/91/115   | -       |
| 14  | CLA  | H     | 1701 | 3    | 1/1/11/20 | 10/20/96/115  | -       |
| 14  | CLA  | A     | 834  | 2    | 1/1/12/20 | 6/26/102/115  | -       |
| 14  | CLA  | G     | 816  | 2    | 1/1/13/20 | 10/32/108/115 | -       |
| 14  | CLA  | B     | 837  | 4    | 1/1/14/20 | 11/33/109/115 | -       |
| 14  | CLA  | b     | 833  | 4    | 1/1/15/20 | 13/39/115/115 | -       |
| 14  | CLA  | n     | 840  | 4    | 1/1/15/20 | 15/39/115/115 | -       |
| 17  | BCR  | B     | 845  | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 14  | CLA  | b     | 834  | 4    | 1/1/12/20 | 6/26/102/115  | -       |
| 17  | BCR  | I     | 101  | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 14  | CLA  | A     | 809  | 2    | 1/1/11/20 | 5/15/91/115   | -       |
| 17  | BCR  | a     | 843  | -    | -         | 2/29/63/63    | 0/2/2/2 |
| 14  | CLA  | g     | 819  | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 14  | CLA  | A     | 806  | 2    | 1/1/14/20 | 8/33/109/115  | -       |
| 14  | CLA  | N     | 816  | 4    | 1/1/12/20 | 3/21/97/115   | -       |
| 14  | CLA  | G     | 819  | 2    | 1/1/12/20 | 5/26/102/115  | -       |
| 14  | CLA  | B     | 819  | 4    | 1/1/15/20 | 13/39/115/115 | -       |
| 17  | BCR  | k     | 102  | -    | -         | 0/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 807  | 2    | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CLA  | n     | 829  | 4    | 1/1/15/20 | 9/39/115/115  | -       |
| 14  | CLA  | A     | 817  | 2    | 1/1/14/20 | 11/33/109/115 | -       |
| 14  | CLA  | N     | 811  | 4    | 1/1/15/20 | 13/39/115/115 | -       |
| 14  | CLA  | N     | 819  | 4    | 1/1/15/20 | 12/39/115/115 | -       |
| 14  | CLA  | g     | 820  | 2    | 1/1/11/20 | 7/15/91/115   | -       |
| 14  | CLA  | A     | 818  | 2    | 1/1/15/20 | 16/39/115/115 | -       |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 14  | CLA  | g     | 808 | 2    | 1/1/11/20 | 7/15/91/115   | -       |
| 17  | BCR  | g     | 844 | -    | -         | 1/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 834 | 2    | 1/1/12/20 | 1/26/102/115  | -       |
| 14  | CLA  | A     | 836 | 2    | 1/1/12/20 | 7/23/99/115   | -       |
| 14  | CLA  | a     | 833 | 2    | 1/1/12/20 | 3/26/102/115  | -       |
| 17  | BCR  | b     | 843 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 14  | CLA  | a     | 830 | 2    | 1/1/15/20 | 14/39/115/115 | -       |
| 14  | CLA  | n     | 827 | 4    | 1/1/15/20 | 15/39/115/115 | -       |
| 14  | CLA  | A     | 824 | -    | 1/1/15/20 | 7/39/115/115  | -       |
| 17  | BCR  | m     | 102 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 17  | BCR  | B     | 844 | -    | -         | 11/29/63/63   | 0/2/2/2 |
| 14  | CLA  | G     | 823 | 2    | 1/1/11/20 | 8/15/91/115   | -       |
| 14  | CLA  | b     | 814 | 4    | 1/1/15/20 | 12/39/115/115 | -       |
| 14  | CLA  | b     | 822 | 4    | 1/1/11/20 | 5/15/91/115   | -       |
| 14  | CLA  | B     | 823 | -    | 1/1/13/20 | 10/27/103/115 | -       |
| 17  | BCR  | i     | 101 | -    | -         | 3/29/63/63    | 0/2/2/2 |
| 14  | CLA  | N     | 838 | 4    | 1/1/14/20 | 13/33/109/115 | -       |
| 14  | CLA  | B     | 820 | -    | 1/1/15/20 | 5/39/115/115  | -       |
| 17  | BCR  | b     | 847 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 14  | CLA  | G     | 839 | 2    | 1/1/15/20 | 12/39/115/115 | -       |
| 14  | CLA  | B     | 818 | 4    | 1/1/15/20 | 21/39/115/115 | -       |
| 14  | CLA  | l     | 202 | 12   | 1/1/11/20 | 5/15/91/115   | -       |
| 14  | CLA  | G     | 818 | 2    | 1/1/15/20 | 8/39/115/115  | -       |
| 14  | CLA  | N     | 803 | -    | 1/1/15/20 | 14/39/115/115 | -       |
| 17  | BCR  | a     | 847 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 14  | CLA  | N     | 818 | 4    | 1/1/11/20 | 5/15/91/115   | -       |
| 15  | PQN  | n     | 841 | -    | -         | 2/23/43/43    | 0/2/2/2 |
| 14  | CLA  | a     | 804 | 2    | 1/1/15/20 | 18/39/115/115 | -       |
| 18  | LHG  | g     | 850 | -    | -         | 22/53/53/53   | -       |
| 14  | CLA  | b     | 830 | 4    | 1/1/15/20 | 10/39/115/115 | -       |
| 14  | CLA  | g     | 825 | 2    | 1/1/15/20 | 11/39/115/115 | -       |
| 14  | CLA  | G     | 815 | -    | 1/1/11/20 | 3/15/91/115   | -       |
| 14  | CLA  | N     | 833 | 4    | 1/1/14/20 | 13/33/109/115 | -       |
| 20  | SQD  | n     | 801 | -    | -         | 21/49/69/69   | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals   | Torsions      | Rings   |
|-----|------|-------|-----|------|-----------|---------------|---------|
| 14  | CLA  | B     | 812 | 4    | 1/1/12/20 | 7/26/102/115  | -       |
| 17  | BCR  | l     | 205 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 14  | CLA  | g     | 840 | -    | 1/1/12/20 | 5/21/97/115   | -       |
| 17  | BCR  | I     | 103 | -    | -         | 8/29/63/63    | 0/2/2/2 |
| 14  | CLA  | B     | 806 | 4    | 1/1/15/20 | 13/39/115/115 | -       |
| 14  | CLA  | B     | 816 | 4    | 1/1/11/20 | 6/20/96/115   | -       |
| 14  | CLA  | B     | 824 | 4    | 1/1/15/20 | 13/39/115/115 | -       |
| 14  | CLA  | b     | 825 | 4    | 1/1/15/20 | 7/39/115/115  | -       |
| 17  | BCR  | G     | 846 | -    | -         | 4/29/63/63    | 0/2/2/2 |
| 14  | CLA  | a     | 817 | 2    | 1/1/15/20 | 10/39/115/115 | -       |
| 16  | SF4  | p     | 102 | 5    | -         | -             | 0/6/5/5 |
| 14  | CLA  | a     | 835 | 2    | 1/1/12/20 | 6/23/99/115   | -       |
| 14  | CLA  | G     | 827 | 2    | 1/1/15/20 | 12/39/115/115 | -       |
| 20  | SQD  | b     | 801 | -    | -         | 18/49/69/69   | 0/1/1/1 |
| 14  | CLA  | b     | 840 | -    | 1/1/15/20 | 9/39/115/115  | -       |

All (3314) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 19  | g     | 851 | CL0  | C3B-C4B | 8.63 | 1.49        | 1.41     |
| 19  | a     | 851 | CL0  | C3B-C4B | 8.62 | 1.49        | 1.41     |
| 19  | G     | 851 | CL0  | C3B-C4B | 8.24 | 1.49        | 1.41     |
| 19  | A     | 852 | CL0  | C3B-C4B | 8.12 | 1.49        | 1.41     |
| 19  | g     | 851 | CL0  | C1D-C2D | 8.00 | 1.48        | 1.39     |
| 19  | G     | 851 | CL0  | C1B-C2B | 7.89 | 1.48        | 1.39     |
| 19  | A     | 852 | CL0  | C1B-C2B | 7.87 | 1.48        | 1.39     |
| 19  | g     | 851 | CL0  | C1B-C2B | 7.73 | 1.48        | 1.39     |
| 19  | G     | 851 | CL0  | C1D-C2D | 7.72 | 1.48        | 1.39     |
| 15  | a     | 841 | PQN  | C3-C2   | 7.71 | 1.49        | 1.35     |
| 19  | A     | 852 | CL0  | C1D-C2D | 7.68 | 1.48        | 1.39     |
| 15  | g     | 841 | PQN  | C3-C2   | 7.66 | 1.48        | 1.35     |
| 15  | A     | 842 | PQN  | C3-C2   | 7.65 | 1.48        | 1.35     |
| 15  | N     | 843 | PQN  | C3-C2   | 7.62 | 1.48        | 1.35     |
| 15  | b     | 842 | PQN  | C3-C2   | 7.61 | 1.48        | 1.35     |
| 15  | B     | 842 | PQN  | C3-C2   | 7.61 | 1.48        | 1.35     |
| 15  | G     | 841 | PQN  | C3-C2   | 7.58 | 1.48        | 1.35     |
| 15  | n     | 841 | PQN  | C3-C2   | 7.55 | 1.48        | 1.35     |
| 19  | a     | 851 | CL0  | C1B-C2B | 7.52 | 1.48        | 1.39     |
| 19  | a     | 851 | CL0  | C1D-C2D | 7.52 | 1.48        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 19  | a     | 851  | CL0  | C1A-CHA | 7.40  | 1.48        | 1.40     |
| 19  | A     | 852  | CL0  | C1A-CHA | 7.39  | 1.48        | 1.40     |
| 19  | G     | 851  | CL0  | C1A-CHA | 7.36  | 1.48        | 1.40     |
| 19  | g     | 851  | CL0  | C1A-CHA | 7.18  | 1.48        | 1.40     |
| 19  | a     | 851  | CL0  | O2D-CGD | 5.45  | 1.46        | 1.33     |
| 19  | a     | 851  | CL0  | C3D-C2D | 5.39  | 1.48        | 1.39     |
| 19  | A     | 852  | CL0  | C3D-C2D | 5.35  | 1.48        | 1.39     |
| 19  | G     | 851  | CL0  | C3D-C2D | 5.29  | 1.48        | 1.39     |
| 19  | g     | 851  | CL0  | C3D-C2D | 5.28  | 1.48        | 1.39     |
| 19  | g     | 851  | CL0  | C3B-C2B | 5.25  | 1.47        | 1.40     |
| 19  | a     | 851  | CL0  | C3B-C2B | 5.22  | 1.47        | 1.40     |
| 19  | g     | 851  | CL0  | CHB-C4A | -5.08 | 1.32        | 1.38     |
| 19  | A     | 852  | CL0  | C3B-C2B | 5.02  | 1.47        | 1.40     |
| 19  | G     | 851  | CL0  | O2D-CGD | 5.00  | 1.45        | 1.33     |
| 15  | N     | 843  | PQN  | C10-C5  | 4.98  | 1.48        | 1.40     |
| 15  | B     | 842  | PQN  | C10-C5  | 4.98  | 1.48        | 1.40     |
| 19  | g     | 851  | CL0  | OBD-CAD | 4.97  | 1.28        | 1.22     |
| 15  | G     | 841  | PQN  | C10-C5  | 4.97  | 1.48        | 1.40     |
| 19  | A     | 852  | CL0  | O2D-CGD | 4.95  | 1.45        | 1.33     |
| 19  | G     | 851  | CL0  | C3B-C2B | 4.94  | 1.47        | 1.40     |
| 19  | A     | 852  | CL0  | CHB-C4A | -4.94 | 1.32        | 1.38     |
| 15  | A     | 842  | PQN  | C10-C5  | 4.94  | 1.48        | 1.40     |
| 19  | G     | 851  | CL0  | OBD-CAD | 4.92  | 1.28        | 1.22     |
| 15  | a     | 841  | PQN  | C10-C5  | 4.91  | 1.48        | 1.40     |
| 15  | g     | 841  | PQN  | C10-C5  | 4.89  | 1.48        | 1.40     |
| 19  | A     | 852  | CL0  | OBD-CAD | 4.88  | 1.28        | 1.22     |
| 19  | g     | 851  | CL0  | O2D-CGD | 4.87  | 1.45        | 1.33     |
| 15  | n     | 841  | PQN  | C10-C5  | 4.86  | 1.48        | 1.40     |
| 15  | b     | 842  | PQN  | C10-C5  | 4.86  | 1.48        | 1.40     |
| 19  | a     | 851  | CL0  | OBD-CAD | 4.84  | 1.28        | 1.22     |
| 19  | G     | 851  | CL0  | CHB-C4A | -4.81 | 1.32        | 1.38     |
| 20  | b     | 801  | SQD  | O48-C23 | 4.72  | 1.47        | 1.33     |
| 20  | n     | 801  | SQD  | O48-C23 | 4.68  | 1.47        | 1.33     |
| 20  | l     | 201  | SQD  | O48-C23 | 4.68  | 1.47        | 1.33     |
| 20  | h     | 1702 | SQD  | O48-C23 | 4.68  | 1.47        | 1.33     |
| 20  | H     | 1702 | SQD  | O48-C23 | 4.67  | 1.47        | 1.33     |
| 20  | w     | 202  | SQD  | O48-C23 | 4.66  | 1.46        | 1.33     |
| 19  | a     | 851  | CL0  | CHC-C4B | 4.66  | 1.47        | 1.39     |
| 20  | x     | 1702 | SQD  | O48-C23 | 4.66  | 1.46        | 1.33     |
| 20  | B     | 801  | SQD  | O48-C23 | 4.64  | 1.46        | 1.33     |
| 19  | A     | 852  | CL0  | C3A-C2A | -4.62 | 1.50        | 1.54     |
| 19  | g     | 851  | CL0  | C3A-C2A | -4.60 | 1.50        | 1.54     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 19  | a     | 851  | CL0  | CHB-C4A | -4.54 | 1.33        | 1.38     |
| 19  | A     | 852  | CL0  | O2A-CGA | 4.49  | 1.45        | 1.30     |
| 19  | G     | 851  | CL0  | C3A-C2A | -4.48 | 1.50        | 1.54     |
| 19  | A     | 852  | CL0  | CHC-C4B | 4.48  | 1.46        | 1.39     |
| 19  | a     | 851  | CL0  | CHB-C1B | 4.46  | 1.46        | 1.39     |
| 19  | G     | 851  | CL0  | CHC-C4B | 4.39  | 1.46        | 1.39     |
| 19  | a     | 851  | CL0  | C3A-C2A | -4.39 | 1.50        | 1.54     |
| 19  | g     | 851  | CL0  | CHC-C4B | 4.35  | 1.46        | 1.39     |
| 19  | g     | 851  | CL0  | O2A-CGA | 4.23  | 1.45        | 1.33     |
| 19  | G     | 851  | CL0  | CHB-C1B | 4.23  | 1.46        | 1.39     |
| 19  | g     | 851  | CL0  | CHB-C1B | 4.20  | 1.46        | 1.39     |
| 19  | a     | 851  | CL0  | O2A-CGA | 4.19  | 1.45        | 1.33     |
| 19  | a     | 851  | CL0  | CHD-C1D | 4.18  | 1.46        | 1.39     |
| 19  | A     | 852  | CL0  | CHB-C1B | 4.16  | 1.46        | 1.39     |
| 19  | g     | 851  | CL0  | CHD-C4C | 4.16  | 1.47        | 1.39     |
| 19  | G     | 851  | CL0  | O2A-CGA | 4.16  | 1.45        | 1.33     |
| 19  | a     | 851  | CL0  | CHD-C4C | 4.09  | 1.47        | 1.39     |
| 14  | A     | 826  | CLA  | C1D-ND  | 4.04  | 1.43        | 1.37     |
| 19  | a     | 851  | CL0  | CHC-C1C | 4.04  | 1.47        | 1.39     |
| 19  | G     | 851  | CL0  | CHD-C4C | 4.03  | 1.47        | 1.39     |
| 19  | A     | 852  | CL0  | CHD-C1D | 4.03  | 1.46        | 1.39     |
| 19  | g     | 851  | CL0  | CHD-C1D | 4.02  | 1.46        | 1.39     |
| 19  | G     | 851  | CL0  | CHD-C1D | 4.02  | 1.46        | 1.39     |
| 19  | A     | 852  | CL0  | CHD-C4C | 4.00  | 1.47        | 1.39     |
| 19  | A     | 852  | CL0  | CHC-C1C | 3.95  | 1.46        | 1.39     |
| 19  | G     | 851  | CL0  | CHC-C1C | 3.83  | 1.46        | 1.39     |
| 19  | g     | 851  | CL0  | CHC-C1C | 3.80  | 1.46        | 1.39     |
| 20  | w     | 202  | SQD  | O47-C45 | -3.75 | 1.37        | 1.46     |
| 20  | h     | 1702 | SQD  | O47-C45 | -3.74 | 1.37        | 1.46     |
| 20  | n     | 801  | SQD  | O47-C45 | -3.74 | 1.37        | 1.46     |
| 20  | B     | 801  | SQD  | O47-C45 | -3.70 | 1.37        | 1.46     |
| 20  | l     | 201  | SQD  | O47-C45 | -3.70 | 1.37        | 1.46     |
| 20  | b     | 801  | SQD  | O47-C45 | -3.69 | 1.37        | 1.46     |
| 20  | H     | 1702 | SQD  | O47-C45 | -3.68 | 1.37        | 1.46     |
| 20  | x     | 1702 | SQD  | O47-C45 | -3.68 | 1.37        | 1.46     |
| 14  | j     | 101  | CLA  | C1D-ND  | 3.67  | 1.42        | 1.37     |
| 14  | t     | 102  | CLA  | C1D-ND  | 3.64  | 1.42        | 1.37     |
| 14  | A     | 838  | CLA  | C1D-ND  | 3.62  | 1.42        | 1.37     |
| 14  | N     | 828  | CLA  | C1D-ND  | 3.61  | 1.42        | 1.37     |
| 14  | g     | 853  | CLA  | C1D-ND  | 3.61  | 1.42        | 1.37     |
| 14  | u     | 102  | CLA  | C1D-ND  | 3.60  | 1.42        | 1.37     |
| 14  | J     | 101  | CLA  | C1D-ND  | 3.60  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14  | k     | 101  | CLA  | C1D-ND | 3.60 | 1.42        | 1.37     |
| 14  | g     | 812  | CLA  | C1D-ND | 3.59 | 1.42        | 1.37     |
| 14  | h     | 1701 | CLA  | C1D-ND | 3.58 | 1.42        | 1.37     |
| 14  | f     | 202  | CLA  | C1D-ND | 3.58 | 1.42        | 1.37     |
| 14  | a     | 832  | CLA  | C1D-ND | 3.58 | 1.42        | 1.37     |
| 14  | n     | 826  | CLA  | C1D-ND | 3.58 | 1.42        | 1.37     |
| 14  | g     | 805  | CLA  | C1D-ND | 3.57 | 1.42        | 1.37     |
| 14  | n     | 820  | CLA  | C1D-ND | 3.57 | 1.42        | 1.37     |
| 14  | G     | 823  | CLA  | C1D-ND | 3.57 | 1.42        | 1.37     |
| 14  | n     | 821  | CLA  | C1D-ND | 3.57 | 1.42        | 1.37     |
| 14  | A     | 820  | CLA  | C1D-ND | 3.57 | 1.42        | 1.37     |
| 14  | g     | 818  | CLA  | C1D-ND | 3.57 | 1.42        | 1.37     |
| 14  | A     | 825  | CLA  | C1D-ND | 3.57 | 1.42        | 1.37     |
| 14  | A     | 836  | CLA  | C1D-ND | 3.57 | 1.42        | 1.37     |
| 14  | b     | 827  | CLA  | C1D-ND | 3.57 | 1.42        | 1.37     |
| 14  | T     | 101  | CLA  | C1D-ND | 3.57 | 1.42        | 1.37     |
| 14  | n     | 835  | CLA  | C1D-ND | 3.57 | 1.42        | 1.37     |
| 14  | G     | 840  | CLA  | C1D-ND | 3.57 | 1.42        | 1.37     |
| 14  | N     | 823  | CLA  | C1D-ND | 3.57 | 1.42        | 1.37     |
| 14  | K     | 101  | CLA  | C1D-ND | 3.57 | 1.42        | 1.37     |
| 14  | A     | 815  | CLA  | C1D-ND | 3.57 | 1.42        | 1.37     |
| 14  | b     | 822  | CLA  | C1D-ND | 3.56 | 1.42        | 1.37     |
| 14  | s     | 202  | CLA  | C1D-ND | 3.56 | 1.42        | 1.37     |
| 14  | A     | 832  | CLA  | C1D-ND | 3.56 | 1.42        | 1.37     |
| 14  | a     | 826  | CLA  | C1D-ND | 3.56 | 1.42        | 1.37     |
| 14  | B     | 818  | CLA  | C1D-ND | 3.56 | 1.42        | 1.37     |
| 14  | b     | 823  | CLA  | C1D-ND | 3.56 | 1.42        | 1.37     |
| 14  | N     | 830  | CLA  | C1D-ND | 3.56 | 1.42        | 1.37     |
| 14  | G     | 822  | CLA  | C1D-ND | 3.56 | 1.42        | 1.37     |
| 14  | A     | 802  | CLA  | C1D-ND | 3.56 | 1.42        | 1.37     |
| 14  | G     | 811  | CLA  | C1D-ND | 3.55 | 1.42        | 1.37     |
| 14  | b     | 828  | CLA  | C1D-ND | 3.55 | 1.42        | 1.37     |
| 14  | b     | 837  | CLA  | C1D-ND | 3.55 | 1.42        | 1.37     |
| 14  | j     | 102  | CLA  | C1D-ND | 3.55 | 1.42        | 1.37     |
| 14  | B     | 810  | CLA  | C1D-ND | 3.54 | 1.42        | 1.37     |
| 14  | a     | 814  | CLA  | C1D-ND | 3.54 | 1.42        | 1.37     |
| 14  | S     | 203  | CLA  | C1D-ND | 3.54 | 1.42        | 1.37     |
| 14  | n     | 828  | CLA  | C1D-ND | 3.54 | 1.42        | 1.37     |
| 14  | U     | 102  | CLA  | C1D-ND | 3.54 | 1.42        | 1.37     |
| 14  | B     | 813  | CLA  | C1D-ND | 3.54 | 1.42        | 1.37     |
| 14  | u     | 101  | CLA  | C1D-ND | 3.54 | 1.42        | 1.37     |
| 14  | U     | 101  | CLA  | C1D-ND | 3.54 | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14  | T     | 102  | CLA  | C1D-ND | 3.54 | 1.42        | 1.37     |
| 14  | A     | 814  | CLA  | C1D-ND | 3.54 | 1.42        | 1.37     |
| 14  | A     | 839  | CLA  | C1D-ND | 3.54 | 1.42        | 1.37     |
| 14  | N     | 827  | CLA  | C1D-ND | 3.54 | 1.42        | 1.37     |
| 14  | N     | 813  | CLA  | C1D-ND | 3.53 | 1.42        | 1.37     |
| 14  | N     | 814  | CLA  | C1D-ND | 3.53 | 1.42        | 1.37     |
| 14  | g     | 811  | CLA  | C1D-ND | 3.53 | 1.42        | 1.37     |
| 14  | A     | 823  | CLA  | C1D-ND | 3.53 | 1.42        | 1.37     |
| 14  | B     | 841  | CLA  | C1D-ND | 3.53 | 1.42        | 1.37     |
| 14  | g     | 814  | CLA  | C1D-ND | 3.53 | 1.42        | 1.37     |
| 14  | A     | 801  | CLA  | C1D-ND | 3.53 | 1.42        | 1.37     |
| 14  | n     | 827  | CLA  | C1D-ND | 3.53 | 1.42        | 1.37     |
| 14  | a     | 805  | CLA  | C1D-ND | 3.53 | 1.42        | 1.37     |
| 14  | a     | 840  | CLA  | C1D-ND | 3.53 | 1.42        | 1.37     |
| 14  | g     | 834  | CLA  | C1D-ND | 3.53 | 1.42        | 1.37     |
| 14  | X     | 1701 | CLA  | C1D-ND | 3.53 | 1.42        | 1.37     |
| 14  | a     | 834  | CLA  | C1D-ND | 3.53 | 1.42        | 1.37     |
| 14  | n     | 815  | CLA  | C1D-ND | 3.53 | 1.42        | 1.37     |
| 14  | b     | 832  | CLA  | C1D-ND | 3.53 | 1.42        | 1.37     |
| 14  | G     | 836  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | g     | 820  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | B     | 827  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | F     | 202  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | A     | 806  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | B     | 822  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | G     | 815  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | g     | 816  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | B     | 807  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | G     | 805  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | G     | 818  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | B     | 839  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | G     | 839  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | g     | 825  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | A     | 830  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | a     | 825  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | n     | 831  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | g     | 817  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | n     | 823  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | g     | 826  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | n     | 833  | CLA  | C1D-ND | 3.52 | 1.42        | 1.37     |
| 14  | L     | 1501 | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | a     | 822  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14  | A     | 821  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | g     | 801  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | n     | 812  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | G     | 825  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | n     | 838  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | B     | 819  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | N     | 833  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | a     | 808  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | b     | 853  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | b     | 841  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | G     | 806  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | A     | 812  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | G     | 835  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | N     | 815  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | n     | 824  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | A     | 824  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | N     | 817  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | A     | 857  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | F     | 201  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | b     | 840  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | g     | 807  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | A     | 811  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | b     | 821  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | b     | 836  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | b     | 839  | CLA  | C1D-ND | 3.51 | 1.42        | 1.37     |
| 14  | n     | 808  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | w     | 205  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | N     | 822  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | N     | 842  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | g     | 832  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | a     | 829  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | x     | 1701 | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | g     | 829  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | g     | 838  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | n     | 836  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | a     | 854  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | N     | 825  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | n     | 840  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | A     | 808  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | A     | 816  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | B     | 825  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | A     | 833  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14  | A     | 835  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | J     | 102  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | a     | 812  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | G     | 814  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | n     | 830  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | A     | 819  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | l     | 204  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | g     | 837  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | G     | 803  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | g     | 808  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | n     | 811  | CLA  | C1D-ND | 3.50 | 1.42        | 1.37     |
| 14  | N     | 840  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | A     | 841  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | B     | 823  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | a     | 837  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | G     | 821  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | G     | 812  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | B     | 809  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | b     | 813  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | B     | 820  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | B     | 834  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | G     | 827  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | H     | 1701 | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | A     | 813  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | G     | 837  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | A     | 817  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | b     | 819  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | g     | 802  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | N     | 810  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | l     | 202  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | n     | 834  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | G     | 801  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | n     | 806  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | n     | 816  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | B     | 836  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | a     | 801  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | n     | 832  | CLA  | C1D-ND | 3.49 | 1.42        | 1.37     |
| 14  | G     | 832  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | t     | 101  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | A     | 810  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | G     | 819  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | a     | 811  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14  | N     | 824  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | w     | 203  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | a     | 810  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | a     | 816  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | b     | 816  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | b     | 802  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | b     | 808  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | a     | 835  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | A     | 837  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | n     | 814  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | N     | 811  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | g     | 835  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | n     | 822  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | B     | 837  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | b     | 807  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | N     | 819  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | b     | 817  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | B     | 812  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | a     | 809  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | b     | 811  | CLA  | C1D-ND | 3.48 | 1.42        | 1.37     |
| 14  | N     | 836  | CLA  | C1D-ND | 3.47 | 1.42        | 1.37     |
| 14  | b     | 831  | CLA  | C1D-ND | 3.47 | 1.42        | 1.37     |
| 14  | n     | 825  | CLA  | C1D-ND | 3.47 | 1.42        | 1.37     |
| 14  | a     | 819  | CLA  | C1D-ND | 3.47 | 1.42        | 1.37     |
| 14  | b     | 824  | CLA  | C1D-ND | 3.47 | 1.42        | 1.37     |
| 14  | G     | 810  | CLA  | C1D-ND | 3.47 | 1.42        | 1.37     |
| 14  | A     | 807  | CLA  | C1D-ND | 3.47 | 1.42        | 1.37     |
| 14  | n     | 813  | CLA  | C1D-ND | 3.47 | 1.42        | 1.37     |
| 14  | B     | 826  | CLA  | C1D-ND | 3.47 | 1.42        | 1.37     |
| 14  | L     | 1503 | CLA  | C1D-ND | 3.47 | 1.42        | 1.37     |
| 14  | a     | 813  | CLA  | C1D-ND | 3.47 | 1.42        | 1.37     |
| 14  | g     | 821  | CLA  | C1D-ND | 3.47 | 1.42        | 1.37     |
| 14  | G     | 813  | CLA  | C1D-ND | 3.47 | 1.42        | 1.37     |
| 14  | b     | 825  | CLA  | C1D-ND | 3.47 | 1.42        | 1.37     |
| 14  | G     | 838  | CLA  | C1D-ND | 3.47 | 1.42        | 1.37     |
| 14  | N     | 829  | CLA  | C1D-ND | 3.47 | 1.42        | 1.37     |
| 14  | B     | 805  | CLA  | C1D-ND | 3.47 | 1.42        | 1.37     |
| 14  | a     | 821  | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | B     | 850  | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | a     | 828  | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | a     | 803  | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | G     | 817  | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 14  | b     | 829 | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | a     | 802 | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | a     | 817 | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | a     | 853 | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | g     | 815 | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | g     | 831 | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | n     | 818 | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | W     | 204 | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | s     | 201 | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | n     | 810 | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | n     | 819 | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | G     | 830 | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | a     | 836 | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | b     | 833 | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | N     | 837 | CLA  | C1D-ND | 3.46 | 1.42        | 1.37     |
| 14  | G     | 833 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | g     | 813 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | A     | 822 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | A     | 831 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | a     | 839 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | N     | 851 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | A     | 805 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | B     | 840 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | b     | 806 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | A     | 829 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | S     | 201 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | a     | 815 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | a     | 820 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | G     | 809 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | g     | 806 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | g     | 822 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | B     | 831 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | b     | 815 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | N     | 816 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | A     | 827 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | B     | 833 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | g     | 823 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | A     | 854 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | A     | 818 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | a     | 824 | CLA  | C1D-ND | 3.45 | 1.42        | 1.37     |
| 14  | b     | 814 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | b     | 835 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 14  | g     | 840 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | g     | 824 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | A     | 828 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | W     | 202 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | a     | 831 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | N     | 821 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | n     | 839 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | B     | 808 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | G     | 834 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | N     | 838 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | G     | 820 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | g     | 828 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | A     | 809 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | b     | 818 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | A     | 803 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | B     | 817 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | b     | 851 | CLA  | C1D-ND | 3.44 | 1.42        | 1.37     |
| 14  | N     | 809 | CLA  | C1D-ND | 3.43 | 1.42        | 1.37     |
| 14  | N     | 818 | CLA  | C1D-ND | 3.43 | 1.42        | 1.37     |
| 14  | g     | 810 | CLA  | C1D-ND | 3.43 | 1.42        | 1.37     |
| 14  | b     | 809 | CLA  | C1D-ND | 3.43 | 1.42        | 1.37     |
| 14  | b     | 834 | CLA  | C1D-ND | 3.43 | 1.42        | 1.37     |
| 14  | G     | 807 | CLA  | C1D-ND | 3.43 | 1.42        | 1.37     |
| 14  | g     | 804 | CLA  | C1D-ND | 3.43 | 1.42        | 1.37     |
| 14  | B     | 816 | CLA  | C1D-ND | 3.43 | 1.42        | 1.37     |
| 14  | n     | 837 | CLA  | C1D-ND | 3.43 | 1.42        | 1.37     |
| 14  | B     | 835 | CLA  | C1D-ND | 3.43 | 1.42        | 1.37     |
| 14  | B     | 806 | CLA  | C1D-ND | 3.43 | 1.42        | 1.37     |
| 14  | N     | 841 | CLA  | C1D-ND | 3.43 | 1.42        | 1.37     |
| 14  | A     | 804 | CLA  | C1D-ND | 3.43 | 1.42        | 1.37     |
| 14  | a     | 823 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |
| 14  | n     | 805 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |
| 14  | a     | 806 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |
| 14  | g     | 833 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |
| 14  | G     | 804 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |
| 14  | B     | 804 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |
| 14  | b     | 820 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |
| 14  | g     | 836 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |
| 14  | B     | 815 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |
| 14  | N     | 808 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |
| 14  | g     | 819 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |
| 14  | g     | 830 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 14  | B     | 829 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |
| 14  | n     | 850 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |
| 14  | a     | 827 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |
| 14  | N     | 812 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |
| 14  | B     | 838 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |
| 14  | a     | 833 | CLA  | C1D-ND | 3.42 | 1.42        | 1.37     |
| 14  | G     | 808 | CLA  | C1D-ND | 3.41 | 1.42        | 1.37     |
| 14  | n     | 852 | CLA  | C1D-ND | 3.41 | 1.42        | 1.37     |
| 14  | b     | 810 | CLA  | C1D-ND | 3.41 | 1.42        | 1.37     |
| 14  | g     | 809 | CLA  | C1D-ND | 3.41 | 1.42        | 1.37     |
| 14  | B     | 821 | CLA  | C1D-ND | 3.41 | 1.42        | 1.37     |
| 14  | b     | 838 | CLA  | C1D-ND | 3.41 | 1.42        | 1.37     |
| 14  | N     | 831 | CLA  | C1D-ND | 3.41 | 1.42        | 1.37     |
| 14  | B     | 824 | CLA  | C1D-ND | 3.41 | 1.42        | 1.37     |
| 14  | B     | 814 | CLA  | C1D-ND | 3.41 | 1.42        | 1.37     |
| 14  | f     | 201 | CLA  | C1D-ND | 3.41 | 1.42        | 1.37     |
| 14  | B     | 828 | CLA  | C1D-ND | 3.41 | 1.42        | 1.37     |
| 14  | G     | 831 | CLA  | C1D-ND | 3.41 | 1.42        | 1.37     |
| 14  | a     | 830 | CLA  | C1D-ND | 3.41 | 1.42        | 1.37     |
| 14  | N     | 807 | CLA  | C1D-ND | 3.40 | 1.42        | 1.37     |
| 14  | N     | 801 | CLA  | C1D-ND | 3.40 | 1.42        | 1.37     |
| 14  | n     | 817 | CLA  | C1D-ND | 3.40 | 1.42        | 1.37     |
| 14  | b     | 804 | CLA  | C1D-ND | 3.40 | 1.42        | 1.37     |
| 14  | G     | 802 | CLA  | C1D-ND | 3.40 | 1.42        | 1.37     |
| 14  | g     | 854 | CLA  | C1D-ND | 3.40 | 1.42        | 1.37     |
| 14  | b     | 826 | CLA  | C1D-ND | 3.40 | 1.42        | 1.37     |
| 14  | N     | 835 | CLA  | C1D-ND | 3.40 | 1.42        | 1.37     |
| 14  | a     | 804 | CLA  | C1D-ND | 3.40 | 1.42        | 1.37     |
| 14  | N     | 820 | CLA  | C1D-ND | 3.39 | 1.42        | 1.37     |
| 14  | B     | 811 | CLA  | C1D-ND | 3.39 | 1.42        | 1.37     |
| 14  | B     | 832 | CLA  | C1D-ND | 3.39 | 1.42        | 1.37     |
| 14  | g     | 827 | CLA  | C1D-ND | 3.39 | 1.42        | 1.37     |
| 14  | n     | 809 | CLA  | C1D-ND | 3.39 | 1.42        | 1.37     |
| 14  | b     | 812 | CLA  | C1D-ND | 3.39 | 1.42        | 1.37     |
| 14  | N     | 806 | CLA  | C1D-ND | 3.39 | 1.42        | 1.37     |
| 14  | G     | 816 | CLA  | C1D-ND | 3.39 | 1.42        | 1.37     |
| 14  | n     | 807 | CLA  | C1D-ND | 3.38 | 1.42        | 1.37     |
| 14  | g     | 803 | CLA  | C1D-ND | 3.38 | 1.42        | 1.37     |
| 14  | N     | 839 | CLA  | C1D-ND | 3.38 | 1.42        | 1.37     |
| 14  | a     | 807 | CLA  | C1D-ND | 3.38 | 1.42        | 1.37     |
| 14  | g     | 839 | CLA  | C1D-ND | 3.38 | 1.42        | 1.37     |
| 14  | G     | 853 | CLA  | C1D-ND | 3.38 | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 828  | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 14  | N     | 832  | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 14  | n     | 804  | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 14  | G     | 826  | CLA  | C1D-ND  | 3.37  | 1.42        | 1.37     |
| 14  | N     | 826  | CLA  | C1D-ND  | 3.36  | 1.42        | 1.37     |
| 14  | A     | 834  | CLA  | C1D-ND  | 3.36  | 1.42        | 1.37     |
| 14  | n     | 803  | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 14  | G     | 829  | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 14  | a     | 838  | CLA  | C1D-ND  | 3.35  | 1.42        | 1.37     |
| 14  | N     | 804  | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |
| 14  | l     | 203  | CLA  | C1D-ND  | 3.34  | 1.42        | 1.37     |
| 14  | n     | 829  | CLA  | C1D-ND  | 3.33  | 1.42        | 1.37     |
| 20  | h     | 1702 | SQD  | O5-C1   | 3.33  | 1.50        | 1.41     |
| 14  | B     | 830  | CLA  | C1D-ND  | 3.33  | 1.42        | 1.37     |
| 20  | w     | 202  | SQD  | O47-C7  | 3.33  | 1.43        | 1.34     |
| 14  | a     | 818  | CLA  | C1D-ND  | 3.32  | 1.42        | 1.37     |
| 20  | w     | 202  | SQD  | O5-C1   | 3.31  | 1.50        | 1.41     |
| 20  | b     | 801  | SQD  | O5-C1   | 3.31  | 1.50        | 1.41     |
| 14  | L     | 1502 | CLA  | C1D-ND  | 3.31  | 1.42        | 1.37     |
| 14  | B     | 803  | CLA  | C1D-ND  | 3.31  | 1.42        | 1.37     |
| 14  | b     | 803  | CLA  | C1D-ND  | 3.30  | 1.42        | 1.37     |
| 20  | l     | 201  | SQD  | O5-C1   | 3.30  | 1.50        | 1.41     |
| 14  | b     | 830  | CLA  | C1D-ND  | 3.30  | 1.42        | 1.37     |
| 14  | A     | 853  | CLA  | C1D-ND  | 3.29  | 1.42        | 1.37     |
| 20  | b     | 801  | SQD  | O47-C7  | 3.29  | 1.43        | 1.34     |
| 20  | H     | 1702 | SQD  | O47-C7  | 3.29  | 1.43        | 1.34     |
| 20  | x     | 1702 | SQD  | O5-C1   | 3.29  | 1.50        | 1.41     |
| 14  | A     | 840  | CLA  | C1D-ND  | 3.29  | 1.42        | 1.37     |
| 20  | n     | 801  | SQD  | O47-C7  | 3.28  | 1.43        | 1.34     |
| 14  | W     | 203  | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 14  | b     | 805  | CLA  | C1D-ND  | 3.27  | 1.42        | 1.37     |
| 20  | l     | 201  | SQD  | O47-C7  | 3.26  | 1.43        | 1.34     |
| 20  | n     | 801  | SQD  | O5-C1   | 3.26  | 1.50        | 1.41     |
| 18  | A     | 850  | LHG  | C26-C25 | -3.25 | 1.35        | 1.51     |
| 18  | a     | 850  | LHG  | C26-C25 | -3.25 | 1.35        | 1.51     |
| 14  | G     | 824  | CLA  | C1D-ND  | 3.25  | 1.42        | 1.37     |
| 18  | a     | 849  | LHG  | C26-C25 | -3.25 | 1.35        | 1.51     |
| 18  | G     | 850  | LHG  | C26-C25 | -3.25 | 1.35        | 1.51     |
| 20  | x     | 1702 | SQD  | O47-C7  | 3.24  | 1.43        | 1.34     |
| 14  | n     | 802  | CLA  | C1D-ND  | 3.24  | 1.42        | 1.37     |
| 14  | A     | 801  | CLA  | C4B-NB  | 3.24  | 1.42        | 1.37     |
| 14  | N     | 803  | CLA  | C1D-ND  | 3.24  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | A     | 851  | LHG  | C26-C25 | -3.24 | 1.35        | 1.51     |
| 20  | B     | 801  | SQD  | O5-C1   | 3.24  | 1.50        | 1.41     |
| 18  | g     | 849  | LHG  | C26-C25 | -3.23 | 1.35        | 1.51     |
| 18  | g     | 850  | LHG  | C26-C25 | -3.23 | 1.35        | 1.51     |
| 14  | G     | 815  | CLA  | C4B-NB  | 3.23  | 1.42        | 1.37     |
| 18  | G     | 849  | LHG  | C26-C25 | -3.22 | 1.35        | 1.51     |
| 14  | N     | 805  | CLA  | C1D-ND  | 3.21  | 1.42        | 1.37     |
| 14  | B     | 804  | CLA  | C4B-NB  | 3.21  | 1.42        | 1.37     |
| 18  | X     | 1702 | LHG  | C26-C25 | -3.21 | 1.35        | 1.51     |
| 18  | S     | 202  | LHG  | C26-C25 | -3.21 | 1.35        | 1.51     |
| 14  | b     | 833  | CLA  | C4B-NB  | 3.21  | 1.42        | 1.37     |
| 20  | H     | 1702 | SQD  | O5-C1   | 3.20  | 1.50        | 1.41     |
| 20  | B     | 801  | SQD  | O47-C7  | 3.20  | 1.43        | 1.34     |
| 18  | v     | 102  | LHG  | C26-C25 | -3.19 | 1.35        | 1.51     |
| 18  | m     | 101  | LHG  | C26-C25 | -3.19 | 1.35        | 1.51     |
| 14  | g     | 805  | CLA  | C4B-NB  | 3.19  | 1.42        | 1.37     |
| 14  | A     | 805  | CLA  | C4B-NB  | 3.19  | 1.42        | 1.37     |
| 20  | h     | 1702 | SQD  | O47-C7  | 3.19  | 1.43        | 1.34     |
| 14  | A     | 836  | CLA  | C4B-NB  | 3.19  | 1.42        | 1.37     |
| 14  | b     | 802  | CLA  | C4B-NB  | 3.18  | 1.42        | 1.37     |
| 14  | A     | 820  | CLA  | C4B-NB  | 3.18  | 1.42        | 1.37     |
| 14  | B     | 850  | CLA  | C4B-NB  | 3.18  | 1.42        | 1.37     |
| 14  | w     | 204  | CLA  | C1D-ND  | 3.18  | 1.42        | 1.37     |
| 14  | N     | 821  | CLA  | C4B-NB  | 3.18  | 1.42        | 1.37     |
| 14  | n     | 832  | CLA  | C4B-NB  | 3.17  | 1.42        | 1.37     |
| 14  | A     | 806  | CLA  | C4B-NB  | 3.16  | 1.42        | 1.37     |
| 14  | N     | 837  | CLA  | C4B-NB  | 3.15  | 1.42        | 1.37     |
| 14  | g     | 819  | CLA  | C4B-NB  | 3.15  | 1.42        | 1.37     |
| 14  | a     | 837  | CLA  | C4B-NB  | 3.14  | 1.42        | 1.37     |
| 14  | g     | 810  | CLA  | C4B-NB  | 3.14  | 1.42        | 1.37     |
| 14  | A     | 812  | CLA  | C4B-NB  | 3.14  | 1.42        | 1.37     |
| 14  | b     | 823  | CLA  | C4B-NB  | 3.14  | 1.42        | 1.37     |
| 14  | N     | 851  | CLA  | C4B-NB  | 3.14  | 1.42        | 1.37     |
| 14  | B     | 839  | CLA  | C4B-NB  | 3.13  | 1.42        | 1.37     |
| 14  | b     | 824  | CLA  | C4B-NB  | 3.13  | 1.42        | 1.37     |
| 14  | g     | 854  | CLA  | C4B-NB  | 3.13  | 1.42        | 1.37     |
| 14  | K     | 101  | CLA  | C4B-NB  | 3.13  | 1.42        | 1.37     |
| 14  | G     | 806  | CLA  | C4B-NB  | 3.13  | 1.42        | 1.37     |
| 14  | n     | 816  | CLA  | C4B-NB  | 3.13  | 1.42        | 1.37     |
| 14  | A     | 853  | CLA  | C4B-NB  | 3.13  | 1.42        | 1.37     |
| 14  | a     | 853  | CLA  | C4B-NB  | 3.13  | 1.42        | 1.37     |
| 14  | A     | 833  | CLA  | C4B-NB  | 3.12  | 1.42        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | h     | 1701 | CLA  | C4B-NB  | 3.12 | 1.42        | 1.37     |
| 14  | B     | 813  | CLA  | C4B-NB  | 3.12 | 1.42        | 1.37     |
| 14  | b     | 812  | CLA  | C4B-NB  | 3.12 | 1.42        | 1.37     |
| 14  | n     | 834  | CLA  | C4B-NB  | 3.12 | 1.42        | 1.37     |
| 14  | N     | 801  | CLA  | C4B-NB  | 3.12 | 1.42        | 1.37     |
| 14  | G     | 852  | CLA  | C1D-ND  | 3.11 | 1.42        | 1.37     |
| 14  | N     | 840  | CLA  | C4B-NB  | 3.11 | 1.42        | 1.37     |
| 14  | X     | 1701 | CLA  | C4B-NB  | 3.11 | 1.42        | 1.37     |
| 14  | g     | 809  | CLA  | C4B-NB  | 3.11 | 1.41        | 1.37     |
| 14  | a     | 805  | CLA  | C4B-NB  | 3.11 | 1.41        | 1.37     |
| 14  | T     | 101  | CLA  | C4B-NB  | 3.11 | 1.41        | 1.37     |
| 20  | n     | 801  | SQD  | C24-C23 | 3.11 | 1.59        | 1.50     |
| 14  | n     | 835  | CLA  | C4B-NB  | 3.11 | 1.41        | 1.37     |
| 14  | s     | 202  | CLA  | C4B-NB  | 3.11 | 1.41        | 1.37     |
| 14  | g     | 837  | CLA  | C4B-NB  | 3.10 | 1.41        | 1.37     |
| 14  | B     | 841  | CLA  | C4B-NB  | 3.10 | 1.41        | 1.37     |
| 20  | b     | 801  | SQD  | C24-C23 | 3.10 | 1.59        | 1.50     |
| 14  | g     | 804  | CLA  | C4B-NB  | 3.10 | 1.41        | 1.37     |
| 14  | n     | 833  | CLA  | C4B-NB  | 3.10 | 1.41        | 1.37     |
| 14  | a     | 821  | CLA  | C4B-NB  | 3.10 | 1.41        | 1.37     |
| 14  | t     | 102  | CLA  | C4B-NB  | 3.10 | 1.41        | 1.37     |
| 14  | b     | 841  | CLA  | C4B-NB  | 3.10 | 1.41        | 1.37     |
| 14  | g     | 853  | CLA  | C4B-NB  | 3.10 | 1.41        | 1.37     |
| 14  | a     | 852  | CLA  | C1D-ND  | 3.10 | 1.41        | 1.37     |
| 14  | G     | 812  | CLA  | C4B-NB  | 3.09 | 1.41        | 1.37     |
| 14  | N     | 836  | CLA  | C4B-NB  | 3.09 | 1.41        | 1.37     |
| 14  | n     | 831  | CLA  | C4B-NB  | 3.09 | 1.41        | 1.37     |
| 14  | g     | 821  | CLA  | C4B-NB  | 3.09 | 1.41        | 1.37     |
| 14  | A     | 838  | CLA  | C4B-NB  | 3.09 | 1.41        | 1.37     |
| 20  | h     | 1702 | SQD  | C24-C23 | 3.09 | 1.59        | 1.50     |
| 14  | n     | 838  | CLA  | C4B-NB  | 3.09 | 1.41        | 1.37     |
| 14  | b     | 836  | CLA  | C4B-NB  | 3.09 | 1.41        | 1.37     |
| 14  | b     | 853  | CLA  | C4B-NB  | 3.09 | 1.41        | 1.37     |
| 14  | N     | 842  | CLA  | C4B-NB  | 3.09 | 1.41        | 1.37     |
| 14  | j     | 101  | CLA  | C4B-NB  | 3.08 | 1.41        | 1.37     |
| 14  | l     | 204  | CLA  | C4B-NB  | 3.08 | 1.41        | 1.37     |
| 14  | f     | 202  | CLA  | C4B-NB  | 3.08 | 1.41        | 1.37     |
| 14  | G     | 803  | CLA  | C4B-NB  | 3.08 | 1.41        | 1.37     |
| 14  | a     | 809  | CLA  | C4B-NB  | 3.08 | 1.41        | 1.37     |
| 14  | N     | 833  | CLA  | C4B-NB  | 3.08 | 1.41        | 1.37     |
| 14  | a     | 854  | CLA  | C4B-NB  | 3.08 | 1.41        | 1.37     |
| 14  | b     | 821  | CLA  | C4B-NB  | 3.08 | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14  | n     | 812  | CLA  | C4B-NB | 3.08 | 1.41        | 1.37     |
| 14  | k     | 101  | CLA  | C4B-NB | 3.08 | 1.41        | 1.37     |
| 14  | G     | 835  | CLA  | C4B-NB | 3.07 | 1.41        | 1.37     |
| 14  | j     | 102  | CLA  | C4B-NB | 3.07 | 1.41        | 1.37     |
| 14  | B     | 828  | CLA  | C4B-NB | 3.07 | 1.41        | 1.37     |
| 14  | G     | 816  | CLA  | C4B-NB | 3.07 | 1.41        | 1.37     |
| 14  | B     | 811  | CLA  | C4B-NB | 3.07 | 1.41        | 1.37     |
| 14  | U     | 101  | CLA  | C4B-NB | 3.07 | 1.41        | 1.37     |
| 14  | A     | 803  | CLA  | C4B-NB | 3.07 | 1.41        | 1.37     |
| 14  | N     | 834  | CLA  | C1D-ND | 3.07 | 1.41        | 1.37     |
| 14  | F     | 202  | CLA  | C4B-NB | 3.07 | 1.41        | 1.37     |
| 14  | n     | 810  | CLA  | C4B-NB | 3.07 | 1.41        | 1.37     |
| 14  | g     | 820  | CLA  | C4B-NB | 3.07 | 1.41        | 1.37     |
| 14  | b     | 805  | CLA  | C4B-NB | 3.07 | 1.41        | 1.37     |
| 14  | B     | 836  | CLA  | C4B-NB | 3.06 | 1.41        | 1.37     |
| 14  | G     | 801  | CLA  | C4B-NB | 3.06 | 1.41        | 1.37     |
| 14  | B     | 805  | CLA  | C4B-NB | 3.06 | 1.41        | 1.37     |
| 14  | a     | 840  | CLA  | C4B-NB | 3.06 | 1.41        | 1.37     |
| 14  | g     | 831  | CLA  | C4B-NB | 3.06 | 1.41        | 1.37     |
| 14  | b     | 839  | CLA  | C4B-NB | 3.06 | 1.41        | 1.37     |
| 14  | B     | 840  | CLA  | C4B-NB | 3.06 | 1.41        | 1.37     |
| 14  | g     | 817  | CLA  | C4B-NB | 3.06 | 1.41        | 1.37     |
| 14  | n     | 821  | CLA  | C4B-NB | 3.06 | 1.41        | 1.37     |
| 14  | B     | 832  | CLA  | C4B-NB | 3.06 | 1.41        | 1.37     |
| 14  | B     | 835  | CLA  | C4B-NB | 3.06 | 1.41        | 1.37     |
| 14  | J     | 101  | CLA  | C4B-NB | 3.06 | 1.41        | 1.37     |
| 14  | N     | 838  | CLA  | C4B-NB | 3.06 | 1.41        | 1.37     |
| 14  | G     | 811  | CLA  | C4B-NB | 3.05 | 1.41        | 1.37     |
| 14  | b     | 851  | CLA  | C4B-NB | 3.05 | 1.41        | 1.37     |
| 14  | n     | 806  | CLA  | C4B-NB | 3.05 | 1.41        | 1.37     |
| 14  | H     | 1701 | CLA  | C4B-NB | 3.05 | 1.41        | 1.37     |
| 14  | N     | 841  | CLA  | C4B-NB | 3.05 | 1.41        | 1.37     |
| 14  | a     | 817  | CLA  | C4B-NB | 3.05 | 1.41        | 1.37     |
| 14  | N     | 822  | CLA  | C4B-NB | 3.05 | 1.41        | 1.37     |
| 14  | U     | 102  | CLA  | C4B-NB | 3.05 | 1.41        | 1.37     |
| 14  | w     | 203  | CLA  | C4B-NB | 3.05 | 1.41        | 1.37     |
| 14  | g     | 839  | CLA  | C4B-NB | 3.05 | 1.41        | 1.37     |
| 14  | b     | 840  | CLA  | C4B-NB | 3.05 | 1.41        | 1.37     |
| 14  | A     | 855  | CLA  | C1D-ND | 3.05 | 1.41        | 1.37     |
| 14  | a     | 836  | CLA  | C4B-NB | 3.05 | 1.41        | 1.37     |
| 14  | A     | 810  | CLA  | C4B-NB | 3.05 | 1.41        | 1.37     |
| 14  | B     | 803  | CLA  | C4B-NB | 3.05 | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | G     | 819  | CLA  | C4B-NB  | 3.05 | 1.41        | 1.37     |
| 14  | n     | 827  | CLA  | C4B-NB  | 3.04 | 1.41        | 1.37     |
| 14  | n     | 850  | CLA  | C4B-NB  | 3.04 | 1.41        | 1.37     |
| 14  | T     | 102  | CLA  | C4B-NB  | 3.04 | 1.41        | 1.37     |
| 20  | l     | 201  | SQD  | C24-C23 | 3.04 | 1.59        | 1.50     |
| 14  | N     | 814  | CLA  | C4B-NB  | 3.04 | 1.41        | 1.37     |
| 14  | A     | 837  | CLA  | C4B-NB  | 3.04 | 1.41        | 1.37     |
| 14  | B     | 812  | CLA  | C4B-NB  | 3.04 | 1.41        | 1.37     |
| 14  | g     | 808  | CLA  | C4B-NB  | 3.04 | 1.41        | 1.37     |
| 14  | A     | 813  | CLA  | C4B-NB  | 3.04 | 1.41        | 1.37     |
| 14  | n     | 840  | CLA  | C4B-NB  | 3.04 | 1.41        | 1.37     |
| 14  | L     | 1502 | CLA  | C4B-NB  | 3.04 | 1.41        | 1.37     |
| 14  | b     | 809  | CLA  | C4B-NB  | 3.04 | 1.41        | 1.37     |
| 14  | g     | 815  | CLA  | C4B-NB  | 3.04 | 1.41        | 1.37     |
| 14  | n     | 819  | CLA  | C4B-NB  | 3.04 | 1.41        | 1.37     |
| 14  | a     | 812  | CLA  | C4B-NB  | 3.04 | 1.41        | 1.37     |
| 14  | u     | 101  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 14  | a     | 808  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 14  | b     | 803  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 14  | n     | 823  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 20  | B     | 801  | SQD  | C24-C23 | 3.03 | 1.59        | 1.50     |
| 14  | g     | 807  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 14  | n     | 830  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 14  | u     | 102  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 14  | G     | 838  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 14  | S     | 203  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 14  | g     | 832  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 20  | w     | 202  | SQD  | C24-C23 | 3.03 | 1.59        | 1.50     |
| 14  | g     | 812  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 14  | g     | 818  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 14  | N     | 812  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 14  | n     | 826  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 14  | w     | 205  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 14  | A     | 832  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 14  | a     | 834  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 14  | x     | 1701 | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 14  | b     | 831  | CLA  | C4B-NB  | 3.03 | 1.41        | 1.37     |
| 20  | H     | 1702 | SQD  | C24-C23 | 3.02 | 1.59        | 1.50     |
| 14  | N     | 808  | CLA  | C4B-NB  | 3.02 | 1.41        | 1.37     |
| 14  | F     | 201  | CLA  | C4B-NB  | 3.02 | 1.41        | 1.37     |
| 14  | G     | 840  | CLA  | C4B-NB  | 3.02 | 1.41        | 1.37     |
| 14  | A     | 826  | CLA  | C4B-NB  | 3.02 | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | A     | 835  | CLA  | C4B-NB  | 3.02 | 1.41        | 1.37     |
| 14  | n     | 803  | CLA  | C4B-NB  | 3.02 | 1.41        | 1.37     |
| 14  | G     | 833  | CLA  | C4B-NB  | 3.02 | 1.41        | 1.37     |
| 14  | A     | 839  | CLA  | C4B-NB  | 3.02 | 1.41        | 1.37     |
| 14  | b     | 834  | CLA  | C4B-NB  | 3.02 | 1.41        | 1.37     |
| 14  | a     | 815  | CLA  | C4B-NB  | 3.02 | 1.41        | 1.37     |
| 14  | b     | 822  | CLA  | C4B-NB  | 3.02 | 1.41        | 1.37     |
| 14  | b     | 828  | CLA  | C4B-NB  | 3.02 | 1.41        | 1.37     |
| 14  | b     | 835  | CLA  | C4B-NB  | 3.02 | 1.41        | 1.37     |
| 14  | A     | 811  | CLA  | C4B-NB  | 3.02 | 1.41        | 1.37     |
| 14  | b     | 827  | CLA  | C4B-NB  | 3.02 | 1.41        | 1.37     |
| 14  | b     | 811  | CLA  | C4B-NB  | 3.02 | 1.41        | 1.37     |
| 14  | A     | 828  | CLA  | C4B-NB  | 3.01 | 1.41        | 1.37     |
| 14  | A     | 857  | CLA  | C4B-NB  | 3.01 | 1.41        | 1.37     |
| 14  | A     | 834  | CLA  | C4B-NB  | 3.01 | 1.41        | 1.37     |
| 14  | a     | 802  | CLA  | C4B-NB  | 3.01 | 1.41        | 1.37     |
| 14  | g     | 816  | CLA  | C4B-NB  | 3.01 | 1.41        | 1.37     |
| 14  | N     | 806  | CLA  | C4B-NB  | 3.01 | 1.41        | 1.37     |
| 14  | N     | 805  | CLA  | C4B-NB  | 3.01 | 1.41        | 1.37     |
| 14  | A     | 823  | CLA  | C4B-NB  | 3.01 | 1.41        | 1.37     |
| 14  | a     | 816  | CLA  | C4B-NB  | 3.01 | 1.41        | 1.37     |
| 20  | x     | 1702 | SQD  | C24-C23 | 3.01 | 1.59        | 1.50     |
| 14  | g     | 840  | CLA  | C4B-NB  | 3.01 | 1.41        | 1.37     |
| 14  | A     | 818  | CLA  | C4B-NB  | 3.01 | 1.41        | 1.37     |
| 14  | G     | 814  | CLA  | C4B-NB  | 3.01 | 1.41        | 1.37     |
| 14  | G     | 824  | CLA  | C4B-NB  | 3.01 | 1.41        | 1.37     |
| 14  | G     | 839  | CLA  | C4B-NB  | 3.01 | 1.41        | 1.37     |
| 14  | N     | 828  | CLA  | C4B-NB  | 3.01 | 1.41        | 1.37     |
| 14  | N     | 834  | CLA  | C4B-NB  | 3.01 | 1.41        | 1.37     |
| 14  | n     | 820  | CLA  | C4B-NB  | 3.01 | 1.41        | 1.37     |
| 14  | n     | 815  | CLA  | C4B-NB  | 3.00 | 1.41        | 1.37     |
| 14  | G     | 809  | CLA  | C4B-NB  | 3.00 | 1.41        | 1.37     |
| 14  | s     | 201  | CLA  | C4B-NB  | 3.00 | 1.41        | 1.37     |
| 14  | b     | 817  | CLA  | C4B-NB  | 3.00 | 1.41        | 1.37     |
| 14  | B     | 817  | CLA  | C4B-NB  | 3.00 | 1.41        | 1.37     |
| 14  | B     | 819  | CLA  | C4B-NB  | 3.00 | 1.41        | 1.37     |
| 14  | J     | 102  | CLA  | C4B-NB  | 3.00 | 1.41        | 1.37     |
| 14  | n     | 811  | CLA  | C4B-NB  | 3.00 | 1.41        | 1.37     |
| 14  | B     | 815  | CLA  | C4B-NB  | 3.00 | 1.41        | 1.37     |
| 14  | g     | 834  | CLA  | C4B-NB  | 3.00 | 1.41        | 1.37     |
| 14  | a     | 810  | CLA  | C4B-NB  | 3.00 | 1.41        | 1.37     |
| 14  | N     | 804  | CLA  | C4B-NB  | 3.00 | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 14  | G     | 818 | CLA  | C4B-NB | 3.00 | 1.41        | 1.37     |
| 14  | b     | 820 | CLA  | C4B-NB | 3.00 | 1.41        | 1.37     |
| 14  | G     | 829 | CLA  | C4B-NB | 2.99 | 1.41        | 1.37     |
| 14  | G     | 810 | CLA  | C4B-NB | 2.99 | 1.41        | 1.37     |
| 14  | g     | 802 | CLA  | C4B-NB | 2.99 | 1.41        | 1.37     |
| 14  | g     | 827 | CLA  | C4B-NB | 2.99 | 1.41        | 1.37     |
| 14  | N     | 835 | CLA  | C4B-NB | 2.99 | 1.41        | 1.37     |
| 14  | B     | 833 | CLA  | C4B-NB | 2.99 | 1.41        | 1.37     |
| 14  | N     | 825 | CLA  | C4B-NB | 2.99 | 1.41        | 1.37     |
| 14  | a     | 832 | CLA  | C4B-NB | 2.99 | 1.41        | 1.37     |
| 14  | b     | 819 | CLA  | C4B-NB | 2.99 | 1.41        | 1.37     |
| 14  | b     | 825 | CLA  | C4B-NB | 2.99 | 1.41        | 1.37     |
| 14  | B     | 822 | CLA  | C4B-NB | 2.99 | 1.41        | 1.37     |
| 14  | N     | 839 | CLA  | C4B-NB | 2.99 | 1.41        | 1.37     |
| 14  | G     | 828 | CLA  | C4B-NB | 2.99 | 1.41        | 1.37     |
| 14  | A     | 815 | CLA  | C4B-NB | 2.99 | 1.41        | 1.37     |
| 14  | G     | 820 | CLA  | C4B-NB | 2.99 | 1.41        | 1.37     |
| 14  | G     | 834 | CLA  | C4B-NB | 2.99 | 1.41        | 1.37     |
| 14  | b     | 832 | CLA  | C4B-NB | 2.99 | 1.41        | 1.37     |
| 14  | g     | 814 | CLA  | C4B-NB | 2.98 | 1.41        | 1.37     |
| 14  | B     | 816 | CLA  | C4B-NB | 2.98 | 1.41        | 1.37     |
| 14  | N     | 818 | CLA  | C4B-NB | 2.98 | 1.41        | 1.37     |
| 14  | N     | 824 | CLA  | C4B-NB | 2.98 | 1.41        | 1.37     |
| 14  | a     | 825 | CLA  | C4B-NB | 2.98 | 1.41        | 1.37     |
| 14  | A     | 829 | CLA  | C4B-NB | 2.98 | 1.41        | 1.37     |
| 14  | B     | 831 | CLA  | C4B-NB | 2.98 | 1.41        | 1.37     |
| 14  | g     | 811 | CLA  | C4B-NB | 2.98 | 1.41        | 1.37     |
| 14  | a     | 827 | CLA  | C4B-NB | 2.98 | 1.41        | 1.37     |
| 14  | a     | 807 | CLA  | C4B-NB | 2.98 | 1.41        | 1.37     |
| 14  | n     | 822 | CLA  | C4B-NB | 2.98 | 1.41        | 1.37     |
| 14  | n     | 802 | CLA  | C4B-NB | 2.98 | 1.41        | 1.37     |
| 14  | B     | 820 | CLA  | C4B-NB | 2.98 | 1.41        | 1.37     |
| 14  | G     | 826 | CLA  | C4B-NB | 2.98 | 1.41        | 1.37     |
| 14  | a     | 829 | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | W     | 203 | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | b     | 804 | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | g     | 826 | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | A     | 814 | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | a     | 813 | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | b     | 838 | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | l     | 203 | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | A     | 802 | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |

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| Mol | Chain | Res  | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|------|-------------|----------|
| 14  | g     | 813  | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | n     | 852  | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | n     | 818  | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | A     | 840  | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | B     | 821  | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | a     | 833  | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | N     | 813  | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | N     | 832  | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | L     | 1503 | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | a     | 826  | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | G     | 817  | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | n     | 837  | CLA  | C4B-NB | 2.97 | 1.41        | 1.37     |
| 14  | G     | 853  | CLA  | C4B-NB | 2.96 | 1.41        | 1.37     |
| 14  | A     | 804  | CLA  | C4B-NB | 2.96 | 1.41        | 1.37     |
| 14  | g     | 829  | CLA  | C4B-NB | 2.96 | 1.41        | 1.37     |
| 14  | a     | 828  | CLA  | C4B-NB | 2.96 | 1.41        | 1.37     |
| 14  | L     | 1501 | CLA  | C4B-NB | 2.96 | 1.41        | 1.37     |
| 14  | S     | 201  | CLA  | C4B-NB | 2.96 | 1.41        | 1.37     |
| 14  | A     | 821  | CLA  | C4B-NB | 2.96 | 1.41        | 1.37     |
| 14  | a     | 818  | CLA  | C4B-NB | 2.96 | 1.41        | 1.37     |
| 14  | N     | 829  | CLA  | C4B-NB | 2.96 | 1.41        | 1.37     |
| 14  | A     | 807  | CLA  | C4B-NB | 2.96 | 1.41        | 1.37     |
| 14  | b     | 810  | CLA  | C4B-NB | 2.96 | 1.41        | 1.37     |
| 14  | B     | 824  | CLA  | C4B-NB | 2.96 | 1.41        | 1.37     |
| 14  | A     | 841  | CLA  | C4B-NB | 2.96 | 1.41        | 1.37     |
| 14  | g     | 828  | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |
| 14  | A     | 827  | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |
| 14  | N     | 816  | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |
| 14  | t     | 101  | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |
| 14  | A     | 830  | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |
| 14  | B     | 829  | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |
| 14  | G     | 832  | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |
| 14  | n     | 839  | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |
| 14  | a     | 814  | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |
| 14  | A     | 808  | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |
| 14  | a     | 831  | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |
| 14  | b     | 816  | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |
| 14  | n     | 814  | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |
| 14  | a     | 822  | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |
| 14  | G     | 802  | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |
| 14  | A     | 819  | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |
| 14  | G     | 827  | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 14  | W     | 204 | CLA  | C4B-NB | 2.95 | 1.41        | 1.37     |
| 14  | B     | 818 | CLA  | C4B-NB | 2.94 | 1.41        | 1.37     |
| 14  | a     | 819 | CLA  | C4B-NB | 2.94 | 1.41        | 1.37     |
| 14  | N     | 811 | CLA  | C4B-NB | 2.94 | 1.41        | 1.37     |
| 14  | A     | 854 | CLA  | C4B-NB | 2.94 | 1.41        | 1.37     |
| 14  | N     | 803 | CLA  | C4B-NB | 2.94 | 1.41        | 1.37     |
| 14  | l     | 202 | CLA  | C4B-NB | 2.94 | 1.41        | 1.37     |
| 14  | G     | 813 | CLA  | C4B-NB | 2.94 | 1.41        | 1.37     |
| 14  | B     | 827 | CLA  | C4B-NB | 2.94 | 1.41        | 1.37     |
| 14  | b     | 837 | CLA  | C4B-NB | 2.94 | 1.41        | 1.37     |
| 14  | G     | 808 | CLA  | C4B-NB | 2.94 | 1.41        | 1.37     |
| 14  | N     | 826 | CLA  | C4B-NB | 2.94 | 1.41        | 1.37     |
| 14  | W     | 202 | CLA  | C4B-NB | 2.94 | 1.41        | 1.37     |
| 14  | B     | 808 | CLA  | C4B-NB | 2.94 | 1.41        | 1.37     |
| 14  | a     | 830 | CLA  | C4B-NB | 2.94 | 1.41        | 1.37     |
| 14  | N     | 817 | CLA  | C4B-NB | 2.94 | 1.41        | 1.37     |
| 14  | A     | 817 | CLA  | C4B-NB | 2.94 | 1.41        | 1.37     |
| 14  | N     | 823 | CLA  | C4B-NB | 2.93 | 1.41        | 1.37     |
| 14  | N     | 807 | CLA  | C4B-NB | 2.93 | 1.41        | 1.37     |
| 14  | n     | 824 | CLA  | C4B-NB | 2.93 | 1.41        | 1.37     |
| 14  | N     | 810 | CLA  | C4B-NB | 2.93 | 1.41        | 1.37     |
| 14  | b     | 808 | CLA  | C4B-NB | 2.93 | 1.41        | 1.37     |
| 14  | g     | 836 | CLA  | C4B-NB | 2.93 | 1.41        | 1.37     |
| 14  | a     | 820 | CLA  | C4B-NB | 2.93 | 1.41        | 1.37     |
| 14  | g     | 833 | CLA  | C4B-NB | 2.92 | 1.41        | 1.37     |
| 14  | B     | 834 | CLA  | C4B-NB | 2.92 | 1.41        | 1.37     |
| 14  | a     | 838 | CLA  | C4B-NB | 2.92 | 1.41        | 1.37     |
| 14  | n     | 829 | CLA  | C4B-NB | 2.92 | 1.41        | 1.37     |
| 14  | a     | 801 | CLA  | C4B-NB | 2.92 | 1.41        | 1.37     |
| 14  | a     | 803 | CLA  | C4B-NB | 2.92 | 1.41        | 1.37     |
| 14  | B     | 806 | CLA  | C4B-NB | 2.92 | 1.41        | 1.37     |
| 14  | N     | 820 | CLA  | C4B-NB | 2.92 | 1.41        | 1.37     |
| 14  | B     | 809 | CLA  | C4B-NB | 2.92 | 1.41        | 1.37     |
| 14  | B     | 810 | CLA  | C4B-NB | 2.92 | 1.41        | 1.37     |
| 14  | g     | 806 | CLA  | C4B-NB | 2.91 | 1.41        | 1.37     |
| 14  | f     | 201 | CLA  | C4B-NB | 2.91 | 1.41        | 1.37     |
| 14  | N     | 830 | CLA  | C4B-NB | 2.91 | 1.41        | 1.37     |
| 14  | n     | 808 | CLA  | C4B-NB | 2.91 | 1.41        | 1.37     |
| 14  | B     | 837 | CLA  | C4B-NB | 2.91 | 1.41        | 1.37     |
| 14  | a     | 804 | CLA  | C4B-NB | 2.91 | 1.41        | 1.37     |
| 14  | g     | 801 | CLA  | C4B-NB | 2.91 | 1.41        | 1.37     |
| 14  | A     | 816 | CLA  | C4B-NB | 2.91 | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 14  | g     | 822 | CLA  | C4B-NB  | 2.91 | 1.41        | 1.37     |
| 14  | n     | 805 | CLA  | C4B-NB  | 2.91 | 1.41        | 1.37     |
| 14  | G     | 823 | CLA  | C4B-NB  | 2.90 | 1.41        | 1.37     |
| 14  | n     | 828 | CLA  | C4B-NB  | 2.90 | 1.41        | 1.37     |
| 14  | A     | 825 | CLA  | C4B-NB  | 2.90 | 1.41        | 1.37     |
| 14  | A     | 822 | CLA  | C4B-NB  | 2.90 | 1.41        | 1.37     |
| 14  | G     | 805 | CLA  | C4B-NB  | 2.90 | 1.41        | 1.37     |
| 14  | G     | 831 | CLA  | C4B-NB  | 2.90 | 1.41        | 1.37     |
| 14  | B     | 823 | CLA  | C4B-NB  | 2.90 | 1.41        | 1.37     |
| 14  | b     | 830 | CLA  | C4B-NB  | 2.90 | 1.41        | 1.37     |
| 14  | n     | 809 | CLA  | C4B-NB  | 2.90 | 1.41        | 1.37     |
| 14  | B     | 838 | CLA  | C4B-NB  | 2.90 | 1.41        | 1.37     |
| 14  | g     | 803 | CLA  | C4B-NB  | 2.90 | 1.41        | 1.37     |
| 14  | a     | 828 | CLA  | C1B-C2B | 2.90 | 1.49        | 1.43     |
| 14  | G     | 830 | CLA  | C4B-NB  | 2.89 | 1.41        | 1.37     |
| 14  | N     | 809 | CLA  | C4B-NB  | 2.89 | 1.41        | 1.37     |
| 14  | A     | 809 | CLA  | C4B-NB  | 2.89 | 1.41        | 1.37     |
| 14  | B     | 807 | CLA  | C4B-NB  | 2.89 | 1.41        | 1.37     |
| 14  | b     | 815 | CLA  | C4B-NB  | 2.89 | 1.41        | 1.37     |
| 14  | b     | 813 | CLA  | C4B-NB  | 2.89 | 1.41        | 1.37     |
| 14  | n     | 807 | CLA  | C4B-NB  | 2.89 | 1.41        | 1.37     |
| 14  | A     | 824 | CLA  | C4B-NB  | 2.89 | 1.41        | 1.37     |
| 14  | G     | 822 | CLA  | C4B-NB  | 2.88 | 1.41        | 1.37     |
| 14  | B     | 825 | CLA  | C4B-NB  | 2.88 | 1.41        | 1.37     |
| 14  | G     | 821 | CLA  | C4B-NB  | 2.88 | 1.41        | 1.37     |
| 14  | G     | 804 | CLA  | C4B-NB  | 2.88 | 1.41        | 1.37     |
| 14  | A     | 831 | CLA  | C4B-NB  | 2.88 | 1.41        | 1.37     |
| 14  | b     | 807 | CLA  | C4B-NB  | 2.87 | 1.41        | 1.37     |
| 14  | G     | 825 | CLA  | C4B-NB  | 2.87 | 1.41        | 1.37     |
| 14  | g     | 852 | CLA  | C1D-ND  | 2.87 | 1.41        | 1.37     |
| 14  | N     | 831 | CLA  | C4B-NB  | 2.87 | 1.41        | 1.37     |
| 14  | a     | 824 | CLA  | C4B-NB  | 2.87 | 1.41        | 1.37     |
| 14  | G     | 836 | CLA  | C4B-NB  | 2.87 | 1.41        | 1.37     |
| 14  | a     | 835 | CLA  | C4B-NB  | 2.87 | 1.41        | 1.37     |
| 14  | N     | 815 | CLA  | C4B-NB  | 2.86 | 1.41        | 1.37     |
| 14  | w     | 204 | CLA  | C4B-NB  | 2.86 | 1.41        | 1.37     |
| 14  | b     | 829 | CLA  | C4B-NB  | 2.86 | 1.41        | 1.37     |
| 14  | a     | 823 | CLA  | C4B-NB  | 2.86 | 1.41        | 1.37     |
| 14  | b     | 806 | CLA  | C4B-NB  | 2.86 | 1.41        | 1.37     |
| 14  | B     | 814 | CLA  | C4B-NB  | 2.86 | 1.41        | 1.37     |
| 14  | g     | 823 | CLA  | C4B-NB  | 2.86 | 1.41        | 1.37     |
| 14  | g     | 838 | CLA  | C4B-NB  | 2.86 | 1.41        | 1.37     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 14  | g     | 824 | CLA  | C4B-NB  | 2.85 | 1.41        | 1.37     |
| 14  | b     | 818 | CLA  | C4B-NB  | 2.85 | 1.41        | 1.37     |
| 14  | g     | 825 | CLA  | C4B-NB  | 2.85 | 1.41        | 1.37     |
| 14  | b     | 814 | CLA  | C4B-NB  | 2.85 | 1.41        | 1.37     |
| 14  | B     | 830 | CLA  | C4B-NB  | 2.85 | 1.41        | 1.37     |
| 14  | a     | 839 | CLA  | C4B-NB  | 2.85 | 1.41        | 1.37     |
| 14  | G     | 837 | CLA  | C4B-NB  | 2.84 | 1.41        | 1.37     |
| 14  | n     | 829 | CLA  | C1B-C2B | 2.84 | 1.49        | 1.43     |
| 14  | N     | 831 | CLA  | C1B-C2B | 2.83 | 1.49        | 1.43     |
| 14  | N     | 819 | CLA  | C4B-NB  | 2.83 | 1.41        | 1.37     |
| 14  | n     | 813 | CLA  | C4B-NB  | 2.83 | 1.41        | 1.37     |
| 14  | B     | 826 | CLA  | C4B-NB  | 2.83 | 1.41        | 1.37     |
| 14  | a     | 807 | CLA  | C1B-C2B | 2.82 | 1.49        | 1.43     |
| 14  | B     | 830 | CLA  | C1B-C2B | 2.82 | 1.49        | 1.43     |
| 14  | g     | 830 | CLA  | C4B-NB  | 2.82 | 1.41        | 1.37     |
| 14  | n     | 817 | CLA  | C4B-NB  | 2.82 | 1.41        | 1.37     |
| 14  | n     | 804 | CLA  | C4B-NB  | 2.82 | 1.41        | 1.37     |
| 14  | g     | 835 | CLA  | C4B-NB  | 2.82 | 1.41        | 1.37     |
| 14  | a     | 811 | CLA  | C4B-NB  | 2.81 | 1.41        | 1.37     |
| 14  | G     | 807 | CLA  | C4B-NB  | 2.80 | 1.41        | 1.37     |
| 14  | N     | 834 | CLA  | C1B-C2B | 2.79 | 1.49        | 1.43     |
| 14  | A     | 808 | CLA  | C1B-C2B | 2.79 | 1.49        | 1.43     |
| 14  | G     | 808 | CLA  | C1B-C2B | 2.79 | 1.49        | 1.43     |
| 14  | n     | 833 | CLA  | C1B-C2B | 2.78 | 1.49        | 1.43     |
| 14  | n     | 803 | CLA  | C1B-C2B | 2.78 | 1.49        | 1.43     |
| 14  | N     | 818 | CLA  | C1B-C2B | 2.78 | 1.49        | 1.43     |
| 14  | b     | 826 | CLA  | C4B-NB  | 2.78 | 1.41        | 1.37     |
| 14  | N     | 827 | CLA  | C4B-NB  | 2.77 | 1.41        | 1.37     |
| 14  | g     | 807 | CLA  | C1B-C2B | 2.77 | 1.49        | 1.43     |
| 14  | B     | 827 | CLA  | C1B-C2B | 2.77 | 1.49        | 1.43     |
| 14  | B     | 822 | CLA  | C1B-C2B | 2.77 | 1.49        | 1.43     |
| 14  | j     | 102 | CLA  | C1B-C2B | 2.77 | 1.49        | 1.43     |
| 14  | A     | 802 | CLA  | C1B-C2B | 2.76 | 1.49        | 1.43     |
| 14  | n     | 836 | CLA  | C4B-NB  | 2.76 | 1.41        | 1.37     |
| 14  | S     | 201 | CLA  | C1B-C2B | 2.76 | 1.49        | 1.43     |
| 14  | G     | 809 | CLA  | C1B-C2B | 2.76 | 1.49        | 1.43     |
| 14  | a     | 806 | CLA  | C4B-NB  | 2.76 | 1.41        | 1.37     |
| 14  | g     | 801 | CLA  | C1B-C2B | 2.76 | 1.49        | 1.43     |
| 14  | b     | 817 | CLA  | C1B-C2B | 2.76 | 1.49        | 1.43     |
| 14  | B     | 812 | CLA  | C1B-C2B | 2.75 | 1.49        | 1.43     |
| 14  | T     | 102 | CLA  | C1B-C2B | 2.75 | 1.49        | 1.43     |
| 14  | g     | 814 | CLA  | C1B-C2B | 2.75 | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 14  | N     | 842 | CLA  | C1B-C2B | 2.75 | 1.49        | 1.43     |
| 14  | A     | 823 | CLA  | C1B-C2B | 2.75 | 1.49        | 1.43     |
| 14  | a     | 813 | CLA  | C1B-C2B | 2.75 | 1.49        | 1.43     |
| 14  | n     | 825 | CLA  | C4B-NB  | 2.75 | 1.41        | 1.37     |
| 14  | t     | 102 | CLA  | C1B-C2B | 2.75 | 1.49        | 1.43     |
| 14  | B     | 814 | CLA  | C1B-C2B | 2.75 | 1.49        | 1.43     |
| 14  | A     | 835 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | a     | 814 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | g     | 808 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | B     | 807 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | g     | 831 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | J     | 102 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | u     | 102 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | G     | 823 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | B     | 834 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | b     | 816 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | n     | 816 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | N     | 835 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | G     | 822 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | n     | 813 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | n     | 850 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | A     | 857 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | N     | 824 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | n     | 824 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | b     | 806 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | a     | 852 | CLA  | C4B-NB  | 2.74 | 1.41        | 1.37     |
| 14  | N     | 804 | CLA  | C1B-C2B | 2.74 | 1.49        | 1.43     |
| 14  | A     | 814 | CLA  | C1B-C2B | 2.73 | 1.49        | 1.43     |
| 14  | K     | 101 | CLA  | C1B-C2B | 2.73 | 1.49        | 1.43     |
| 14  | n     | 811 | CLA  | C1B-C2B | 2.73 | 1.49        | 1.43     |
| 14  | n     | 840 | CLA  | C1B-C2B | 2.73 | 1.49        | 1.43     |
| 14  | b     | 804 | CLA  | C1B-C2B | 2.73 | 1.49        | 1.43     |
| 14  | n     | 822 | CLA  | C1B-C2B | 2.73 | 1.49        | 1.43     |
| 14  | A     | 813 | CLA  | C1B-C2B | 2.73 | 1.49        | 1.43     |
| 14  | G     | 804 | CLA  | C1B-C2B | 2.73 | 1.49        | 1.43     |
| 14  | n     | 837 | CLA  | C1B-C2B | 2.73 | 1.49        | 1.43     |
| 14  | a     | 818 | CLA  | C1B-C2B | 2.73 | 1.49        | 1.43     |
| 14  | A     | 815 | CLA  | C1B-C2B | 2.73 | 1.49        | 1.43     |
| 14  | b     | 851 | CLA  | C1B-C2B | 2.73 | 1.49        | 1.43     |
| 14  | a     | 801 | CLA  | C1B-C2B | 2.73 | 1.49        | 1.43     |
| 14  | G     | 835 | CLA  | C1B-C2B | 2.72 | 1.49        | 1.43     |
| 14  | t     | 101 | CLA  | C1B-C2B | 2.72 | 1.49        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 833  | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 14  | A     | 819  | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 14  | B     | 836  | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 14  | b     | 836  | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 14  | G     | 811  | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 14  | G     | 819  | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 14  | B     | 804  | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 14  | a     | 821  | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 14  | L     | 1501 | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 14  | b     | 807  | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 14  | g     | 822  | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 14  | B     | 816  | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 14  | N     | 837  | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 14  | G     | 805  | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 14  | g     | 832  | CLA  | C1B-C2B | 2.72  | 1.49        | 1.43     |
| 14  | B     | 824  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | W     | 202  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | j     | 101  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | n     | 820  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | g     | 821  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | A     | 822  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | a     | 812  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | a     | 831  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | n     | 838  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | s     | 201  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | N     | 823  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | N     | 826  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | n     | 835  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | k     | 101  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | A     | 804  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | A     | 833  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | N     | 813  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | A     | 810  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | N     | 807  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 14  | b     | 822  | CLA  | C1B-C2B | 2.71  | 1.49        | 1.43     |
| 19  | g     | 851  | CL0  | CHA-CBD | -2.71 | 1.48        | 1.51     |
| 14  | N     | 839  | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 14  | a     | 839  | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 14  | h     | 1701 | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 14  | G     | 813  | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 14  | w     | 205  | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |
| 14  | n     | 809  | CLA  | C1B-C2B | 2.70  | 1.49        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | a     | 808  | CLA  | C1B-C2B | 2.70 | 1.49        | 1.43     |
| 14  | a     | 809  | CLA  | C1B-C2B | 2.70 | 1.49        | 1.43     |
| 14  | B     | 832  | CLA  | C1B-C2B | 2.70 | 1.49        | 1.43     |
| 14  | B     | 841  | CLA  | C1B-C2B | 2.70 | 1.49        | 1.43     |
| 14  | a     | 840  | CLA  | C1B-C2B | 2.70 | 1.49        | 1.43     |
| 14  | G     | 802  | CLA  | C1B-C2B | 2.70 | 1.49        | 1.43     |
| 14  | U     | 101  | CLA  | C1B-C2B | 2.70 | 1.49        | 1.43     |
| 14  | G     | 832  | CLA  | C1B-C2B | 2.70 | 1.49        | 1.43     |
| 14  | T     | 101  | CLA  | C1B-C2B | 2.70 | 1.49        | 1.43     |
| 14  | W     | 204  | CLA  | C1B-C2B | 2.70 | 1.49        | 1.43     |
| 14  | B     | 831  | CLA  | C1B-C2B | 2.70 | 1.49        | 1.43     |
| 14  | L     | 1503 | CLA  | C1B-C2B | 2.70 | 1.49        | 1.43     |
| 14  | a     | 822  | CLA  | C1B-C2B | 2.70 | 1.49        | 1.43     |
| 14  | N     | 815  | CLA  | C1B-C2B | 2.70 | 1.49        | 1.43     |
| 14  | N     | 828  | CLA  | C1B-C2B | 2.70 | 1.49        | 1.43     |
| 14  | A     | 821  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | B     | 823  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | A     | 832  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | u     | 101  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | n     | 806  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | B     | 806  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | l     | 202  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | B     | 821  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | b     | 834  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | A     | 811  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | b     | 813  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | N     | 810  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | g     | 806  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | A     | 809  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | g     | 839  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | A     | 841  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | a     | 833  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | a     | 834  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | A     | 816  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | a     | 805  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | b     | 811  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | N     | 816  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | N     | 817  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | B     | 838  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | G     | 830  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | N     | 809  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |
| 14  | a     | 810  | CLA  | C1B-C2B | 2.69 | 1.49        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 840  | CLA  | C1B-C2B | 2.69  | 1.49        | 1.43     |
| 14  | g     | 812  | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 14  | g     | 816  | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 14  | w     | 203  | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 14  | x     | 1701 | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 14  | b     | 819  | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 14  | a     | 820  | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 14  | b     | 821  | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 14  | N     | 811  | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 14  | n     | 817  | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 14  | g     | 818  | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 14  | n     | 852  | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 14  | B     | 817  | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 14  | n     | 815  | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 14  | g     | 852  | CLA  | C4B-NB  | 2.68  | 1.41        | 1.37     |
| 14  | n     | 821  | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 14  | N     | 822  | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 14  | g     | 838  | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 14  | f     | 201  | CLA  | C1B-C2B | 2.68  | 1.49        | 1.43     |
| 14  | G     | 853  | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 14  | H     | 1701 | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 14  | G     | 839  | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 14  | n     | 810  | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 19  | A     | 852  | CL0  | CHA-CBD | -2.67 | 1.48        | 1.51     |
| 14  | b     | 839  | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 14  | a     | 826  | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 14  | a     | 835  | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 14  | g     | 837  | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 14  | g     | 805  | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 14  | A     | 817  | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 14  | a     | 838  | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 14  | b     | 827  | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 14  | B     | 825  | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 14  | a     | 815  | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 14  | b     | 838  | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 14  | n     | 805  | CLA  | C1B-C2B | 2.67  | 1.49        | 1.43     |
| 14  | G     | 815  | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 14  | N     | 808  | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 14  | A     | 854  | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 14  | A     | 820  | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 14  | f     | 202  | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |
| 14  | G     | 806  | CLA  | C1B-C2B | 2.66  | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 14  | b     | 832 | CLA  | C1B-C2B | 2.66 | 1.49        | 1.43     |
| 14  | g     | 803 | CLA  | C1B-C2B | 2.66 | 1.49        | 1.43     |
| 14  | B     | 813 | CLA  | C1B-C2B | 2.66 | 1.49        | 1.43     |
| 14  | n     | 827 | CLA  | C1B-C2B | 2.66 | 1.49        | 1.43     |
| 14  | G     | 814 | CLA  | C1B-C2B | 2.66 | 1.49        | 1.43     |
| 14  | U     | 102 | CLA  | C1B-C2B | 2.66 | 1.49        | 1.43     |
| 14  | b     | 818 | CLA  | C1B-C2B | 2.66 | 1.49        | 1.43     |
| 14  | A     | 839 | CLA  | C1B-C2B | 2.66 | 1.49        | 1.43     |
| 14  | n     | 831 | CLA  | C1B-C2B | 2.66 | 1.49        | 1.43     |
| 14  | a     | 832 | CLA  | C1B-C2B | 2.66 | 1.49        | 1.43     |
| 14  | s     | 202 | CLA  | C1B-C2B | 2.66 | 1.49        | 1.43     |
| 14  | A     | 826 | CLA  | C1B-C2B | 2.66 | 1.49        | 1.43     |
| 14  | A     | 838 | CLA  | C1B-C2B | 2.66 | 1.49        | 1.43     |
| 14  | b     | 803 | CLA  | C1B-C2B | 2.66 | 1.49        | 1.43     |
| 14  | g     | 813 | CLA  | C1B-C2B | 2.66 | 1.49        | 1.43     |
| 14  | a     | 824 | CLA  | C1B-C2B | 2.66 | 1.49        | 1.43     |
| 14  | b     | 840 | CLA  | C1B-C2B | 2.66 | 1.49        | 1.43     |
| 14  | J     | 101 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | B     | 810 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | b     | 823 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | l     | 204 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | b     | 826 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | G     | 810 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | g     | 824 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | G     | 836 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | a     | 837 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | b     | 810 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | a     | 804 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | B     | 819 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | g     | 827 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | B     | 815 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | b     | 814 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | b     | 828 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | G     | 834 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | N     | 814 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | g     | 834 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | a     | 825 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | G     | 840 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | N     | 838 | CLA  | C1B-C2B | 2.65 | 1.49        | 1.43     |
| 14  | N     | 806 | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | g     | 840 | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | g     | 835 | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |

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| Mol | Chain | Res  | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 14  | G     | 828  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | N     | 830  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | X     | 1701 | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | N     | 840  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | G     | 838  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | G     | 833  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | N     | 836  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | g     | 815  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | G     | 816  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | n     | 839  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | b     | 825  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | b     | 853  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | a     | 854  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | G     | 807  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | g     | 823  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | F     | 201  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | b     | 837  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | A     | 803  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | B     | 809  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | N     | 825  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | g     | 825  | CLA  | C1B-C2B | 2.64 | 1.49        | 1.43     |
| 14  | A     | 853  | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | n     | 807  | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | n     | 814  | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | a     | 816  | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | g     | 836  | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | a     | 819  | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | B     | 808  | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | g     | 833  | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | b     | 815  | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | N     | 833  | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | A     | 837  | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | G     | 837  | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | B     | 839  | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | L     | 1502 | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | n     | 825  | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | G     | 825  | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | a     | 830  | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | a     | 803  | CLA  | C1B-C2B | 2.63 | 1.49        | 1.43     |
| 14  | A     | 828  | CLA  | C1B-C2B | 2.62 | 1.49        | 1.43     |
| 14  | S     | 203  | CLA  | C1B-C2B | 2.62 | 1.49        | 1.43     |
| 14  | B     | 811  | CLA  | C1B-C2B | 2.62 | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 14  | b     | 808 | CLA  | C1B-C2B | 2.62 | 1.49        | 1.43     |
| 14  | n     | 812 | CLA  | C1B-C2B | 2.62 | 1.49        | 1.43     |
| 14  | B     | 828 | CLA  | C1B-C2B | 2.62 | 1.49        | 1.43     |
| 14  | b     | 824 | CLA  | C1B-C2B | 2.62 | 1.49        | 1.43     |
| 14  | g     | 830 | CLA  | C1B-C2B | 2.62 | 1.49        | 1.43     |
| 14  | n     | 823 | CLA  | C1B-C2B | 2.62 | 1.49        | 1.43     |
| 14  | N     | 832 | CLA  | C1B-C2B | 2.62 | 1.49        | 1.43     |
| 14  | b     | 809 | CLA  | C1B-C2B | 2.62 | 1.49        | 1.43     |
| 14  | g     | 802 | CLA  | C1B-C2B | 2.62 | 1.49        | 1.43     |
| 14  | b     | 835 | CLA  | C1B-C2B | 2.62 | 1.49        | 1.43     |
| 14  | b     | 841 | CLA  | C1B-C2B | 2.62 | 1.49        | 1.43     |
| 14  | N     | 829 | CLA  | C1B-C2B | 2.62 | 1.49        | 1.43     |
| 14  | a     | 817 | CLA  | C1B-C2B | 2.62 | 1.49        | 1.43     |
| 14  | A     | 805 | CLA  | C1B-C2B | 2.61 | 1.49        | 1.43     |
| 14  | b     | 805 | CLA  | CHC-C1C | 2.61 | 1.43        | 1.38     |
| 14  | G     | 824 | CLA  | C1B-C2B | 2.61 | 1.49        | 1.43     |
| 14  | A     | 824 | CLA  | C1B-C2B | 2.61 | 1.49        | 1.43     |
| 14  | A     | 829 | CLA  | C1B-C2B | 2.61 | 1.49        | 1.43     |
| 14  | b     | 812 | CLA  | C1B-C2B | 2.61 | 1.49        | 1.43     |
| 14  | F     | 202 | CLA  | C1B-C2B | 2.61 | 1.49        | 1.43     |
| 14  | N     | 820 | CLA  | C1B-C2B | 2.61 | 1.49        | 1.43     |
| 14  | g     | 820 | CLA  | C1B-C2B | 2.61 | 1.49        | 1.43     |
| 14  | A     | 825 | CLA  | C1B-C2B | 2.61 | 1.49        | 1.43     |
| 14  | a     | 806 | CLA  | C1B-C2B | 2.61 | 1.49        | 1.43     |
| 14  | B     | 850 | CLA  | C3B-C4B | 2.61 | 1.50        | 1.42     |
| 14  | A     | 807 | CLA  | C1B-C2B | 2.61 | 1.49        | 1.43     |
| 14  | N     | 819 | CLA  | C1B-C2B | 2.61 | 1.49        | 1.43     |
| 14  | A     | 834 | CLA  | C1B-C2B | 2.61 | 1.49        | 1.43     |
| 14  | A     | 827 | CLA  | C1B-C2B | 2.60 | 1.49        | 1.43     |
| 14  | b     | 829 | CLA  | C1B-C2B | 2.60 | 1.49        | 1.43     |
| 14  | g     | 819 | CLA  | C1B-C2B | 2.60 | 1.49        | 1.43     |
| 14  | G     | 827 | CLA  | C1B-C2B | 2.60 | 1.49        | 1.43     |
| 14  | a     | 811 | CLA  | C1B-C2B | 2.60 | 1.49        | 1.43     |
| 14  | n     | 826 | CLA  | C1B-C2B | 2.60 | 1.49        | 1.43     |
| 14  | n     | 808 | CLA  | C1B-C2B | 2.60 | 1.49        | 1.43     |
| 14  | n     | 818 | CLA  | C1B-C2B | 2.60 | 1.49        | 1.43     |
| 14  | B     | 805 | CLA  | C1B-C2B | 2.60 | 1.49        | 1.43     |
| 14  | N     | 821 | CLA  | C1B-C2B | 2.60 | 1.49        | 1.43     |
| 14  | N     | 841 | CLA  | C1B-C2B | 2.60 | 1.49        | 1.43     |
| 14  | n     | 802 | CLA  | C1B-C2B | 2.60 | 1.49        | 1.43     |
| 14  | A     | 830 | CLA  | C1B-C2B | 2.60 | 1.49        | 1.43     |
| 14  | B     | 826 | CLA  | C1B-C2B | 2.60 | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | n     | 832 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 14  | A     | 806 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 14  | a     | 836 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 14  | a     | 853 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 14  | N     | 812 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 14  | n     | 819 | CLA  | C1B-C2B | 2.60  | 1.49        | 1.43     |
| 14  | a     | 827 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 14  | N     | 851 | CLA  | C3B-C4B | 2.59  | 1.50        | 1.42     |
| 14  | g     | 828 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 14  | n     | 830 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 14  | w     | 204 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 14  | n     | 828 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 14  | a     | 823 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 14  | B     | 835 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 14  | G     | 826 | CLA  | C1B-C2B | 2.59  | 1.49        | 1.43     |
| 14  | G     | 803 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 14  | g     | 811 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 14  | b     | 833 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 14  | g     | 826 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 14  | n     | 836 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 14  | A     | 836 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 14  | g     | 809 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 14  | n     | 834 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 14  | B     | 818 | CLA  | C1B-C2B | 2.58  | 1.49        | 1.43     |
| 14  | b     | 830 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 14  | A     | 840 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 14  | b     | 833 | CLA  | C3B-C4B | 2.57  | 1.50        | 1.42     |
| 14  | g     | 804 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 14  | g     | 810 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 14  | G     | 820 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 14  | A     | 812 | CLA  | C1B-C2B | 2.57  | 1.49        | 1.43     |
| 14  | A     | 831 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 14  | B     | 803 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 14  | G     | 818 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 14  | G     | 831 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 14  | a     | 802 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 14  | l     | 203 | CLA  | C1B-C2B | 2.56  | 1.49        | 1.43     |
| 18  | a     | 850 | LHG  | O8-C6   | -2.55 | 1.39        | 1.45     |
| 14  | G     | 812 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 14  | G     | 829 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 14  | N     | 827 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 14  | g     | 817 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | B     | 829 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 14  | b     | 802 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 19  | G     | 851 | CL0  | CHA-CBD | -2.55 | 1.48        | 1.51     |
| 14  | a     | 852 | CLA  | C1B-C2B | 2.55  | 1.49        | 1.43     |
| 14  | B     | 837 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 14  | n     | 804 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 14  | G     | 801 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 14  | b     | 831 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 14  | a     | 829 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 14  | G     | 821 | CLA  | C1B-C2B | 2.54  | 1.49        | 1.43     |
| 14  | G     | 817 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 14  | G     | 812 | CLA  | C3B-C4B | 2.53  | 1.50        | 1.42     |
| 14  | g     | 829 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 14  | b     | 805 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 14  | N     | 805 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 14  | b     | 820 | CLA  | C1B-C2B | 2.53  | 1.49        | 1.43     |
| 14  | N     | 851 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 14  | B     | 850 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 14  | g     | 852 | CLA  | CMD-C2D | -2.52 | 1.45        | 1.50     |
| 14  | W     | 203 | CLA  | C1B-C2B | 2.52  | 1.49        | 1.43     |
| 14  | A     | 806 | CLA  | C3B-C4B | 2.50  | 1.50        | 1.42     |
| 14  | G     | 852 | CLA  | C4B-NB  | 2.50  | 1.41        | 1.37     |
| 14  | G     | 815 | CLA  | C3B-C4B | 2.50  | 1.50        | 1.42     |
| 17  | I     | 102 | BCR  | C30-C25 | -2.50 | 1.50        | 1.53     |
| 14  | A     | 855 | CLA  | C4B-NB  | 2.50  | 1.41        | 1.37     |
| 14  | g     | 853 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 14  | G     | 806 | CLA  | C3B-C4B | 2.50  | 1.50        | 1.42     |
| 14  | A     | 818 | CLA  | C1B-C2B | 2.50  | 1.49        | 1.43     |
| 14  | n     | 832 | CLA  | C3B-C4B | 2.50  | 1.50        | 1.42     |
| 14  | B     | 804 | CLA  | C3B-C4B | 2.49  | 1.50        | 1.42     |
| 18  | g     | 850 | LHG  | O8-C6   | -2.49 | 1.39        | 1.45     |
| 14  | A     | 855 | CLA  | MG-NB   | -2.49 | 2.00        | 2.05     |
| 14  | g     | 852 | CLA  | CMB-C2B | -2.49 | 1.45        | 1.50     |
| 14  | A     | 801 | CLA  | C1B-C2B | 2.48  | 1.49        | 1.43     |
| 18  | A     | 850 | LHG  | O7-C5   | -2.48 | 1.40        | 1.46     |
| 14  | N     | 832 | CLA  | CMD-C2D | -2.48 | 1.45        | 1.50     |
| 14  | A     | 826 | CLA  | C3B-C4B | 2.47  | 1.49        | 1.42     |
| 14  | g     | 810 | CLA  | C3B-C4B | 2.47  | 1.49        | 1.42     |
| 14  | N     | 803 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 14  | N     | 801 | CLA  | C1B-C2B | 2.47  | 1.48        | 1.43     |
| 14  | n     | 804 | CLA  | CHC-C1C | 2.46  | 1.43        | 1.38     |
| 14  | b     | 830 | CLA  | CMD-C2D | -2.46 | 1.45        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | G     | 850  | LHG  | O8-C6   | -2.46 | 1.39        | 1.45     |
| 14  | A     | 812  | CLA  | C3B-C4B | 2.46  | 1.49        | 1.42     |
| 14  | N     | 814  | CLA  | C3B-C4B | 2.46  | 1.49        | 1.42     |
| 14  | n     | 812  | CLA  | C3B-C4B | 2.45  | 1.49        | 1.42     |
| 18  | a     | 849  | LHG  | O8-C6   | -2.45 | 1.39        | 1.45     |
| 14  | B     | 820  | CLA  | C3B-C4B | 2.45  | 1.49        | 1.42     |
| 14  | a     | 805  | CLA  | C3B-C4B | 2.45  | 1.49        | 1.42     |
| 14  | A     | 855  | CLA  | C1B-C2B | 2.45  | 1.48        | 1.43     |
| 14  | N     | 805  | CLA  | CHC-C1C | 2.45  | 1.43        | 1.38     |
| 18  | A     | 851  | LHG  | O8-C6   | -2.44 | 1.39        | 1.45     |
| 14  | g     | 805  | CLA  | C3B-C4B | 2.44  | 1.49        | 1.42     |
| 14  | g     | 804  | CLA  | C3B-C4B | 2.44  | 1.49        | 1.42     |
| 18  | G     | 849  | LHG  | O8-C6   | -2.44 | 1.39        | 1.45     |
| 14  | N     | 827  | CLA  | C3B-C4B | 2.44  | 1.49        | 1.42     |
| 14  | N     | 803  | CLA  | CHC-C1C | 2.44  | 1.43        | 1.38     |
| 14  | n     | 810  | CLA  | C3B-C4B | 2.44  | 1.49        | 1.42     |
| 18  | g     | 849  | LHG  | O8-C6   | -2.43 | 1.39        | 1.45     |
| 17  | n     | 847  | BCR  | C30-C25 | -2.43 | 1.50        | 1.53     |
| 14  | N     | 821  | CLA  | C3B-C4B | 2.43  | 1.49        | 1.42     |
| 18  | X     | 1702 | LHG  | O8-C6   | -2.43 | 1.39        | 1.45     |
| 14  | g     | 854  | CLA  | C1B-C2B | 2.43  | 1.48        | 1.43     |
| 14  | b     | 823  | CLA  | C3B-C4B | 2.43  | 1.49        | 1.42     |
| 14  | g     | 852  | CLA  | MG-NB   | -2.42 | 2.01        | 2.05     |
| 14  | b     | 841  | CLA  | CMB-C2B | -2.42 | 1.45        | 1.50     |
| 14  | G     | 833  | CLA  | C3B-C4B | 2.42  | 1.49        | 1.42     |
| 14  | N     | 803  | CLA  | C3B-C4B | 2.42  | 1.49        | 1.42     |
| 14  | B     | 803  | CLA  | C3B-C4B | 2.42  | 1.49        | 1.42     |
| 18  | a     | 850  | LHG  | O7-C5   | -2.42 | 1.40        | 1.46     |
| 14  | B     | 803  | CLA  | CHC-C1C | 2.41  | 1.43        | 1.38     |
| 14  | G     | 840  | CLA  | C3B-C4B | 2.41  | 1.49        | 1.42     |
| 14  | a     | 821  | CLA  | C3B-C4B | 2.41  | 1.49        | 1.42     |
| 17  | g     | 847  | BCR  | C1-C6   | -2.41 | 1.50        | 1.53     |
| 14  | B     | 837  | CLA  | CHC-C1C | 2.41  | 1.43        | 1.38     |
| 14  | B     | 820  | CLA  | CHC-C1C | 2.41  | 1.43        | 1.38     |
| 18  | A     | 850  | LHG  | O8-C6   | -2.41 | 1.39        | 1.45     |
| 14  | A     | 836  | CLA  | C3B-C4B | 2.41  | 1.49        | 1.42     |
| 14  | b     | 802  | CLA  | C3B-C4B | 2.41  | 1.49        | 1.42     |
| 14  | H     | 1701 | CLA  | C3B-C4B | 2.41  | 1.49        | 1.42     |
| 14  | b     | 811  | CLA  | C3B-C4B | 2.41  | 1.49        | 1.42     |
| 14  | N     | 812  | CLA  | C3B-C4B | 2.40  | 1.49        | 1.42     |
| 14  | A     | 853  | CLA  | C3B-C4B | 2.40  | 1.49        | 1.42     |
| 14  | g     | 828  | CLA  | CMB-C2B | -2.40 | 1.45        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 821  | CLA  | C3B-C4B | 2.40  | 1.49        | 1.42     |
| 14  | a     | 819  | CLA  | C3B-C4B | 2.40  | 1.49        | 1.42     |
| 14  | B     | 813  | CLA  | C3B-C4B | 2.40  | 1.49        | 1.42     |
| 14  | A     | 807  | CLA  | C3B-C4B | 2.40  | 1.49        | 1.42     |
| 14  | b     | 824  | CLA  | C3B-C4B | 2.40  | 1.49        | 1.42     |
| 14  | b     | 805  | CLA  | C3B-C4B | 2.39  | 1.49        | 1.42     |
| 18  | m     | 101  | LHG  | O8-C6   | -2.39 | 1.39        | 1.45     |
| 14  | G     | 826  | CLA  | C3B-C4B | 2.39  | 1.49        | 1.42     |
| 14  | G     | 803  | CLA  | C3B-C4B | 2.39  | 1.49        | 1.42     |
| 14  | N     | 834  | CLA  | CMD-C2D | -2.39 | 1.45        | 1.50     |
| 14  | B     | 808  | CLA  | C3B-C4B | 2.39  | 1.49        | 1.42     |
| 14  | a     | 809  | CLA  | C3B-C4B | 2.39  | 1.49        | 1.42     |
| 14  | A     | 803  | CLA  | C3B-C4B | 2.39  | 1.49        | 1.42     |
| 14  | g     | 811  | CLA  | C3B-C4B | 2.39  | 1.49        | 1.42     |
| 14  | b     | 820  | CLA  | C3B-C4B | 2.39  | 1.49        | 1.42     |
| 18  | G     | 850  | LHG  | O7-C5   | -2.39 | 1.41        | 1.46     |
| 14  | g     | 854  | CLA  | CMB-C2B | -2.39 | 1.45        | 1.50     |
| 14  | B     | 805  | CLA  | CHC-C1C | 2.38  | 1.43        | 1.38     |
| 14  | l     | 204  | CLA  | C3B-C4B | 2.38  | 1.49        | 1.42     |
| 14  | G     | 852  | CLA  | MG-NB   | -2.38 | 2.01        | 2.05     |
| 14  | X     | 1701 | CLA  | C3B-C4B | 2.38  | 1.49        | 1.42     |
| 17  | a     | 847  | BCR  | C30-C25 | -2.38 | 1.50        | 1.53     |
| 14  | B     | 837  | CLA  | C3B-C4B | 2.38  | 1.49        | 1.42     |
| 18  | v     | 102  | LHG  | O8-C6   | -2.38 | 1.39        | 1.45     |
| 14  | g     | 840  | CLA  | C3B-C4B | 2.38  | 1.49        | 1.42     |
| 14  | a     | 815  | CLA  | C3B-C4B | 2.38  | 1.49        | 1.42     |
| 18  | X     | 1702 | LHG  | O7-C5   | -2.38 | 1.41        | 1.46     |
| 14  | G     | 820  | CLA  | C3B-C4B | 2.38  | 1.49        | 1.42     |
| 14  | b     | 832  | CLA  | C3B-C4B | 2.38  | 1.49        | 1.42     |
| 14  | B     | 811  | CLA  | C3B-C4B | 2.38  | 1.49        | 1.42     |
| 18  | g     | 850  | LHG  | O7-C5   | -2.38 | 1.41        | 1.46     |
| 14  | B     | 805  | CLA  | C3B-C4B | 2.38  | 1.49        | 1.42     |
| 14  | f     | 202  | CLA  | C3B-C4B | 2.38  | 1.49        | 1.42     |
| 14  | b     | 820  | CLA  | CHC-C1C | 2.38  | 1.43        | 1.38     |
| 14  | g     | 815  | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 14  | a     | 802  | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 14  | n     | 814  | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 14  | a     | 837  | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 14  | g     | 802  | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 14  | T     | 101  | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 14  | n     | 802  | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 14  | G     | 803  | CLA  | CHC-C1C | 2.37  | 1.43        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | W     | 203 | CLA  | CHC-C1C | 2.37  | 1.43        | 1.38     |
| 14  | b     | 824 | CLA  | CHC-C1C | 2.37  | 1.43        | 1.38     |
| 14  | n     | 822 | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 14  | a     | 836 | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 14  | B     | 830 | CLA  | CMD-C2D | -2.37 | 1.45        | 1.50     |
| 14  | j     | 101 | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 14  | a     | 854 | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 14  | g     | 819 | CLA  | C3B-C4B | 2.37  | 1.49        | 1.42     |
| 18  | S     | 202 | LHG  | O7-C5   | -2.37 | 1.41        | 1.46     |
| 14  | B     | 817 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 14  | J     | 101 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 14  | a     | 802 | CLA  | CHC-C1C | 2.36  | 1.43        | 1.38     |
| 14  | F     | 202 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 14  | n     | 852 | CLA  | CHC-C1C | 2.36  | 1.43        | 1.38     |
| 14  | A     | 833 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 14  | N     | 837 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 18  | S     | 202 | LHG  | O8-C6   | -2.36 | 1.39        | 1.45     |
| 14  | N     | 805 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 14  | g     | 839 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 14  | g     | 809 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 18  | v     | 102 | LHG  | O8-C23  | 2.36  | 1.40        | 1.33     |
| 14  | B     | 830 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 14  | n     | 840 | CLA  | CMB-C2B | -2.36 | 1.45        | 1.50     |
| 14  | G     | 811 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 14  | G     | 838 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 18  | G     | 849 | LHG  | O7-C5   | -2.36 | 1.41        | 1.46     |
| 14  | b     | 837 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 14  | g     | 813 | CLA  | C3B-C4B | 2.36  | 1.49        | 1.42     |
| 14  | B     | 815 | CLA  | CHC-C1C | 2.36  | 1.43        | 1.38     |
| 14  | A     | 826 | CLA  | CHC-C1C | 2.36  | 1.43        | 1.38     |
| 14  | A     | 805 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | A     | 831 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | a     | 832 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | b     | 812 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | A     | 825 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 18  | v     | 102 | LHG  | O7-C5   | -2.35 | 1.41        | 1.46     |
| 14  | s     | 202 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | u     | 101 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 18  | S     | 202 | LHG  | O8-C23  | 2.35  | 1.40        | 1.33     |
| 14  | W     | 203 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | N     | 801 | CLA  | CMB-C2B | -2.35 | 1.45        | 1.50     |
| 14  | B     | 834 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | G     | 826 | CLA  | CHC-C1C | 2.35  | 1.43        | 1.38     |
| 14  | N     | 822 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | A     | 818 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | N     | 827 | CLA  | CHC-C1C | 2.35  | 1.43        | 1.38     |
| 14  | n     | 816 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | A     | 813 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | A     | 837 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 18  | a     | 849 | LHG  | O7-C5   | -2.35 | 1.41        | 1.46     |
| 14  | U     | 101 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | G     | 829 | CLA  | CMB-C2B | -2.35 | 1.46        | 1.50     |
| 14  | N     | 801 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | n     | 821 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | g     | 821 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | n     | 829 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | g     | 802 | CLA  | CHC-C1C | 2.35  | 1.43        | 1.38     |
| 14  | g     | 826 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | A     | 811 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | A     | 841 | CLA  | C3B-C4B | 2.35  | 1.49        | 1.42     |
| 14  | G     | 852 | CLA  | C1B-C2B | 2.35  | 1.48        | 1.43     |
| 14  | b     | 808 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 14  | b     | 827 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 14  | N     | 826 | CLA  | CMC-C2C | -2.34 | 1.46        | 1.50     |
| 14  | g     | 819 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.38     |
| 14  | n     | 815 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 14  | a     | 804 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 14  | a     | 812 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 14  | N     | 825 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 14  | B     | 820 | CLA  | C1B-C2B | 2.34  | 1.48        | 1.43     |
| 14  | N     | 831 | CLA  | CMD-C2D | -2.34 | 1.46        | 1.50     |
| 14  | G     | 853 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 14  | B     | 839 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 14  | b     | 812 | CLA  | CMB-C2B | -2.34 | 1.46        | 1.50     |
| 14  | n     | 819 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 14  | a     | 825 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 14  | A     | 803 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.38     |
| 14  | N     | 806 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.38     |
| 14  | b     | 853 | CLA  | CHC-C1C | 2.34  | 1.43        | 1.38     |
| 14  | N     | 809 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 18  | g     | 849 | LHG  | O7-C5   | -2.34 | 1.41        | 1.46     |
| 14  | G     | 810 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 14  | B     | 836 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 14  | G     | 831 | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 18  | A     | 851  | LHG  | O7-C5   | -2.34 | 1.41        | 1.46     |
| 14  | N     | 806  | CLA  | C3B-C4B | 2.34  | 1.49        | 1.42     |
| 14  | k     | 101  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | b     | 853  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | G     | 814  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | b     | 826  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | g     | 838  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | l     | 203  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | n     | 832  | CLA  | CHC-C1C | 2.33  | 1.43        | 1.38     |
| 14  | n     | 802  | CLA  | CHC-C1C | 2.33  | 1.43        | 1.38     |
| 14  | B     | 806  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | B     | 840  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | B     | 827  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | J     | 102  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | b     | 834  | CLA  | CHC-C1C | 2.33  | 1.43        | 1.38     |
| 14  | A     | 854  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | G     | 801  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | N     | 807  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | g     | 801  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | a     | 838  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | b     | 815  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | b     | 825  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 18  | X     | 1702 | LHG  | O8-C23  | 2.33  | 1.40        | 1.33     |
| 14  | N     | 825  | CLA  | CHC-C1C | 2.33  | 1.43        | 1.38     |
| 14  | A     | 853  | CLA  | CHC-C1C | 2.33  | 1.43        | 1.38     |
| 14  | g     | 834  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | F     | 201  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | N     | 807  | CLA  | CHC-C1C | 2.33  | 1.43        | 1.38     |
| 14  | N     | 838  | CLA  | CHC-C1C | 2.33  | 1.43        | 1.38     |
| 14  | N     | 851  | CLA  | CHC-C1C | 2.33  | 1.43        | 1.38     |
| 14  | h     | 1701 | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | n     | 820  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | n     | 834  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | n     | 823  | CLA  | C3B-C4B | 2.33  | 1.49        | 1.42     |
| 14  | G     | 816  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | A     | 834  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | A     | 813  | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 14  | g     | 825  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | g     | 836  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | a     | 826  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | a     | 828  | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 14  | N     | 842  | CLA  | CMB-C2B | -2.32 | 1.46        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | t     | 101  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | b     | 834  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | a     | 854  | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 14  | N     | 816  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | b     | 822  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | K     | 101  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | x     | 1701 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | b     | 836  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | A     | 804  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | N     | 831  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | a     | 833  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | a     | 852  | CLA  | MG-NB   | -2.32 | 2.01        | 2.05     |
| 14  | g     | 854  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | A     | 839  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | a     | 811  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | N     | 838  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | L     | 1503 | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | a     | 814  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | B     | 809  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | a     | 813  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | G     | 820  | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 14  | a     | 828  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | g     | 824  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | A     | 831  | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 14  | A     | 838  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | b     | 809  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | N     | 841  | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 14  | g     | 825  | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 18  | m     | 101  | LHG  | O8-C23  | 2.32  | 1.40        | 1.33     |
| 14  | g     | 852  | CLA  | CMC-C2C | -2.32 | 1.46        | 1.50     |
| 14  | B     | 815  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | a     | 806  | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 14  | G     | 807  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | T     | 102  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | b     | 803  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | G     | 825  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | N     | 841  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | n     | 852  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | n     | 838  | CLA  | C3B-C4B | 2.32  | 1.49        | 1.42     |
| 14  | g     | 803  | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 14  | a     | 819  | CLA  | CHC-C1C | 2.32  | 1.43        | 1.38     |
| 14  | a     | 803  | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | G     | 817 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 14  | n     | 808 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | g     | 837 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | A     | 827 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | B     | 840 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 14  | a     | 853 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 14  | b     | 815 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 14  | N     | 833 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 14  | N     | 813 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | b     | 835 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | a     | 807 | CLA  | CMD-C2D | -2.31 | 1.46        | 1.50     |
| 14  | A     | 801 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | N     | 821 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 18  | A     | 850 | LHG  | O8-C23  | 2.31  | 1.40        | 1.33     |
| 14  | J     | 102 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 14  | b     | 851 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | a     | 804 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 14  | G     | 821 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | S     | 203 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | b     | 830 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | b     | 825 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 14  | n     | 824 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | n     | 822 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 14  | n     | 837 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 17  | a     | 847 | BCR  | C1-C6   | -2.31 | 1.50        | 1.53     |
| 14  | u     | 102 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | b     | 838 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | g     | 814 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | n     | 835 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | a     | 803 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 14  | a     | 825 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 14  | A     | 826 | CLA  | CMC-C2C | -2.31 | 1.46        | 1.50     |
| 14  | N     | 804 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 14  | g     | 804 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 14  | b     | 802 | CLA  | CMB-C2B | -2.31 | 1.46        | 1.50     |
| 14  | U     | 102 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 18  | g     | 849 | LHG  | O8-C23  | 2.31  | 1.40        | 1.33     |
| 14  | N     | 817 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | A     | 819 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | t     | 102 | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | A     | 807 | CLA  | CHC-C1C | 2.31  | 1.43        | 1.38     |
| 14  | G     | 830 | CLA  | CMD-C2D | -2.31 | 1.46        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 857  | CLA  | C3B-C4B | 2.31  | 1.49        | 1.42     |
| 14  | n     | 833  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | B     | 823  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | A     | 809  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | b     | 832  | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 14  | b     | 803  | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 14  | G     | 839  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | n     | 831  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | w     | 203  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | g     | 818  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | B     | 826  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | A     | 820  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | j     | 102  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | b     | 817  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | g     | 808  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | l     | 203  | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 14  | N     | 840  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | N     | 818  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | N     | 835  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | b     | 813  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | B     | 836  | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 14  | N     | 810  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | L     | 1502 | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | G     | 811  | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 14  | N     | 828  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | n     | 814  | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 14  | A     | 810  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | n     | 833  | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 18  | G     | 849  | LHG  | O7-C7   | 2.30  | 1.40        | 1.34     |
| 14  | N     | 804  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | W     | 204  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | g     | 833  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | N     | 833  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | b     | 823  | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 14  | a     | 824  | CLA  | C3B-C4B | 2.30  | 1.49        | 1.42     |
| 14  | n     | 829  | CLA  | CHC-C1C | 2.30  | 1.43        | 1.38     |
| 14  | B     | 841  | CLA  | CMB-C2B | -2.29 | 1.46        | 1.50     |
| 14  | a     | 816  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | N     | 816  | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 14  | n     | 815  | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 14  | n     | 834  | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 14  | A     | 818  | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 818  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | w     | 205  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | N     | 818  | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 14  | N     | 824  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | B     | 812  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 18  | m     | 101  | LHG  | O7-C7   | 2.29  | 1.40        | 1.34     |
| 14  | B     | 827  | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 14  | n     | 803  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | G     | 819  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | b     | 839  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 18  | m     | 101  | LHG  | O7-C5   | -2.29 | 1.41        | 1.46     |
| 14  | n     | 829  | CLA  | CMD-C2D | -2.29 | 1.46        | 1.50     |
| 14  | n     | 823  | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 14  | g     | 806  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | s     | 201  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | a     | 801  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | a     | 808  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | g     | 813  | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 14  | w     | 204  | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 14  | b     | 840  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | a     | 817  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | g     | 816  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | a     | 820  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | l     | 202  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | n     | 818  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | G     | 804  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | B     | 816  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | H     | 1701 | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 14  | T     | 102  | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 14  | A     | 820  | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 14  | B     | 824  | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 14  | g     | 832  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | n     | 850  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | B     | 807  | CLA  | CHC-C1C | 2.29  | 1.43        | 1.38     |
| 14  | B     | 832  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | a     | 853  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | A     | 814  | CLA  | C3B-C4B | 2.29  | 1.49        | 1.42     |
| 14  | g     | 803  | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | n     | 811  | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | g     | 812  | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | a     | 809  | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | A     | 808  | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | G     | 810 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | b     | 826 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | a     | 831 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | G     | 827 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | F     | 201 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | G     | 825 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | w     | 204 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | B     | 807 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | B     | 826 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 18  | a     | 849 | LHG  | O7-C7   | 2.28  | 1.40        | 1.34     |
| 14  | A     | 816 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | a     | 806 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | A     | 829 | CLA  | CMB-C2B | -2.28 | 1.46        | 1.50     |
| 14  | j     | 102 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | G     | 813 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | g     | 820 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | n     | 804 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | b     | 831 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 18  | A     | 851 | LHG  | O8-C23  | 2.28  | 1.40        | 1.33     |
| 14  | G     | 836 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | n     | 837 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | B     | 823 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | G     | 807 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | b     | 822 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | G     | 821 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | n     | 819 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | w     | 205 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | A     | 854 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | b     | 806 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | n     | 807 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | A     | 815 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | b     | 807 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | g     | 826 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | g     | 830 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | g     | 833 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | b     | 816 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 18  | G     | 849 | LHG  | O8-C23  | 2.28  | 1.40        | 1.33     |
| 14  | n     | 831 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | G     | 822 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | G     | 802 | CLA  | C3B-C4B | 2.28  | 1.49        | 1.42     |
| 14  | N     | 819 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | n     | 824 | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | t     | 101  | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 14  | j     | 101  | CLA  | CHC-C1C | 2.28  | 1.43        | 1.38     |
| 18  | G     | 850  | LHG  | O7-C7   | 2.28  | 1.40        | 1.34     |
| 14  | B     | 824  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 18  | S     | 202  | LHG  | O7-C7   | 2.27  | 1.40        | 1.34     |
| 18  | A     | 851  | LHG  | O7-C7   | 2.27  | 1.40        | 1.34     |
| 14  | b     | 828  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | B     | 821  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | a     | 810  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | L     | 1502 | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 14  | N     | 823  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | a     | 827  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | f     | 201  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | A     | 802  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | b     | 816  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | G     | 809  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | A     | 835  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | a     | 820  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 14  | b     | 817  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 14  | b     | 833  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 14  | B     | 825  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 14  | b     | 807  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 14  | g     | 836  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 14  | n     | 803  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 14  | n     | 828  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | b     | 814  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | b     | 830  | CLA  | CMB-C2B | -2.27 | 1.46        | 1.50     |
| 14  | n     | 821  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 14  | B     | 834  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 14  | B     | 810  | CLA  | CMB-C2B | -2.27 | 1.46        | 1.50     |
| 14  | G     | 814  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 14  | S     | 201  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 14  | n     | 835  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 18  | g     | 849  | LHG  | O7-C7   | 2.27  | 1.40        | 1.34     |
| 18  | a     | 849  | LHG  | O8-C23  | 2.27  | 1.40        | 1.33     |
| 14  | N     | 829  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | n     | 805  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | B     | 838  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | b     | 836  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 14  | N     | 836  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | g     | 835  | CLA  | MG-NB   | -2.27 | 2.01        | 2.05     |
| 14  | G     | 817  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | A     | 823  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | B     | 822  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | G     | 809  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 14  | a     | 834  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 18  | v     | 102  | LHG  | O7-C7   | 2.27  | 1.40        | 1.34     |
| 14  | A     | 834  | CLA  | CMB-C2B | -2.27 | 1.46        | 1.50     |
| 14  | g     | 840  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 14  | A     | 806  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 14  | G     | 828  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | a     | 834  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | G     | 806  | CLA  | CHC-C1C | 2.27  | 1.43        | 1.38     |
| 14  | b     | 819  | CLA  | C3B-C4B | 2.27  | 1.49        | 1.42     |
| 14  | G     | 824  | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 14  | N     | 837  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | B     | 818  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | B     | 821  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | B     | 830  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | N     | 839  | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 14  | a     | 830  | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 14  | u     | 101  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | a     | 829  | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 14  | A     | 857  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | G     | 804  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | B     | 806  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | b     | 829  | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 14  | n     | 806  | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 14  | A     | 841  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 18  | g     | 850  | LHG  | O8-C23  | 2.26  | 1.39        | 1.33     |
| 14  | S     | 201  | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 14  | B     | 819  | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 14  | a     | 810  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | n     | 836  | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 14  | g     | 806  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | b     | 837  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 18  | G     | 850  | LHG  | O8-C23  | 2.26  | 1.39        | 1.33     |
| 14  | J     | 101  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | a     | 829  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | x     | 1701 | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | N     | 820  | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 14  | n     | 806  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | A     | 821  | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 14  | B     | 825  | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | n     | 816  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | A     | 855  | CLA  | CMD-C2D | -2.26 | 1.46        | 1.50     |
| 20  | h     | 1702 | SQD  | O9-S    | 2.26  | 1.51        | 1.45     |
| 14  | n     | 836  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 20  | l     | 201  | SQD  | O9-S    | 2.26  | 1.51        | 1.45     |
| 20  | b     | 801  | SQD  | O9-S    | 2.26  | 1.51        | 1.45     |
| 14  | g     | 817  | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 14  | n     | 808  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | a     | 826  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | b     | 821  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | a     | 822  | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 14  | g     | 837  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | l     | 204  | CLA  | CHC-C1C | 2.26  | 1.43        | 1.38     |
| 14  | a     | 840  | CLA  | C3B-C4B | 2.26  | 1.49        | 1.42     |
| 14  | G     | 852  | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 14  | g     | 853  | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 14  | s     | 202  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | N     | 826  | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 14  | A     | 840  | CLA  | MG-NB   | -2.25 | 2.01        | 2.05     |
| 14  | U     | 101  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | U     | 102  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | B     | 839  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | B     | 818  | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 14  | N     | 813  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | n     | 811  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | a     | 833  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | n     | 826  | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 14  | b     | 810  | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 14  | n     | 805  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | N     | 830  | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 14  | A     | 805  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | G     | 813  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | g     | 812  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | n     | 838  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | n     | 830  | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 14  | B     | 835  | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 14  | g     | 834  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | a     | 836  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | G     | 852  | CLA  | CMB-C2B | -2.25 | 1.46        | 1.50     |
| 14  | N     | 832  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | N     | 835  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | W     | 204  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 802  | CLA  | CMD-C2D | -2.25 | 1.46        | 1.50     |
| 14  | A     | 810  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | n     | 839  | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 14  | w     | 203  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | G     | 826  | CLA  | CMC-C2C | -2.25 | 1.46        | 1.50     |
| 14  | G     | 828  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | A     | 839  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | b     | 827  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | n     | 809  | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 14  | b     | 809  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 17  | g     | 847  | BCR  | C30-C25 | -2.25 | 1.50        | 1.53     |
| 14  | N     | 832  | CLA  | C3B-C4B | 2.25  | 1.49        | 1.42     |
| 14  | B     | 817  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | a     | 816  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | b     | 835  | CLA  | CHC-C1C | 2.25  | 1.43        | 1.38     |
| 14  | g     | 816  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | h     | 1701 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | n     | 825  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | t     | 102  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | B     | 831  | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 14  | N     | 811  | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 14  | b     | 841  | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 14  | T     | 101  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | A     | 801  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 20  | n     | 801  | SQD  | O9-S    | 2.24  | 1.51        | 1.45     |
| 14  | L     | 1503 | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | n     | 827  | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 14  | G     | 833  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | n     | 830  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | A     | 828  | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 14  | N     | 822  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | G     | 835  | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 14  | a     | 835  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | N     | 808  | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 14  | n     | 817  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | g     | 827  | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 14  | G     | 837  | CLA  | MG-NB   | -2.24 | 2.01        | 2.05     |
| 14  | G     | 805  | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 14  | u     | 102  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | B     | 850  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 18  | g     | 850  | LHG  | O7-C7   | 2.24  | 1.40        | 1.34     |
| 14  | g     | 809  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | g     | 810  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | N     | 811  | CLA  | CMB-C2B | -2.24 | 1.46        | 1.50     |
| 14  | G     | 853  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | N     | 829  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | A     | 811  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | G     | 827  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | g     | 838  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | A     | 830  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | a     | 815  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 18  | X     | 1702 | LHG  | O7-C7   | 2.24  | 1.40        | 1.34     |
| 14  | n     | 825  | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 14  | A     | 830  | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 14  | B     | 828  | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 14  | B     | 816  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | b     | 819  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | n     | 826  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | b     | 813  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | B     | 833  | CLA  | C3B-C4B | 2.24  | 1.49        | 1.42     |
| 14  | N     | 817  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | N     | 823  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | n     | 839  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | b     | 804  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | g     | 818  | CLA  | CHC-C1C | 2.24  | 1.43        | 1.38     |
| 14  | A     | 840  | CLA  | CMB-C2B | -2.23 | 1.46        | 1.50     |
| 14  | G     | 823  | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 14  | b     | 818  | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 14  | B     | 811  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | a     | 827  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | W     | 202  | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 14  | A     | 840  | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 14  | B     | 829  | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 14  | b     | 818  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | G     | 831  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | S     | 203  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | A     | 809  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | B     | 835  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | G     | 839  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | G     | 808  | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 14  | N     | 815  | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 14  | G     | 824  | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 14  | N     | 839  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | B     | 831  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 824  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | B     | 813  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | b     | 828  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | g     | 854  | CLA  | CMD-C2D | -2.23 | 1.46        | 1.50     |
| 14  | A     | 833  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | a     | 812  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | b     | 839  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | a     | 837  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | a     | 852  | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 17  | N     | 853  | BCR  | C30-C25 | -2.23 | 1.50        | 1.53     |
| 14  | g     | 831  | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 14  | A     | 822  | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 14  | a     | 840  | CLA  | CMB-C2B | -2.23 | 1.46        | 1.50     |
| 14  | a     | 818  | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 14  | n     | 812  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | a     | 830  | CLA  | CHC-C1C | 2.23  | 1.43        | 1.38     |
| 14  | a     | 835  | CLA  | MG-NB   | -2.23 | 2.01        | 2.05     |
| 14  | A     | 829  | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 14  | B     | 814  | CLA  | C3B-C4B | 2.23  | 1.49        | 1.42     |
| 14  | n     | 820  | CLA  | CHC-C1C | 2.23  | 1.42        | 1.38     |
| 20  | B     | 801  | SQD  | O9-S    | 2.23  | 1.51        | 1.45     |
| 14  | K     | 101  | CLA  | CHC-C1C | 2.23  | 1.42        | 1.38     |
| 14  | n     | 804  | CLA  | CMC-C2C | -2.23 | 1.46        | 1.50     |
| 14  | G     | 815  | CLA  | CHC-C1C | 2.23  | 1.42        | 1.38     |
| 14  | n     | 827  | CLA  | CHC-C1C | 2.23  | 1.42        | 1.38     |
| 14  | A     | 815  | CLA  | CHC-C1C | 2.23  | 1.42        | 1.38     |
| 14  | G     | 835  | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | g     | 824  | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | a     | 817  | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 20  | x     | 1702 | SQD  | O9-S    | 2.22  | 1.51        | 1.45     |
| 14  | b     | 838  | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | G     | 834  | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 14  | g     | 820  | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | s     | 201  | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | A     | 825  | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | f     | 201  | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | g     | 829  | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 14  | a     | 821  | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | a     | 827  | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 14  | n     | 813  | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 14  | a     | 852  | CLA  | CMB-C2B | -2.22 | 1.46        | 1.50     |
| 14  | b     | 806  | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | G     | 808 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 14  | A     | 836 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | a     | 814 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | A     | 821 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | b     | 808 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | N     | 809 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | g     | 814 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | g     | 822 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 14  | G     | 830 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 14  | N     | 828 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | n     | 817 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 14  | g     | 831 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | A     | 832 | CLA  | C3B-C4B | 2.22  | 1.49        | 1.42     |
| 14  | b     | 814 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | B     | 812 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | F     | 202 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | b     | 831 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | n     | 836 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 14  | N     | 826 | CLA  | CMD-C2D | -2.22 | 1.46        | 1.50     |
| 14  | N     | 824 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | A     | 832 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | B     | 829 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 14  | a     | 801 | CLA  | CHC-C1C | 2.22  | 1.42        | 1.38     |
| 20  | w     | 202 | SQD  | O9-S    | 2.22  | 1.51        | 1.45     |
| 14  | N     | 819 | CLA  | MG-NB   | -2.22 | 2.01        | 2.05     |
| 14  | N     | 801 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | B     | 818 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 14  | B     | 829 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 14  | A     | 827 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | G     | 819 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | G     | 836 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | a     | 818 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 14  | g     | 823 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 14  | b     | 804 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 14  | G     | 805 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | a     | 822 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | a     | 838 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | g     | 829 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 14  | N     | 831 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | N     | 821 | CLA  | CMB-C2B | -2.21 | 1.46        | 1.50     |
| 14  | B     | 828 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | a     | 852 | CLA  | CMD-C2D | -2.21 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | a     | 808 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | G     | 818 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | G     | 829 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 18  | A     | 850 | LHG  | O7-C7   | 2.21  | 1.40        | 1.34     |
| 14  | A     | 828 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | B     | 808 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | N     | 836 | CLA  | CMB-C2B | -2.21 | 1.46        | 1.50     |
| 14  | g     | 852 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 14  | G     | 801 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | a     | 835 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 14  | G     | 832 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | N     | 808 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | N     | 840 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | g     | 801 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | g     | 817 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | A     | 817 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | A     | 830 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 14  | n     | 826 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 14  | G     | 802 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | A     | 819 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | a     | 803 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 14  | a     | 839 | CLA  | C3B-C4B | 2.21  | 1.49        | 1.42     |
| 14  | A     | 840 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | B     | 806 | CLA  | MG-NB   | -2.21 | 2.01        | 2.05     |
| 14  | G     | 816 | CLA  | CHC-C1C | 2.21  | 1.42        | 1.38     |
| 14  | g     | 808 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | A     | 817 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 14  | G     | 840 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | g     | 815 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | A     | 824 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 14  | B     | 841 | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 14  | g     | 835 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | A     | 838 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | a     | 805 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | A     | 834 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | g     | 840 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 14  | g     | 854 | CLA  | MG-NB   | -2.20 | 2.01        | 2.05     |
| 14  | G     | 822 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | n     | 807 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | n     | 813 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | a     | 831 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | N     | 816 | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | N     | 810  | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | A     | 804  | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | n     | 840  | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 14  | g     | 853  | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | l     | 202  | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | G     | 852  | CLA  | CMD-C2D | -2.20 | 1.46        | 1.50     |
| 14  | g     | 817  | CLA  | CMB-C2B | -2.20 | 1.46        | 1.50     |
| 14  | g     | 835  | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 14  | A     | 835  | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 18  | a     | 850  | LHG  | O7-C7   | 2.20  | 1.40        | 1.34     |
| 14  | g     | 807  | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 14  | X     | 1701 | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 17  | G     | 847  | BCR  | C30-C25 | -2.20 | 1.51        | 1.53     |
| 14  | N     | 820  | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | B     | 819  | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | g     | 828  | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 14  | N     | 819  | CLA  | C3B-C4B | 2.20  | 1.49        | 1.42     |
| 14  | N     | 826  | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | b     | 811  | CLA  | CHC-C1C | 2.20  | 1.42        | 1.38     |
| 14  | g     | 829  | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 14  | A     | 808  | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 14  | a     | 823  | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 14  | n     | 828  | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 14  | G     | 826  | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 14  | G     | 831  | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 14  | n     | 803  | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 14  | n     | 830  | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |
| 14  | g     | 821  | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 14  | G     | 829  | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 14  | N     | 842  | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 14  | B     | 835  | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |
| 14  | g     | 809  | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 14  | b     | 810  | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |
| 14  | G     | 836  | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 14  | n     | 813  | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 14  | n     | 807  | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 14  | b     | 818  | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 20  | H     | 1702 | SQD  | O9-S    | 2.19  | 1.51        | 1.45     |
| 14  | L     | 1501 | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 14  | b     | 829  | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 14  | g     | 825  | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 14  | b     | 814  | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 810  | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 14  | B     | 833  | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |
| 14  | N     | 814  | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 14  | N     | 834  | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 14  | A     | 831  | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 14  | g     | 832  | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 14  | g     | 828  | CLA  | MG-NB   | -2.19 | 2.01        | 2.05     |
| 14  | g     | 839  | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 14  | g     | 822  | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 14  | A     | 814  | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 14  | B     | 815  | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 14  | L     | 1501 | CLA  | CMB-C2B | -2.19 | 1.46        | 1.50     |
| 14  | g     | 852  | CLA  | C1B-C2B | 2.19  | 1.48        | 1.43     |
| 14  | g     | 805  | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 14  | G     | 834  | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 14  | g     | 827  | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 14  | g     | 807  | CLA  | CMD-C2D | -2.19 | 1.46        | 1.50     |
| 14  | B     | 822  | CLA  | CHC-C1C | 2.19  | 1.42        | 1.38     |
| 14  | G     | 837  | CLA  | C3B-C4B | 2.19  | 1.49        | 1.42     |
| 14  | B     | 814  | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 14  | g     | 811  | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 14  | N     | 815  | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 14  | b     | 840  | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 14  | N     | 834  | CLA  | CMB-C2B | -2.18 | 1.46        | 1.50     |
| 14  | A     | 822  | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 14  | b     | 812  | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 14  | G     | 824  | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 14  | g     | 852  | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 14  | a     | 829  | CLA  | CMB-C2B | -2.18 | 1.46        | 1.50     |
| 14  | g     | 854  | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 14  | a     | 839  | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 14  | n     | 818  | CLA  | CMB-C2B | -2.18 | 1.46        | 1.50     |
| 14  | b     | 820  | CLA  | CMB-C2B | -2.18 | 1.46        | 1.50     |
| 14  | g     | 803  | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 18  | a     | 850  | LHG  | O8-C23  | 2.18  | 1.39        | 1.33     |
| 14  | G     | 830  | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 14  | b     | 810  | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 14  | B     | 832  | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 14  | B     | 838  | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 14  | k     | 101  | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 14  | a     | 813  | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 14  | B     | 820  | CLA  | CMB-C2B | -2.18 | 1.46        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 807  | CLA  | C3B-C4B | 2.18  | 1.49        | 1.42     |
| 14  | g     | 823  | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 14  | A     | 823  | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 14  | f     | 202  | CLA  | CHC-C1C | 2.18  | 1.42        | 1.38     |
| 14  | N     | 839  | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 14  | N     | 841  | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 14  | g     | 823  | CLA  | CMB-C2B | -2.18 | 1.46        | 1.50     |
| 14  | B     | 810  | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 14  | N     | 801  | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 14  | N     | 832  | CLA  | MG-NB   | -2.18 | 2.01        | 2.05     |
| 14  | N     | 801  | CLA  | CMD-C2D | -2.18 | 1.46        | 1.50     |
| 14  | a     | 811  | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 14  | A     | 855  | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 14  | g     | 819  | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 14  | A     | 816  | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 14  | a     | 806  | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 14  | g     | 827  | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 14  | g     | 830  | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 14  | A     | 837  | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 14  | g     | 823  | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 14  | B     | 840  | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 14  | b     | 809  | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 14  | A     | 802  | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 14  | a     | 827  | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 14  | G     | 837  | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 14  | N     | 812  | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 14  | b     | 818  | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 14  | A     | 804  | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 14  | G     | 826  | CLA  | CMD-C2D | -2.17 | 1.46        | 1.50     |
| 14  | N     | 811  | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 14  | a     | 824  | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 14  | a     | 816  | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 20  | h     | 1702 | SQD  | O7-S    | 2.17  | 1.51        | 1.45     |
| 14  | n     | 809  | CLA  | CMB-C2B | -2.17 | 1.46        | 1.50     |
| 14  | n     | 810  | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 14  | b     | 851  | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 14  | A     | 837  | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 20  | w     | 202  | SQD  | O7-S    | 2.17  | 1.51        | 1.45     |
| 14  | a     | 840  | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 14  | G     | 812  | CLA  | CHC-C1C | 2.17  | 1.42        | 1.38     |
| 14  | N     | 839  | CLA  | MG-NB   | -2.17 | 2.01        | 2.05     |
| 14  | A     | 829  | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 809  | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 14  | G     | 821  | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 14  | G     | 820  | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 14  | n     | 817  | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 14  | L     | 1503 | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 14  | a     | 829  | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 14  | N     | 834  | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 14  | N     | 806  | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 14  | G     | 830  | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 14  | A     | 837  | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 20  | B     | 801  | SQD  | O7-S    | 2.16  | 1.51        | 1.45     |
| 20  | l     | 201  | SQD  | O7-S    | 2.16  | 1.51        | 1.45     |
| 14  | A     | 818  | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 14  | n     | 850  | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 14  | n     | 826  | CLA  | CMC-C2C | -2.16 | 1.46        | 1.50     |
| 14  | N     | 834  | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 14  | n     | 828  | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 14  | b     | 812  | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 14  | a     | 809  | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 14  | a     | 813  | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 14  | A     | 824  | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 14  | N     | 836  | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 14  | n     | 818  | CLA  | CHC-C1C | 2.16  | 1.42        | 1.38     |
| 14  | G     | 832  | CLA  | C3B-C4B | 2.16  | 1.49        | 1.42     |
| 14  | G     | 828  | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 14  | g     | 833  | CLA  | CMB-C2B | -2.16 | 1.46        | 1.50     |
| 14  | n     | 810  | CLA  | CMD-C2D | -2.16 | 1.46        | 1.50     |
| 14  | g     | 816  | CLA  | MG-NB   | -2.16 | 2.01        | 2.05     |
| 14  | B     | 804  | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 14  | B     | 810  | CLA  | C3B-C4B | 2.15  | 1.49        | 1.42     |
| 14  | G     | 817  | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 14  | N     | 832  | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 14  | A     | 812  | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 14  | N     | 806  | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 14  | a     | 808  | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 20  | b     | 801  | SQD  | O7-S    | 2.15  | 1.51        | 1.45     |
| 14  | A     | 808  | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 14  | b     | 831  | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 14  | n     | 825  | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 14  | a     | 853  | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 14  | b     | 831  | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 14  | g     | 820  | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 20  | H     | 1702 | SQD  | O7-S    | 2.15  | 1.51        | 1.45     |
| 14  | N     | 830  | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 14  | G     | 802  | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 14  | a     | 836  | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 14  | b     | 806  | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 14  | l     | 203  | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 17  | N     | 852  | BCR  | C1-C6   | -2.15 | 1.51        | 1.53     |
| 14  | W     | 203  | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 14  | g     | 831  | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 14  | a     | 823  | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 14  | n     | 818  | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 14  | b     | 827  | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 14  | A     | 836  | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 14  | B     | 804  | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 14  | b     | 803  | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 14  | g     | 839  | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 14  | G     | 809  | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 14  | W     | 202  | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 14  | g     | 831  | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 14  | b     | 830  | CLA  | CHC-C1C | 2.15  | 1.42        | 1.38     |
| 14  | a     | 819  | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 14  | A     | 824  | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 14  | g     | 827  | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 14  | A     | 812  | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 20  | n     | 801  | SQD  | O7-S    | 2.15  | 1.51        | 1.45     |
| 14  | g     | 824  | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 14  | A     | 840  | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 14  | g     | 839  | CLA  | MG-NB   | -2.15 | 2.01        | 2.05     |
| 19  | g     | 851  | CL0  | CBD-CGD | -2.15 | 1.49        | 1.52     |
| 18  | v     | 102  | LHG  | P-O6    | 2.15  | 1.67        | 1.59     |
| 14  | g     | 825  | CLA  | CMC-C2C | -2.15 | 1.46        | 1.50     |
| 14  | g     | 839  | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 14  | B     | 818  | CLA  | CMD-C2D | -2.15 | 1.46        | 1.50     |
| 14  | b     | 819  | CLA  | CMB-C2B | -2.15 | 1.46        | 1.50     |
| 14  | b     | 840  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | W     | 202  | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 14  | a     | 852  | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 14  | B     | 841  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | g     | 824  | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 14  | B     | 809  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | G     | 827  | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 14  | n     | 805  | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | n     | 804  | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 14  | b     | 841  | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 14  | N     | 812  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | B     | 833  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | a     | 803  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | a     | 832  | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 14  | A     | 837  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | L     | 1501 | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | A     | 829  | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 14  | g     | 810  | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 14  | n     | 802  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | G     | 808  | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 14  | a     | 827  | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 14  | b     | 851  | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 14  | A     | 810  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | b     | 827  | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 14  | n     | 839  | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 14  | a     | 822  | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 14  | a     | 817  | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 14  | b     | 835  | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 14  | A     | 818  | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 14  | N     | 830  | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 14  | a     | 839  | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 14  | A     | 807  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | a     | 823  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | g     | 833  | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 14  | n     | 809  | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 14  | g     | 807  | CLA  | CHC-C1C | 2.14  | 1.42        | 1.38     |
| 14  | n     | 852  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | B     | 838  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | A     | 817  | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 14  | B     | 820  | CLA  | MG-NB   | -2.14 | 2.01        | 2.05     |
| 14  | N     | 820  | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 14  | N     | 841  | CLA  | CMC-C2C | -2.14 | 1.46        | 1.50     |
| 14  | G     | 836  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | N     | 830  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | g     | 829  | CLA  | CMB-C2B | -2.14 | 1.46        | 1.50     |
| 18  | m     | 101  | LHG  | P-O6    | 2.14  | 1.67        | 1.59     |
| 14  | N     | 836  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 14  | g     | 828  | CLA  | CMD-C2D | -2.14 | 1.46        | 1.50     |
| 17  | g     | 848  | BCR  | C1-C6   | -2.13 | 1.51        | 1.53     |
| 14  | n     | 852  | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | a     | 807 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 14  | a     | 823 | CLA  | C3B-C4B | 2.13  | 1.49        | 1.42     |
| 14  | g     | 827 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 14  | A     | 833 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 14  | g     | 817 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 14  | G     | 804 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 14  | N     | 820 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 14  | B     | 831 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 14  | g     | 806 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 14  | s     | 201 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 14  | g     | 836 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 14  | B     | 814 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 14  | G     | 834 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 14  | W     | 203 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 14  | b     | 810 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 14  | a     | 807 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 14  | G     | 852 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 14  | N     | 819 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 14  | b     | 804 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 18  | S     | 202 | LHG  | P-O6    | 2.13  | 1.67        | 1.59     |
| 14  | n     | 808 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 14  | g     | 822 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 14  | a     | 853 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 14  | b     | 812 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 14  | n     | 817 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 14  | g     | 811 | CLA  | CHC-C1C | 2.13  | 1.42        | 1.38     |
| 14  | k     | 101 | CLA  | CBD-CAD | 2.13  | 1.56        | 1.51     |
| 14  | g     | 803 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 14  | w     | 204 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 14  | b     | 815 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 14  | N     | 815 | CLA  | MG-NB   | -2.13 | 2.01        | 2.05     |
| 14  | G     | 828 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 14  | g     | 809 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 14  | a     | 801 | CLA  | CMD-C2D | -2.13 | 1.46        | 1.50     |
| 14  | f     | 202 | CLA  | CMB-C2B | -2.13 | 1.46        | 1.50     |
| 14  | N     | 840 | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 14  | B     | 821 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | B     | 835 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 17  | b     | 848 | BCR  | C30-C25 | -2.12 | 1.51        | 1.53     |
| 14  | U     | 101 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | B     | 811 | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | A     | 822 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | w     | 203  | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 14  | A     | 824  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | a     | 825  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 18  | X     | 1702 | LHG  | P-O6    | 2.12  | 1.67        | 1.59     |
| 14  | G     | 808  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | N     | 809  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | A     | 824  | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 14  | u     | 101  | CLA  | CBD-CAD | 2.12  | 1.56        | 1.51     |
| 14  | a     | 837  | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 14  | B     | 827  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | j     | 102  | CLA  | CBD-CAD | 2.12  | 1.56        | 1.51     |
| 14  | G     | 834  | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | N     | 837  | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | B     | 838  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | F     | 201  | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 17  | A     | 848  | BCR  | C30-C25 | -2.12 | 1.51        | 1.53     |
| 14  | a     | 824  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | n     | 839  | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | K     | 101  | CLA  | CBD-CAD | 2.12  | 1.56        | 1.51     |
| 14  | a     | 807  | CLA  | CHC-C1C | 2.12  | 1.42        | 1.38     |
| 14  | G     | 824  | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 14  | N     | 824  | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | b     | 830  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | F     | 202  | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 14  | A     | 828  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | G     | 830  | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 14  | B     | 832  | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | G     | 823  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | g     | 810  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | n     | 814  | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | A     | 828  | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 14  | N     | 826  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | a     | 812  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | A     | 853  | CLA  | CMB-C2B | -2.12 | 1.46        | 1.50     |
| 14  | B     | 825  | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | N     | 823  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | t     | 102  | CLA  | CBD-CAD | 2.12  | 1.56        | 1.51     |
| 14  | b     | 841  | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | a     | 830  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | a     | 831  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | G     | 853  | CLA  | CMD-C2D | -2.12 | 1.46        | 1.50     |
| 14  | N     | 829  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | N     | 841  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | g     | 832  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | L     | 1502 | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | b     | 840  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | l     | 204  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | b     | 829  | CLA  | MG-NB   | -2.12 | 2.01        | 2.05     |
| 14  | a     | 821  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | T     | 102  | CLA  | CBD-CAD | 2.11  | 1.56        | 1.51     |
| 14  | n     | 834  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | B     | 839  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | g     | 822  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | b     | 835  | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 14  | A     | 801  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | A     | 821  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | G     | 820  | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 14  | N     | 827  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | n     | 850  | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 14  | A     | 834  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | A     | 836  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | g     | 837  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 20  | x     | 1702 | SQD  | O7-S    | 2.11  | 1.51        | 1.45     |
| 14  | S     | 201  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | n     | 837  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 17  | i     | 102  | BCR  | C30-C25 | -2.11 | 1.51        | 1.53     |
| 14  | N     | 812  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | n     | 820  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | a     | 801  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | G     | 831  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 18  | g     | 849  | LHG  | P-O6    | 2.11  | 1.67        | 1.59     |
| 14  | S     | 201  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | n     | 811  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | B     | 825  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | B     | 832  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | N     | 807  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | N     | 838  | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 14  | G     | 838  | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 14  | g     | 816  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | n     | 819  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | B     | 824  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | G     | 823  | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 14  | n     | 819  | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 14  | g     | 806  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | H     | 1701 | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | B     | 821  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | a     | 817  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 18  | A     | 851  | LHG  | P-O6    | 2.11  | 1.67        | 1.59     |
| 14  | L     | 1501 | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 14  | g     | 820  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | a     | 816  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | w     | 203  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 17  | b     | 844  | BCR  | C30-C25 | -2.11 | 1.51        | 1.53     |
| 14  | N     | 805  | CLA  | CMC-C2C | -2.11 | 1.46        | 1.50     |
| 14  | N     | 818  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | n     | 809  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | s     | 201  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | n     | 809  | CLA  | CHC-C1C | 2.11  | 1.42        | 1.38     |
| 14  | N     | 819  | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 14  | A     | 805  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | n     | 838  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | W     | 202  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | g     | 805  | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 14  | a     | 853  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | b     | 826  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | N     | 805  | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 14  | G     | 832  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | A     | 825  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | G     | 812  | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 14  | g     | 820  | CLA  | CMB-C2B | -2.11 | 1.46        | 1.50     |
| 14  | A     | 828  | CLA  | CMD-C2D | -2.11 | 1.46        | 1.50     |
| 14  | A     | 855  | CLA  | C3B-C4B | 2.11  | 1.48        | 1.42     |
| 14  | G     | 801  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | G     | 828  | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | L     | 1501 | CLA  | MG-NB   | -2.11 | 2.01        | 2.05     |
| 14  | G     | 819  | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | g     | 823  | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | n     | 839  | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 14  | X     | 1701 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | G     | 825  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | b     | 832  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | k     | 101  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | N     | 811  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | a     | 838  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | b     | 831  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | L     | 1502 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | a     | 830 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 14  | l     | 203 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 14  | g     | 804 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | b     | 822 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | a     | 823 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 18  | G     | 849 | LHG  | P-O6    | 2.10  | 1.67        | 1.59     |
| 14  | N     | 841 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 14  | B     | 819 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 14  | b     | 838 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | N     | 805 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | B     | 808 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | a     | 811 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 14  | G     | 801 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 14  | G     | 802 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | B     | 823 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | N     | 804 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | A     | 817 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 14  | A     | 839 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 14  | n     | 815 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | A     | 808 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | A     | 839 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | n     | 828 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | a     | 840 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | g     | 832 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | A     | 819 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | B     | 809 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 14  | b     | 811 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | b     | 825 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | N     | 830 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | G     | 816 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 14  | N     | 805 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | A     | 806 | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 14  | G     | 817 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | U     | 102 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | A     | 816 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | a     | 821 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | a     | 818 | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 14  | G     | 852 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |
| 14  | N     | 824 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | b     | 807 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | b     | 838 | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | A     | 819 | CLA  | CMC-C2C | -2.10 | 1.46        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 832  | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | J     | 102  | CLA  | CBD-CAD | 2.10  | 1.56        | 1.51     |
| 14  | G     | 834  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | g     | 812  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | g     | 830  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | u     | 102  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | A     | 810  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | a     | 810  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | g     | 836  | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | n     | 834  | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 14  | A     | 830  | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 14  | B     | 833  | CLA  | CHC-C1C | 2.10  | 1.42        | 1.38     |
| 14  | N     | 828  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | N     | 836  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | b     | 826  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | s     | 201  | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 14  | L     | 1503 | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | G     | 818  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | N     | 808  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | B     | 833  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | a     | 854  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | G     | 840  | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | g     | 816  | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 14  | k     | 101  | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | g     | 853  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | n     | 825  | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | a     | 802  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | g     | 801  | CLA  | CMD-C2D | -2.10 | 1.46        | 1.50     |
| 14  | A     | 821  | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 14  | B     | 811  | CLA  | CMB-C2B | -2.10 | 1.46        | 1.50     |
| 14  | g     | 801  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | b     | 802  | CLA  | MG-NB   | -2.10 | 2.01        | 2.05     |
| 14  | N     | 815  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | A     | 812  | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 14  | B     | 829  | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | B     | 819  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | G     | 827  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | G     | 839  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | K     | 101  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | b     | 840  | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | N     | 807  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | B     | 811  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | g     | 811 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | A     | 802 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | A     | 807 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | a     | 832 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | a     | 838 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | b     | 851 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | g     | 808 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | n     | 827 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | g     | 840 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | G     | 815 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | G     | 838 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | A     | 855 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 14  | B     | 803 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | a     | 811 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | b     | 809 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | b     | 834 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | b     | 838 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | A     | 802 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | G     | 825 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | A     | 820 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | n     | 810 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | G     | 818 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | G     | 832 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | N     | 815 | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 14  | B     | 810 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | b     | 802 | CLA  | CHC-C1C | 2.09  | 1.42        | 1.38     |
| 14  | B     | 803 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | G     | 821 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | n     | 810 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 17  | n     | 842 | BCR  | C30-C25 | -2.09 | 1.51        | 1.53     |
| 14  | G     | 829 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | g     | 804 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | g     | 853 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | A     | 830 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | a     | 820 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | A     | 838 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | b     | 807 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | b     | 829 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | B     | 828 | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | N     | 839 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | n     | 831 | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | A     | 816 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | n     | 802  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | g     | 814  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 18  | a     | 849  | LHG  | P-O6    | 2.09  | 1.67        | 1.59     |
| 14  | G     | 807  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | N     | 803  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | n     | 837  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | N     | 810  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | u     | 101  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | G     | 823  | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | N     | 812  | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | n     | 823  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | A     | 816  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | b     | 816  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | N     | 821  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | G     | 811  | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | G     | 838  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 17  | B     | 851  | BCR  | C1-C6   | -2.09 | 1.51        | 1.53     |
| 17  | I     | 101  | BCR  | C30-C25 | -2.09 | 1.51        | 1.53     |
| 14  | f     | 201  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | N     | 838  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | B     | 826  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | b     | 819  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | B     | 829  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | a     | 824  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | G     | 817  | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | L     | 1503 | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | a     | 819  | CLA  | CMC-C2C | -2.09 | 1.46        | 1.50     |
| 17  | B     | 846  | BCR  | C30-C25 | -2.09 | 1.51        | 1.53     |
| 14  | B     | 831  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | b     | 809  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | b     | 828  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | g     | 833  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | n     | 820  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | J     | 101  | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | u     | 101  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | A     | 841  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | b     | 820  | CLA  | MG-NB   | -2.09 | 2.01        | 2.05     |
| 14  | g     | 837  | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | n     | 811  | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | A     | 805  | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |
| 14  | B     | 816  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | b     | 811  | CLA  | CMB-C2B | -2.09 | 1.46        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | f     | 201  | CLA  | CMD-C2D | -2.09 | 1.46        | 1.50     |
| 14  | b     | 804  | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | G     | 816  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | n     | 830  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | B     | 805  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | g     | 821  | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | w     | 205  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | B     | 837  | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 14  | b     | 824  | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | n     | 830  | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | A     | 857  | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | G     | 822  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | H     | 1701 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | a     | 809  | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | a     | 833  | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | G     | 838  | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | G     | 839  | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | A     | 838  | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | B     | 812  | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | n     | 808  | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 14  | A     | 834  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 17  | j     | 103  | BCR  | C1-C6   | -2.08 | 1.51        | 1.53     |
| 14  | B     | 822  | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | B     | 836  | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | B     | 837  | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | g     | 812  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | n     | 805  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | B     | 850  | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | L     | 1502 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | a     | 820  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | a     | 835  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | n     | 824  | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | b     | 853  | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | N     | 826  | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | B     | 806  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | a     | 828  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | j     | 101  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | B     | 840  | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | g     | 838  | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | A     | 815  | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | b     | 803  | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | B     | 817  | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | a     | 826 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | g     | 821 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 18  | A     | 850 | LHG  | P-O6    | 2.08  | 1.67        | 1.59     |
| 14  | G     | 831 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | s     | 202 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | A     | 833 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | G     | 812 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | U     | 101 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | G     | 833 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | S     | 201 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 14  | n     | 833 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | A     | 811 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | B     | 834 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | b     | 824 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | g     | 831 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | n     | 823 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | a     | 818 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | G     | 819 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | n     | 803 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | A     | 854 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | B     | 807 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | G     | 821 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | n     | 815 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | T     | 102 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | b     | 837 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | S     | 201 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | b     | 808 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | w     | 205 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | N     | 822 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | B     | 839 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | N     | 835 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | N     | 851 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | a     | 832 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | a     | 839 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | G     | 803 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 14  | B     | 835 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | G     | 816 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | g     | 837 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | n     | 814 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | A     | 823 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | A     | 838 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | a     | 817 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | a     | 821 | CLA  | CMB-C2B | -2.08 | 1.46        | 1.50     |
| 14  | b     | 809 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 14  | g     | 802 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | G     | 835 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | g     | 803 | CLA  | CMC-C2C | -2.08 | 1.46        | 1.50     |
| 14  | g     | 830 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | a     | 805 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | N     | 825 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | A     | 804 | CLA  | MG-NB   | -2.08 | 2.01        | 2.05     |
| 14  | B     | 824 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | B     | 827 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | a     | 840 | CLA  | CMD-C2D | -2.08 | 1.46        | 1.50     |
| 14  | N     | 814 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | A     | 820 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | a     | 814 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | b     | 822 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | g     | 807 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 14  | n     | 824 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | A     | 809 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 14  | B     | 805 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 14  | N     | 806 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 14  | U     | 101 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 14  | n     | 836 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | N     | 842 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 17  | n     | 843 | BCR  | C30-C25 | -2.07 | 1.51        | 1.53     |
| 14  | n     | 850 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 14  | A     | 854 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | a     | 806 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | g     | 828 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 14  | w     | 204 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | B     | 810 | CLA  | CHC-C1C | 2.07  | 1.42        | 1.38     |
| 14  | G     | 809 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | G     | 832 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 14  | N     | 838 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | A     | 812 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 14  | A     | 832 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | b     | 806 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | A     | 823 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 14  | b     | 815 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 14  | n     | 835 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | G     | 805 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 14  | n     | 827 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | h     | 1701 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | b     | 814  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | G     | 840  | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 14  | W     | 204  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | A     | 829  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | A     | 854  | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 14  | a     | 815  | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 14  | a     | 829  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | a     | 837  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | a     | 854  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | G     | 810  | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 14  | A     | 809  | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 14  | a     | 826  | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 14  | b     | 817  | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 14  | G     | 818  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | g     | 838  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | B     | 837  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | a     | 822  | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 14  | a     | 825  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | a     | 833  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | l     | 204  | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 17  | N     | 848  | BCR  | C30-C25 | -2.07 | 1.51        | 1.53     |
| 14  | N     | 804  | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 14  | f     | 202  | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 14  | g     | 802  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | G     | 807  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | n     | 838  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | K     | 101  | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 14  | n     | 834  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | B     | 831  | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 14  | a     | 802  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | j     | 102  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | l     | 203  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | a     | 804  | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 14  | N     | 824  | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 14  | g     | 825  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | A     | 823  | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 14  | a     | 818  | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 14  | b     | 835  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | l     | 202  | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 14  | J     | 102  | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | u     | 102  | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | B     | 813 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | b     | 829 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 14  | J     | 101 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | N     | 837 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 14  | A     | 804 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 14  | N     | 818 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 14  | S     | 203 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 14  | n     | 852 | CLA  | CMC-C2C | -2.07 | 1.46        | 1.50     |
| 14  | B     | 823 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | a     | 836 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | G     | 814 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 14  | A     | 814 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 18  | g     | 850 | LHG  | P-O6    | 2.07  | 1.67        | 1.59     |
| 14  | N     | 809 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | n     | 813 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | b     | 808 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 14  | G     | 823 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | n     | 817 | CLA  | CMB-C2B | -2.07 | 1.46        | 1.50     |
| 14  | A     | 825 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | B     | 836 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | b     | 817 | CLA  | CMD-C2D | -2.07 | 1.46        | 1.50     |
| 14  | g     | 813 | CLA  | MG-NB   | -2.07 | 2.01        | 2.05     |
| 14  | g     | 822 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 14  | B     | 839 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | F     | 201 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 14  | A     | 832 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | a     | 836 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | N     | 811 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | n     | 809 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | N     | 814 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 14  | U     | 102 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 14  | n     | 840 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | n     | 850 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | a     | 815 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | B     | 815 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | b     | 825 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | N     | 804 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | S     | 203 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | g     | 804 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | g     | 805 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | g     | 811 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | g     | 853 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | n     | 828 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 14  | B     | 841 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | b     | 851 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | U     | 101 | CLA  | CBD-CAD | 2.06  | 1.56        | 1.51     |
| 14  | G     | 829 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | A     | 811 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | G     | 853 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | N     | 813 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | b     | 813 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | n     | 819 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | w     | 204 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 14  | B     | 808 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | B     | 819 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | a     | 830 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | b     | 810 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | N     | 817 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | B     | 834 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | G     | 809 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 14  | N     | 808 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 14  | B     | 817 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 14  | a     | 831 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | F     | 202 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | T     | 102 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | g     | 813 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | w     | 203 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | a     | 825 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | a     | 815 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | n     | 832 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 14  | B     | 814 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 19  | G     | 851 | CL0  | CBD-CGD | -2.06 | 1.49        | 1.52     |
| 14  | B     | 803 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | b     | 821 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | b     | 833 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | n     | 831 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | a     | 814 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | G     | 840 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | g     | 810 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | A     | 839 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | G     | 801 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | n     | 813 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | B     | 814 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | a     | 808 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | a     | 839 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | g     | 821 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | g     | 838 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 14  | A     | 857 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | a     | 813 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | b     | 820 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | b     | 828 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | N     | 825 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | a     | 806 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 14  | W     | 204 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | g     | 818 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | j     | 102 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | G     | 839 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 14  | A     | 804 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 14  | A     | 835 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | B     | 812 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | G     | 814 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | g     | 811 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | n     | 826 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 14  | B     | 817 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | a     | 824 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 14  | b     | 813 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | T     | 101 | CLA  | CMB-C2B | -2.06 | 1.46        | 1.50     |
| 14  | B     | 822 | CLA  | CMD-C2D | -2.06 | 1.46        | 1.50     |
| 14  | b     | 804 | CLA  | CMC-C2C | -2.06 | 1.46        | 1.50     |
| 14  | g     | 814 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | G     | 803 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | N     | 827 | CLA  | MG-NB   | -2.06 | 2.01        | 2.05     |
| 14  | n     | 811 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | t     | 101 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | J     | 102 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | g     | 835 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | A     | 813 | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | A     | 814 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | b     | 824 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | g     | 829 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | a     | 810 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 18  | G     | 850 | LHG  | P-O6    | 2.05  | 1.67        | 1.59     |
| 14  | n     | 823 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | l     | 202 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | G     | 806 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | G     | 853 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | b     | 827  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | b     | 853  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | b     | 821  | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | N     | 813  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | N     | 821  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | B     | 850  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | F     | 201  | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | N     | 803  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | U     | 102  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | g     | 819  | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | g     | 832  | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | A     | 831  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | A     | 853  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | n     | 812  | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | N     | 837  | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | W     | 202  | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | A     | 812  | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | a     | 833  | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | N     | 817  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | A     | 801  | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | A     | 827  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | l     | 203  | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | n     | 806  | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | g     | 807  | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | A     | 810  | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | B     | 813  | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | a     | 805  | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | f     | 201  | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | G     | 835  | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | N     | 834  | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | A     | 826  | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | x     | 1701 | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | T     | 101  | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | n     | 808  | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | A     | 817  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | A     | 822  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | n     | 812  | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 17  | B     | 852  | BCR  | C30-C25 | -2.05 | 1.51        | 1.53     |
| 14  | n     | 816  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | u     | 102  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | B     | 807  | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | h     | 1701 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 817  | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | A     | 809  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | N     | 816  | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | A     | 803  | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | x     | 1701 | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | N     | 808  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | N     | 828  | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | N     | 838  | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | N     | 840  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | a     | 852  | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | G     | 814  | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | g     | 815  | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | t     | 101  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | b     | 839  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 19  | a     | 851  | CL0  | CHA-CBD | -2.05 | 1.49        | 1.51     |
| 14  | g     | 818  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | g     | 836  | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | n     | 822  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | n     | 826  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | B     | 804  | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | B     | 826  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | a     | 812  | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | N     | 808  | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | n     | 831  | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | B     | 840  | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | l     | 204  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | X     | 1701 | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | T     | 101  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | A     | 818  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 18  | a     | 850  | LHG  | P-O6    | 2.05  | 1.67        | 1.59     |
| 14  | n     | 816  | CLA  | MG-NB   | -2.05 | 2.01        | 2.05     |
| 14  | G     | 805  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | g     | 817  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | A     | 806  | CLA  | CMD-C2D | -2.05 | 1.46        | 1.50     |
| 14  | A     | 853  | CLA  | CMC-C2C | -2.05 | 1.46        | 1.50     |
| 14  | a     | 819  | CLA  | CMB-C2B | -2.05 | 1.46        | 1.50     |
| 14  | a     | 837  | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | G     | 820  | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | A     | 836  | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | B     | 807  | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | B     | 815  | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | A     | 811  | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | B     | 816 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | G     | 827 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | N     | 817 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | g     | 826 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | n     | 807 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | A     | 801 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | K     | 101 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | N     | 828 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | N     | 829 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | g     | 818 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | g     | 819 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | b     | 830 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | n     | 822 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | N     | 823 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | s     | 202 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | A     | 841 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | B     | 820 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | a     | 834 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | b     | 837 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | B     | 833 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | b     | 839 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | B     | 805 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | G     | 833 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | n     | 812 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | b     | 828 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | N     | 822 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | n     | 821 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | n     | 840 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | G     | 813 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | b     | 821 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | b     | 838 | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | N     | 833 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | a     | 810 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | g     | 826 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | G     | 806 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | g     | 815 | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | B     | 826 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | a     | 816 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | S     | 203 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | A     | 819 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | F     | 201 | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | B     | 809 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | B     | 810  | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | B     | 821  | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | b     | 836  | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 17  | b     | 843  | BCR  | C30-C25 | -2.04 | 1.51        | 1.53     |
| 14  | G     | 840  | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | a     | 839  | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | f     | 202  | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | G     | 837  | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | N     | 842  | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | X     | 1701 | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | a     | 815  | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | b     | 803  | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | G     | 804  | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | g     | 809  | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | b     | 853  | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | N     | 833  | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | a     | 832  | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | B     | 829  | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | B     | 838  | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | a     | 819  | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | a     | 829  | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | a     | 816  | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | G     | 803  | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | g     | 808  | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | n     | 808  | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | A     | 813  | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | b     | 819  | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | G     | 804  | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | N     | 835  | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | g     | 839  | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | B     | 840  | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | G     | 808  | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | n     | 836  | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | A     | 819  | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | B     | 818  | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | B     | 837  | CLA  | CMB-C2B | -2.04 | 1.46        | 1.50     |
| 14  | A     | 805  | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | N     | 839  | CLA  | CMC-C2C | -2.04 | 1.46        | 1.50     |
| 14  | g     | 834  | CLA  | CMD-C2D | -2.04 | 1.46        | 1.50     |
| 14  | b     | 834  | CLA  | MG-NB   | -2.04 | 2.01        | 2.05     |
| 14  | a     | 811  | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | N     | 840  | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | B     | 809 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | B     | 850 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | G     | 811 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 14  | G     | 812 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 14  | N     | 807 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | n     | 821 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | B     | 815 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | a     | 808 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 14  | g     | 815 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 20  | b     | 801 | SQD  | C8-C7   | 2.03  | 1.56        | 1.50     |
| 14  | G     | 829 | CLA  | CHC-C1C | 2.03  | 1.42        | 1.38     |
| 14  | N     | 825 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | A     | 841 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | a     | 809 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | b     | 839 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | G     | 819 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | G     | 853 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | n     | 821 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 14  | a     | 812 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 14  | b     | 811 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | g     | 824 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | g     | 835 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 14  | K     | 101 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | b     | 805 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | W     | 203 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | B     | 836 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | A     | 813 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | B     | 830 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | b     | 816 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | t     | 102 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | N     | 820 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 14  | g     | 830 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | A     | 802 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | A     | 841 | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | A     | 827 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | b     | 805 | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 14  | A     | 807 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | N     | 823 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | n     | 814 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | n     | 827 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | w     | 205 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | B     | 834 | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | a     | 804  | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 14  | g     | 834  | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | F     | 202  | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | a     | 834  | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | g     | 802  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | N     | 835  | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | B     | 841  | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | N     | 821  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | g     | 808  | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | t     | 102  | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 14  | J     | 101  | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | G     | 839  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | A     | 831  | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | a     | 809  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 20  | n     | 801  | SQD  | C8-C7   | 2.03  | 1.56        | 1.50     |
| 14  | N     | 806  | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | N     | 833  | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 14  | n     | 804  | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 14  | A     | 829  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | a     | 820  | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | s     | 202  | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | t     | 102  | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | b     | 813  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | a     | 805  | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | G     | 812  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | N     | 810  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | A     | 815  | CLA  | CMD-C2D | -2.03 | 1.46        | 1.50     |
| 14  | G     | 816  | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | G     | 819  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | n     | 802  | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | n     | 807  | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | A     | 813  | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | A     | 820  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | b     | 828  | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | G     | 826  | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | g     | 818  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | n     | 806  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | n     | 822  | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | b     | 834  | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | G     | 822  | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | H     | 1701 | CLA  | MG-NB   | -2.03 | 2.01        | 2.05     |
| 14  | N     | 822  | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | u     | 101  | CLA  | CMB-C2B | -2.03 | 1.46        | 1.50     |
| 14  | N     | 829  | CLA  | CMC-C2C | -2.03 | 1.46        | 1.50     |
| 14  | G     | 807  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | n     | 838  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | A     | 857  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | b     | 817  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | G     | 813  | CLA  | MG-NB   | -2.02 | 2.01        | 2.05     |
| 14  | a     | 822  | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 14  | b     | 833  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | b     | 818  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | A     | 806  | CLA  | MG-NB   | -2.02 | 2.01        | 2.05     |
| 14  | n     | 813  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | n     | 817  | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | a     | 825  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | l     | 202  | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 14  | G     | 802  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | t     | 101  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | n     | 852  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | A     | 821  | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 14  | G     | 802  | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | g     | 816  | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | n     | 833  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | k     | 101  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | n     | 803  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | n     | 806  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | G     | 836  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | h     | 1701 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | B     | 828  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | n     | 806  | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 14  | A     | 824  | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | A     | 857  | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | B     | 828  | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 14  | b     | 805  | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | b     | 814  | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | G     | 817  | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | N     | 804  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | A     | 803  | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | b     | 808  | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | b     | 827  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | G     | 805  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | N     | 815  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | n     | 805  | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | a     | 806 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | N     | 842 | CLA  | CHC-C1C | 2.02  | 1.42        | 1.38     |
| 14  | N     | 851 | CLA  | CMD-C2D | -2.02 | 1.46        | 1.50     |
| 14  | A     | 839 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | G     | 833 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | a     | 804 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | b     | 851 | CLA  | MG-NB   | -2.02 | 2.01        | 2.05     |
| 14  | N     | 828 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | g     | 801 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | B     | 808 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | B     | 832 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | a     | 802 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | G     | 833 | CLA  | MG-NB   | -2.02 | 2.01        | 2.05     |
| 14  | G     | 805 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | T     | 102 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | n     | 837 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | l     | 204 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | N     | 810 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | A     | 835 | CLA  | CMC-C2C | -2.02 | 1.46        | 1.50     |
| 14  | B     | 816 | CLA  | CMB-C2B | -2.02 | 1.46        | 1.50     |
| 14  | A     | 855 | CLA  | CHC-C1C | 2.02  | 1.42        | 1.38     |
| 14  | W     | 204 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | g     | 803 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | g     | 807 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | n     | 816 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | B     | 824 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | N     | 813 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | g     | 802 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | n     | 832 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 14  | A     | 803 | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 14  | a     | 826 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | a     | 838 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | G     | 813 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | N     | 803 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | N     | 833 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | A     | 817 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | B     | 830 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | G     | 837 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | a     | 854 | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | G     | 813 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | G     | 818 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | N     | 818 | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 14  | G     | 825  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | W     | 204  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | A     | 832  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | B     | 811  | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | j     | 101  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | N     | 831  | CLA  | MG-NB   | -2.01 | 2.01        | 2.05     |
| 14  | g     | 825  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | n     | 802  | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | n     | 818  | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 14  | B     | 823  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | B     | 827  | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | a     | 833  | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | G     | 837  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | A     | 822  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | N     | 812  | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | N     | 816  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | b     | 840  | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | j     | 102  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | n     | 825  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | B     | 812  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | G     | 810  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | G     | 835  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | N     | 811  | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | g     | 806  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | n     | 837  | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | b     | 826  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | a     | 804  | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | b     | 804  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | x     | 1701 | CLA  | MG-NB   | -2.01 | 2.01        | 2.05     |
| 14  | A     | 814  | CLA  | CMB-C2B | -2.01 | 1.46        | 1.50     |
| 14  | B     | 822  | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | G     | 803  | CLA  | CMD-C2D | -2.01 | 1.46        | 1.50     |
| 14  | n     | 812  | CLA  | CMC-C2C | -2.01 | 1.46        | 1.50     |
| 14  | n     | 815  | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |
| 14  | A     | 830  | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 14  | a     | 813  | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |
| 14  | A     | 803  | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |
| 14  | b     | 823  | CLA  | CMD-C2D | -2.00 | 1.46        | 1.50     |
| 14  | b     | 833  | CLA  | MG-NB   | -2.00 | 2.01        | 2.05     |
| 14  | G     | 808  | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |
| 14  | A     | 816  | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 14  | B     | 825  | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 14  | n     | 850 | CLA  | MG-NB   | -2.00 | 2.01        | 2.05     |
| 14  | b     | 836 | CLA  | MG-NB   | -2.00 | 2.01        | 2.05     |
| 14  | A     | 835 | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |
| 14  | b     | 815 | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |
| 14  | G     | 852 | CLA  | MG-ND   | -2.00 | 2.01        | 2.05     |
| 14  | n     | 831 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 14  | N     | 825 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 14  | b     | 823 | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |
| 20  | B     | 801 | SQD  | C8-C7   | 2.00  | 1.56        | 1.50     |
| 14  | A     | 808 | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |
| 14  | b     | 803 | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |
| 14  | G     | 825 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 14  | B     | 822 | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |
| 14  | a     | 803 | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |
| 14  | G     | 831 | CLA  | CMC-C2C | -2.00 | 1.46        | 1.50     |
| 14  | b     | 816 | CLA  | CMB-C2B | -2.00 | 1.46        | 1.50     |
| 14  | N     | 810 | CLA  | MG-NB   | -2.00 | 2.01        | 2.05     |
| 14  | j     | 101 | CLA  | MG-NB   | -2.00 | 2.01        | 2.05     |

All (3742) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|--------|-------------|----------|
| 17  | I     | 102 | BCR  | C16-C17-C18 | -10.42 | 112.67      | 127.28   |
| 17  | a     | 846 | BCR  | C24-C23-C22 | -9.84  | 111.68      | 126.23   |
| 17  | I     | 102 | BCR  | C24-C23-C22 | -9.64  | 111.97      | 126.23   |
| 17  | a     | 846 | BCR  | C16-C17-C18 | -9.21  | 114.36      | 127.28   |
| 17  | W     | 201 | BCR  | C20-C21-C22 | -8.85  | 114.86      | 127.28   |
| 17  | b     | 846 | BCR  | C15-C14-C13 | -8.04  | 116.00      | 127.28   |
| 17  | g     | 846 | BCR  | C7-C8-C9    | -7.86  | 114.60      | 126.23   |
| 17  | W     | 201 | BCR  | C24-C23-C22 | -7.48  | 115.17      | 126.23   |
| 14  | a     | 807 | CLA  | C4A-NA-C1A  | 7.24   | 109.98      | 106.68   |
| 17  | B     | 844 | BCR  | C16-C17-C18 | -7.21  | 117.17      | 127.28   |
| 14  | B     | 827 | CLA  | C4A-NA-C1A  | 7.02   | 109.88      | 106.68   |
| 14  | n     | 840 | CLA  | C4A-NA-C1A  | 7.01   | 109.88      | 106.68   |
| 14  | B     | 809 | CLA  | C4A-NA-C1A  | 6.96   | 109.86      | 106.68   |
| 17  | g     | 846 | BCR  | C15-C14-C13 | -6.96  | 117.51      | 127.28   |
| 14  | N     | 831 | CLA  | C4A-NA-C1A  | 6.94   | 109.84      | 106.68   |
| 14  | N     | 828 | CLA  | C4A-NA-C1A  | 6.92   | 109.84      | 106.68   |
| 14  | W     | 202 | CLA  | C4A-NA-C1A  | 6.91   | 109.83      | 106.68   |
| 14  | N     | 834 | CLA  | C4A-NA-C1A  | 6.87   | 109.81      | 106.68   |
| 14  | A     | 826 | CLA  | C4A-NA-C1A  | 6.87   | 109.81      | 106.68   |
| 14  | a     | 818 | CLA  | C4A-NA-C1A  | 6.87   | 109.81      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | N     | 810  | CLA  | C4A-NA-C1A  | 6.87  | 109.81      | 106.68   |
| 14  | B     | 838  | CLA  | C4A-NA-C1A  | 6.86  | 109.81      | 106.68   |
| 14  | N     | 842  | CLA  | C4A-NA-C1A  | 6.86  | 109.81      | 106.68   |
| 14  | A     | 804  | CLA  | C4A-NA-C1A  | 6.85  | 109.80      | 106.68   |
| 14  | n     | 816  | CLA  | C4A-NA-C1A  | 6.81  | 109.79      | 106.68   |
| 14  | b     | 841  | CLA  | C4A-NA-C1A  | 6.80  | 109.78      | 106.68   |
| 14  | G     | 824  | CLA  | C4A-NA-C1A  | 6.80  | 109.78      | 106.68   |
| 14  | g     | 807  | CLA  | C4A-NA-C1A  | 6.78  | 109.77      | 106.68   |
| 14  | a     | 820  | CLA  | C4A-NA-C1A  | 6.77  | 109.77      | 106.68   |
| 14  | a     | 830  | CLA  | C4A-NA-C1A  | 6.77  | 109.77      | 106.68   |
| 14  | b     | 803  | CLA  | C4A-NA-C1A  | 6.75  | 109.76      | 106.68   |
| 14  | G     | 823  | CLA  | C4A-NA-C1A  | 6.74  | 109.75      | 106.68   |
| 14  | B     | 841  | CLA  | C4A-NA-C1A  | 6.73  | 109.75      | 106.68   |
| 14  | a     | 828  | CLA  | C4A-NA-C1A  | 6.73  | 109.75      | 106.68   |
| 14  | G     | 821  | CLA  | C4A-NA-C1A  | 6.72  | 109.75      | 106.68   |
| 14  | b     | 851  | CLA  | C4A-NA-C1A  | 6.72  | 109.75      | 106.68   |
| 14  | B     | 817  | CLA  | C4A-NA-C1A  | 6.72  | 109.75      | 106.68   |
| 14  | B     | 833  | CLA  | C4A-NA-C1A  | 6.71  | 109.74      | 106.68   |
| 14  | a     | 812  | CLA  | C4A-NA-C1A  | 6.71  | 109.74      | 106.68   |
| 14  | B     | 830  | CLA  | C4A-NA-C1A  | 6.71  | 109.74      | 106.68   |
| 14  | A     | 819  | CLA  | C4A-NA-C1A  | 6.70  | 109.74      | 106.68   |
| 14  | b     | 817  | CLA  | C4A-NA-C1A  | 6.70  | 109.74      | 106.68   |
| 14  | G     | 819  | CLA  | C4A-NA-C1A  | 6.70  | 109.73      | 106.68   |
| 14  | A     | 838  | CLA  | C4A-NA-C1A  | 6.70  | 109.73      | 106.68   |
| 14  | B     | 822  | CLA  | C4A-NA-C1A  | 6.70  | 109.73      | 106.68   |
| 14  | G     | 822  | CLA  | C4A-NA-C1A  | 6.69  | 109.73      | 106.68   |
| 14  | A     | 815  | CLA  | C4A-NA-C1A  | 6.68  | 109.73      | 106.68   |
| 14  | A     | 823  | CLA  | C4A-NA-C1A  | 6.68  | 109.73      | 106.68   |
| 14  | a     | 838  | CLA  | C4A-NA-C1A  | 6.68  | 109.73      | 106.68   |
| 14  | W     | 203  | CLA  | C4A-NA-C1A  | 6.67  | 109.72      | 106.68   |
| 14  | H     | 1701 | CLA  | C4A-NA-C1A  | 6.67  | 109.72      | 106.68   |
| 17  | B     | 851  | BCR  | C24-C23-C22 | -6.67 | 116.37      | 126.23   |
| 14  | g     | 801  | CLA  | C4A-NA-C1A  | 6.67  | 109.72      | 106.68   |
| 14  | a     | 839  | CLA  | C4A-NA-C1A  | 6.66  | 109.72      | 106.68   |
| 14  | N     | 816  | CLA  | C4A-NA-C1A  | 6.66  | 109.72      | 106.68   |
| 14  | n     | 829  | CLA  | C4A-NA-C1A  | 6.66  | 109.72      | 106.68   |
| 14  | A     | 822  | CLA  | C4A-NA-C1A  | 6.65  | 109.71      | 106.68   |
| 14  | g     | 828  | CLA  | C4A-NA-C1A  | 6.64  | 109.71      | 106.68   |
| 14  | g     | 830  | CLA  | C4A-NA-C1A  | 6.64  | 109.71      | 106.68   |
| 14  | b     | 827  | CLA  | C4A-NA-C1A  | 6.64  | 109.71      | 106.68   |
| 14  | g     | 814  | CLA  | C4A-NA-C1A  | 6.64  | 109.71      | 106.68   |
| 14  | g     | 812  | CLA  | C4A-NA-C1A  | 6.63  | 109.71      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 816  | CLA  | C4A-NA-C1A  | 6.63  | 109.71      | 106.68   |
| 14  | A     | 806  | CLA  | C4A-NA-C1A  | 6.63  | 109.70      | 106.68   |
| 14  | B     | 821  | CLA  | C4A-NA-C1A  | 6.63  | 109.70      | 106.68   |
| 14  | A     | 813  | CLA  | C4A-NA-C1A  | 6.62  | 109.70      | 106.68   |
| 14  | G     | 808  | CLA  | C4A-NA-C1A  | 6.62  | 109.70      | 106.68   |
| 14  | G     | 816  | CLA  | C4A-NA-C1A  | 6.62  | 109.70      | 106.68   |
| 14  | A     | 814  | CLA  | C4A-NA-C1A  | 6.62  | 109.70      | 106.68   |
| 14  | B     | 812  | CLA  | C4A-NA-C1A  | 6.62  | 109.70      | 106.68   |
| 14  | A     | 854  | CLA  | C4A-NA-C1A  | 6.61  | 109.69      | 106.68   |
| 14  | N     | 839  | CLA  | C4A-NA-C1A  | 6.61  | 109.69      | 106.68   |
| 14  | x     | 1701 | CLA  | C4A-NA-C1A  | 6.61  | 109.69      | 106.68   |
| 14  | b     | 821  | CLA  | C4A-NA-C1A  | 6.61  | 109.69      | 106.68   |
| 14  | L     | 1501 | CLA  | C4A-NA-C1A  | 6.60  | 109.69      | 106.68   |
| 14  | g     | 837  | CLA  | C4A-NA-C1A  | 6.60  | 109.69      | 106.68   |
| 14  | g     | 840  | CLA  | C4A-NA-C1A  | 6.60  | 109.69      | 106.68   |
| 14  | A     | 807  | CLA  | C4A-NA-C1A  | 6.60  | 109.69      | 106.68   |
| 14  | a     | 815  | CLA  | C4A-NA-C1A  | 6.60  | 109.69      | 106.68   |
| 14  | B     | 816  | CLA  | C4A-NA-C1A  | 6.59  | 109.69      | 106.68   |
| 14  | a     | 806  | CLA  | C4A-NA-C1A  | 6.59  | 109.69      | 106.68   |
| 17  | i     | 102  | BCR  | C24-C23-C22 | -6.59 | 116.49      | 126.23   |
| 14  | A     | 835  | CLA  | C4A-NA-C1A  | 6.59  | 109.69      | 106.68   |
| 17  | w     | 206  | BCR  | C24-C23-C22 | -6.59 | 116.49      | 126.23   |
| 14  | A     | 836  | CLA  | C4A-NA-C1A  | 6.59  | 109.68      | 106.68   |
| 14  | B     | 815  | CLA  | C4A-NA-C1A  | 6.58  | 109.68      | 106.68   |
| 14  | a     | 840  | CLA  | C4A-NA-C1A  | 6.58  | 109.68      | 106.68   |
| 14  | A     | 829  | CLA  | C4A-NA-C1A  | 6.58  | 109.68      | 106.68   |
| 14  | a     | 805  | CLA  | C4A-NA-C1A  | 6.58  | 109.68      | 106.68   |
| 14  | b     | 834  | CLA  | C4A-NA-C1A  | 6.58  | 109.68      | 106.68   |
| 14  | G     | 829  | CLA  | C4A-NA-C1A  | 6.57  | 109.68      | 106.68   |
| 14  | b     | 838  | CLA  | C4A-NA-C1A  | 6.57  | 109.68      | 106.68   |
| 14  | g     | 816  | CLA  | C4A-NA-C1A  | 6.57  | 109.68      | 106.68   |
| 14  | s     | 201  | CLA  | C4A-NA-C1A  | 6.57  | 109.68      | 106.68   |
| 14  | G     | 835  | CLA  | C4A-NA-C1A  | 6.57  | 109.67      | 106.68   |
| 14  | N     | 836  | CLA  | C4A-NA-C1A  | 6.57  | 109.67      | 106.68   |
| 14  | G     | 830  | CLA  | C4A-NA-C1A  | 6.56  | 109.67      | 106.68   |
| 14  | G     | 838  | CLA  | C4A-NA-C1A  | 6.56  | 109.67      | 106.68   |
| 14  | N     | 823  | CLA  | C4A-NA-C1A  | 6.56  | 109.67      | 106.68   |
| 14  | b     | 822  | CLA  | C4A-NA-C1A  | 6.56  | 109.67      | 106.68   |
| 14  | G     | 809  | CLA  | C4A-NA-C1A  | 6.56  | 109.67      | 106.68   |
| 14  | g     | 806  | CLA  | C4A-NA-C1A  | 6.55  | 109.67      | 106.68   |
| 14  | b     | 809  | CLA  | C4A-NA-C1A  | 6.55  | 109.67      | 106.68   |
| 14  | X     | 1701 | CLA  | C4A-NA-C1A  | 6.55  | 109.67      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 813  | CLA  | C4A-NA-C1A  | 6.55  | 109.67      | 106.68   |
| 14  | A     | 808  | CLA  | C4A-NA-C1A  | 6.55  | 109.67      | 106.68   |
| 14  | N     | 824  | CLA  | C4A-NA-C1A  | 6.55  | 109.67      | 106.68   |
| 14  | g     | 838  | CLA  | C4A-NA-C1A  | 6.55  | 109.67      | 106.68   |
| 14  | N     | 822  | CLA  | C4A-NA-C1A  | 6.54  | 109.66      | 106.68   |
| 14  | G     | 826  | CLA  | C4A-NA-C1A  | 6.54  | 109.66      | 106.68   |
| 14  | N     | 815  | CLA  | C4A-NA-C1A  | 6.54  | 109.66      | 106.68   |
| 14  | n     | 826  | CLA  | C4A-NA-C1A  | 6.54  | 109.66      | 106.68   |
| 14  | A     | 857  | CLA  | C4A-NA-C1A  | 6.54  | 109.66      | 106.68   |
| 14  | a     | 834  | CLA  | C4A-NA-C1A  | 6.54  | 109.66      | 106.68   |
| 14  | A     | 803  | CLA  | C4A-NA-C1A  | 6.53  | 109.66      | 106.68   |
| 14  | S     | 201  | CLA  | C4A-NA-C1A  | 6.53  | 109.66      | 106.68   |
| 14  | g     | 805  | CLA  | C4A-NA-C1A  | 6.53  | 109.66      | 106.68   |
| 14  | a     | 813  | CLA  | C4A-NA-C1A  | 6.53  | 109.66      | 106.68   |
| 14  | G     | 853  | CLA  | C4A-NA-C1A  | 6.53  | 109.66      | 106.68   |
| 14  | n     | 833  | CLA  | C4A-NA-C1A  | 6.52  | 109.66      | 106.68   |
| 14  | l     | 202  | CLA  | C4A-NA-C1A  | 6.52  | 109.66      | 106.68   |
| 14  | a     | 822  | CLA  | C4A-NA-C1A  | 6.52  | 109.65      | 106.68   |
| 14  | B     | 835  | CLA  | C4A-NA-C1A  | 6.52  | 109.65      | 106.68   |
| 17  | t     | 104  | BCR  | C20-C21-C22 | -6.51 | 118.14      | 127.28   |
| 14  | A     | 817  | CLA  | C4A-NA-C1A  | 6.51  | 109.65      | 106.68   |
| 14  | a     | 816  | CLA  | C4A-NA-C1A  | 6.51  | 109.65      | 106.68   |
| 14  | A     | 821  | CLA  | C4A-NA-C1A  | 6.51  | 109.65      | 106.68   |
| 14  | n     | 813  | CLA  | C4A-NA-C1A  | 6.51  | 109.65      | 106.68   |
| 14  | A     | 839  | CLA  | C4A-NA-C1A  | 6.51  | 109.65      | 106.68   |
| 14  | g     | 834  | CLA  | C4A-NA-C1A  | 6.51  | 109.65      | 106.68   |
| 14  | a     | 825  | CLA  | C4A-NA-C1A  | 6.51  | 109.65      | 106.68   |
| 14  | A     | 820  | CLA  | C4A-NA-C1A  | 6.50  | 109.64      | 106.68   |
| 17  | i     | 101  | BCR  | C7-C8-C9    | -6.50 | 116.62      | 126.23   |
| 14  | g     | 818  | CLA  | C4A-NA-C1A  | 6.50  | 109.64      | 106.68   |
| 14  | g     | 839  | CLA  | C4A-NA-C1A  | 6.50  | 109.64      | 106.68   |
| 14  | a     | 802  | CLA  | C4A-NA-C1A  | 6.50  | 109.64      | 106.68   |
| 14  | G     | 814  | CLA  | C4A-NA-C1A  | 6.49  | 109.64      | 106.68   |
| 14  | t     | 101  | CLA  | C4A-NA-C1A  | 6.49  | 109.64      | 106.68   |
| 14  | g     | 815  | CLA  | C4A-NA-C1A  | 6.49  | 109.64      | 106.68   |
| 14  | n     | 837  | CLA  | C4A-NA-C1A  | 6.49  | 109.64      | 106.68   |
| 14  | U     | 101  | CLA  | C4A-NA-C1A  | 6.48  | 109.64      | 106.68   |
| 14  | h     | 1701 | CLA  | C4A-NA-C1A  | 6.48  | 109.64      | 106.68   |
| 14  | n     | 820  | CLA  | C4A-NA-C1A  | 6.48  | 109.64      | 106.68   |
| 14  | a     | 814  | CLA  | C4A-NA-C1A  | 6.48  | 109.63      | 106.68   |
| 17  | t     | 104  | BCR  | C24-C23-C22 | -6.48 | 116.66      | 126.23   |
| 14  | u     | 101  | CLA  | C4A-NA-C1A  | 6.47  | 109.63      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | g     | 825 | CLA  | C4A-NA-C1A  | 6.47  | 109.63      | 106.68   |
| 14  | N     | 837 | CLA  | C4A-NA-C1A  | 6.47  | 109.63      | 106.68   |
| 14  | g     | 823 | CLA  | C4A-NA-C1A  | 6.47  | 109.63      | 106.68   |
| 14  | w     | 204 | CLA  | C4A-NA-C1A  | 6.47  | 109.63      | 106.68   |
| 14  | B     | 840 | CLA  | C4A-NA-C1A  | 6.47  | 109.63      | 106.68   |
| 14  | A     | 809 | CLA  | C4A-NA-C1A  | 6.47  | 109.63      | 106.68   |
| 14  | N     | 835 | CLA  | C4A-NA-C1A  | 6.46  | 109.63      | 106.68   |
| 14  | G     | 839 | CLA  | C4A-NA-C1A  | 6.46  | 109.63      | 106.68   |
| 14  | f     | 201 | CLA  | C4A-NA-C1A  | 6.46  | 109.63      | 106.68   |
| 14  | A     | 811 | CLA  | C4A-NA-C1A  | 6.46  | 109.62      | 106.68   |
| 14  | B     | 813 | CLA  | C4A-NA-C1A  | 6.46  | 109.62      | 106.68   |
| 14  | G     | 807 | CLA  | C4A-NA-C1A  | 6.45  | 109.62      | 106.68   |
| 14  | J     | 101 | CLA  | C4A-NA-C1A  | 6.45  | 109.62      | 106.68   |
| 14  | G     | 827 | CLA  | C4A-NA-C1A  | 6.45  | 109.62      | 106.68   |
| 14  | A     | 802 | CLA  | C4A-NA-C1A  | 6.44  | 109.62      | 106.68   |
| 14  | G     | 813 | CLA  | C4A-NA-C1A  | 6.44  | 109.62      | 106.68   |
| 14  | A     | 841 | CLA  | C4A-NA-C1A  | 6.44  | 109.62      | 106.68   |
| 14  | G     | 836 | CLA  | C4A-NA-C1A  | 6.44  | 109.62      | 106.68   |
| 14  | N     | 814 | CLA  | C4A-NA-C1A  | 6.44  | 109.61      | 106.68   |
| 14  | G     | 832 | CLA  | C4A-NA-C1A  | 6.43  | 109.61      | 106.68   |
| 14  | n     | 809 | CLA  | C4A-NA-C1A  | 6.43  | 109.61      | 106.68   |
| 14  | a     | 837 | CLA  | C4A-NA-C1A  | 6.43  | 109.61      | 106.68   |
| 14  | B     | 832 | CLA  | C4A-NA-C1A  | 6.43  | 109.61      | 106.68   |
| 17  | g     | 843 | BCR  | C11-C10-C9  | -6.43 | 118.26      | 127.28   |
| 14  | N     | 840 | CLA  | C4A-NA-C1A  | 6.43  | 109.61      | 106.68   |
| 14  | N     | 826 | CLA  | C4A-NA-C1A  | 6.43  | 109.61      | 106.68   |
| 14  | B     | 819 | CLA  | C4A-NA-C1A  | 6.43  | 109.61      | 106.68   |
| 14  | G     | 802 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 14  | b     | 832 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 14  | n     | 808 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 14  | A     | 825 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 14  | g     | 822 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 14  | G     | 804 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 14  | G     | 810 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 14  | g     | 835 | CLA  | C4A-NA-C1A  | 6.42  | 109.61      | 106.68   |
| 17  | j     | 104 | BCR  | C20-C21-C22 | -6.41 | 118.28      | 127.28   |
| 14  | G     | 833 | CLA  | C4A-NA-C1A  | 6.41  | 109.61      | 106.68   |
| 14  | b     | 811 | CLA  | C4A-NA-C1A  | 6.41  | 109.61      | 106.68   |
| 14  | b     | 816 | CLA  | C4A-NA-C1A  | 6.41  | 109.61      | 106.68   |
| 14  | b     | 823 | CLA  | C4A-NA-C1A  | 6.41  | 109.61      | 106.68   |
| 14  | T     | 101 | CLA  | C4A-NA-C1A  | 6.41  | 109.60      | 106.68   |
| 14  | b     | 806 | CLA  | C4A-NA-C1A  | 6.41  | 109.60      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms      | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|------|-------------|----------|
| 14  | N     | 811  | CLA  | C4A-NA-C1A | 6.41 | 109.60      | 106.68   |
| 14  | N     | 813  | CLA  | C4A-NA-C1A | 6.41 | 109.60      | 106.68   |
| 14  | g     | 808  | CLA  | C4A-NA-C1A | 6.41 | 109.60      | 106.68   |
| 14  | g     | 832  | CLA  | C4A-NA-C1A | 6.41 | 109.60      | 106.68   |
| 14  | n     | 821  | CLA  | C4A-NA-C1A | 6.41 | 109.60      | 106.68   |
| 14  | A     | 810  | CLA  | C4A-NA-C1A | 6.41 | 109.60      | 106.68   |
| 14  | g     | 827  | CLA  | C4A-NA-C1A | 6.40 | 109.60      | 106.68   |
| 14  | u     | 102  | CLA  | C4A-NA-C1A | 6.40 | 109.60      | 106.68   |
| 14  | n     | 822  | CLA  | C4A-NA-C1A | 6.40 | 109.60      | 106.68   |
| 14  | A     | 832  | CLA  | C4A-NA-C1A | 6.40 | 109.60      | 106.68   |
| 14  | B     | 834  | CLA  | C4A-NA-C1A | 6.40 | 109.60      | 106.68   |
| 14  | b     | 830  | CLA  | C4A-NA-C1A | 6.40 | 109.60      | 106.68   |
| 14  | a     | 852  | CLA  | C4A-NA-C1A | 6.40 | 109.60      | 106.68   |
| 14  | G     | 811  | CLA  | C4A-NA-C1A | 6.39 | 109.60      | 106.68   |
| 14  | U     | 102  | CLA  | C4A-NA-C1A | 6.39 | 109.60      | 106.68   |
| 14  | B     | 823  | CLA  | C4A-NA-C1A | 6.39 | 109.59      | 106.68   |
| 14  | b     | 808  | CLA  | C4A-NA-C1A | 6.39 | 109.59      | 106.68   |
| 14  | g     | 836  | CLA  | C4A-NA-C1A | 6.39 | 109.59      | 106.68   |
| 14  | g     | 833  | CLA  | C4A-NA-C1A | 6.38 | 109.59      | 106.68   |
| 14  | a     | 823  | CLA  | C4A-NA-C1A | 6.38 | 109.59      | 106.68   |
| 14  | N     | 809  | CLA  | C4A-NA-C1A | 6.38 | 109.59      | 106.68   |
| 14  | n     | 806  | CLA  | C4A-NA-C1A | 6.38 | 109.59      | 106.68   |
| 14  | n     | 834  | CLA  | C4A-NA-C1A | 6.38 | 109.59      | 106.68   |
| 14  | g     | 820  | CLA  | C4A-NA-C1A | 6.38 | 109.59      | 106.68   |
| 14  | B     | 831  | CLA  | C4A-NA-C1A | 6.38 | 109.59      | 106.68   |
| 14  | n     | 835  | CLA  | C4A-NA-C1A | 6.37 | 109.59      | 106.68   |
| 14  | b     | 807  | CLA  | C4A-NA-C1A | 6.37 | 109.59      | 106.68   |
| 14  | b     | 839  | CLA  | C4A-NA-C1A | 6.37 | 109.59      | 106.68   |
| 14  | n     | 807  | CLA  | C4A-NA-C1A | 6.37 | 109.58      | 106.68   |
| 14  | a     | 826  | CLA  | C4A-NA-C1A | 6.37 | 109.58      | 106.68   |
| 14  | L     | 1502 | CLA  | C4A-NA-C1A | 6.37 | 109.58      | 106.68   |
| 14  | n     | 811  | CLA  | C4A-NA-C1A | 6.36 | 109.58      | 106.68   |
| 14  | n     | 830  | CLA  | C4A-NA-C1A | 6.36 | 109.58      | 106.68   |
| 14  | B     | 807  | CLA  | C4A-NA-C1A | 6.36 | 109.58      | 106.68   |
| 14  | a     | 832  | CLA  | C4A-NA-C1A | 6.36 | 109.58      | 106.68   |
| 14  | b     | 812  | CLA  | C4A-NA-C1A | 6.36 | 109.58      | 106.68   |
| 14  | a     | 801  | CLA  | C4A-NA-C1A | 6.36 | 109.58      | 106.68   |
| 14  | n     | 839  | CLA  | C4A-NA-C1A | 6.35 | 109.58      | 106.68   |
| 14  | n     | 815  | CLA  | C4A-NA-C1A | 6.35 | 109.58      | 106.68   |
| 14  | B     | 814  | CLA  | C4A-NA-C1A | 6.35 | 109.58      | 106.68   |
| 14  | k     | 101  | CLA  | C4A-NA-C1A | 6.35 | 109.58      | 106.68   |
| 14  | n     | 819  | CLA  | C4A-NA-C1A | 6.35 | 109.57      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | b     | 819 | CLA  | C4A-NA-C1A  | 6.35  | 109.57      | 106.68   |
| 14  | N     | 829 | CLA  | C4A-NA-C1A  | 6.34  | 109.57      | 106.68   |
| 14  | n     | 805 | CLA  | C4A-NA-C1A  | 6.34  | 109.57      | 106.68   |
| 14  | a     | 809 | CLA  | C4A-NA-C1A  | 6.34  | 109.57      | 106.68   |
| 14  | a     | 833 | CLA  | C4A-NA-C1A  | 6.34  | 109.57      | 106.68   |
| 14  | G     | 805 | CLA  | C4A-NA-C1A  | 6.34  | 109.57      | 106.68   |
| 17  | A     | 847 | BCR  | C15-C14-C13 | -6.34 | 118.39      | 127.28   |
| 14  | N     | 818 | CLA  | C4A-NA-C1A  | 6.34  | 109.57      | 106.68   |
| 14  | N     | 821 | CLA  | C4A-NA-C1A  | 6.34  | 109.57      | 106.68   |
| 14  | n     | 825 | CLA  | C4A-NA-C1A  | 6.34  | 109.57      | 106.68   |
| 14  | a     | 819 | CLA  | C4A-NA-C1A  | 6.34  | 109.57      | 106.68   |
| 14  | N     | 817 | CLA  | C4A-NA-C1A  | 6.33  | 109.57      | 106.68   |
| 14  | g     | 802 | CLA  | C4A-NA-C1A  | 6.33  | 109.57      | 106.68   |
| 14  | b     | 815 | CLA  | C4A-NA-C1A  | 6.33  | 109.57      | 106.68   |
| 14  | G     | 806 | CLA  | C4A-NA-C1A  | 6.33  | 109.57      | 106.68   |
| 14  | b     | 835 | CLA  | C4A-NA-C1A  | 6.33  | 109.57      | 106.68   |
| 14  | G     | 812 | CLA  | C4A-NA-C1A  | 6.33  | 109.56      | 106.68   |
| 14  | B     | 828 | CLA  | C4A-NA-C1A  | 6.32  | 109.56      | 106.68   |
| 14  | g     | 821 | CLA  | C4A-NA-C1A  | 6.32  | 109.56      | 106.68   |
| 14  | n     | 850 | CLA  | C4A-NA-C1A  | 6.32  | 109.56      | 106.68   |
| 14  | a     | 835 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 14  | J     | 102 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 14  | j     | 102 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 14  | n     | 831 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 14  | w     | 203 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 14  | b     | 853 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 14  | A     | 824 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 14  | T     | 102 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 14  | F     | 201 | CLA  | C4A-NA-C1A  | 6.31  | 109.56      | 106.68   |
| 14  | g     | 810 | CLA  | C4A-NA-C1A  | 6.30  | 109.55      | 106.68   |
| 14  | n     | 824 | CLA  | C4A-NA-C1A  | 6.30  | 109.55      | 106.68   |
| 14  | b     | 831 | CLA  | C4A-NA-C1A  | 6.30  | 109.55      | 106.68   |
| 17  | B     | 846 | BCR  | C24-C23-C22 | -6.30 | 116.92      | 126.23   |
| 14  | b     | 840 | CLA  | C4A-NA-C1A  | 6.30  | 109.55      | 106.68   |
| 14  | G     | 837 | CLA  | C4A-NA-C1A  | 6.29  | 109.55      | 106.68   |
| 14  | N     | 838 | CLA  | C4A-NA-C1A  | 6.29  | 109.55      | 106.68   |
| 14  | g     | 813 | CLA  | C4A-NA-C1A  | 6.28  | 109.55      | 106.68   |
| 14  | n     | 803 | CLA  | C4A-NA-C1A  | 6.28  | 109.54      | 106.68   |
| 14  | w     | 205 | CLA  | C4A-NA-C1A  | 6.28  | 109.54      | 106.68   |
| 14  | g     | 819 | CLA  | C4A-NA-C1A  | 6.28  | 109.54      | 106.68   |
| 14  | b     | 836 | CLA  | C4A-NA-C1A  | 6.28  | 109.54      | 106.68   |
| 14  | G     | 828 | CLA  | C4A-NA-C1A  | 6.27  | 109.54      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | g     | 826 | CLA  | C4A-NA-C1A  | 6.27  | 109.54      | 106.68   |
| 14  | n     | 817 | CLA  | C4A-NA-C1A  | 6.27  | 109.54      | 106.68   |
| 14  | A     | 853 | CLA  | C4A-NA-C1A  | 6.27  | 109.54      | 106.68   |
| 14  | b     | 810 | CLA  | C4A-NA-C1A  | 6.27  | 109.54      | 106.68   |
| 14  | G     | 817 | CLA  | C4A-NA-C1A  | 6.27  | 109.54      | 106.68   |
| 14  | A     | 827 | CLA  | C4A-NA-C1A  | 6.27  | 109.54      | 106.68   |
| 14  | K     | 101 | CLA  | C4A-NA-C1A  | 6.27  | 109.54      | 106.68   |
| 14  | l     | 204 | CLA  | C4A-NA-C1A  | 6.27  | 109.54      | 106.68   |
| 14  | a     | 810 | CLA  | C4A-NA-C1A  | 6.26  | 109.54      | 106.68   |
| 14  | A     | 812 | CLA  | C4A-NA-C1A  | 6.26  | 109.53      | 106.68   |
| 14  | a     | 824 | CLA  | C4A-NA-C1A  | 6.26  | 109.53      | 106.68   |
| 14  | g     | 831 | CLA  | C4A-NA-C1A  | 6.26  | 109.53      | 106.68   |
| 14  | n     | 838 | CLA  | C4A-NA-C1A  | 6.26  | 109.53      | 106.68   |
| 14  | a     | 836 | CLA  | C4A-NA-C1A  | 6.25  | 109.53      | 106.68   |
| 14  | N     | 841 | CLA  | C4A-NA-C1A  | 6.25  | 109.53      | 106.68   |
| 14  | n     | 810 | CLA  | C4A-NA-C1A  | 6.25  | 109.53      | 106.68   |
| 14  | l     | 203 | CLA  | C4A-NA-C1A  | 6.25  | 109.53      | 106.68   |
| 14  | b     | 825 | CLA  | C4A-NA-C1A  | 6.25  | 109.53      | 106.68   |
| 14  | n     | 812 | CLA  | C4A-NA-C1A  | 6.25  | 109.53      | 106.68   |
| 14  | N     | 833 | CLA  | C4A-NA-C1A  | 6.24  | 109.53      | 106.68   |
| 14  | t     | 102 | CLA  | C4A-NA-C1A  | 6.24  | 109.53      | 106.68   |
| 14  | A     | 837 | CLA  | C4A-NA-C1A  | 6.24  | 109.53      | 106.68   |
| 17  | A     | 856 | BCR  | C15-C14-C13 | -6.24 | 118.53      | 127.28   |
| 14  | b     | 814 | CLA  | C4A-NA-C1A  | 6.24  | 109.52      | 106.68   |
| 14  | G     | 834 | CLA  | C4A-NA-C1A  | 6.23  | 109.52      | 106.68   |
| 14  | a     | 804 | CLA  | C4A-NA-C1A  | 6.23  | 109.52      | 106.68   |
| 14  | B     | 808 | CLA  | C4A-NA-C1A  | 6.23  | 109.52      | 106.68   |
| 14  | s     | 202 | CLA  | C4A-NA-C1A  | 6.23  | 109.52      | 106.68   |
| 14  | B     | 825 | CLA  | C4A-NA-C1A  | 6.23  | 109.52      | 106.68   |
| 17  | n     | 845 | BCR  | C15-C14-C13 | -6.23 | 118.54      | 127.28   |
| 14  | n     | 818 | CLA  | C4A-NA-C1A  | 6.23  | 109.52      | 106.68   |
| 14  | N     | 820 | CLA  | C4A-NA-C1A  | 6.22  | 109.52      | 106.68   |
| 14  | S     | 203 | CLA  | C4A-NA-C1A  | 6.21  | 109.51      | 106.68   |
| 14  | G     | 803 | CLA  | C4A-NA-C1A  | 6.21  | 109.51      | 106.68   |
| 14  | G     | 831 | CLA  | C4A-NA-C1A  | 6.21  | 109.51      | 106.68   |
| 14  | b     | 837 | CLA  | C4A-NA-C1A  | 6.21  | 109.51      | 106.68   |
| 14  | A     | 834 | CLA  | C4A-NA-C1A  | 6.21  | 109.51      | 106.68   |
| 14  | B     | 804 | CLA  | C4A-NA-C1A  | 6.20  | 109.51      | 106.68   |
| 14  | n     | 836 | CLA  | C4A-NA-C1A  | 6.20  | 109.51      | 106.68   |
| 14  | g     | 803 | CLA  | C4A-NA-C1A  | 6.19  | 109.50      | 106.68   |
| 14  | A     | 833 | CLA  | C4A-NA-C1A  | 6.19  | 109.50      | 106.68   |
| 14  | n     | 832 | CLA  | C4A-NA-C1A  | 6.19  | 109.50      | 106.68   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | N     | 807  | CLA  | C4A-NA-C1A  | 6.19  | 109.50      | 106.68   |
| 14  | N     | 819  | CLA  | C4A-NA-C1A  | 6.19  | 109.50      | 106.68   |
| 14  | b     | 829  | CLA  | C4A-NA-C1A  | 6.18  | 109.50      | 106.68   |
| 14  | B     | 810  | CLA  | C4A-NA-C1A  | 6.18  | 109.50      | 106.68   |
| 14  | G     | 840  | CLA  | C4A-NA-C1A  | 6.17  | 109.50      | 106.68   |
| 14  | B     | 836  | CLA  | C4A-NA-C1A  | 6.17  | 109.50      | 106.68   |
| 14  | a     | 854  | CLA  | C4A-NA-C1A  | 6.17  | 109.50      | 106.68   |
| 14  | a     | 808  | CLA  | C4A-NA-C1A  | 6.17  | 109.49      | 106.68   |
| 14  | G     | 818  | CLA  | C4A-NA-C1A  | 6.16  | 109.49      | 106.68   |
| 14  | L     | 1503 | CLA  | C4A-NA-C1A  | 6.16  | 109.49      | 106.68   |
| 14  | n     | 804  | CLA  | C4A-NA-C1A  | 6.16  | 109.49      | 106.68   |
| 14  | B     | 839  | CLA  | C4A-NA-C1A  | 6.15  | 109.49      | 106.68   |
| 14  | G     | 815  | CLA  | C4A-NA-C1A  | 6.15  | 109.48      | 106.68   |
| 14  | g     | 817  | CLA  | C4A-NA-C1A  | 6.15  | 109.48      | 106.68   |
| 14  | b     | 818  | CLA  | C4A-NA-C1A  | 6.15  | 109.48      | 106.68   |
| 17  | N     | 844  | BCR  | C24-C23-C22 | -6.14 | 117.15      | 126.23   |
| 14  | n     | 827  | CLA  | C4A-NA-C1A  | 6.14  | 109.48      | 106.68   |
| 14  | b     | 826  | CLA  | C4A-NA-C1A  | 6.14  | 109.48      | 106.68   |
| 14  | N     | 812  | CLA  | C4A-NA-C1A  | 6.14  | 109.48      | 106.68   |
| 14  | W     | 204  | CLA  | C4A-NA-C1A  | 6.14  | 109.48      | 106.68   |
| 14  | N     | 808  | CLA  | C4A-NA-C1A  | 6.13  | 109.47      | 106.68   |
| 14  | b     | 828  | CLA  | C4A-NA-C1A  | 6.13  | 109.47      | 106.68   |
| 14  | g     | 824  | CLA  | C4A-NA-C1A  | 6.12  | 109.47      | 106.68   |
| 14  | n     | 828  | CLA  | C4A-NA-C1A  | 6.12  | 109.47      | 106.68   |
| 14  | B     | 811  | CLA  | C4A-NA-C1A  | 6.12  | 109.47      | 106.68   |
| 14  | a     | 831  | CLA  | C4A-NA-C1A  | 6.12  | 109.47      | 106.68   |
| 14  | G     | 825  | CLA  | C4A-NA-C1A  | 6.12  | 109.47      | 106.68   |
| 14  | N     | 806  | CLA  | C4A-NA-C1A  | 6.12  | 109.47      | 106.68   |
| 14  | B     | 806  | CLA  | C4A-NA-C1A  | 6.12  | 109.47      | 106.68   |
| 14  | f     | 202  | CLA  | C4A-NA-C1A  | 6.12  | 109.47      | 106.68   |
| 14  | N     | 825  | CLA  | C4A-NA-C1A  | 6.09  | 109.46      | 106.68   |
| 14  | a     | 829  | CLA  | C4A-NA-C1A  | 6.09  | 109.46      | 106.68   |
| 14  | N     | 830  | CLA  | C4A-NA-C1A  | 6.09  | 109.46      | 106.68   |
| 17  | t     | 104  | BCR  | C16-C17-C18 | -6.09 | 118.74      | 127.28   |
| 14  | B     | 805  | CLA  | C4A-NA-C1A  | 6.09  | 109.46      | 106.68   |
| 14  | A     | 818  | CLA  | C4A-NA-C1A  | 6.08  | 109.45      | 106.68   |
| 14  | A     | 830  | CLA  | C4A-NA-C1A  | 6.08  | 109.45      | 106.68   |
| 17  | V     | 101  | BCR  | C11-C10-C9  | -6.08 | 118.75      | 127.28   |
| 14  | A     | 855  | CLA  | C4A-NA-C1A  | 6.07  | 109.45      | 106.68   |
| 17  | j     | 104  | BCR  | C11-C10-C9  | -6.07 | 118.77      | 127.28   |
| 14  | g     | 809  | CLA  | C4A-NA-C1A  | 6.07  | 109.45      | 106.68   |
| 17  | a     | 848  | BCR  | C20-C21-C22 | -6.07 | 118.77      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | N     | 832 | CLA  | C4A-NA-C1A  | 6.06  | 109.44      | 106.68   |
| 14  | B     | 826 | CLA  | C4A-NA-C1A  | 6.06  | 109.44      | 106.68   |
| 14  | F     | 202 | CLA  | C4A-NA-C1A  | 6.06  | 109.44      | 106.68   |
| 14  | n     | 814 | CLA  | C4A-NA-C1A  | 6.05  | 109.44      | 106.68   |
| 14  | a     | 811 | CLA  | C4A-NA-C1A  | 6.05  | 109.44      | 106.68   |
| 14  | a     | 821 | CLA  | C4A-NA-C1A  | 6.05  | 109.44      | 106.68   |
| 14  | b     | 833 | CLA  | C4A-NA-C1A  | 6.05  | 109.44      | 106.68   |
| 17  | j     | 104 | BCR  | C24-C23-C22 | -6.05 | 117.29      | 126.23   |
| 14  | A     | 831 | CLA  | C4A-NA-C1A  | 6.05  | 109.44      | 106.68   |
| 14  | B     | 837 | CLA  | C4A-NA-C1A  | 6.04  | 109.44      | 106.68   |
| 14  | A     | 840 | CLA  | C4A-NA-C1A  | 6.04  | 109.44      | 106.68   |
| 17  | G     | 843 | BCR  | C16-C17-C18 | -6.02 | 118.83      | 127.28   |
| 14  | b     | 820 | CLA  | C4A-NA-C1A  | 6.02  | 109.43      | 106.68   |
| 14  | g     | 804 | CLA  | C4A-NA-C1A  | 6.02  | 109.42      | 106.68   |
| 17  | T     | 104 | BCR  | C15-C14-C13 | -6.02 | 118.84      | 127.28   |
| 14  | b     | 824 | CLA  | C4A-NA-C1A  | 6.01  | 109.42      | 106.68   |
| 14  | N     | 801 | CLA  | C4A-NA-C1A  | 6.01  | 109.42      | 106.68   |
| 14  | g     | 852 | CLA  | C4A-NA-C1A  | 6.00  | 109.42      | 106.68   |
| 17  | I     | 101 | BCR  | C24-C23-C22 | -6.00 | 117.36      | 126.23   |
| 14  | b     | 802 | CLA  | C4A-NA-C1A  | 5.99  | 109.41      | 106.68   |
| 14  | N     | 851 | CLA  | C4A-NA-C1A  | 5.99  | 109.41      | 106.68   |
| 14  | n     | 852 | CLA  | C4A-NA-C1A  | 5.99  | 109.41      | 106.68   |
| 14  | a     | 817 | CLA  | C4A-NA-C1A  | 5.99  | 109.41      | 106.68   |
| 14  | G     | 820 | CLA  | C4A-NA-C1A  | 5.98  | 109.41      | 106.68   |
| 14  | B     | 818 | CLA  | C4A-NA-C1A  | 5.98  | 109.41      | 106.68   |
| 14  | g     | 811 | CLA  | C4A-NA-C1A  | 5.98  | 109.41      | 106.68   |
| 14  | A     | 805 | CLA  | C4A-NA-C1A  | 5.98  | 109.41      | 106.68   |
| 14  | g     | 829 | CLA  | C4A-NA-C1A  | 5.97  | 109.40      | 106.68   |
| 17  | g     | 848 | BCR  | C7-C8-C9    | -5.97 | 117.40      | 126.23   |
| 17  | V     | 101 | BCR  | C7-C8-C9    | -5.97 | 117.40      | 126.23   |
| 14  | b     | 804 | CLA  | C4A-NA-C1A  | 5.97  | 109.40      | 106.68   |
| 14  | N     | 804 | CLA  | C4A-NA-C1A  | 5.96  | 109.40      | 106.68   |
| 17  | B     | 851 | BCR  | C16-C17-C18 | -5.95 | 118.94      | 127.28   |
| 17  | a     | 848 | BCR  | C7-C8-C9    | -5.95 | 117.44      | 126.23   |
| 17  | f     | 203 | BCR  | C15-C14-C13 | -5.94 | 118.94      | 127.28   |
| 14  | n     | 823 | CLA  | C4A-NA-C1A  | 5.94  | 109.39      | 106.68   |
| 14  | B     | 850 | CLA  | C4A-NA-C1A  | 5.93  | 109.39      | 106.68   |
| 14  | N     | 805 | CLA  | C4A-NA-C1A  | 5.92  | 109.38      | 106.68   |
| 14  | g     | 854 | CLA  | C4A-NA-C1A  | 5.89  | 109.37      | 106.68   |
| 17  | G     | 843 | BCR  | C11-C10-C9  | -5.89 | 119.01      | 127.28   |
| 14  | B     | 824 | CLA  | C4A-NA-C1A  | 5.89  | 109.36      | 106.68   |
| 17  | v     | 101 | BCR  | C20-C21-C22 | -5.88 | 119.04      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | a     | 827 | CLA  | C4A-NA-C1A  | 5.87  | 109.36      | 106.68   |
| 14  | A     | 828 | CLA  | C4A-NA-C1A  | 5.87  | 109.36      | 106.68   |
| 17  | s     | 203 | BCR  | C15-C14-C13 | -5.86 | 119.06      | 127.28   |
| 17  | n     | 846 | BCR  | C15-C14-C13 | -5.86 | 119.06      | 127.28   |
| 17  | A     | 844 | BCR  | C11-C10-C9  | -5.85 | 119.08      | 127.28   |
| 17  | B     | 846 | BCR  | C16-C17-C18 | -5.82 | 119.11      | 127.28   |
| 14  | j     | 101 | CLA  | C4A-NA-C1A  | 5.82  | 109.33      | 106.68   |
| 17  | A     | 849 | BCR  | C7-C8-C9    | -5.78 | 117.68      | 126.23   |
| 14  | B     | 829 | CLA  | C4A-NA-C1A  | 5.78  | 109.32      | 106.68   |
| 17  | n     | 845 | BCR  | C20-C21-C22 | -5.76 | 119.20      | 127.28   |
| 17  | B     | 846 | BCR  | C20-C21-C22 | -5.75 | 119.21      | 127.28   |
| 17  | w     | 201 | BCR  | C24-C23-C22 | -5.74 | 117.74      | 126.23   |
| 14  | n     | 802 | CLA  | C4A-NA-C1A  | 5.72  | 109.29      | 106.68   |
| 14  | B     | 820 | CLA  | C4A-NA-C1A  | 5.72  | 109.29      | 106.68   |
| 14  | G     | 852 | CLA  | C4A-NA-C1A  | 5.72  | 109.29      | 106.68   |
| 17  | G     | 848 | BCR  | C7-C8-C9    | -5.70 | 117.81      | 126.23   |
| 17  | i     | 101 | BCR  | C11-C10-C9  | -5.70 | 119.29      | 127.28   |
| 14  | a     | 803 | CLA  | C4A-NA-C1A  | 5.69  | 109.28      | 106.68   |
| 17  | j     | 104 | BCR  | C16-C17-C18 | -5.67 | 119.33      | 127.28   |
| 17  | B     | 845 | BCR  | C24-C23-C22 | -5.67 | 117.85      | 126.23   |
| 17  | b     | 845 | BCR  | C24-C23-C22 | -5.66 | 117.86      | 126.23   |
| 14  | N     | 803 | CLA  | C4A-NA-C1A  | 5.66  | 109.26      | 106.68   |
| 17  | n     | 845 | BCR  | C11-C10-C9  | -5.65 | 119.35      | 127.28   |
| 17  | a     | 846 | BCR  | C3-C4-C5    | -5.64 | 104.00      | 114.06   |
| 17  | T     | 104 | BCR  | C16-C17-C18 | -5.64 | 119.37      | 127.28   |
| 17  | l     | 205 | BCR  | C24-C23-C22 | -5.62 | 117.92      | 126.23   |
| 17  | B     | 843 | BCR  | C20-C21-C22 | -5.62 | 119.40      | 127.28   |
| 19  | G     | 851 | CL0  | CHA-C1A-C2A | -5.62 | 120.12      | 133.31   |
| 17  | B     | 845 | BCR  | C7-C8-C9    | -5.61 | 117.94      | 126.23   |
| 14  | a     | 853 | CLA  | C4A-NA-C1A  | 5.61  | 109.24      | 106.68   |
| 17  | v     | 101 | BCR  | C24-C23-C22 | -5.61 | 117.94      | 126.23   |
| 17  | N     | 852 | BCR  | C16-C17-C18 | -5.60 | 119.43      | 127.28   |
| 17  | a     | 844 | BCR  | C16-C17-C18 | -5.59 | 119.44      | 127.28   |
| 14  | g     | 853 | CLA  | C4A-NA-C1A  | 5.58  | 109.23      | 106.68   |
| 17  | n     | 849 | BCR  | C16-C17-C18 | -5.58 | 119.45      | 127.28   |
| 17  | n     | 844 | BCR  | C24-C23-C22 | -5.57 | 117.99      | 126.23   |
| 17  | N     | 847 | BCR  | C15-C14-C13 | -5.56 | 119.47      | 127.28   |
| 14  | N     | 827 | CLA  | C4A-NA-C1A  | 5.56  | 109.22      | 106.68   |
| 17  | g     | 846 | BCR  | C20-C21-C22 | -5.56 | 119.48      | 127.28   |
| 17  | B     | 848 | BCR  | C16-C17-C18 | -5.55 | 119.49      | 127.28   |
| 17  | I     | 101 | BCR  | C16-C17-C18 | -5.55 | 119.49      | 127.28   |
| 17  | B     | 848 | BCR  | C24-C23-C22 | -5.54 | 118.04      | 126.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | v     | 101 | BCR  | C3-C4-C5    | -5.50 | 104.25      | 114.06   |
| 17  | A     | 849 | BCR  | C20-C21-C22 | -5.48 | 119.59      | 127.28   |
| 17  | n     | 842 | BCR  | C24-C23-C22 | -5.48 | 118.13      | 126.23   |
| 17  | n     | 842 | BCR  | C20-C21-C22 | -5.48 | 119.60      | 127.28   |
| 17  | u     | 103 | BCR  | C16-C17-C18 | -5.47 | 119.61      | 127.28   |
| 17  | B     | 843 | BCR  | C24-C23-C22 | -5.45 | 118.17      | 126.23   |
| 17  | N     | 852 | BCR  | C20-C19-C18 | -5.43 | 111.46      | 126.36   |
| 14  | G     | 801 | CLA  | C4A-NA-C1A  | 5.43  | 109.16      | 106.68   |
| 17  | F     | 203 | BCR  | C15-C14-C13 | -5.42 | 119.67      | 127.28   |
| 14  | B     | 803 | CLA  | C4A-NA-C1A  | 5.41  | 109.15      | 106.68   |
| 17  | a     | 845 | BCR  | C3-C4-C5    | -5.41 | 104.41      | 114.06   |
| 17  | G     | 848 | BCR  | C20-C21-C22 | -5.41 | 119.69      | 127.28   |
| 17  | a     | 843 | BCR  | C11-C10-C9  | -5.39 | 119.72      | 127.28   |
| 17  | N     | 846 | BCR  | C24-C23-C22 | -5.37 | 118.28      | 126.23   |
| 17  | S     | 204 | BCR  | C15-C14-C13 | -5.36 | 119.76      | 127.28   |
| 17  | W     | 206 | BCR  | C7-C8-C9    | -5.35 | 118.33      | 126.23   |
| 19  | A     | 852 | CL0  | CHA-C1A-C2A | -5.34 | 120.78      | 133.31   |
| 17  | v     | 101 | BCR  | C16-C17-C18 | -5.33 | 119.81      | 127.28   |
| 17  | b     | 850 | BCR  | C20-C21-C22 | -5.32 | 119.82      | 127.28   |
| 17  | G     | 845 | BCR  | C3-C4-C5    | -5.31 | 104.59      | 114.06   |
| 17  | g     | 845 | BCR  | C3-C4-C5    | -5.30 | 104.60      | 114.06   |
| 17  | a     | 846 | BCR  | C16-C15-C14 | -5.30 | 112.67      | 123.52   |
| 17  | I     | 102 | BCR  | C21-C20-C19 | -5.30 | 107.84      | 123.20   |
| 19  | a     | 851 | CL0  | CHA-C1A-C2A | -5.30 | 120.86      | 133.31   |
| 17  | V     | 101 | BCR  | C15-C14-C13 | -5.30 | 119.85      | 127.28   |
| 17  | N     | 844 | BCR  | C20-C21-C22 | -5.29 | 119.86      | 127.28   |
| 17  | B     | 848 | BCR  | C20-C21-C22 | -5.29 | 119.86      | 127.28   |
| 17  | g     | 848 | BCR  | C20-C21-C22 | -5.29 | 119.86      | 127.28   |
| 17  | B     | 847 | BCR  | C24-C23-C22 | -5.28 | 118.42      | 126.23   |
| 17  | A     | 846 | BCR  | C15-C14-C13 | -5.28 | 119.87      | 127.28   |
| 17  | N     | 848 | BCR  | C15-C14-C13 | -5.28 | 119.87      | 127.28   |
| 17  | G     | 846 | BCR  | C15-C14-C13 | -5.28 | 119.88      | 127.28   |
| 17  | B     | 851 | BCR  | C20-C21-C22 | -5.26 | 119.90      | 127.28   |
| 17  | n     | 847 | BCR  | C16-C17-C18 | -5.25 | 119.91      | 127.28   |
| 17  | k     | 102 | BCR  | C16-C17-C18 | -5.25 | 119.92      | 127.28   |
| 14  | b     | 805 | CLA  | C4A-NA-C1A  | 5.24  | 109.07      | 106.68   |
| 17  | b     | 846 | BCR  | C11-C10-C9  | -5.24 | 119.94      | 127.28   |
| 17  | n     | 845 | BCR  | C24-C23-C22 | -5.22 | 118.52      | 126.23   |
| 17  | n     | 843 | BCR  | C7-C8-C9    | -5.22 | 118.52      | 126.23   |
| 17  | g     | 846 | BCR  | C8-C9-C10   | 5.19  | 127.17      | 119.01   |
| 17  | n     | 846 | BCR  | C11-C10-C9  | -5.18 | 120.02      | 127.28   |
| 14  | A     | 801 | CLA  | C4A-NA-C1A  | 5.18  | 109.04      | 106.68   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | b     | 847 | BCR  | C11-C10-C9  | -5.17 | 120.03      | 127.28   |
| 17  | A     | 847 | BCR  | C20-C21-C22 | -5.16 | 120.04      | 127.28   |
| 17  | S     | 204 | BCR  | C11-C10-C9  | -5.15 | 120.06      | 127.28   |
| 17  | G     | 844 | BCR  | C16-C17-C18 | -5.12 | 120.10      | 127.28   |
| 17  | F     | 203 | BCR  | C11-C10-C9  | -5.07 | 120.17      | 127.28   |
| 17  | N     | 847 | BCR  | C20-C21-C22 | -5.07 | 120.17      | 127.28   |
| 17  | m     | 102 | BCR  | C20-C21-C22 | -5.06 | 120.18      | 127.28   |
| 17  | f     | 203 | BCR  | C11-C10-C9  | -5.05 | 120.19      | 127.28   |
| 17  | w     | 206 | BCR  | C20-C21-C22 | -5.05 | 120.20      | 127.28   |
| 17  | Y     | 101 | BCR  | C16-C17-C18 | -5.04 | 120.21      | 127.28   |
| 17  | m     | 102 | BCR  | C16-C17-C18 | -5.03 | 120.22      | 127.28   |
| 17  | b     | 847 | BCR  | C15-C14-C13 | -5.03 | 120.22      | 127.28   |
| 17  | N     | 847 | BCR  | C24-C23-C22 | -5.03 | 118.80      | 126.23   |
| 17  | N     | 848 | BCR  | C11-C10-C9  | -5.02 | 120.24      | 127.28   |
| 17  | A     | 844 | BCR  | C16-C17-C18 | -5.01 | 120.25      | 127.28   |
| 17  | g     | 848 | BCR  | C38-C26-C25 | -5.00 | 119.03      | 124.48   |
| 17  | m     | 102 | BCR  | C33-C5-C6   | -4.99 | 119.03      | 124.48   |
| 17  | I     | 101 | BCR  | C7-C8-C9    | -4.99 | 118.85      | 126.23   |
| 17  | b     | 844 | BCR  | C7-C8-C9    | -4.99 | 118.86      | 126.23   |
| 17  | V     | 101 | BCR  | C16-C17-C18 | -4.98 | 120.29      | 127.28   |
| 17  | i     | 101 | BCR  | C3-C4-C5    | -4.98 | 105.17      | 114.06   |
| 19  | g     | 851 | CL0  | CHA-C1A-C2A | -4.98 | 121.62      | 133.31   |
| 17  | I     | 101 | BCR  | C20-C21-C22 | -4.97 | 120.31      | 127.28   |
| 17  | I     | 103 | BCR  | C16-C17-C18 | -4.96 | 120.32      | 127.28   |
| 17  | G     | 843 | BCR  | C15-C14-C13 | -4.95 | 120.33      | 127.28   |
| 17  | N     | 846 | BCR  | C15-C14-C13 | -4.95 | 120.33      | 127.28   |
| 17  | J     | 103 | BCR  | C15-C14-C13 | -4.95 | 120.34      | 127.28   |
| 17  | I     | 102 | BCR  | C16-C15-C14 | -4.94 | 113.42      | 123.52   |
| 17  | G     | 847 | BCR  | C16-C17-C18 | -4.93 | 120.36      | 127.28   |
| 17  | k     | 102 | BCR  | C20-C21-C22 | -4.93 | 120.36      | 127.28   |
| 17  | g     | 844 | BCR  | C16-C17-C18 | -4.93 | 120.37      | 127.28   |
| 17  | y     | 101 | BCR  | C33-C5-C6   | -4.93 | 119.11      | 124.48   |
| 17  | b     | 850 | BCR  | C7-C8-C9    | -4.92 | 118.96      | 126.23   |
| 17  | l     | 206 | BCR  | C3-C4-C5    | -4.91 | 105.30      | 114.06   |
| 17  | N     | 846 | BCR  | C11-C10-C9  | -4.91 | 120.39      | 127.28   |
| 17  | n     | 845 | BCR  | C16-C17-C18 | -4.91 | 120.40      | 127.28   |
| 17  | a     | 847 | BCR  | C15-C14-C13 | -4.90 | 120.40      | 127.28   |
| 17  | g     | 847 | BCR  | C15-C14-C13 | -4.90 | 120.41      | 127.28   |
| 17  | g     | 847 | BCR  | C16-C17-C18 | -4.89 | 120.42      | 127.28   |
| 17  | w     | 206 | BCR  | C15-C14-C13 | -4.89 | 120.42      | 127.28   |
| 17  | N     | 853 | BCR  | C11-C10-C9  | -4.89 | 120.42      | 127.28   |
| 17  | B     | 847 | BCR  | C15-C14-C13 | -4.89 | 120.42      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | n     | 844 | BCR  | C7-C8-C9    | -4.89 | 119.00      | 126.23   |
| 17  | s     | 203 | BCR  | C11-C10-C9  | -4.89 | 120.43      | 127.28   |
| 17  | G     | 848 | BCR  | C38-C26-C25 | -4.88 | 119.16      | 124.48   |
| 17  | B     | 847 | BCR  | C11-C10-C9  | -4.88 | 120.44      | 127.28   |
| 17  | N     | 845 | BCR  | C24-C23-C22 | -4.88 | 119.02      | 126.23   |
| 17  | T     | 104 | BCR  | C38-C26-C25 | -4.87 | 119.17      | 124.48   |
| 17  | W     | 201 | BCR  | C38-C26-C25 | -4.87 | 119.17      | 124.48   |
| 17  | i     | 102 | BCR  | C33-C5-C6   | -4.87 | 119.17      | 124.48   |
| 17  | A     | 845 | BCR  | C16-C17-C18 | -4.86 | 120.46      | 127.28   |
| 17  | a     | 844 | BCR  | C20-C21-C22 | -4.86 | 120.47      | 127.28   |
| 17  | g     | 848 | BCR  | C33-C5-C6   | -4.86 | 119.18      | 124.48   |
| 17  | Y     | 101 | BCR  | C33-C5-C6   | -4.86 | 119.19      | 124.48   |
| 17  | j     | 103 | BCR  | C11-C10-C9  | -4.86 | 120.47      | 127.28   |
| 17  | b     | 845 | BCR  | C7-C8-C9    | -4.85 | 119.06      | 126.23   |
| 17  | w     | 207 | BCR  | C3-C4-C5    | -4.85 | 105.40      | 114.06   |
| 17  | A     | 849 | BCR  | C38-C26-C25 | -4.84 | 119.20      | 124.48   |
| 17  | a     | 845 | BCR  | C15-C14-C13 | -4.84 | 120.49      | 127.28   |
| 17  | g     | 843 | BCR  | C16-C17-C18 | -4.83 | 120.50      | 127.28   |
| 17  | n     | 842 | BCR  | C16-C17-C18 | -4.83 | 120.50      | 127.28   |
| 17  | j     | 103 | BCR  | C33-C5-C6   | -4.83 | 119.21      | 124.48   |
| 17  | G     | 845 | BCR  | C15-C14-C13 | -4.82 | 120.51      | 127.28   |
| 17  | N     | 844 | BCR  | C16-C17-C18 | -4.82 | 120.52      | 127.28   |
| 17  | n     | 845 | BCR  | C36-C18-C19 | 4.82  | 125.45      | 118.09   |
| 17  | n     | 846 | BCR  | C24-C23-C22 | -4.82 | 119.11      | 126.23   |
| 17  | B     | 843 | BCR  | C16-C17-C18 | -4.81 | 120.53      | 127.28   |
| 17  | B     | 852 | BCR  | C15-C14-C13 | -4.80 | 120.54      | 127.28   |
| 17  | g     | 847 | BCR  | C7-C8-C9    | -4.80 | 119.14      | 126.23   |
| 17  | B     | 852 | BCR  | C11-C10-C9  | -4.80 | 120.55      | 127.28   |
| 17  | M     | 101 | BCR  | C20-C21-C22 | -4.80 | 120.55      | 127.28   |
| 17  | a     | 848 | BCR  | C38-C26-C25 | -4.79 | 119.26      | 124.48   |
| 17  | W     | 201 | BCR  | C3-C4-C5    | -4.79 | 105.52      | 114.06   |
| 17  | a     | 847 | BCR  | C7-C8-C9    | -4.78 | 119.17      | 126.23   |
| 17  | y     | 101 | BCR  | C20-C21-C22 | -4.78 | 120.58      | 127.28   |
| 17  | n     | 844 | BCR  | C15-C14-C13 | -4.77 | 120.58      | 127.28   |
| 17  | t     | 103 | BCR  | C15-C14-C13 | -4.77 | 120.58      | 127.28   |
| 17  | g     | 845 | BCR  | C15-C14-C13 | -4.77 | 120.58      | 127.28   |
| 17  | A     | 846 | BCR  | C7-C8-C9    | -4.77 | 119.17      | 126.23   |
| 17  | n     | 847 | BCR  | C24-C23-C22 | -4.77 | 119.17      | 126.23   |
| 17  | T     | 103 | BCR  | C16-C17-C18 | -4.77 | 120.59      | 127.28   |
| 17  | T     | 103 | BCR  | C15-C14-C13 | -4.76 | 120.60      | 127.28   |
| 17  | N     | 848 | BCR  | C24-C23-C22 | -4.76 | 119.19      | 126.23   |
| 17  | N     | 853 | BCR  | C15-C14-C13 | -4.76 | 120.61      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | A     | 856 | BCR  | C16-C17-C18 | -4.75 | 120.61      | 127.28   |
| 17  | A     | 845 | BCR  | C20-C21-C22 | -4.74 | 120.63      | 127.28   |
| 17  | T     | 104 | BCR  | C33-C5-C6   | -4.73 | 119.33      | 124.48   |
| 17  | N     | 847 | BCR  | C11-C10-C9  | -4.71 | 120.67      | 127.28   |
| 17  | N     | 853 | BCR  | C16-C17-C18 | -4.71 | 120.67      | 127.28   |
| 17  | b     | 846 | BCR  | C16-C17-C18 | -4.71 | 120.67      | 127.28   |
| 17  | A     | 846 | BCR  | C3-C4-C5    | -4.70 | 105.67      | 114.06   |
| 17  | U     | 103 | BCR  | C16-C17-C18 | -4.69 | 120.69      | 127.28   |
| 17  | b     | 852 | BCR  | C15-C14-C13 | -4.69 | 120.70      | 127.28   |
| 17  | g     | 846 | BCR  | C34-C9-C10  | -4.69 | 115.22      | 122.82   |
| 17  | s     | 203 | BCR  | C16-C17-C18 | -4.69 | 120.70      | 127.28   |
| 17  | n     | 843 | BCR  | C15-C14-C13 | -4.69 | 120.70      | 127.28   |
| 17  | A     | 845 | BCR  | C15-C14-C13 | -4.69 | 120.70      | 127.28   |
| 17  | n     | 851 | BCR  | C11-C10-C9  | -4.69 | 120.71      | 127.28   |
| 17  | g     | 846 | BCR  | C33-C5-C6   | -4.68 | 119.38      | 124.48   |
| 17  | N     | 844 | BCR  | C15-C14-C13 | -4.68 | 120.72      | 127.28   |
| 17  | f     | 203 | BCR  | C16-C17-C18 | -4.67 | 120.73      | 127.28   |
| 17  | b     | 843 | BCR  | C16-C17-C18 | -4.66 | 120.75      | 127.28   |
| 17  | b     | 843 | BCR  | C20-C21-C22 | -4.66 | 120.75      | 127.28   |
| 17  | t     | 103 | BCR  | C16-C17-C18 | -4.64 | 120.77      | 127.28   |
| 17  | N     | 849 | BCR  | C15-C14-C13 | -4.63 | 120.78      | 127.28   |
| 17  | U     | 103 | BCR  | C15-C14-C13 | -4.63 | 120.78      | 127.28   |
| 17  | N     | 853 | BCR  | C7-C8-C9    | -4.63 | 119.38      | 126.23   |
| 17  | B     | 845 | BCR  | C15-C14-C13 | -4.63 | 120.78      | 127.28   |
| 17  | K     | 102 | BCR  | C16-C17-C18 | -4.63 | 120.78      | 127.28   |
| 17  | j     | 103 | BCR  | C7-C8-C9    | -4.63 | 119.39      | 126.23   |
| 17  | W     | 206 | BCR  | C20-C21-C22 | -4.62 | 120.79      | 127.28   |
| 17  | G     | 846 | BCR  | C7-C8-C9    | -4.62 | 119.40      | 126.23   |
| 17  | n     | 845 | BCR  | C7-C8-C9    | -4.62 | 119.40      | 126.23   |
| 17  | Y     | 101 | BCR  | C20-C21-C22 | -4.61 | 120.81      | 127.28   |
| 17  | j     | 104 | BCR  | C15-C14-C13 | -4.61 | 120.81      | 127.28   |
| 17  | b     | 847 | BCR  | C24-C23-C22 | -4.61 | 119.41      | 126.23   |
| 17  | n     | 842 | BCR  | C15-C14-C13 | -4.61 | 120.81      | 127.28   |
| 17  | l     | 205 | BCR  | C15-C14-C13 | -4.61 | 120.82      | 127.28   |
| 17  | b     | 846 | BCR  | C7-C8-C9    | -4.60 | 119.43      | 126.23   |
| 17  | G     | 848 | BCR  | C16-C17-C18 | -4.59 | 120.83      | 127.28   |
| 17  | A     | 847 | BCR  | C3-C4-C5    | -4.58 | 105.89      | 114.06   |
| 17  | j     | 104 | BCR  | C3-C4-C5    | -4.58 | 105.89      | 114.06   |
| 17  | B     | 845 | BCR  | C33-C5-C6   | -4.58 | 119.49      | 124.48   |
| 17  | A     | 848 | BCR  | C16-C17-C18 | -4.57 | 120.86      | 127.28   |
| 17  | n     | 846 | BCR  | C7-C8-C9    | -4.57 | 119.47      | 126.23   |
| 17  | G     | 844 | BCR  | C20-C21-C22 | -4.57 | 120.87      | 127.28   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | N     | 847 | BCR  | C7-C8-C9    | -4.57 | 119.48      | 126.23   |
| 17  | g     | 844 | BCR  | C20-C21-C22 | -4.57 | 120.88      | 127.28   |
| 17  | b     | 847 | BCR  | C38-C26-C25 | -4.56 | 119.51      | 124.48   |
| 17  | a     | 844 | BCR  | C15-C14-C13 | -4.56 | 120.89      | 127.28   |
| 17  | w     | 207 | BCR  | C20-C21-C22 | -4.55 | 120.89      | 127.28   |
| 17  | i     | 101 | BCR  | C15-C14-C13 | -4.55 | 120.89      | 127.28   |
| 17  | N     | 853 | BCR  | C20-C21-C22 | -4.55 | 120.90      | 127.28   |
| 17  | B     | 844 | BCR  | C33-C5-C6   | -4.55 | 119.52      | 124.48   |
| 17  | n     | 849 | BCR  | C15-C14-C13 | -4.54 | 120.91      | 127.28   |
| 17  | u     | 103 | BCR  | C20-C21-C22 | -4.54 | 120.91      | 127.28   |
| 17  | U     | 103 | BCR  | C20-C21-C22 | -4.54 | 120.91      | 127.28   |
| 17  | b     | 845 | BCR  | C15-C14-C13 | -4.54 | 120.92      | 127.28   |
| 17  | B     | 852 | BCR  | C7-C8-C9    | -4.53 | 119.53      | 126.23   |
| 17  | A     | 856 | BCR  | C20-C21-C22 | -4.53 | 120.93      | 127.28   |
| 17  | A     | 847 | BCR  | C38-C26-C25 | -4.52 | 119.55      | 124.48   |
| 17  | b     | 844 | BCR  | C15-C14-C13 | -4.52 | 120.94      | 127.28   |
| 17  | n     | 851 | BCR  | C15-C14-C13 | -4.51 | 120.95      | 127.28   |
| 17  | W     | 201 | BCR  | C20-C19-C18 | -4.50 | 114.03      | 126.36   |
| 17  | A     | 847 | BCR  | C16-C17-C18 | -4.50 | 120.97      | 127.28   |
| 17  | a     | 845 | BCR  | C16-C17-C18 | -4.50 | 120.97      | 127.28   |
| 17  | b     | 852 | BCR  | C16-C17-C18 | -4.50 | 120.97      | 127.28   |
| 17  | a     | 847 | BCR  | C16-C17-C18 | -4.50 | 120.97      | 127.28   |
| 17  | B     | 843 | BCR  | C15-C14-C13 | -4.50 | 120.97      | 127.28   |
| 17  | i     | 101 | BCR  | C24-C23-C22 | -4.48 | 119.60      | 126.23   |
| 17  | b     | 843 | BCR  | C11-C10-C9  | -4.48 | 120.99      | 127.28   |
| 17  | W     | 205 | BCR  | C38-C26-C25 | -4.48 | 119.60      | 124.48   |
| 17  | n     | 847 | BCR  | C33-C5-C6   | -4.48 | 119.60      | 124.48   |
| 17  | A     | 846 | BCR  | C11-C10-C9  | -4.47 | 121.00      | 127.28   |
| 17  | g     | 845 | BCR  | C16-C17-C18 | -4.47 | 121.01      | 127.28   |
| 17  | w     | 207 | BCR  | C16-C17-C18 | -4.47 | 121.02      | 127.28   |
| 17  | a     | 847 | BCR  | C11-C10-C9  | -4.46 | 121.02      | 127.28   |
| 17  | N     | 845 | BCR  | C15-C14-C13 | -4.46 | 121.03      | 127.28   |
| 17  | m     | 102 | BCR  | C15-C14-C13 | -4.46 | 121.03      | 127.28   |
| 17  | S     | 204 | BCR  | C7-C8-C9    | -4.44 | 119.67      | 126.23   |
| 17  | j     | 103 | BCR  | C15-C14-C13 | -4.44 | 121.05      | 127.28   |
| 17  | B     | 852 | BCR  | C16-C17-C18 | -4.43 | 121.06      | 127.28   |
| 17  | G     | 847 | BCR  | C15-C14-C13 | -4.43 | 121.07      | 127.28   |
| 17  | n     | 845 | BCR  | C3-C4-C5    | -4.43 | 106.16      | 114.06   |
| 17  | j     | 103 | BCR  | C16-C17-C18 | -4.43 | 121.07      | 127.28   |
| 17  | M     | 101 | BCR  | C16-C17-C18 | -4.43 | 121.07      | 127.28   |
| 17  | n     | 846 | BCR  | C20-C21-C22 | -4.42 | 121.08      | 127.28   |
| 17  | w     | 206 | BCR  | C38-C26-C25 | -4.42 | 119.66      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | n     | 842 | BCR  | C33-C5-C6   | -4.41 | 119.67      | 124.48   |
| 17  | M     | 101 | BCR  | C15-C14-C13 | -4.41 | 121.09      | 127.28   |
| 17  | N     | 844 | BCR  | C33-C5-C6   | -4.40 | 119.68      | 124.48   |
| 17  | b     | 850 | BCR  | C15-C14-C13 | -4.40 | 121.11      | 127.28   |
| 17  | b     | 848 | BCR  | C33-C5-C6   | -4.40 | 119.68      | 124.48   |
| 17  | g     | 846 | BCR  | C24-C23-C22 | -4.40 | 119.73      | 126.23   |
| 17  | b     | 852 | BCR  | C11-C10-C9  | -4.39 | 121.12      | 127.28   |
| 17  | b     | 843 | BCR  | C24-C23-C22 | -4.39 | 119.74      | 126.23   |
| 17  | n     | 851 | BCR  | C7-C8-C9    | -4.39 | 119.75      | 126.23   |
| 17  | N     | 846 | BCR  | C7-C8-C9    | -4.38 | 119.75      | 126.23   |
| 17  | A     | 849 | BCR  | C16-C17-C18 | -4.38 | 121.13      | 127.28   |
| 17  | b     | 848 | BCR  | C16-C17-C18 | -4.38 | 121.13      | 127.28   |
| 17  | G     | 846 | BCR  | C3-C4-C5    | -4.38 | 106.25      | 114.06   |
| 17  | I     | 103 | BCR  | C38-C26-C25 | -4.38 | 119.71      | 124.48   |
| 17  | n     | 851 | BCR  | C16-C17-C18 | -4.37 | 121.15      | 127.28   |
| 17  | i     | 102 | BCR  | C7-C8-C9    | -4.37 | 119.77      | 126.23   |
| 17  | F     | 203 | BCR  | C7-C8-C9    | -4.37 | 119.77      | 126.23   |
| 17  | b     | 845 | BCR  | C16-C17-C18 | -4.37 | 121.15      | 127.28   |
| 17  | g     | 847 | BCR  | C11-C10-C9  | -4.37 | 121.15      | 127.28   |
| 17  | B     | 845 | BCR  | C16-C17-C18 | -4.37 | 121.15      | 127.28   |
| 17  | F     | 203 | BCR  | C16-C17-C18 | -4.37 | 121.15      | 127.28   |
| 17  | w     | 206 | BCR  | C16-C17-C18 | -4.36 | 121.17      | 127.28   |
| 17  | l     | 206 | BCR  | C15-C14-C13 | -4.36 | 121.17      | 127.28   |
| 17  | n     | 844 | BCR  | C16-C17-C18 | -4.36 | 121.17      | 127.28   |
| 17  | y     | 101 | BCR  | C16-C17-C18 | -4.36 | 121.17      | 127.28   |
| 17  | u     | 103 | BCR  | C11-C10-C9  | -4.35 | 121.17      | 127.28   |
| 17  | I     | 101 | BCR  | C11-C10-C9  | -4.35 | 121.17      | 127.28   |
| 17  | j     | 104 | BCR  | C38-C26-C25 | -4.34 | 119.75      | 124.48   |
| 17  | A     | 847 | BCR  | C11-C10-C9  | -4.34 | 121.20      | 127.28   |
| 17  | n     | 847 | BCR  | C20-C21-C22 | -4.34 | 121.20      | 127.28   |
| 17  | J     | 103 | BCR  | C16-C17-C18 | -4.33 | 121.20      | 127.28   |
| 17  | N     | 844 | BCR  | C11-C10-C9  | -4.33 | 121.21      | 127.28   |
| 17  | B     | 846 | BCR  | C15-C14-C13 | -4.32 | 121.21      | 127.28   |
| 17  | b     | 843 | BCR  | C15-C14-C13 | -4.32 | 121.22      | 127.28   |
| 17  | g     | 844 | BCR  | C15-C14-C13 | -4.32 | 121.22      | 127.28   |
| 17  | G     | 844 | BCR  | C15-C14-C13 | -4.31 | 121.23      | 127.28   |
| 17  | f     | 203 | BCR  | C7-C8-C9    | -4.31 | 119.85      | 126.23   |
| 17  | k     | 102 | BCR  | C15-C14-C13 | -4.31 | 121.23      | 127.28   |
| 17  | b     | 850 | BCR  | C11-C10-C9  | -4.31 | 121.24      | 127.28   |
| 17  | G     | 847 | BCR  | C20-C21-C22 | -4.31 | 121.24      | 127.28   |
| 17  | A     | 844 | BCR  | C7-C8-C9    | -4.31 | 119.86      | 126.23   |
| 17  | A     | 847 | BCR  | C24-C23-C22 | -4.30 | 119.87      | 126.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | a     | 844  | BCR  | C11-C10-C9  | -4.30 | 121.25      | 127.28   |
| 17  | w     | 207  | BCR  | C38-C26-C25 | -4.30 | 119.80      | 124.48   |
| 17  | N     | 845  | BCR  | C16-C17-C18 | -4.29 | 121.26      | 127.28   |
| 17  | a     | 843  | BCR  | C16-C17-C18 | -4.29 | 121.26      | 127.28   |
| 17  | g     | 844  | BCR  | C11-C10-C9  | -4.29 | 121.26      | 127.28   |
| 17  | b     | 852  | BCR  | C20-C21-C22 | -4.29 | 121.27      | 127.28   |
| 17  | B     | 851  | BCR  | C28-C27-C26 | -4.29 | 106.41      | 114.06   |
| 17  | n     | 843  | BCR  | C33-C5-C6   | -4.28 | 119.81      | 124.48   |
| 17  | N     | 846  | BCR  | C16-C17-C18 | -4.28 | 121.28      | 127.28   |
| 17  | w     | 206  | BCR  | C11-C10-C9  | -4.28 | 121.28      | 127.28   |
| 17  | G     | 843  | BCR  | C20-C21-C22 | -4.28 | 121.28      | 127.28   |
| 17  | a     | 848  | BCR  | C16-C17-C18 | -4.27 | 121.28      | 127.28   |
| 17  | K     | 102  | BCR  | C15-C14-C13 | -4.27 | 121.29      | 127.28   |
| 17  | u     | 103  | BCR  | C15-C14-C13 | -4.26 | 121.30      | 127.28   |
| 17  | w     | 201  | BCR  | C7-C8-C9    | -4.26 | 119.93      | 126.23   |
| 17  | w     | 206  | BCR  | C7-C8-C9    | -4.26 | 119.93      | 126.23   |
| 17  | A     | 849  | BCR  | C24-C23-C22 | -4.26 | 119.93      | 126.23   |
| 17  | n     | 844  | BCR  | C11-C10-C9  | -4.25 | 121.31      | 127.28   |
| 17  | I     | 101  | BCR  | C3-C4-C5    | -4.25 | 106.48      | 114.06   |
| 17  | L     | 1504 | BCR  | C15-C14-C13 | -4.25 | 121.32      | 127.28   |
| 17  | l     | 205  | BCR  | C38-C26-C25 | -4.25 | 119.85      | 124.48   |
| 17  | b     | 847  | BCR  | C7-C8-C9    | -4.25 | 119.95      | 126.23   |
| 17  | w     | 207  | BCR  | C15-C14-C13 | -4.24 | 121.33      | 127.28   |
| 17  | W     | 201  | BCR  | C8-C7-C6    | -4.24 | 115.68      | 127.00   |
| 17  | g     | 845  | BCR  | C4-C5-C6    | -4.24 | 116.98      | 122.70   |
| 17  | J     | 103  | BCR  | C11-C10-C9  | -4.24 | 121.34      | 127.28   |
| 17  | g     | 844  | BCR  | C33-C5-C6   | -4.24 | 119.86      | 124.48   |
| 17  | A     | 847  | BCR  | C7-C8-C9    | -4.23 | 119.97      | 126.23   |
| 17  | G     | 848  | BCR  | C33-C5-C6   | -4.23 | 119.87      | 124.48   |
| 17  | t     | 103  | BCR  | C11-C10-C9  | -4.23 | 121.35      | 127.28   |
| 17  | b     | 850  | BCR  | C24-C23-C22 | -4.23 | 119.98      | 126.23   |
| 17  | W     | 206  | BCR  | C11-C10-C9  | -4.23 | 121.35      | 127.28   |
| 17  | n     | 851  | BCR  | C24-C23-C22 | -4.23 | 119.98      | 126.23   |
| 17  | N     | 849  | BCR  | C16-C17-C18 | -4.23 | 121.35      | 127.28   |
| 17  | n     | 842  | BCR  | C11-C10-C9  | -4.22 | 121.35      | 127.28   |
| 17  | A     | 848  | BCR  | C15-C14-C13 | -4.22 | 121.35      | 127.28   |
| 17  | n     | 846  | BCR  | C16-C17-C18 | -4.22 | 121.36      | 127.28   |
| 17  | y     | 101  | BCR  | C38-C26-C25 | -4.22 | 119.88      | 124.48   |
| 17  | N     | 848  | BCR  | C38-C26-C25 | -4.21 | 119.89      | 124.48   |
| 17  | K     | 102  | BCR  | C20-C21-C22 | -4.21 | 121.37      | 127.28   |
| 17  | A     | 856  | BCR  | C28-C27-C26 | -4.21 | 106.55      | 114.06   |
| 17  | l     | 205  | BCR  | C16-C17-C18 | -4.20 | 121.38      | 127.28   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | b     | 845  | BCR  | C11-C10-C9  | -4.20 | 121.39      | 127.28   |
| 17  | M     | 101  | BCR  | C38-C26-C25 | -4.20 | 119.90      | 124.48   |
| 17  | G     | 846  | BCR  | C16-C17-C18 | -4.19 | 121.40      | 127.28   |
| 17  | N     | 849  | BCR  | C33-C5-C6   | -4.19 | 119.92      | 124.48   |
| 17  | m     | 102  | BCR  | C38-C26-C25 | -4.18 | 119.92      | 124.48   |
| 17  | a     | 843  | BCR  | C7-C8-C9    | -4.18 | 120.05      | 126.23   |
| 17  | A     | 856  | BCR  | C33-C5-C6   | -4.18 | 119.93      | 124.48   |
| 17  | k     | 102  | BCR  | C11-C10-C9  | -4.17 | 121.44      | 127.28   |
| 17  | w     | 201  | BCR  | C15-C14-C13 | -4.17 | 121.44      | 127.28   |
| 17  | G     | 845  | BCR  | C11-C10-C9  | -4.16 | 121.44      | 127.28   |
| 17  | w     | 201  | BCR  | C33-C5-C6   | -4.16 | 119.94      | 124.48   |
| 17  | B     | 852  | BCR  | C20-C21-C22 | -4.16 | 121.45      | 127.28   |
| 17  | N     | 848  | BCR  | C16-C17-C18 | -4.16 | 121.45      | 127.28   |
| 17  | A     | 846  | BCR  | C20-C21-C22 | -4.15 | 121.46      | 127.28   |
| 17  | b     | 844  | BCR  | C16-C17-C18 | -4.14 | 121.47      | 127.28   |
| 17  | G     | 843  | BCR  | C7-C8-C9    | -4.14 | 120.11      | 126.23   |
| 17  | g     | 847  | BCR  | C20-C21-C22 | -4.13 | 121.49      | 127.28   |
| 17  | n     | 846  | BCR  | C38-C26-C25 | -4.11 | 120.00      | 124.48   |
| 17  | a     | 845  | BCR  | C4-C5-C6    | -4.11 | 117.15      | 122.70   |
| 17  | g     | 843  | BCR  | C7-C8-C9    | -4.11 | 120.15      | 126.23   |
| 20  | l     | 201  | SQD  | O47-C7-C8   | 4.11  | 120.36      | 111.48   |
| 17  | B     | 847  | BCR  | C20-C21-C22 | -4.10 | 121.52      | 127.28   |
| 17  | G     | 845  | BCR  | C4-C5-C6    | -4.10 | 117.16      | 122.70   |
| 17  | B     | 847  | BCR  | C7-C8-C9    | -4.10 | 120.16      | 126.23   |
| 17  | n     | 849  | BCR  | C20-C19-C18 | -4.10 | 115.11      | 126.36   |
| 17  | g     | 845  | BCR  | C11-C10-C9  | -4.10 | 121.53      | 127.28   |
| 17  | b     | 843  | BCR  | C33-C5-C6   | -4.10 | 120.01      | 124.48   |
| 17  | L     | 1504 | BCR  | C16-C17-C18 | -4.09 | 121.54      | 127.28   |
| 17  | s     | 203  | BCR  | C7-C8-C9    | -4.09 | 120.19      | 126.23   |
| 17  | t     | 104  | BCR  | C38-C26-C25 | -4.08 | 120.03      | 124.48   |
| 17  | B     | 848  | BCR  | C33-C5-C6   | -4.08 | 120.03      | 124.48   |
| 17  | B     | 847  | BCR  | C38-C26-C25 | -4.08 | 120.03      | 124.48   |
| 17  | Y     | 101  | BCR  | C15-C14-C13 | -4.08 | 121.56      | 127.28   |
| 17  | a     | 844  | BCR  | C33-C5-C6   | -4.08 | 120.03      | 124.48   |
| 17  | a     | 844  | BCR  | C38-C26-C25 | -4.07 | 120.04      | 124.48   |
| 17  | w     | 201  | BCR  | C38-C26-C25 | -4.07 | 120.04      | 124.48   |
| 18  | a     | 850  | LHG  | O7-C7-C8    | 4.07  | 120.28      | 111.48   |
| 17  | A     | 845  | BCR  | C38-C26-C25 | -4.06 | 120.05      | 124.48   |
| 17  | L     | 1504 | BCR  | C20-C21-C22 | -4.06 | 121.58      | 127.28   |
| 17  | a     | 845  | BCR  | C11-C10-C9  | -4.06 | 121.58      | 127.28   |
| 17  | l     | 206  | BCR  | C16-C17-C18 | -4.06 | 121.58      | 127.28   |
| 17  | s     | 203  | BCR  | C20-C21-C22 | -4.06 | 121.59      | 127.28   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | g     | 844  | BCR  | C38-C26-C25 | -4.06 | 120.06      | 124.48   |
| 17  | n     | 851  | BCR  | C20-C21-C22 | -4.05 | 121.59      | 127.28   |
| 17  | B     | 848  | BCR  | C15-C14-C13 | -4.05 | 121.59      | 127.28   |
| 17  | a     | 846  | BCR  | C20-C19-C18 | -4.05 | 115.25      | 126.36   |
| 17  | N     | 852  | BCR  | C15-C14-C13 | -4.05 | 121.60      | 127.28   |
| 17  | G     | 848  | BCR  | C24-C23-C22 | -4.05 | 120.25      | 126.23   |
| 17  | A     | 849  | BCR  | C33-C5-C6   | -4.05 | 120.07      | 124.48   |
| 17  | u     | 103  | BCR  | C24-C23-C22 | -4.05 | 120.25      | 126.23   |
| 17  | g     | 848  | BCR  | C24-C23-C22 | -4.05 | 120.25      | 126.23   |
| 20  | n     | 801  | SQD  | O47-C7-C8   | 4.05  | 120.23      | 111.48   |
| 17  | l     | 206  | BCR  | C11-C10-C9  | -4.05 | 121.61      | 127.28   |
| 17  | b     | 852  | BCR  | C24-C23-C22 | -4.04 | 120.26      | 126.23   |
| 17  | B     | 846  | BCR  | C11-C10-C9  | -4.04 | 121.61      | 127.28   |
| 17  | b     | 844  | BCR  | C11-C10-C9  | -4.04 | 121.62      | 127.28   |
| 17  | b     | 848  | BCR  | C15-C14-C13 | -4.03 | 121.62      | 127.28   |
| 20  | x     | 1702 | SQD  | O47-C7-C8   | 4.03  | 120.21      | 111.48   |
| 17  | W     | 206  | BCR  | C16-C17-C18 | -4.03 | 121.62      | 127.28   |
| 17  | a     | 848  | BCR  | C33-C5-C6   | -4.03 | 120.09      | 124.48   |
| 17  | W     | 206  | BCR  | C3-C4-C5    | -4.03 | 106.88      | 114.06   |
| 17  | l     | 206  | BCR  | C20-C21-C22 | -4.02 | 121.64      | 127.28   |
| 17  | g     | 848  | BCR  | C16-C17-C18 | -4.02 | 121.64      | 127.28   |
| 17  | f     | 203  | BCR  | C20-C21-C22 | -4.02 | 121.65      | 127.28   |
| 17  | N     | 847  | BCR  | C33-C5-C6   | -4.01 | 120.10      | 124.48   |
| 17  | G     | 845  | BCR  | C16-C17-C18 | -4.01 | 121.65      | 127.28   |
| 17  | g     | 843  | BCR  | C15-C14-C13 | -4.01 | 121.66      | 127.28   |
| 17  | n     | 851  | BCR  | C3-C4-C5    | -4.01 | 106.91      | 114.06   |
| 20  | b     | 801  | SQD  | O47-C7-C8   | 4.00  | 120.14      | 111.48   |
| 17  | a     | 843  | BCR  | C33-C5-C6   | -4.00 | 120.12      | 124.48   |
| 17  | g     | 846  | BCR  | C38-C26-C25 | -4.00 | 120.12      | 124.48   |
| 17  | b     | 847  | BCR  | C20-C21-C22 | -3.99 | 121.68      | 127.28   |
| 17  | A     | 845  | BCR  | C33-C5-C6   | -3.99 | 120.13      | 124.48   |
| 20  | B     | 801  | SQD  | O9-S-O7     | -3.99 | 100.84      | 113.82   |
| 17  | B     | 846  | BCR  | C33-C5-C6   | -3.98 | 120.14      | 124.48   |
| 17  | k     | 102  | BCR  | C24-C23-C22 | -3.98 | 120.35      | 126.23   |
| 17  | B     | 852  | BCR  | C24-C23-C22 | -3.97 | 120.36      | 126.23   |
| 20  | H     | 1702 | SQD  | O47-C7-C8   | 3.97  | 120.07      | 111.48   |
| 17  | t     | 103  | BCR  | C20-C21-C22 | -3.97 | 121.71      | 127.28   |
| 17  | a     | 846  | BCR  | C38-C26-C25 | -3.97 | 120.15      | 124.48   |
| 17  | L     | 1504 | BCR  | C3-C4-C5    | -3.97 | 106.98      | 114.06   |
| 17  | T     | 104  | BCR  | C11-C10-C9  | -3.96 | 121.72      | 127.28   |
| 17  | y     | 101  | BCR  | C15-C14-C13 | -3.96 | 121.72      | 127.28   |
| 18  | X     | 1702 | LHG  | O7-C7-C8    | 3.96  | 120.05      | 111.48   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | g     | 843  | BCR  | C33-C5-C6   | -3.96 | 120.17      | 124.48   |
| 17  | G     | 845  | BCR  | C7-C8-C9    | -3.95 | 120.39      | 126.23   |
| 17  | b     | 846  | BCR  | C33-C5-C6   | -3.95 | 120.17      | 124.48   |
| 17  | v     | 101  | BCR  | C4-C5-C6    | -3.95 | 117.36      | 122.70   |
| 20  | B     | 801  | SQD  | O47-C7-C8   | 3.95  | 120.02      | 111.48   |
| 17  | b     | 843  | BCR  | C7-C8-C9    | -3.95 | 120.40      | 126.23   |
| 17  | W     | 205  | BCR  | C16-C17-C18 | -3.95 | 121.74      | 127.28   |
| 20  | w     | 202  | SQD  | O47-C7-C8   | 3.94  | 120.01      | 111.48   |
| 20  | H     | 1702 | SQD  | O9-S-O7     | -3.94 | 101.00      | 113.82   |
| 18  | S     | 202  | LHG  | O7-C7-C8    | 3.94  | 120.01      | 111.48   |
| 17  | i     | 101  | BCR  | C16-C17-C18 | -3.94 | 121.75      | 127.28   |
| 17  | b     | 846  | BCR  | C15-C16-C17 | -3.94 | 115.46      | 123.52   |
| 18  | g     | 850  | LHG  | O7-C7-C8    | 3.94  | 120.00      | 111.48   |
| 18  | v     | 102  | LHG  | O7-C7-C8    | 3.93  | 119.99      | 111.48   |
| 17  | b     | 844  | BCR  | C33-C5-C6   | -3.93 | 120.19      | 124.48   |
| 17  | I     | 102  | BCR  | C7-C8-C9    | -3.93 | 120.42      | 126.23   |
| 17  | G     | 844  | BCR  | C33-C5-C6   | -3.92 | 120.21      | 124.48   |
| 17  | Y     | 101  | BCR  | C38-C26-C25 | -3.92 | 120.21      | 124.48   |
| 20  | l     | 201  | SQD  | O9-S-O7     | -3.91 | 101.09      | 113.82   |
| 20  | w     | 202  | SQD  | O9-S-O7     | -3.91 | 101.09      | 113.82   |
| 18  | g     | 849  | LHG  | O7-C7-C8    | 3.91  | 119.94      | 111.48   |
| 17  | A     | 848  | BCR  | C33-C5-C6   | -3.91 | 120.22      | 124.48   |
| 18  | A     | 851  | LHG  | O7-C7-C8    | 3.90  | 119.92      | 111.48   |
| 20  | h     | 1702 | SQD  | O9-S-O7     | -3.89 | 101.17      | 113.82   |
| 20  | n     | 801  | SQD  | O9-S-O7     | -3.89 | 101.17      | 113.82   |
| 17  | T     | 103  | BCR  | C11-C10-C9  | -3.89 | 121.83      | 127.28   |
| 17  | B     | 851  | BCR  | C33-C5-C6   | -3.89 | 120.24      | 124.48   |
| 17  | l     | 205  | BCR  | C20-C21-C22 | -3.88 | 121.83      | 127.28   |
| 17  | A     | 844  | BCR  | C33-C5-C6   | -3.88 | 120.25      | 124.48   |
| 17  | B     | 847  | BCR  | C16-C17-C18 | -3.87 | 121.84      | 127.28   |
| 17  | G     | 843  | BCR  | C33-C5-C6   | -3.87 | 120.26      | 124.48   |
| 17  | w     | 201  | BCR  | C16-C17-C18 | -3.87 | 121.85      | 127.28   |
| 20  | h     | 1702 | SQD  | O47-C7-C8   | 3.87  | 119.85      | 111.48   |
| 18  | G     | 849  | LHG  | O7-C7-C8    | 3.85  | 119.82      | 111.48   |
| 17  | G     | 844  | BCR  | C38-C26-C25 | -3.85 | 120.28      | 124.48   |
| 17  | I     | 102  | BCR  | C19-C18-C17 | 3.85  | 125.06      | 119.01   |
| 17  | k     | 102  | BCR  | C7-C8-C9    | -3.84 | 120.55      | 126.23   |
| 17  | N     | 848  | BCR  | C20-C21-C22 | -3.84 | 121.89      | 127.28   |
| 17  | K     | 102  | BCR  | C3-C4-C5    | -3.84 | 107.21      | 114.06   |
| 17  | I     | 102  | BCR  | C33-C5-C6   | -3.84 | 120.30      | 124.48   |
| 20  | x     | 1702 | SQD  | O9-S-O7     | -3.84 | 101.35      | 113.82   |
| 17  | S     | 204  | BCR  | C16-C17-C18 | -3.84 | 121.90      | 127.28   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | A     | 844  | BCR  | C15-C14-C13 | -3.84 | 121.90      | 127.28   |
| 17  | B     | 851  | BCR  | C11-C10-C9  | -3.83 | 121.91      | 127.28   |
| 17  | N     | 853  | BCR  | C24-C23-C22 | -3.83 | 120.57      | 126.23   |
| 17  | i     | 101  | BCR  | C4-C5-C6    | -3.82 | 117.54      | 122.70   |
| 17  | U     | 103  | BCR  | C24-C23-C22 | -3.82 | 120.58      | 126.23   |
| 17  | M     | 101  | BCR  | C33-C5-C6   | -3.82 | 120.31      | 124.48   |
| 18  | G     | 850  | LHG  | O7-C7-C8    | 3.82  | 119.74      | 111.48   |
| 17  | N     | 848  | BCR  | C7-C8-C9    | -3.82 | 120.59      | 126.23   |
| 17  | n     | 849  | BCR  | C24-C23-C22 | -3.82 | 120.59      | 126.23   |
| 17  | V     | 101  | BCR  | C3-C4-C5    | -3.82 | 107.25      | 114.06   |
| 17  | N     | 848  | BCR  | C33-C5-C6   | -3.82 | 120.32      | 124.48   |
| 17  | a     | 848  | BCR  | C3-C4-C5    | -3.81 | 107.25      | 114.06   |
| 17  | a     | 847  | BCR  | C20-C21-C22 | -3.81 | 121.93      | 127.28   |
| 17  | N     | 845  | BCR  | C33-C5-C6   | -3.81 | 120.33      | 124.48   |
| 17  | A     | 856  | BCR  | C38-C26-C25 | -3.80 | 120.33      | 124.48   |
| 17  | u     | 103  | BCR  | C7-C8-C9    | -3.80 | 120.61      | 126.23   |
| 17  | n     | 849  | BCR  | C20-C21-C22 | -3.80 | 121.95      | 127.28   |
| 17  | K     | 102  | BCR  | C38-C26-C25 | -3.80 | 120.34      | 124.48   |
| 17  | W     | 206  | BCR  | C38-C26-C25 | -3.80 | 120.34      | 124.48   |
| 17  | g     | 845  | BCR  | C20-C21-C22 | -3.80 | 121.95      | 127.28   |
| 17  | a     | 843  | BCR  | C15-C14-C13 | -3.79 | 121.96      | 127.28   |
| 17  | G     | 847  | BCR  | C11-C10-C9  | -3.79 | 121.96      | 127.28   |
| 17  | N     | 852  | BCR  | C33-C5-C6   | -3.79 | 120.35      | 124.48   |
| 15  | b     | 842  | PQN  | C11-C12-C13 | -3.79 | 120.30      | 126.83   |
| 17  | N     | 853  | BCR  | C3-C4-C5    | -3.79 | 107.30      | 114.06   |
| 17  | G     | 844  | BCR  | C11-C10-C9  | -3.79 | 121.97      | 127.28   |
| 17  | A     | 849  | BCR  | C3-C4-C5    | -3.78 | 107.31      | 114.06   |
| 15  | B     | 842  | PQN  | C11-C12-C13 | -3.78 | 120.31      | 126.83   |
| 17  | n     | 842  | BCR  | C7-C8-C9    | -3.78 | 120.64      | 126.23   |
| 17  | n     | 847  | BCR  | C15-C14-C13 | -3.78 | 121.97      | 127.28   |
| 17  | B     | 847  | BCR  | C3-C4-C5    | -3.78 | 107.32      | 114.06   |
| 17  | t     | 104  | BCR  | C15-C14-C13 | -3.78 | 121.98      | 127.28   |
| 17  | L     | 1504 | BCR  | C38-C26-C25 | -3.77 | 120.37      | 124.48   |
| 17  | g     | 844  | BCR  | C7-C8-C9    | -3.77 | 120.66      | 126.23   |
| 17  | w     | 207  | BCR  | C24-C23-C22 | -3.77 | 120.66      | 126.23   |
| 17  | a     | 844  | BCR  | C7-C8-C9    | -3.77 | 120.66      | 126.23   |
| 17  | l     | 205  | BCR  | C7-C8-C9    | -3.77 | 120.66      | 126.23   |
| 20  | b     | 801  | SQD  | O9-S-O7     | -3.77 | 101.57      | 113.82   |
| 17  | V     | 101  | BCR  | C20-C21-C22 | -3.77 | 121.99      | 127.28   |
| 17  | G     | 847  | BCR  | C24-C23-C22 | -3.76 | 120.67      | 126.23   |
| 17  | I     | 102  | BCR  | C11-C10-C9  | -3.76 | 122.01      | 127.28   |
| 17  | A     | 844  | BCR  | C24-C23-C22 | -3.76 | 120.68      | 126.23   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | b     | 848  | BCR  | C20-C21-C22 | -3.75 | 122.02      | 127.28   |
| 18  | m     | 101  | LHG  | O7-C7-C8    | 3.74  | 119.57      | 111.48   |
| 17  | A     | 845  | BCR  | C11-C10-C9  | -3.74 | 122.03      | 127.28   |
| 17  | i     | 102  | BCR  | C15-C16-C17 | -3.74 | 115.87      | 123.52   |
| 17  | a     | 846  | BCR  | C7-C8-C9    | -3.73 | 120.71      | 126.23   |
| 17  | B     | 851  | BCR  | C15-C14-C13 | -3.73 | 122.04      | 127.28   |
| 17  | V     | 101  | BCR  | C24-C23-C22 | -3.73 | 120.72      | 126.23   |
| 17  | i     | 101  | BCR  | C20-C21-C22 | -3.73 | 122.05      | 127.28   |
| 17  | t     | 103  | BCR  | C3-C4-C5    | -3.73 | 107.41      | 114.06   |
| 19  | a     | 851  | CL0  | C1-C2-C3    | -3.72 | 120.09      | 126.20   |
| 17  | A     | 856  | BCR  | C11-C10-C9  | -3.72 | 122.05      | 127.28   |
| 17  | w     | 207  | BCR  | C11-C10-C9  | -3.72 | 122.06      | 127.28   |
| 15  | G     | 841  | PQN  | C11-C12-C13 | -3.71 | 120.44      | 126.83   |
| 17  | W     | 201  | BCR  | C16-C15-C14 | -3.71 | 115.92      | 123.52   |
| 17  | W     | 206  | BCR  | C15-C14-C13 | -3.71 | 122.08      | 127.28   |
| 17  | n     | 845  | BCR  | C38-C26-C25 | -3.71 | 120.44      | 124.48   |
| 17  | N     | 844  | BCR  | C7-C8-C9    | -3.71 | 120.75      | 126.23   |
| 17  | A     | 846  | BCR  | C16-C17-C18 | -3.70 | 122.08      | 127.28   |
| 17  | L     | 1504 | BCR  | C24-C23-C22 | -3.70 | 120.76      | 126.23   |
| 17  | f     | 203  | BCR  | C24-C23-C22 | -3.70 | 120.76      | 126.23   |
| 17  | l     | 205  | BCR  | C11-C10-C9  | -3.70 | 122.09      | 127.28   |
| 17  | B     | 846  | BCR  | C7-C8-C9    | -3.70 | 120.76      | 126.23   |
| 17  | v     | 101  | BCR  | C7-C8-C9    | -3.70 | 120.76      | 126.23   |
| 17  | l     | 206  | BCR  | C38-C26-C25 | -3.70 | 120.45      | 124.48   |
| 15  | A     | 842  | PQN  | C11-C12-C13 | -3.69 | 120.47      | 126.83   |
| 17  | N     | 845  | BCR  | C11-C10-C9  | -3.69 | 122.10      | 127.28   |
| 15  | N     | 843  | PQN  | C11-C12-C13 | -3.69 | 120.48      | 126.83   |
| 17  | j     | 103  | BCR  | C20-C21-C22 | -3.69 | 122.11      | 127.28   |
| 17  | a     | 844  | BCR  | C24-C23-C22 | -3.68 | 120.79      | 126.23   |
| 17  | i     | 102  | BCR  | C21-C20-C19 | -3.68 | 112.53      | 123.20   |
| 17  | B     | 843  | BCR  | C11-C10-C9  | -3.68 | 122.12      | 127.28   |
| 18  | a     | 849  | LHG  | O7-C7-C8    | 3.68  | 119.44      | 111.48   |
| 17  | a     | 845  | BCR  | C20-C21-C22 | -3.67 | 122.13      | 127.28   |
| 17  | N     | 846  | BCR  | C33-C5-C6   | -3.67 | 120.48      | 124.48   |
| 17  | l     | 206  | BCR  | C24-C23-C22 | -3.67 | 120.80      | 126.23   |
| 17  | a     | 848  | BCR  | C24-C23-C22 | -3.67 | 120.81      | 126.23   |
| 17  | b     | 852  | BCR  | C7-C8-C9    | -3.66 | 120.82      | 126.23   |
| 17  | U     | 103  | BCR  | C38-C26-C25 | -3.66 | 120.49      | 124.48   |
| 17  | a     | 845  | BCR  | C38-C26-C25 | -3.65 | 120.50      | 124.48   |
| 17  | W     | 206  | BCR  | C24-C23-C22 | -3.65 | 120.83      | 126.23   |
| 17  | t     | 104  | BCR  | C3-C4-C5    | -3.65 | 107.55      | 114.06   |
| 17  | g     | 845  | BCR  | C7-C8-C9    | -3.65 | 120.84      | 126.23   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | B     | 845 | BCR  | C11-C10-C9  | -3.64 | 122.17      | 127.28   |
| 17  | j     | 104 | BCR  | C33-C5-C6   | -3.64 | 120.52      | 124.48   |
| 17  | k     | 102 | BCR  | C38-C26-C25 | -3.63 | 120.52      | 124.48   |
| 17  | N     | 849 | BCR  | C20-C21-C22 | -3.63 | 122.19      | 127.28   |
| 17  | g     | 844 | BCR  | C24-C23-C22 | -3.62 | 120.88      | 126.23   |
| 17  | N     | 846 | BCR  | C20-C21-C22 | -3.62 | 122.20      | 127.28   |
| 17  | A     | 844 | BCR  | C20-C21-C22 | -3.62 | 122.20      | 127.28   |
| 17  | g     | 843 | BCR  | C28-C27-C26 | -3.61 | 107.61      | 114.06   |
| 17  | N     | 852 | BCR  | C20-C21-C22 | -3.61 | 122.21      | 127.28   |
| 17  | K     | 102 | BCR  | C24-C23-C22 | -3.61 | 120.89      | 126.23   |
| 17  | J     | 103 | BCR  | C20-C21-C22 | -3.61 | 122.22      | 127.28   |
| 17  | G     | 847 | BCR  | C33-C5-C6   | -3.60 | 120.55      | 124.48   |
| 17  | m     | 102 | BCR  | C24-C23-C22 | -3.60 | 120.91      | 126.23   |
| 17  | B     | 843 | BCR  | C38-C26-C25 | -3.60 | 120.56      | 124.48   |
| 17  | U     | 103 | BCR  | C33-C5-C6   | -3.60 | 120.56      | 124.48   |
| 17  | B     | 851 | BCR  | C27-C26-C25 | -3.59 | 117.85      | 122.70   |
| 17  | b     | 848 | BCR  | C24-C23-C22 | -3.59 | 120.92      | 126.23   |
| 17  | A     | 856 | BCR  | C11-C12-C13 | -3.59 | 116.52      | 126.36   |
| 17  | U     | 103 | BCR  | C3-C4-C5    | -3.58 | 107.67      | 114.06   |
| 17  | A     | 846 | BCR  | C4-C5-C6    | -3.57 | 117.87      | 122.70   |
| 17  | n     | 843 | BCR  | C16-C17-C18 | -3.57 | 122.27      | 127.28   |
| 17  | I     | 103 | BCR  | C15-C14-C13 | -3.56 | 122.28      | 127.28   |
| 17  | u     | 103 | BCR  | C3-C4-C5    | -3.56 | 107.70      | 114.06   |
| 17  | t     | 103 | BCR  | C24-C23-C22 | -3.56 | 120.97      | 126.23   |
| 17  | G     | 845 | BCR  | C38-C26-C25 | -3.55 | 120.61      | 124.48   |
| 17  | j     | 103 | BCR  | C24-C23-C22 | -3.55 | 120.98      | 126.23   |
| 17  | a     | 846 | BCR  | C15-C14-C13 | -3.55 | 122.30      | 127.28   |
| 17  | T     | 103 | BCR  | C3-C4-C5    | -3.55 | 107.73      | 114.06   |
| 17  | b     | 847 | BCR  | C16-C17-C18 | -3.54 | 122.31      | 127.28   |
| 17  | k     | 102 | BCR  | C33-C5-C6   | -3.54 | 120.62      | 124.48   |
| 17  | I     | 103 | BCR  | C11-C10-C9  | -3.54 | 122.31      | 127.28   |
| 18  | A     | 850 | LHG  | O7-C7-C8    | 3.54  | 119.14      | 111.48   |
| 17  | b     | 850 | BCR  | C16-C17-C18 | -3.53 | 122.32      | 127.28   |
| 17  | U     | 103 | BCR  | C11-C10-C9  | -3.53 | 122.32      | 127.28   |
| 17  | Y     | 101 | BCR  | C24-C23-C22 | -3.53 | 121.01      | 126.23   |
| 17  | K     | 102 | BCR  | C11-C10-C9  | -3.53 | 122.33      | 127.28   |
| 17  | B     | 844 | BCR  | C16-C15-C14 | -3.53 | 116.30      | 123.52   |
| 17  | g     | 848 | BCR  | C15-C14-C13 | -3.52 | 122.34      | 127.28   |
| 17  | a     | 843 | BCR  | C28-C27-C26 | -3.52 | 107.78      | 114.06   |
| 17  | I     | 102 | BCR  | C28-C27-C26 | -3.52 | 107.79      | 114.06   |
| 17  | a     | 843 | BCR  | C20-C21-C22 | -3.52 | 122.35      | 127.28   |
| 17  | u     | 103 | BCR  | C38-C26-C25 | -3.51 | 120.65      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | J     | 103 | BCR  | C3-C4-C5    | -3.51 | 107.79      | 114.06   |
| 17  | G     | 846 | BCR  | C11-C10-C9  | -3.51 | 122.35      | 127.28   |
| 17  | W     | 201 | BCR  | C10-C11-C12 | -3.51 | 113.04      | 123.20   |
| 17  | n     | 847 | BCR  | C30-C25-C26 | -3.50 | 117.85      | 122.64   |
| 17  | u     | 103 | BCR  | C33-C5-C6   | -3.50 | 120.67      | 124.48   |
| 17  | I     | 102 | BCR  | C27-C26-C25 | -3.49 | 117.99      | 122.70   |
| 17  | t     | 104 | BCR  | C11-C10-C9  | -3.49 | 122.39      | 127.28   |
| 17  | N     | 847 | BCR  | C16-C17-C18 | -3.49 | 122.39      | 127.28   |
| 17  | G     | 846 | BCR  | C28-C27-C26 | -3.49 | 107.84      | 114.06   |
| 17  | G     | 847 | BCR  | C7-C8-C9    | -3.49 | 121.08      | 126.23   |
| 17  | n     | 849 | BCR  | C33-C5-C6   | -3.48 | 120.68      | 124.48   |
| 17  | Y     | 101 | BCR  | C28-C27-C26 | -3.48 | 107.85      | 114.06   |
| 17  | J     | 103 | BCR  | C33-C5-C6   | -3.48 | 120.69      | 124.48   |
| 14  | N     | 831 | CLA  | O2D-CGD-O1D | -3.48 | 117.08      | 123.85   |
| 17  | K     | 102 | BCR  | C33-C5-C6   | -3.48 | 120.69      | 124.48   |
| 17  | v     | 101 | BCR  | C11-C10-C9  | -3.47 | 122.41      | 127.28   |
| 17  | b     | 847 | BCR  | C33-C5-C6   | -3.47 | 120.70      | 124.48   |
| 17  | A     | 845 | BCR  | C24-C23-C22 | -3.47 | 121.10      | 126.23   |
| 17  | B     | 848 | BCR  | C7-C8-C9    | -3.47 | 121.10      | 126.23   |
| 17  | G     | 844 | BCR  | C7-C8-C9    | -3.47 | 121.11      | 126.23   |
| 20  | n     | 801 | SQD  | O9-S-C6     | 3.47  | 111.93      | 106.76   |
| 17  | n     | 843 | BCR  | C11-C10-C9  | -3.47 | 122.42      | 127.28   |
| 17  | g     | 847 | BCR  | C24-C23-C22 | -3.46 | 121.12      | 126.23   |
| 17  | G     | 845 | BCR  | C20-C21-C22 | -3.46 | 122.43      | 127.28   |
| 17  | N     | 845 | BCR  | C3-C4-C5    | -3.45 | 107.90      | 114.06   |
| 17  | j     | 103 | BCR  | C38-C26-C25 | -3.45 | 120.72      | 124.48   |
| 15  | n     | 841 | PQN  | C11-C12-C13 | -3.45 | 120.89      | 126.83   |
| 17  | B     | 843 | BCR  | C3-C4-C5    | -3.44 | 107.91      | 114.06   |
| 17  | a     | 843 | BCR  | C24-C23-C22 | -3.44 | 121.14      | 126.23   |
| 17  | A     | 845 | BCR  | C7-C8-C9    | -3.44 | 121.14      | 126.23   |
| 17  | s     | 203 | BCR  | C24-C23-C22 | -3.44 | 121.14      | 126.23   |
| 17  | G     | 843 | BCR  | C11-C12-C13 | -3.44 | 116.94      | 126.36   |
| 17  | s     | 203 | BCR  | C38-C26-C25 | -3.44 | 120.73      | 124.48   |
| 17  | g     | 845 | BCR  | C38-C26-C25 | -3.43 | 120.74      | 124.48   |
| 17  | W     | 205 | BCR  | C7-C8-C9    | -3.43 | 121.16      | 126.23   |
| 17  | A     | 848 | BCR  | C7-C8-C9    | -3.42 | 121.17      | 126.23   |
| 17  | J     | 103 | BCR  | C7-C8-C9    | -3.42 | 121.17      | 126.23   |
| 17  | A     | 848 | BCR  | C11-C10-C9  | -3.42 | 122.48      | 127.28   |
| 17  | W     | 206 | BCR  | C28-C27-C26 | -3.42 | 107.96      | 114.06   |
| 17  | G     | 846 | BCR  | C20-C21-C22 | -3.41 | 122.49      | 127.28   |
| 17  | a     | 846 | BCR  | C28-C27-C26 | -3.41 | 107.97      | 114.06   |
| 17  | n     | 845 | BCR  | C4-C5-C6    | -3.41 | 118.10      | 122.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | t     | 103  | BCR  | C7-C8-C9    | -3.41 | 121.20      | 126.23   |
| 17  | B     | 844  | BCR  | C24-C23-C22 | -3.40 | 121.20      | 126.23   |
| 17  | A     | 848  | BCR  | C20-C21-C22 | -3.40 | 122.51      | 127.28   |
| 17  | B     | 844  | BCR  | C11-C10-C9  | -3.40 | 122.51      | 127.28   |
| 14  | L     | 1501 | CLA  | O2D-CGD-O1D | -3.40 | 117.23      | 123.85   |
| 17  | J     | 103  | BCR  | C24-C23-C22 | -3.40 | 121.21      | 126.23   |
| 14  | N     | 819  | CLA  | C3B-C4B-NB  | -3.40 | 107.50      | 110.53   |
| 17  | t     | 103  | BCR  | C38-C26-C25 | -3.39 | 120.78      | 124.48   |
| 17  | n     | 846  | BCR  | C3-C4-C5    | -3.39 | 108.00      | 114.06   |
| 17  | U     | 103  | BCR  | C7-C8-C9    | -3.39 | 121.22      | 126.23   |
| 17  | F     | 203  | BCR  | C20-C21-C22 | -3.39 | 122.53      | 127.28   |
| 17  | B     | 847  | BCR  | C33-C5-C6   | -3.39 | 120.79      | 124.48   |
| 17  | J     | 103  | BCR  | C38-C26-C25 | -3.38 | 120.79      | 124.48   |
| 17  | g     | 846  | BCR  | C16-C17-C18 | -3.38 | 122.53      | 127.28   |
| 17  | s     | 203  | BCR  | C33-C5-C6   | -3.38 | 120.79      | 124.48   |
| 17  | a     | 845  | BCR  | C7-C8-C9    | -3.38 | 121.23      | 126.23   |
| 17  | n     | 845  | BCR  | C33-C5-C4   | 3.38  | 120.80      | 113.60   |
| 17  | b     | 852  | BCR  | C3-C4-C5    | -3.38 | 108.04      | 114.06   |
| 20  | H     | 1702 | SQD  | O7-S-C6     | 3.37  | 111.79      | 106.76   |
| 17  | I     | 101  | BCR  | C15-C14-C13 | -3.37 | 122.55      | 127.28   |
| 17  | f     | 203  | BCR  | C38-C26-C25 | -3.37 | 120.80      | 124.48   |
| 17  | I     | 103  | BCR  | C7-C8-C9    | -3.37 | 121.25      | 126.23   |
| 17  | i     | 102  | BCR  | C38-C26-C25 | -3.37 | 120.81      | 124.48   |
| 14  | N     | 804  | CLA  | O2D-CGD-O1D | -3.37 | 117.30      | 123.85   |
| 19  | g     | 851  | CL0  | CMB-C2B-C3B | 3.37  | 131.41      | 124.68   |
| 19  | G     | 851  | CL0  | C1B-CHB-C4A | 3.36  | 123.48      | 121.32   |
| 17  | l     | 206  | BCR  | C28-C27-C26 | -3.36 | 108.06      | 114.06   |
| 17  | S     | 204  | BCR  | C38-C26-C25 | -3.36 | 120.82      | 124.48   |
| 17  | w     | 201  | BCR  | C11-C10-C9  | -3.36 | 122.56      | 127.28   |
| 17  | F     | 203  | BCR  | C38-C26-C25 | -3.36 | 120.82      | 124.48   |
| 17  | T     | 103  | BCR  | C33-C5-C6   | -3.36 | 120.82      | 124.48   |
| 17  | S     | 204  | BCR  | C20-C21-C22 | -3.36 | 122.57      | 127.28   |
| 17  | W     | 201  | BCR  | C30-C25-C24 | 3.35  | 124.75      | 115.65   |
| 17  | i     | 102  | BCR  | C11-C10-C9  | -3.35 | 122.58      | 127.28   |
| 17  | B     | 851  | BCR  | C7-C8-C9    | -3.34 | 121.29      | 126.23   |
| 17  | N     | 845  | BCR  | C20-C21-C22 | -3.34 | 122.59      | 127.28   |
| 17  | T     | 103  | BCR  | C28-C27-C26 | -3.34 | 108.09      | 114.06   |
| 17  | G     | 844  | BCR  | C28-C27-C26 | -3.34 | 108.09      | 114.06   |
| 17  | B     | 852  | BCR  | C3-C4-C5    | -3.34 | 108.11      | 114.06   |
| 14  | B     | 812  | CLA  | O2D-CGD-O1D | -3.34 | 117.36      | 123.85   |
| 17  | g     | 846  | BCR  | C15-C16-C17 | -3.33 | 116.70      | 123.52   |
| 14  | B     | 811  | CLA  | O2D-CGD-O1D | -3.33 | 117.36      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 19  | a     | 851 | CL0  | CMB-C2B-C3B | 3.33  | 131.34      | 124.68   |
| 14  | B     | 830 | CLA  | O2D-CGD-O1D | -3.33 | 117.37      | 123.85   |
| 17  | n     | 844 | BCR  | C3-C4-C5    | -3.33 | 108.12      | 114.06   |
| 17  | G     | 846 | BCR  | C38-C26-C25 | -3.33 | 120.85      | 124.48   |
| 17  | f     | 203 | BCR  | C33-C5-C6   | -3.33 | 120.86      | 124.48   |
| 17  | g     | 843 | BCR  | C20-C21-C22 | -3.32 | 122.62      | 127.28   |
| 14  | N     | 814 | CLA  | O2D-CGD-O1D | -3.32 | 117.38      | 123.85   |
| 17  | N     | 849 | BCR  | C24-C23-C22 | -3.32 | 121.32      | 126.23   |
| 17  | n     | 844 | BCR  | C20-C21-C22 | -3.32 | 122.63      | 127.28   |
| 14  | N     | 827 | CLA  | O2D-CGD-O1D | -3.32 | 117.39      | 123.85   |
| 17  | v     | 101 | BCR  | C15-C14-C13 | -3.31 | 122.63      | 127.28   |
| 17  | n     | 849 | BCR  | C28-C27-C26 | -3.31 | 108.14      | 114.06   |
| 17  | b     | 845 | BCR  | C38-C26-C25 | -3.31 | 120.87      | 124.48   |
| 17  | B     | 845 | BCR  | C38-C26-C25 | -3.31 | 120.87      | 124.48   |
| 17  | b     | 844 | BCR  | C3-C4-C5    | -3.31 | 108.16      | 114.06   |
| 17  | N     | 852 | BCR  | C28-C27-C26 | -3.31 | 108.16      | 114.06   |
| 17  | m     | 102 | BCR  | C11-C10-C9  | -3.30 | 122.65      | 127.28   |
| 14  | A     | 829 | CLA  | O2D-CGD-O1D | -3.28 | 117.46      | 123.85   |
| 14  | G     | 852 | CLA  | C3B-C4B-NB  | -3.28 | 107.60      | 110.53   |
| 14  | N     | 810 | CLA  | O2D-CGD-O1D | -3.28 | 117.47      | 123.85   |
| 17  | u     | 103 | BCR  | C28-C27-C26 | -3.28 | 108.21      | 114.06   |
| 17  | b     | 844 | BCR  | C30-C25-C26 | -3.28 | 118.16      | 122.64   |
| 17  | I     | 102 | BCR  | C3-C4-C5    | -3.28 | 108.21      | 114.06   |
| 14  | N     | 813 | CLA  | O2D-CGD-O1D | -3.28 | 117.47      | 123.85   |
| 17  | T     | 104 | BCR  | C11-C12-C13 | -3.28 | 117.38      | 126.36   |
| 17  | G     | 848 | BCR  | C15-C14-C13 | -3.27 | 122.69      | 127.28   |
| 17  | k     | 102 | BCR  | C3-C4-C5    | -3.27 | 108.22      | 114.06   |
| 17  | b     | 845 | BCR  | C33-C5-C6   | -3.27 | 120.92      | 124.48   |
| 14  | G     | 826 | CLA  | C3B-C4B-NB  | -3.27 | 107.61      | 110.53   |
| 17  | W     | 201 | BCR  | C28-C27-C26 | -3.27 | 108.23      | 114.06   |
| 17  | b     | 850 | BCR  | C28-C27-C26 | -3.27 | 108.23      | 114.06   |
| 17  | g     | 846 | BCR  | C36-C18-C19 | 3.27  | 123.08      | 118.09   |
| 17  | n     | 844 | BCR  | C38-C26-C25 | -3.26 | 120.93      | 124.48   |
| 17  | S     | 204 | BCR  | C33-C5-C6   | -3.26 | 120.93      | 124.48   |
| 17  | B     | 844 | BCR  | C28-C27-C26 | -3.26 | 108.25      | 114.06   |
| 17  | g     | 847 | BCR  | C33-C5-C6   | -3.25 | 120.94      | 124.48   |
| 20  | B     | 801 | SQD  | O7-S-C6     | 3.24  | 111.60      | 106.76   |
| 17  | t     | 103 | BCR  | C28-C27-C26 | -3.24 | 108.27      | 114.06   |
| 17  | A     | 845 | BCR  | C28-C27-C26 | -3.24 | 108.28      | 114.06   |
| 14  | G     | 837 | CLA  | O2D-CGD-O1D | -3.24 | 117.54      | 123.85   |
| 17  | K     | 102 | BCR  | C7-C8-C9    | -3.24 | 121.44      | 126.23   |
| 17  | W     | 206 | BCR  | C33-C5-C6   | -3.24 | 120.95      | 124.48   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | W     | 203 | CLA  | C3B-C4B-NB  | -3.24 | 107.64      | 110.53   |
| 14  | g     | 811 | CLA  | C3B-C4B-NB  | -3.23 | 107.64      | 110.53   |
| 17  | a     | 848 | BCR  | C20-C19-C18 | -3.23 | 117.50      | 126.36   |
| 17  | v     | 101 | BCR  | C28-C27-C26 | -3.23 | 108.29      | 114.06   |
| 17  | F     | 203 | BCR  | C33-C5-C6   | -3.23 | 120.96      | 124.48   |
| 14  | G     | 818 | CLA  | O2D-CGD-O1D | -3.23 | 117.56      | 123.85   |
| 17  | F     | 203 | BCR  | C28-C27-C26 | -3.23 | 108.30      | 114.06   |
| 17  | T     | 103 | BCR  | C38-C26-C25 | -3.23 | 120.96      | 124.48   |
| 17  | I     | 102 | BCR  | C30-C25-C26 | -3.23 | 118.23      | 122.64   |
| 17  | t     | 103 | BCR  | C33-C5-C6   | -3.22 | 120.97      | 124.48   |
| 17  | N     | 847 | BCR  | C3-C4-C5    | -3.22 | 108.31      | 114.06   |
| 14  | B     | 809 | CLA  | O2D-CGD-O1D | -3.22 | 117.58      | 123.85   |
| 17  | B     | 846 | BCR  | C28-C27-C26 | -3.22 | 108.31      | 114.06   |
| 17  | S     | 204 | BCR  | C24-C23-C22 | -3.22 | 121.47      | 126.23   |
| 14  | A     | 855 | CLA  | C3B-C4B-NB  | -3.22 | 107.66      | 110.53   |
| 17  | N     | 844 | BCR  | C38-C26-C25 | -3.22 | 120.97      | 124.48   |
| 17  | A     | 846 | BCR  | C24-C23-C22 | -3.22 | 121.47      | 126.23   |
| 17  | A     | 849 | BCR  | C15-C14-C13 | -3.22 | 122.77      | 127.28   |
| 19  | A     | 852 | CL0  | CMB-C2B-C3B | 3.21  | 131.10      | 124.68   |
| 15  | a     | 841 | PQN  | C14-C13-C15 | 3.21  | 120.81      | 115.23   |
| 17  | B     | 846 | BCR  | C3-C4-C5    | -3.21 | 108.33      | 114.06   |
| 14  | a     | 811 | CLA  | C3B-C4B-NB  | -3.21 | 107.66      | 110.53   |
| 17  | b     | 845 | BCR  | C3-C4-C5    | -3.21 | 108.33      | 114.06   |
| 19  | A     | 852 | CL0  | O2D-CGD-CBD | 3.21  | 114.47      | 110.95   |
| 14  | N     | 851 | CLA  | C3B-C4B-NB  | -3.20 | 107.67      | 110.53   |
| 14  | n     | 810 | CLA  | O2D-CGD-O1D | -3.20 | 117.61      | 123.85   |
| 17  | K     | 102 | BCR  | C28-C27-C26 | -3.20 | 108.35      | 114.06   |
| 14  | g     | 852 | CLA  | C3B-C4B-NB  | -3.20 | 107.67      | 110.53   |
| 17  | l     | 206 | BCR  | C7-C8-C9    | -3.19 | 121.51      | 126.23   |
| 17  | w     | 201 | BCR  | C20-C21-C22 | -3.19 | 122.80      | 127.28   |
| 17  | A     | 856 | BCR  | C3-C4-C5    | -3.19 | 108.37      | 114.06   |
| 17  | a     | 847 | BCR  | C28-C27-C26 | -3.19 | 108.38      | 114.06   |
| 14  | G     | 812 | CLA  | C3B-C4B-NB  | -3.18 | 107.69      | 110.53   |
| 17  | G     | 844 | BCR  | C24-C23-C22 | -3.18 | 121.53      | 126.23   |
| 14  | B     | 818 | CLA  | C3B-C4B-NB  | -3.18 | 107.69      | 110.53   |
| 19  | a     | 851 | CL0  | CMD-C2D-C3D | 3.18  | 131.03      | 124.68   |
| 19  | A     | 852 | CL0  | CMD-C2D-C3D | 3.18  | 131.03      | 124.68   |
| 14  | a     | 806 | CLA  | O2D-CGD-O1D | -3.17 | 117.67      | 123.85   |
| 17  | g     | 844 | BCR  | C28-C27-C26 | -3.17 | 108.40      | 114.06   |
| 14  | b     | 824 | CLA  | C3B-C4B-NB  | -3.17 | 107.70      | 110.53   |
| 17  | n     | 849 | BCR  | C7-C8-C9    | -3.17 | 121.55      | 126.23   |
| 14  | W     | 203 | CLA  | O2D-CGD-O1D | -3.17 | 117.68      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | n     | 823  | CLA  | O2D-CGD-O1D | -3.16 | 117.69      | 123.85   |
| 17  | M     | 101  | BCR  | C28-C27-C26 | -3.16 | 108.42      | 114.06   |
| 14  | n     | 832  | CLA  | O2D-CGD-O1D | -3.16 | 117.69      | 123.85   |
| 17  | G     | 848  | BCR  | C3-C4-C5    | -3.16 | 108.42      | 114.06   |
| 14  | l     | 202  | CLA  | O2D-CGD-O1D | -3.16 | 117.70      | 123.85   |
| 20  | x     | 1702 | SQD  | O9-S-C6     | 3.16  | 111.47      | 106.76   |
| 17  | i     | 101  | BCR  | C2-C1-C6    | 3.16  | 115.03      | 110.44   |
| 14  | g     | 806  | CLA  | O2D-CGD-O1D | -3.16 | 117.70      | 123.85   |
| 17  | n     | 844  | BCR  | C33-C5-C6   | -3.16 | 121.04      | 124.48   |
| 14  | B     | 834  | CLA  | O2D-CGD-O1D | -3.16 | 117.70      | 123.85   |
| 14  | a     | 836  | CLA  | C3B-C4B-NB  | -3.16 | 107.71      | 110.53   |
| 17  | S     | 204  | BCR  | C28-C27-C26 | -3.16 | 108.43      | 114.06   |
| 14  | b     | 823  | CLA  | O2D-CGD-O1D | -3.15 | 117.71      | 123.85   |
| 17  | f     | 203  | BCR  | C28-C27-C26 | -3.15 | 108.43      | 114.06   |
| 14  | g     | 828  | CLA  | O2D-CGD-O1D | -3.15 | 117.71      | 123.85   |
| 14  | n     | 832  | CLA  | C3B-C4B-NB  | -3.15 | 107.72      | 110.53   |
| 14  | j     | 101  | CLA  | O2D-CGD-O1D | -3.15 | 117.72      | 123.85   |
| 17  | A     | 848  | BCR  | C24-C23-C22 | -3.15 | 121.58      | 126.23   |
| 14  | n     | 833  | CLA  | O2D-CGD-O1D | -3.15 | 117.72      | 123.85   |
| 17  | W     | 205  | BCR  | C11-C10-C9  | -3.15 | 122.86      | 127.28   |
| 17  | n     | 846  | BCR  | C33-C5-C6   | -3.15 | 121.05      | 124.48   |
| 17  | b     | 846  | BCR  | C3-C4-C5    | -3.14 | 108.45      | 114.06   |
| 14  | G     | 829  | CLA  | O2D-CGD-O1D | -3.14 | 117.73      | 123.85   |
| 17  | N     | 852  | BCR  | C8-C7-C6    | -3.14 | 118.60      | 127.00   |
| 17  | W     | 201  | BCR  | C33-C5-C4   | 3.14  | 120.29      | 113.60   |
| 17  | a     | 844  | BCR  | C28-C27-C26 | -3.14 | 108.45      | 114.06   |
| 17  | a     | 846  | BCR  | C10-C11-C12 | -3.14 | 114.10      | 123.20   |
| 14  | b     | 809  | CLA  | O2D-CGD-O1D | -3.14 | 117.73      | 123.85   |
| 14  | l     | 203  | CLA  | C3B-C4B-NB  | -3.14 | 107.73      | 110.53   |
| 14  | g     | 836  | CLA  | O2D-CGD-O1D | -3.14 | 117.74      | 123.85   |
| 14  | w     | 204  | CLA  | C3B-C4B-NB  | -3.14 | 107.73      | 110.53   |
| 14  | A     | 806  | CLA  | C3B-C4B-NB  | -3.14 | 107.73      | 110.53   |
| 17  | a     | 847  | BCR  | C24-C23-C22 | -3.14 | 121.60      | 126.23   |
| 17  | a     | 846  | BCR  | C11-C10-C9  | -3.13 | 122.88      | 127.28   |
| 14  | w     | 203  | CLA  | O2D-CGD-O1D | -3.13 | 117.75      | 123.85   |
| 14  | u     | 102  | CLA  | O2D-CGD-O1D | -3.13 | 117.75      | 123.85   |
| 17  | L     | 1504 | BCR  | C33-C5-C6   | -3.13 | 121.07      | 124.48   |
| 14  | A     | 833  | CLA  | O2D-CGD-O1D | -3.13 | 117.76      | 123.85   |
| 17  | b     | 852  | BCR  | C38-C26-C25 | -3.13 | 121.07      | 124.48   |
| 14  | b     | 834  | CLA  | O2D-CGD-O1D | -3.12 | 117.77      | 123.85   |
| 17  | y     | 101  | BCR  | C11-C10-C9  | -3.12 | 122.90      | 127.28   |
| 14  | B     | 826  | CLA  | O2D-CGD-O1D | -3.12 | 117.77      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | G     | 847  | BCR  | C28-C27-C26 | -3.12 | 108.49      | 114.06   |
| 17  | b     | 847  | BCR  | C3-C4-C5    | -3.12 | 108.49      | 114.06   |
| 17  | m     | 102  | BCR  | C28-C27-C26 | -3.12 | 108.49      | 114.06   |
| 17  | n     | 845  | BCR  | C33-C5-C6   | -3.12 | 121.08      | 124.48   |
| 17  | a     | 848  | BCR  | C33-C5-C4   | 3.12  | 120.25      | 113.60   |
| 14  | N     | 838  | CLA  | C3B-C4B-NB  | -3.12 | 107.75      | 110.53   |
| 14  | L     | 1502 | CLA  | O2D-CGD-O1D | -3.12 | 117.78      | 123.85   |
| 17  | A     | 846  | BCR  | C38-C26-C25 | -3.12 | 121.08      | 124.48   |
| 17  | W     | 205  | BCR  | C16-C15-C14 | -3.12 | 117.14      | 123.52   |
| 17  | W     | 201  | BCR  | C4-C5-C6    | -3.12 | 118.49      | 122.70   |
| 20  | l     | 201  | SQD  | O7-S-C6     | 3.12  | 111.41      | 106.76   |
| 20  | h     | 1702 | SQD  | O9-S-C6     | 3.11  | 111.41      | 106.76   |
| 14  | g     | 832  | CLA  | O2D-CGD-O1D | -3.11 | 117.79      | 123.85   |
| 17  | I     | 102  | BCR  | C38-C26-C27 | 3.11  | 120.23      | 113.60   |
| 14  | b     | 824  | CLA  | O2D-CGD-O1D | -3.11 | 117.79      | 123.85   |
| 14  | A     | 840  | CLA  | O2D-CGD-O1D | -3.11 | 117.79      | 123.85   |
| 14  | G     | 817  | CLA  | C3B-C4B-NB  | -3.11 | 107.75      | 110.53   |
| 14  | U     | 102  | CLA  | O2D-CGD-O1D | -3.11 | 117.80      | 123.85   |
| 17  | t     | 104  | BCR  | C7-C8-C9    | -3.11 | 121.64      | 126.23   |
| 14  | n     | 808  | CLA  | O2D-CGD-O1D | -3.11 | 117.80      | 123.85   |
| 14  | N     | 812  | CLA  | C3B-C4B-NB  | -3.11 | 107.76      | 110.53   |
| 14  | b     | 812  | CLA  | O2D-CGD-O1D | -3.10 | 117.81      | 123.85   |
| 14  | A     | 857  | CLA  | O2D-CGD-O1D | -3.10 | 117.81      | 123.85   |
| 14  | g     | 804  | CLA  | C3B-C4B-NB  | -3.10 | 107.76      | 110.53   |
| 14  | a     | 815  | CLA  | C3B-C4B-NB  | -3.10 | 107.76      | 110.53   |
| 17  | Y     | 101  | BCR  | C11-C10-C9  | -3.10 | 122.93      | 127.28   |
| 17  | G     | 845  | BCR  | C24-C23-C22 | -3.10 | 121.65      | 126.23   |
| 14  | N     | 809  | CLA  | O2D-CGD-O1D | -3.10 | 117.82      | 123.85   |
| 14  | W     | 202  | CLA  | O2D-CGD-O1D | -3.10 | 117.82      | 123.85   |
| 14  | a     | 832  | CLA  | O2D-CGD-O1D | -3.09 | 117.83      | 123.85   |
| 20  | w     | 202  | SQD  | O7-S-C6     | 3.09  | 111.37      | 106.76   |
| 14  | g     | 815  | CLA  | C3B-C4B-NB  | -3.09 | 107.77      | 110.53   |
| 14  | G     | 806  | CLA  | O2D-CGD-O1D | -3.09 | 117.83      | 123.85   |
| 17  | k     | 102  | BCR  | C28-C27-C26 | -3.09 | 108.54      | 114.06   |
| 17  | n     | 847  | BCR  | C7-C8-C9    | -3.09 | 121.66      | 126.23   |
| 14  | A     | 807  | CLA  | O2D-CGD-O1D | -3.09 | 117.83      | 123.85   |
| 14  | T     | 101  | CLA  | O2D-CGD-O1D | -3.09 | 117.83      | 123.85   |
| 14  | B     | 811  | CLA  | C3B-C4B-NB  | -3.09 | 107.77      | 110.53   |
| 17  | j     | 103  | BCR  | C28-C27-C26 | -3.09 | 108.55      | 114.06   |
| 17  | n     | 847  | BCR  | C27-C26-C25 | -3.09 | 118.53      | 122.70   |
| 15  | g     | 841  | PQN  | C14-C13-C15 | 3.09  | 120.59      | 115.23   |
| 20  | w     | 202  | SQD  | O9-S-C6     | 3.09  | 111.36      | 106.76   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | M     | 101 | BCR  | C8-C7-C6    | -3.09 | 118.75      | 127.00   |
| 14  | B     | 825 | CLA  | O2D-CGD-O1D | -3.09 | 117.84      | 123.85   |
| 14  | A     | 825 | CLA  | O2D-CGD-O1D | -3.08 | 117.84      | 123.85   |
| 17  | l     | 205 | BCR  | C33-C5-C6   | -3.08 | 121.12      | 124.48   |
| 17  | I     | 101 | BCR  | C30-C25-C26 | -3.08 | 118.42      | 122.64   |
| 17  | a     | 847 | BCR  | C30-C25-C26 | -3.08 | 118.42      | 122.64   |
| 14  | g     | 810 | CLA  | C3B-C4B-NB  | -3.08 | 107.78      | 110.53   |
| 14  | A     | 836 | CLA  | C3B-C4B-NB  | -3.08 | 107.78      | 110.53   |
| 14  | b     | 838 | CLA  | O2D-CGD-O1D | -3.08 | 117.86      | 123.85   |
| 14  | g     | 834 | CLA  | O2D-CGD-O1D | -3.08 | 117.86      | 123.85   |
| 17  | l     | 206 | BCR  | C4-C5-C6    | -3.08 | 118.55      | 122.70   |
| 17  | B     | 844 | BCR  | C3-C4-C5    | -3.08 | 108.57      | 114.06   |
| 14  | b     | 833 | CLA  | C3B-C4B-NB  | -3.08 | 107.78      | 110.53   |
| 14  | N     | 832 | CLA  | C3B-C4B-NB  | -3.07 | 107.78      | 110.53   |
| 17  | y     | 101 | BCR  | C28-C27-C26 | -3.07 | 108.57      | 114.06   |
| 14  | a     | 822 | CLA  | O2D-CGD-O1D | -3.07 | 117.87      | 123.85   |
| 17  | B     | 848 | BCR  | C28-C27-C26 | -3.07 | 108.58      | 114.06   |
| 17  | T     | 104 | BCR  | C23-C24-C25 | -3.07 | 118.79      | 127.00   |
| 17  | B     | 851 | BCR  | C8-C7-C6    | -3.07 | 118.80      | 127.00   |
| 20  | b     | 801 | SQD  | O9-S-C6     | 3.07  | 111.34      | 106.76   |
| 14  | A     | 830 | CLA  | C3B-C4B-NB  | -3.07 | 107.79      | 110.53   |
| 17  | b     | 846 | BCR  | C11-C12-C13 | -3.07 | 117.96      | 126.36   |
| 17  | I     | 102 | BCR  | C15-C14-C13 | -3.07 | 122.98      | 127.28   |
| 14  | a     | 828 | CLA  | O2D-CGD-O1D | -3.06 | 117.88      | 123.85   |
| 14  | b     | 820 | CLA  | O2D-CGD-O1D | -3.06 | 117.89      | 123.85   |
| 17  | A     | 848 | BCR  | C28-C27-C26 | -3.06 | 108.60      | 114.06   |
| 17  | T     | 103 | BCR  | C20-C21-C22 | -3.06 | 122.98      | 127.28   |
| 14  | g     | 816 | CLA  | C3B-C4B-NB  | -3.06 | 107.80      | 110.53   |
| 14  | g     | 819 | CLA  | C3B-C4B-NB  | -3.06 | 107.80      | 110.53   |
| 17  | G     | 843 | BCR  | C24-C23-C22 | -3.06 | 121.71      | 126.23   |
| 14  | b     | 805 | CLA  | O2D-CGD-O1D | -3.06 | 117.89      | 123.85   |
| 14  | B     | 850 | CLA  | O2D-CGD-O1D | -3.06 | 117.89      | 123.85   |
| 14  | B     | 819 | CLA  | O2D-CGD-O1D | -3.06 | 117.89      | 123.85   |
| 14  | b     | 803 | CLA  | O2D-CGD-O1D | -3.06 | 117.90      | 123.85   |
| 14  | n     | 838 | CLA  | O2D-CGD-O1D | -3.06 | 117.90      | 123.85   |
| 17  | g     | 843 | BCR  | C11-C12-C13 | -3.06 | 117.98      | 126.36   |
| 17  | a     | 848 | BCR  | C15-C14-C13 | -3.06 | 122.99      | 127.28   |
| 19  | A     | 852 | CL0  | O2D-CGD-O1D | -3.05 | 117.90      | 123.85   |
| 14  | B     | 850 | CLA  | C3B-C4B-NB  | -3.05 | 107.80      | 110.53   |
| 17  | N     | 853 | BCR  | C38-C26-C25 | -3.05 | 121.15      | 124.48   |
| 19  | a     | 851 | CL0  | O2D-CGD-O1D | -3.05 | 117.91      | 123.85   |
| 14  | a     | 817 | CLA  | O2D-CGD-O1D | -3.05 | 117.91      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | n     | 829 | CLA  | O2D-CGD-O1D | -3.05 | 117.91      | 123.85   |
| 19  | G     | 851 | CL0  | C1-C2-C3    | -3.05 | 121.20      | 126.20   |
| 14  | N     | 851 | CLA  | O2D-CGD-O1D | -3.05 | 117.92      | 123.85   |
| 14  | n     | 807 | CLA  | O2D-CGD-O1D | -3.05 | 117.92      | 123.85   |
| 14  | N     | 835 | CLA  | O2D-CGD-O1D | -3.04 | 117.92      | 123.85   |
| 14  | a     | 827 | CLA  | O2D-CGD-O1D | -3.04 | 117.92      | 123.85   |
| 14  | a     | 816 | CLA  | C3B-C4B-NB  | -3.04 | 107.81      | 110.53   |
| 17  | T     | 103 | BCR  | C24-C23-C22 | -3.04 | 121.73      | 126.23   |
| 14  | A     | 838 | CLA  | O2D-CGD-O1D | -3.04 | 117.93      | 123.85   |
| 14  | B     | 820 | CLA  | C3B-C4B-NB  | -3.04 | 107.82      | 110.53   |
| 17  | g     | 846 | BCR  | C10-C11-C12 | -3.04 | 114.39      | 123.20   |
| 14  | A     | 826 | CLA  | O2D-CGD-O1D | -3.04 | 117.93      | 123.85   |
| 14  | U     | 101 | CLA  | C3B-C4B-NB  | -3.04 | 107.82      | 110.53   |
| 14  | l     | 203 | CLA  | O2D-CGD-O1D | -3.04 | 117.94      | 123.85   |
| 14  | b     | 833 | CLA  | O2D-CGD-O1D | -3.04 | 117.94      | 123.85   |
| 17  | G     | 845 | BCR  | C33-C5-C4   | 3.04  | 120.07      | 113.60   |
| 17  | l     | 206 | BCR  | C33-C5-C4   | 3.04  | 120.07      | 113.60   |
| 17  | U     | 103 | BCR  | C28-C27-C26 | -3.04 | 108.64      | 114.06   |
| 17  | T     | 103 | BCR  | C7-C8-C9    | -3.04 | 121.74      | 126.23   |
| 17  | M     | 101 | BCR  | C24-C23-C22 | -3.03 | 121.75      | 126.23   |
| 14  | A     | 841 | CLA  | O2D-CGD-O1D | -3.03 | 117.94      | 123.85   |
| 14  | G     | 839 | CLA  | O2D-CGD-O1D | -3.03 | 117.95      | 123.85   |
| 14  | g     | 810 | CLA  | O2D-CGD-O1D | -3.03 | 117.95      | 123.85   |
| 14  | B     | 841 | CLA  | O2D-CGD-O1D | -3.03 | 117.95      | 123.85   |
| 17  | t     | 104 | BCR  | C33-C5-C6   | -3.03 | 121.18      | 124.48   |
| 14  | n     | 818 | CLA  | O2D-CGD-O1D | -3.03 | 117.95      | 123.85   |
| 14  | B     | 839 | CLA  | O2D-CGD-O1D | -3.03 | 117.95      | 123.85   |
| 14  | J     | 101 | CLA  | O2D-CGD-O1D | -3.03 | 117.95      | 123.85   |
| 14  | a     | 805 | CLA  | O2D-CGD-O1D | -3.03 | 117.95      | 123.85   |
| 17  | A     | 844 | BCR  | C28-C27-C26 | -3.03 | 108.66      | 114.06   |
| 17  | n     | 845 | BCR  | C36-C18-C17 | -3.03 | 117.91      | 122.82   |
| 14  | B     | 824 | CLA  | O2D-CGD-O1D | -3.02 | 117.96      | 123.85   |
| 17  | I     | 103 | BCR  | C20-C21-C22 | -3.02 | 123.04      | 127.28   |
| 14  | g     | 825 | CLA  | C3B-C4B-NB  | -3.02 | 107.83      | 110.53   |
| 17  | N     | 845 | BCR  | C7-C8-C9    | -3.02 | 121.76      | 126.23   |
| 14  | b     | 821 | CLA  | C3B-C4B-NB  | -3.02 | 107.83      | 110.53   |
| 14  | n     | 806 | CLA  | O2D-CGD-O1D | -3.02 | 117.97      | 123.85   |
| 14  | A     | 821 | CLA  | O2D-CGD-O1D | -3.02 | 117.97      | 123.85   |
| 14  | a     | 839 | CLA  | O2D-CGD-O1D | -3.02 | 117.97      | 123.85   |
| 14  | b     | 826 | CLA  | O2D-CGD-O1D | -3.02 | 117.98      | 123.85   |
| 17  | A     | 845 | BCR  | C3-C4-C5    | -3.02 | 108.68      | 114.06   |
| 17  | A     | 845 | BCR  | C38-C26-C27 | 3.02  | 120.03      | 113.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 830  | CLA  | O2D-CGD-O1D | -3.02 | 117.98      | 123.85   |
| 14  | A     | 805  | CLA  | O2D-CGD-O1D | -3.02 | 117.98      | 123.85   |
| 14  | b     | 820  | CLA  | C3B-C4B-NB  | -3.02 | 107.84      | 110.53   |
| 17  | A     | 849  | BCR  | C8-C9-C10   | 3.01  | 123.75      | 119.01   |
| 14  | G     | 837  | CLA  | C3B-C4B-NB  | -3.01 | 107.84      | 110.53   |
| 14  | B     | 837  | CLA  | C3B-C4B-NB  | -3.01 | 107.84      | 110.53   |
| 14  | W     | 204  | CLA  | O2D-CGD-O1D | -3.01 | 117.98      | 123.85   |
| 14  | b     | 839  | CLA  | O2D-CGD-O1D | -3.01 | 117.98      | 123.85   |
| 19  | G     | 851  | CL0  | CMD-C2D-C3D | 3.01  | 130.70      | 124.68   |
| 14  | n     | 850  | CLA  | O2D-CGD-O1D | -3.01 | 117.99      | 123.85   |
| 14  | B     | 828  | CLA  | O2D-CGD-O1D | -3.01 | 117.99      | 123.85   |
| 14  | N     | 805  | CLA  | O2D-CGD-O1D | -3.01 | 117.99      | 123.85   |
| 14  | n     | 852  | CLA  | O2D-CGD-O1D | -3.01 | 117.99      | 123.85   |
| 14  | A     | 837  | CLA  | C3B-C4B-NB  | -3.01 | 107.84      | 110.53   |
| 14  | n     | 811  | CLA  | O2D-CGD-O1D | -3.01 | 117.99      | 123.85   |
| 14  | N     | 812  | CLA  | O2D-CGD-O1D | -3.01 | 118.00      | 123.85   |
| 14  | N     | 823  | CLA  | O2D-CGD-O1D | -3.01 | 118.00      | 123.85   |
| 14  | a     | 854  | CLA  | O2D-CGD-O1D | -3.01 | 118.00      | 123.85   |
| 14  | G     | 806  | CLA  | C3B-C4B-NB  | -3.00 | 107.85      | 110.53   |
| 14  | b     | 813  | CLA  | O2D-CGD-O1D | -3.00 | 118.00      | 123.85   |
| 14  | G     | 816  | CLA  | C3B-C4B-NB  | -3.00 | 107.85      | 110.53   |
| 17  | W     | 201  | BCR  | C33-C5-C6   | -3.00 | 121.21      | 124.48   |
| 20  | h     | 1702 | SQD  | O7-S-C6     | 3.00  | 111.24      | 106.76   |
| 14  | g     | 837  | CLA  | O2D-CGD-O1D | -3.00 | 118.01      | 123.85   |
| 14  | A     | 811  | CLA  | O2D-CGD-O1D | -3.00 | 118.01      | 123.85   |
| 14  | n     | 840  | CLA  | O2D-CGD-O1D | -3.00 | 118.01      | 123.85   |
| 14  | A     | 803  | CLA  | O2D-CGD-O1D | -3.00 | 118.01      | 123.85   |
| 17  | L     | 1504 | BCR  | C28-C27-C26 | -3.00 | 108.71      | 114.06   |
| 17  | N     | 852  | BCR  | C11-C10-C9  | -3.00 | 123.07      | 127.28   |
| 14  | a     | 801  | CLA  | O2D-CGD-O1D | -3.00 | 118.01      | 123.85   |
| 17  | A     | 856  | BCR  | C23-C24-C25 | -3.00 | 118.99      | 127.00   |
| 14  | N     | 828  | CLA  | O2D-CGD-O1D | -3.00 | 118.02      | 123.85   |
| 14  | a     | 802  | CLA  | C3B-C4B-NB  | -3.00 | 107.86      | 110.53   |
| 17  | w     | 207  | BCR  | C7-C8-C9    | -3.00 | 121.80      | 126.23   |
| 14  | N     | 815  | CLA  | O2D-CGD-O1D | -3.00 | 118.02      | 123.85   |
| 14  | B     | 818  | CLA  | O2D-CGD-O1D | -3.00 | 118.02      | 123.85   |
| 17  | N     | 845  | BCR  | C8-C7-C6    | -2.99 | 119.00      | 127.00   |
| 14  | n     | 819  | CLA  | C3B-C4B-NB  | -2.99 | 107.86      | 110.53   |
| 17  | W     | 201  | BCR  | C24-C25-C26 | -2.99 | 114.66      | 121.56   |
| 14  | N     | 808  | CLA  | O2D-CGD-O1D | -2.99 | 118.03      | 123.85   |
| 14  | g     | 807  | CLA  | O2D-CGD-O1D | -2.99 | 118.03      | 123.85   |
| 17  | a     | 845  | BCR  | C33-C5-C4   | 2.99  | 119.97      | 113.60   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | N     | 819 | CLA  | O2D-CGD-O1D | -2.99 | 118.03      | 123.85   |
| 14  | B     | 808 | CLA  | O2D-CGD-O1D | -2.99 | 118.03      | 123.85   |
| 19  | g     | 851 | CL0  | O2D-CGD-O1D | -2.99 | 118.03      | 123.85   |
| 17  | I     | 101 | BCR  | C16-C15-C14 | -2.99 | 117.40      | 123.52   |
| 14  | g     | 830 | CLA  | O2D-CGD-O1D | -2.99 | 118.03      | 123.85   |
| 14  | w     | 204 | CLA  | O2D-CGD-O1D | -2.99 | 118.03      | 123.85   |
| 14  | a     | 802 | CLA  | O2D-CGD-O1D | -2.99 | 118.03      | 123.85   |
| 14  | n     | 817 | CLA  | O2D-CGD-O1D | -2.99 | 118.03      | 123.85   |
| 14  | n     | 810 | CLA  | C3B-C4B-NB  | -2.99 | 107.86      | 110.53   |
| 14  | n     | 828 | CLA  | O2D-CGD-O1D | -2.98 | 118.04      | 123.85   |
| 14  | n     | 816 | CLA  | O2D-CGD-O1D | -2.98 | 118.04      | 123.85   |
| 17  | b     | 844 | BCR  | C28-C27-C26 | -2.98 | 108.74      | 114.06   |
| 17  | N     | 853 | BCR  | C2-C1-C6    | 2.98  | 114.77      | 110.44   |
| 17  | y     | 101 | BCR  | C23-C24-C25 | -2.98 | 119.03      | 127.00   |
| 17  | F     | 203 | BCR  | C24-C23-C22 | -2.98 | 121.82      | 126.23   |
| 14  | g     | 853 | CLA  | O2D-CGD-O1D | -2.98 | 118.04      | 123.85   |
| 17  | n     | 843 | BCR  | C3-C4-C5    | -2.98 | 108.74      | 114.06   |
| 14  | b     | 818 | CLA  | C3B-C4B-NB  | -2.98 | 107.87      | 110.53   |
| 20  | n     | 801 | SQD  | O7-S-C6     | 2.98  | 111.21      | 106.76   |
| 14  | g     | 818 | CLA  | O2D-CGD-O1D | -2.98 | 118.05      | 123.85   |
| 14  | N     | 837 | CLA  | O2D-CGD-O1D | -2.98 | 118.05      | 123.85   |
| 14  | A     | 853 | CLA  | O2D-CGD-O1D | -2.98 | 118.05      | 123.85   |
| 17  | G     | 844 | BCR  | C38-C26-C27 | 2.98  | 119.95      | 113.60   |
| 17  | M     | 101 | BCR  | C23-C24-C25 | -2.98 | 119.04      | 127.00   |
| 17  | J     | 103 | BCR  | C28-C27-C26 | -2.98 | 108.74      | 114.06   |
| 14  | u     | 101 | CLA  | C3B-C4B-NB  | -2.98 | 107.87      | 110.53   |
| 14  | a     | 835 | CLA  | C3B-C4B-NB  | -2.98 | 107.87      | 110.53   |
| 14  | N     | 822 | CLA  | O2D-CGD-O1D | -2.98 | 118.05      | 123.85   |
| 17  | n     | 845 | BCR  | C11-C12-C13 | -2.98 | 118.20      | 126.36   |
| 14  | n     | 812 | CLA  | O2D-CGD-O1D | -2.98 | 118.05      | 123.85   |
| 17  | w     | 207 | BCR  | C33-C5-C4   | 2.98  | 119.94      | 113.60   |
| 14  | a     | 818 | CLA  | O2D-CGD-O1D | -2.98 | 118.06      | 123.85   |
| 14  | N     | 818 | CLA  | O2D-CGD-O1D | -2.97 | 118.06      | 123.85   |
| 17  | G     | 844 | BCR  | C23-C24-C25 | -2.97 | 119.05      | 127.00   |
| 14  | A     | 828 | CLA  | O2D-CGD-O1D | -2.97 | 118.06      | 123.85   |
| 17  | N     | 845 | BCR  | C33-C5-C4   | 2.97  | 119.94      | 113.60   |
| 14  | G     | 807 | CLA  | O2D-CGD-O1D | -2.97 | 118.06      | 123.85   |
| 14  | N     | 841 | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 17  | G     | 848 | BCR  | C8-C9-C10   | 2.97  | 123.68      | 119.01   |
| 17  | a     | 845 | BCR  | C24-C23-C22 | -2.97 | 121.84      | 126.23   |
| 14  | g     | 840 | CLA  | O2D-CGD-O1D | -2.97 | 118.07      | 123.85   |
| 14  | G     | 811 | CLA  | O2D-CGD-O1D | -2.97 | 118.07      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | g     | 817  | CLA  | O2D-CGD-O1D | -2.97 | 118.08      | 123.85   |
| 14  | A     | 810  | CLA  | O2D-CGD-O1D | -2.97 | 118.08      | 123.85   |
| 14  | A     | 834  | CLA  | C3B-C4B-NB  | -2.97 | 107.88      | 110.53   |
| 17  | B     | 845  | BCR  | C20-C21-C22 | -2.96 | 123.12      | 127.28   |
| 14  | G     | 819  | CLA  | O2D-CGD-O1D | -2.96 | 118.08      | 123.85   |
| 14  | g     | 854  | CLA  | O2D-CGD-O1D | -2.96 | 118.08      | 123.85   |
| 14  | b     | 823  | CLA  | C3B-C4B-NB  | -2.96 | 107.89      | 110.53   |
| 14  | l     | 204  | CLA  | C3B-C4B-NB  | -2.96 | 107.89      | 110.53   |
| 17  | g     | 845  | BCR  | C23-C24-C25 | -2.96 | 119.09      | 127.00   |
| 14  | a     | 837  | CLA  | O2D-CGD-O1D | -2.96 | 118.08      | 123.85   |
| 14  | A     | 839  | CLA  | O2D-CGD-O1D | -2.96 | 118.09      | 123.85   |
| 14  | b     | 808  | CLA  | O2D-CGD-O1D | -2.96 | 118.09      | 123.85   |
| 14  | N     | 829  | CLA  | O2D-CGD-O1D | -2.96 | 118.09      | 123.85   |
| 17  | y     | 101  | BCR  | C8-C7-C6    | -2.96 | 119.10      | 127.00   |
| 17  | m     | 102  | BCR  | C8-C7-C6    | -2.96 | 119.10      | 127.00   |
| 17  | g     | 847  | BCR  | C30-C25-C26 | -2.96 | 118.59      | 122.64   |
| 17  | W     | 201  | BCR  | C16-C17-C18 | -2.96 | 123.13      | 127.28   |
| 14  | X     | 1701 | CLA  | O2D-CGD-O1D | -2.96 | 118.09      | 123.85   |
| 14  | a     | 805  | CLA  | C3B-C4B-NB  | -2.96 | 107.89      | 110.53   |
| 14  | b     | 832  | CLA  | O2D-CGD-O1D | -2.96 | 118.09      | 123.85   |
| 14  | a     | 821  | CLA  | C3B-C4B-NB  | -2.96 | 107.89      | 110.53   |
| 17  | V     | 101  | BCR  | C4-C5-C6    | -2.96 | 118.71      | 122.70   |
| 14  | N     | 840  | CLA  | O2D-CGD-O1D | -2.96 | 118.09      | 123.85   |
| 14  | n     | 835  | CLA  | O2D-CGD-O1D | -2.96 | 118.09      | 123.85   |
| 14  | b     | 807  | CLA  | O2D-CGD-O1D | -2.96 | 118.09      | 123.85   |
| 14  | n     | 825  | CLA  | O2D-CGD-O1D | -2.95 | 118.10      | 123.85   |
| 14  | s     | 202  | CLA  | O2D-CGD-O1D | -2.95 | 118.10      | 123.85   |
| 14  | n     | 823  | CLA  | C3B-C4B-NB  | -2.95 | 107.89      | 110.53   |
| 14  | B     | 821  | CLA  | C3B-C4B-NB  | -2.95 | 107.89      | 110.53   |
| 17  | N     | 852  | BCR  | C24-C23-C22 | -2.95 | 121.86      | 126.23   |
| 20  | B     | 801  | SQD  | O9-S-C6     | 2.95  | 111.17      | 106.76   |
| 14  | B     | 829  | CLA  | O2D-CGD-O1D | -2.95 | 118.10      | 123.85   |
| 14  | N     | 839  | CLA  | O2D-CGD-O1D | -2.95 | 118.10      | 123.85   |
| 14  | g     | 816  | CLA  | O2D-CGD-O1D | -2.95 | 118.10      | 123.85   |
| 14  | g     | 820  | CLA  | O2D-CGD-O1D | -2.95 | 118.10      | 123.85   |
| 14  | G     | 824  | CLA  | O2D-CGD-O1D | -2.95 | 118.10      | 123.85   |
| 14  | N     | 833  | CLA  | O2D-CGD-O1D | -2.95 | 118.10      | 123.85   |
| 14  | g     | 839  | CLA  | C3B-C4B-NB  | -2.95 | 107.90      | 110.53   |
| 17  | b     | 848  | BCR  | C8-C7-C6    | -2.95 | 119.12      | 127.00   |
| 14  | G     | 833  | CLA  | O2D-CGD-O1D | -2.95 | 118.11      | 123.85   |
| 14  | F     | 201  | CLA  | C3B-C4B-NB  | -2.95 | 107.90      | 110.53   |
| 14  | N     | 834  | CLA  | O2D-CGD-O1D | -2.95 | 118.11      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | N     | 826  | CLA  | O2D-CGD-O1D | -2.95 | 118.11      | 123.85   |
| 17  | L     | 1504 | BCR  | C8-C7-C6    | -2.95 | 119.13      | 127.00   |
| 17  | N     | 846  | BCR  | C38-C26-C25 | -2.95 | 121.27      | 124.48   |
| 14  | G     | 801  | CLA  | O2D-CGD-O1D | -2.95 | 118.11      | 123.85   |
| 14  | j     | 101  | CLA  | C3B-C4B-NB  | -2.95 | 107.90      | 110.53   |
| 17  | N     | 847  | BCR  | C15-C16-C17 | -2.95 | 117.49      | 123.52   |
| 17  | N     | 849  | BCR  | C10-C11-C12 | -2.94 | 114.67      | 123.20   |
| 14  | B     | 807  | CLA  | O2D-CGD-O1D | -2.94 | 118.12      | 123.85   |
| 14  | b     | 811  | CLA  | C3B-C4B-NB  | -2.94 | 107.90      | 110.53   |
| 17  | n     | 849  | BCR  | C11-C10-C9  | -2.94 | 123.15      | 127.28   |
| 14  | N     | 821  | CLA  | C3B-C4B-NB  | -2.94 | 107.90      | 110.53   |
| 14  | B     | 820  | CLA  | O2D-CGD-O1D | -2.94 | 118.12      | 123.85   |
| 17  | N     | 845  | BCR  | C28-C27-C26 | -2.94 | 108.81      | 114.06   |
| 14  | N     | 842  | CLA  | O2D-CGD-O1D | -2.94 | 118.12      | 123.85   |
| 17  | B     | 851  | BCR  | C33-C5-C4   | 2.94  | 119.87      | 113.60   |
| 14  | B     | 817  | CLA  | C3B-C4B-NB  | -2.94 | 107.90      | 110.53   |
| 17  | y     | 101  | BCR  | C24-C23-C22 | -2.94 | 121.88      | 126.23   |
| 17  | w     | 207  | BCR  | C4-C5-C6    | -2.94 | 118.73      | 122.70   |
| 14  | A     | 822  | CLA  | O2D-CGD-O1D | -2.94 | 118.12      | 123.85   |
| 17  | T     | 104  | BCR  | C20-C21-C22 | -2.94 | 123.15      | 127.28   |
| 14  | G     | 821  | CLA  | O2D-CGD-O1D | -2.94 | 118.12      | 123.85   |
| 17  | I     | 102  | BCR  | C36-C18-C17 | -2.94 | 118.05      | 122.82   |
| 17  | b     | 846  | BCR  | C20-C21-C22 | -2.94 | 123.16      | 127.28   |
| 17  | W     | 201  | BCR  | C15-C14-C13 | -2.94 | 123.16      | 127.28   |
| 14  | A     | 837  | CLA  | O2D-CGD-O1D | -2.94 | 118.13      | 123.85   |
| 14  | G     | 828  | CLA  | O2D-CGD-O1D | -2.94 | 118.13      | 123.85   |
| 17  | b     | 845  | BCR  | C20-C21-C22 | -2.94 | 123.16      | 127.28   |
| 14  | n     | 831  | CLA  | O2D-CGD-O1D | -2.94 | 118.13      | 123.85   |
| 14  | n     | 837  | CLA  | O2D-CGD-O1D | -2.94 | 118.13      | 123.85   |
| 17  | G     | 847  | BCR  | C27-C26-C25 | -2.94 | 118.74      | 122.70   |
| 14  | N     | 820  | CLA  | O2D-CGD-O1D | -2.93 | 118.14      | 123.85   |
| 17  | B     | 844  | BCR  | C7-C8-C9    | -2.93 | 121.89      | 126.23   |
| 17  | M     | 101  | BCR  | C10-C11-C12 | -2.93 | 114.70      | 123.20   |
| 14  | a     | 835  | CLA  | O2D-CGD-O1D | -2.93 | 118.14      | 123.85   |
| 14  | g     | 852  | CLA  | C1-C2-C3    | -2.93 | 121.39      | 126.20   |
| 17  | b     | 846  | BCR  | C24-C23-C22 | -2.93 | 121.90      | 126.23   |
| 17  | b     | 848  | BCR  | C11-C10-C9  | -2.93 | 123.17      | 127.28   |
| 17  | G     | 847  | BCR  | C30-C25-C26 | -2.93 | 118.63      | 122.64   |
| 14  | A     | 806  | CLA  | O2D-CGD-O1D | -2.93 | 118.14      | 123.85   |
| 14  | L     | 1502 | CLA  | C3B-C4B-NB  | -2.93 | 107.91      | 110.53   |
| 19  | G     | 851  | CL0  | CMB-C2B-C3B | 2.93  | 130.54      | 124.68   |
| 14  | A     | 812  | CLA  | C3B-C4B-NB  | -2.93 | 107.92      | 110.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | b     | 850  | BCR  | C15-C16-C17 | -2.93 | 117.53      | 123.52   |
| 17  | A     | 847  | BCR  | C4-C5-C6    | -2.93 | 118.75      | 122.70   |
| 14  | n     | 813  | CLA  | O2D-CGD-O1D | -2.93 | 118.15      | 123.85   |
| 17  | A     | 849  | BCR  | C33-C5-C4   | 2.93  | 119.84      | 113.60   |
| 17  | b     | 843  | BCR  | C30-C25-C26 | -2.93 | 118.64      | 122.64   |
| 17  | B     | 848  | BCR  | C11-C10-C9  | -2.92 | 123.18      | 127.28   |
| 14  | b     | 810  | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 14  | a     | 811  | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 14  | G     | 811  | CLA  | C3B-C4B-NB  | -2.92 | 107.92      | 110.53   |
| 14  | A     | 816  | CLA  | C3B-C4B-NB  | -2.92 | 107.92      | 110.53   |
| 14  | B     | 821  | CLA  | O2D-CGD-O1D | -2.92 | 118.16      | 123.85   |
| 14  | G     | 838  | CLA  | O2D-CGD-O1D | -2.92 | 118.17      | 123.85   |
| 14  | A     | 819  | CLA  | O2D-CGD-O1D | -2.92 | 118.17      | 123.85   |
| 20  | x     | 1702 | SQD  | O7-S-C6     | 2.92  | 111.11      | 106.76   |
| 14  | g     | 839  | CLA  | O2D-CGD-O1D | -2.92 | 118.17      | 123.85   |
| 14  | a     | 836  | CLA  | O2D-CGD-O1D | -2.92 | 118.17      | 123.85   |
| 14  | b     | 836  | CLA  | O2D-CGD-O1D | -2.92 | 118.17      | 123.85   |
| 14  | g     | 803  | CLA  | C3B-C4B-NB  | -2.92 | 107.93      | 110.53   |
| 14  | n     | 827  | CLA  | C1-C2-C3    | -2.92 | 121.42      | 126.20   |
| 14  | g     | 803  | CLA  | O2D-CGD-O1D | -2.91 | 118.17      | 123.85   |
| 14  | b     | 818  | CLA  | O2D-CGD-O1D | -2.91 | 118.17      | 123.85   |
| 14  | A     | 807  | CLA  | C3B-C4B-NB  | -2.91 | 107.93      | 110.53   |
| 14  | G     | 830  | CLA  | O2D-CGD-O1D | -2.91 | 118.17      | 123.85   |
| 14  | G     | 836  | CLA  | O2D-CGD-O1D | -2.91 | 118.17      | 123.85   |
| 17  | g     | 845  | BCR  | C33-C5-C4   | 2.91  | 119.81      | 113.60   |
| 14  | G     | 827  | CLA  | O2D-CGD-O1D | -2.91 | 118.18      | 123.85   |
| 14  | N     | 825  | CLA  | O2D-CGD-O1D | -2.91 | 118.18      | 123.85   |
| 14  | B     | 815  | CLA  | C3B-C4B-NB  | -2.91 | 107.93      | 110.53   |
| 14  | a     | 825  | CLA  | O2D-CGD-O1D | -2.91 | 118.18      | 123.85   |
| 14  | A     | 839  | CLA  | C3B-C4B-NB  | -2.91 | 107.93      | 110.53   |
| 14  | a     | 809  | CLA  | C3B-C4B-NB  | -2.91 | 107.93      | 110.53   |
| 17  | W     | 201  | BCR  | C23-C22-C21 | 2.91  | 123.59      | 119.01   |
| 14  | N     | 816  | CLA  | O2D-CGD-O1D | -2.91 | 118.19      | 123.85   |
| 14  | b     | 825  | CLA  | O2D-CGD-O1D | -2.91 | 118.19      | 123.85   |
| 14  | A     | 802  | CLA  | O2D-CGD-O1D | -2.91 | 118.19      | 123.85   |
| 14  | b     | 841  | CLA  | O2D-CGD-O1D | -2.91 | 118.19      | 123.85   |
| 14  | N     | 841  | CLA  | O2D-CGD-O1D | -2.91 | 118.19      | 123.85   |
| 14  | g     | 819  | CLA  | O2D-CGD-O1D | -2.91 | 118.19      | 123.85   |
| 17  | N     | 848  | BCR  | C3-C4-C5    | -2.91 | 108.87      | 114.06   |
| 14  | g     | 805  | CLA  | C3B-C4B-NB  | -2.91 | 107.94      | 110.53   |
| 14  | n     | 821  | CLA  | C3B-C4B-NB  | -2.91 | 107.94      | 110.53   |
| 14  | G     | 803  | CLA  | O2D-CGD-O1D | -2.91 | 118.19      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | a     | 853 | CLA  | O2D-CGD-O1D | -2.91 | 118.19      | 123.85   |
| 17  | a     | 847 | BCR  | C27-C26-C25 | -2.91 | 118.78      | 122.70   |
| 14  | G     | 835 | CLA  | O2D-CGD-O1D | -2.90 | 118.19      | 123.85   |
| 14  | B     | 814 | CLA  | O2D-CGD-O1D | -2.90 | 118.19      | 123.85   |
| 14  | N     | 830 | CLA  | O2D-CGD-O1D | -2.90 | 118.19      | 123.85   |
| 14  | f     | 201 | CLA  | O2D-CGD-O1D | -2.90 | 118.19      | 123.85   |
| 17  | A     | 845 | BCR  | C23-C24-C25 | -2.90 | 119.24      | 127.00   |
| 14  | g     | 835 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 17  | G     | 844 | BCR  | C3-C4-C5    | -2.90 | 108.88      | 114.06   |
| 17  | a     | 846 | BCR  | C38-C26-C27 | 2.90  | 119.78      | 113.60   |
| 14  | b     | 802 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 14  | b     | 817 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 14  | b     | 851 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 14  | n     | 814 | CLA  | C3B-C4B-NB  | -2.90 | 107.94      | 110.53   |
| 17  | w     | 207 | BCR  | C33-C5-C6   | -2.90 | 121.32      | 124.48   |
| 14  | G     | 804 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 14  | g     | 815 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 14  | g     | 835 | CLA  | C3B-C4B-NB  | -2.90 | 107.94      | 110.53   |
| 14  | A     | 816 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 17  | t     | 104 | BCR  | C20-C19-C18 | -2.90 | 118.41      | 126.36   |
| 14  | b     | 814 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 14  | g     | 827 | CLA  | O2D-CGD-O1D | -2.90 | 118.20      | 123.85   |
| 17  | a     | 847 | BCR  | C33-C5-C6   | -2.90 | 121.32      | 124.48   |
| 14  | b     | 827 | CLA  | O2D-CGD-O1D | -2.90 | 118.21      | 123.85   |
| 14  | A     | 813 | CLA  | O2D-CGD-O1D | -2.90 | 118.21      | 123.85   |
| 17  | A     | 847 | BCR  | C33-C5-C4   | 2.90  | 119.78      | 113.60   |
| 14  | s     | 201 | CLA  | C3B-C4B-NB  | -2.90 | 107.94      | 110.53   |
| 15  | G     | 841 | PQN  | C11-C3-C2   | -2.90 | 119.92      | 124.89   |
| 17  | a     | 844 | BCR  | C3-C4-C5    | -2.90 | 108.89      | 114.06   |
| 14  | G     | 826 | CLA  | O2D-CGD-O1D | -2.90 | 118.21      | 123.85   |
| 14  | B     | 837 | CLA  | O2D-CGD-O1D | -2.90 | 118.21      | 123.85   |
| 14  | a     | 820 | CLA  | O2D-CGD-O1D | -2.90 | 118.21      | 123.85   |
| 14  | G     | 813 | CLA  | O2D-CGD-O1D | -2.90 | 118.21      | 123.85   |
| 14  | w     | 205 | CLA  | O2D-CGD-O1D | -2.90 | 118.21      | 123.85   |
| 14  | g     | 801 | CLA  | O2D-CGD-O1D | -2.89 | 118.21      | 123.85   |
| 14  | g     | 804 | CLA  | O2D-CGD-O1D | -2.89 | 118.21      | 123.85   |
| 14  | a     | 804 | CLA  | O2D-CGD-O1D | -2.89 | 118.21      | 123.85   |
| 17  | B     | 852 | BCR  | C38-C26-C25 | -2.89 | 121.33      | 124.48   |
| 14  | g     | 805 | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 14  | A     | 857 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 14  | A     | 801 | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 14  | a     | 819 | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | a     | 840 | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 17  | A     | 849 | BCR  | C20-C19-C18 | -2.89 | 118.43      | 126.36   |
| 14  | G     | 810 | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 14  | A     | 817 | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 14  | B     | 827 | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 14  | N     | 817 | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 17  | A     | 844 | BCR  | C11-C12-C13 | -2.89 | 118.44      | 126.36   |
| 14  | A     | 835 | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 14  | A     | 826 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 14  | A     | 824 | CLA  | O2D-CGD-O1D | -2.89 | 118.22      | 123.85   |
| 14  | b     | 809 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 17  | i     | 102 | BCR  | C10-C11-C12 | -2.89 | 114.83      | 123.20   |
| 19  | g     | 851 | CL0  | C4D-CHA-CBD | -2.89 | 106.06      | 108.97   |
| 14  | n     | 817 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 14  | a     | 810 | CLA  | O2D-CGD-O1D | -2.89 | 118.23      | 123.85   |
| 14  | N     | 814 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 14  | B     | 813 | CLA  | C3B-C4B-NB  | -2.89 | 107.95      | 110.53   |
| 14  | a     | 824 | CLA  | O2D-CGD-O1D | -2.88 | 118.23      | 123.85   |
| 14  | G     | 833 | CLA  | C3B-C4B-NB  | -2.88 | 107.95      | 110.53   |
| 14  | a     | 803 | CLA  | C3B-C4B-NB  | -2.88 | 107.95      | 110.53   |
| 14  | b     | 819 | CLA  | O2D-CGD-O1D | -2.88 | 118.23      | 123.85   |
| 14  | B     | 803 | CLA  | O2D-CGD-O1D | -2.88 | 118.24      | 123.85   |
| 14  | N     | 837 | CLA  | C3B-C4B-NB  | -2.88 | 107.96      | 110.53   |
| 14  | b     | 851 | CLA  | C3B-C4B-NB  | -2.88 | 107.96      | 110.53   |
| 14  | N     | 836 | CLA  | O2D-CGD-O1D | -2.88 | 118.24      | 123.85   |
| 14  | B     | 816 | CLA  | O2D-CGD-O1D | -2.88 | 118.24      | 123.85   |
| 17  | T     | 104 | BCR  | C7-C8-C9    | -2.88 | 121.97      | 126.23   |
| 17  | b     | 848 | BCR  | C7-C8-C9    | -2.88 | 121.97      | 126.23   |
| 14  | g     | 829 | CLA  | O2D-CGD-O1D | -2.88 | 118.24      | 123.85   |
| 14  | b     | 811 | CLA  | O2D-CGD-O1D | -2.88 | 118.24      | 123.85   |
| 14  | B     | 822 | CLA  | O2D-CGD-O1D | -2.88 | 118.24      | 123.85   |
| 14  | B     | 815 | CLA  | O2D-CGD-O1D | -2.88 | 118.24      | 123.85   |
| 14  | g     | 825 | CLA  | O2D-CGD-O1D | -2.88 | 118.25      | 123.85   |
| 14  | N     | 807 | CLA  | C3B-C4B-NB  | -2.88 | 107.96      | 110.53   |
| 14  | n     | 812 | CLA  | C3B-C4B-NB  | -2.88 | 107.96      | 110.53   |
| 17  | A     | 849 | BCR  | C34-C9-C10  | -2.88 | 118.15      | 122.82   |
| 17  | B     | 844 | BCR  | C20-C19-C18 | -2.88 | 118.47      | 126.36   |
| 14  | n     | 808 | CLA  | C3B-C4B-NB  | -2.88 | 107.96      | 110.53   |
| 14  | J     | 101 | CLA  | C3B-C4B-NB  | -2.88 | 107.96      | 110.53   |
| 14  | a     | 852 | CLA  | C3B-C4B-NB  | -2.88 | 107.96      | 110.53   |
| 14  | F     | 202 | CLA  | O2D-CGD-O1D | -2.88 | 118.25      | 123.85   |
| 19  | G     | 851 | CL0  | C4D-CHA-CBD | -2.88 | 106.07      | 108.97   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | N     | 848  | BCR  | C15-C16-C17 | -2.88 | 117.64      | 123.52   |
| 14  | b     | 804  | CLA  | O2D-CGD-O1D | -2.87 | 118.25      | 123.85   |
| 14  | B     | 832  | CLA  | O2D-CGD-O1D | -2.87 | 118.25      | 123.85   |
| 14  | s     | 202  | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 14  | b     | 840  | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 14  | a     | 814  | CLA  | O2D-CGD-O1D | -2.87 | 118.26      | 123.85   |
| 14  | g     | 813  | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 14  | n     | 829  | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 14  | a     | 824  | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 17  | I     | 101  | BCR  | C27-C26-C25 | -2.87 | 118.82      | 122.70   |
| 14  | L     | 1503 | CLA  | O2D-CGD-O1D | -2.87 | 118.26      | 123.85   |
| 14  | A     | 841  | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 14  | n     | 820  | CLA  | O2D-CGD-O1D | -2.87 | 118.26      | 123.85   |
| 14  | B     | 813  | CLA  | O2D-CGD-O1D | -2.87 | 118.26      | 123.85   |
| 14  | G     | 815  | CLA  | O2D-CGD-O1D | -2.87 | 118.26      | 123.85   |
| 14  | b     | 822  | CLA  | O2D-CGD-O1D | -2.87 | 118.26      | 123.85   |
| 14  | G     | 820  | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 14  | A     | 853  | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 14  | k     | 101  | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 14  | n     | 827  | CLA  | O2D-CGD-O1D | -2.87 | 118.26      | 123.85   |
| 14  | g     | 821  | CLA  | O2D-CGD-O1D | -2.87 | 118.27      | 123.85   |
| 14  | n     | 802  | CLA  | O2D-CGD-O1D | -2.87 | 118.27      | 123.85   |
| 14  | g     | 832  | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 14  | n     | 814  | CLA  | O2D-CGD-O1D | -2.87 | 118.27      | 123.85   |
| 14  | A     | 832  | CLA  | O2D-CGD-O1D | -2.87 | 118.27      | 123.85   |
| 14  | a     | 834  | CLA  | O2D-CGD-O1D | -2.87 | 118.27      | 123.85   |
| 14  | H     | 1701 | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 14  | S     | 201  | CLA  | C3B-C4B-NB  | -2.87 | 107.97      | 110.53   |
| 17  | b     | 844  | BCR  | C20-C21-C22 | -2.87 | 123.26      | 127.28   |
| 14  | g     | 823  | CLA  | O2D-CGD-O1D | -2.87 | 118.27      | 123.85   |
| 14  | g     | 824  | CLA  | O2D-CGD-O1D | -2.87 | 118.27      | 123.85   |
| 14  | g     | 813  | CLA  | O2D-CGD-O1D | -2.86 | 118.27      | 123.85   |
| 14  | b     | 840  | CLA  | O2D-CGD-O1D | -2.86 | 118.27      | 123.85   |
| 14  | g     | 809  | CLA  | C3B-C4B-NB  | -2.86 | 107.97      | 110.53   |
| 14  | b     | 815  | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 14  | x     | 1701 | CLA  | C3B-C4B-NB  | -2.86 | 107.97      | 110.53   |
| 14  | N     | 807  | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 14  | b     | 831  | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 14  | b     | 853  | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 14  | G     | 803  | CLA  | C3B-C4B-NB  | -2.86 | 107.98      | 110.53   |
| 17  | g     | 844  | BCR  | C38-C26-C27 | 2.86  | 119.69      | 113.60   |
| 14  | A     | 809  | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 816  | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 14  | G     | 831  | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 14  | S     | 203  | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 14  | n     | 821  | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 14  | A     | 807  | CLA  | CAA-C2A-C1A | -2.86 | 102.61      | 111.97   |
| 17  | j     | 104  | BCR  | C33-C5-C4   | 2.86  | 119.69      | 113.60   |
| 14  | G     | 805  | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 14  | n     | 805  | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 14  | N     | 801  | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 14  | a     | 831  | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 14  | A     | 815  | CLA  | O2D-CGD-O1D | -2.86 | 118.28      | 123.85   |
| 14  | b     | 805  | CLA  | CAC-C3C-C4C | 2.86  | 128.51      | 124.79   |
| 14  | a     | 809  | CLA  | O2D-CGD-O1D | -2.86 | 118.29      | 123.85   |
| 14  | n     | 816  | CLA  | C3B-C4B-NB  | -2.86 | 107.98      | 110.53   |
| 14  | A     | 804  | CLA  | C3B-C4B-NB  | -2.86 | 107.98      | 110.53   |
| 14  | g     | 802  | CLA  | O2D-CGD-O1D | -2.86 | 118.29      | 123.85   |
| 17  | B     | 848  | BCR  | C16-C15-C14 | -2.86 | 117.67      | 123.52   |
| 14  | B     | 805  | CLA  | O2D-CGD-O1D | -2.86 | 118.29      | 123.85   |
| 14  | a     | 806  | CLA  | C3B-C4B-NB  | -2.86 | 107.98      | 110.53   |
| 14  | N     | 801  | CLA  | C3B-C4B-NB  | -2.85 | 107.98      | 110.53   |
| 14  | A     | 818  | CLA  | O2D-CGD-O1D | -2.85 | 118.29      | 123.85   |
| 14  | a     | 830  | CLA  | O2D-CGD-O1D | -2.85 | 118.29      | 123.85   |
| 14  | G     | 816  | CLA  | O2D-CGD-O1D | -2.85 | 118.29      | 123.85   |
| 14  | b     | 815  | CLA  | C3B-C4B-NB  | -2.85 | 107.98      | 110.53   |
| 17  | l     | 206  | BCR  | C33-C5-C6   | -2.85 | 121.37      | 124.48   |
| 17  | A     | 849  | BCR  | C10-C11-C12 | -2.85 | 114.93      | 123.20   |
| 14  | A     | 804  | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 17  | G     | 846  | BCR  | C15-C16-C17 | -2.85 | 117.68      | 123.52   |
| 14  | F     | 202  | CLA  | C3B-C4B-NB  | -2.85 | 107.98      | 110.53   |
| 14  | b     | 812  | CLA  | C3B-C4B-NB  | -2.85 | 107.98      | 110.53   |
| 14  | a     | 803  | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 14  | G     | 808  | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 14  | b     | 806  | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 14  | f     | 201  | CLA  | C3B-C4B-NB  | -2.85 | 107.98      | 110.53   |
| 17  | j     | 104  | BCR  | C20-C19-C18 | -2.85 | 118.55      | 126.36   |
| 14  | g     | 829  | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 14  | a     | 819  | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 14  | b     | 830  | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 14  | H     | 1701 | CLA  | O2D-CGD-O1D | -2.85 | 118.30      | 123.85   |
| 17  | n     | 851  | BCR  | C2-C1-C6    | 2.85  | 114.58      | 110.44   |
| 14  | G     | 836  | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 17  | w     | 206  | BCR  | C33-C5-C6   | -2.85 | 121.38      | 124.48   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | n     | 836  | CLA  | C1-C2-C3    | -2.85 | 121.53      | 126.20   |
| 14  | n     | 825  | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 14  | B     | 840  | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 17  | a     | 846  | BCR  | C19-C18-C17 | 2.85  | 123.49      | 119.01   |
| 17  | N     | 846  | BCR  | C3-C4-C5    | -2.85 | 108.98      | 114.06   |
| 14  | A     | 811  | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 14  | G     | 839  | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 14  | N     | 816  | CLA  | C3B-C4B-NB  | -2.85 | 107.99      | 110.53   |
| 17  | N     | 849  | BCR  | C8-C7-C6    | -2.84 | 119.40      | 127.00   |
| 14  | h     | 1701 | CLA  | C3B-C4B-NB  | -2.84 | 107.99      | 110.53   |
| 14  | n     | 839  | CLA  | C3B-C4B-NB  | -2.84 | 107.99      | 110.53   |
| 14  | n     | 830  | CLA  | O2D-CGD-O1D | -2.84 | 118.31      | 123.85   |
| 14  | n     | 836  | CLA  | O2D-CGD-O1D | -2.84 | 118.31      | 123.85   |
| 17  | b     | 844  | BCR  | C27-C26-C25 | -2.84 | 118.86      | 122.70   |
| 14  | U     | 102  | CLA  | C3B-C4B-NB  | -2.84 | 107.99      | 110.53   |
| 14  | x     | 1701 | CLA  | O2D-CGD-O1D | -2.84 | 118.32      | 123.85   |
| 14  | n     | 815  | CLA  | O2D-CGD-O1D | -2.84 | 118.32      | 123.85   |
| 14  | n     | 826  | CLA  | O2D-CGD-O1D | -2.84 | 118.33      | 123.85   |
| 14  | l     | 204  | CLA  | O2D-CGD-O1D | -2.84 | 118.33      | 123.85   |
| 17  | n     | 842  | BCR  | C38-C26-C25 | -2.84 | 121.39      | 124.48   |
| 14  | B     | 806  | CLA  | O2D-CGD-O1D | -2.84 | 118.33      | 123.85   |
| 17  | F     | 203  | BCR  | C23-C24-C25 | -2.84 | 119.42      | 127.00   |
| 14  | f     | 202  | CLA  | O2D-CGD-O1D | -2.84 | 118.33      | 123.85   |
| 14  | n     | 834  | CLA  | O2D-CGD-O1D | -2.84 | 118.33      | 123.85   |
| 14  | N     | 815  | CLA  | C3B-C4B-NB  | -2.84 | 108.00      | 110.53   |
| 14  | B     | 817  | CLA  | O2D-CGD-O1D | -2.83 | 118.33      | 123.85   |
| 14  | G     | 814  | CLA  | O2D-CGD-O1D | -2.83 | 118.33      | 123.85   |
| 14  | n     | 809  | CLA  | O2D-CGD-O1D | -2.83 | 118.33      | 123.85   |
| 14  | B     | 833  | CLA  | O2D-CGD-O1D | -2.83 | 118.33      | 123.85   |
| 14  | B     | 825  | CLA  | C3B-C4B-NB  | -2.83 | 108.00      | 110.53   |
| 14  | G     | 802  | CLA  | C3B-C4B-NB  | -2.83 | 108.00      | 110.53   |
| 14  | G     | 840  | CLA  | C3B-C4B-NB  | -2.83 | 108.00      | 110.53   |
| 14  | a     | 825  | CLA  | C3B-C4B-NB  | -2.83 | 108.00      | 110.53   |
| 14  | g     | 831  | CLA  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |
| 14  | A     | 812  | CLA  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |
| 14  | A     | 808  | CLA  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |
| 17  | n     | 846  | BCR  | C15-C16-C17 | -2.83 | 117.73      | 123.52   |
| 14  | G     | 840  | CLA  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |
| 17  | g     | 844  | BCR  | C3-C4-C5    | -2.83 | 109.01      | 114.06   |
| 17  | Y     | 101  | BCR  | C8-C7-C6    | -2.83 | 119.44      | 127.00   |
| 14  | G     | 853  | CLA  | C3B-C4B-NB  | -2.83 | 108.00      | 110.53   |
| 14  | t     | 101  | CLA  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | w     | 201  | BCR  | C3-C4-C5    | -2.83 | 109.01      | 114.06   |
| 14  | n     | 819  | CLA  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |
| 14  | n     | 824  | CLA  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |
| 14  | T     | 101  | CLA  | C3B-C4B-NB  | -2.83 | 108.01      | 110.53   |
| 17  | v     | 101  | BCR  | C33-C5-C4   | 2.83  | 119.62      | 113.60   |
| 14  | a     | 821  | CLA  | O2D-CGD-O1D | -2.83 | 118.34      | 123.85   |
| 17  | a     | 844  | BCR  | C38-C26-C27 | 2.83  | 119.62      | 113.60   |
| 14  | G     | 812  | CLA  | O2D-CGD-O1D | -2.83 | 118.35      | 123.85   |
| 14  | n     | 822  | CLA  | O2D-CGD-O1D | -2.83 | 118.35      | 123.85   |
| 14  | g     | 808  | CLA  | O2D-CGD-O1D | -2.83 | 118.35      | 123.85   |
| 17  | b     | 852  | BCR  | C2-C1-C6    | 2.83  | 114.54      | 110.44   |
| 14  | G     | 817  | CLA  | O2D-CGD-O1D | -2.83 | 118.35      | 123.85   |
| 14  | B     | 836  | CLA  | O2D-CGD-O1D | -2.83 | 118.35      | 123.85   |
| 14  | A     | 813  | CLA  | C3B-C4B-NB  | -2.83 | 108.01      | 110.53   |
| 14  | g     | 814  | CLA  | O2D-CGD-O1D | -2.83 | 118.35      | 123.85   |
| 14  | a     | 854  | CLA  | C3B-C4B-NB  | -2.82 | 108.01      | 110.53   |
| 17  | n     | 843  | BCR  | C30-C25-C26 | -2.82 | 118.78      | 122.64   |
| 14  | A     | 820  | CLA  | O2D-CGD-O1D | -2.82 | 118.35      | 123.85   |
| 14  | G     | 823  | CLA  | O2D-CGD-O1D | -2.82 | 118.35      | 123.85   |
| 14  | N     | 805  | CLA  | C3B-C4B-NB  | -2.82 | 108.01      | 110.53   |
| 14  | a     | 822  | CLA  | C3B-C4B-NB  | -2.82 | 108.01      | 110.53   |
| 14  | N     | 824  | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 14  | g     | 822  | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 14  | n     | 839  | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 14  | A     | 854  | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 14  | a     | 812  | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 14  | L     | 1503 | CLA  | C3B-C4B-NB  | -2.82 | 108.01      | 110.53   |
| 14  | a     | 829  | CLA  | C3B-C4B-NB  | -2.82 | 108.01      | 110.53   |
| 20  | H     | 1702 | SQD  | O9-S-C6     | 2.82  | 110.97      | 106.76   |
| 14  | A     | 820  | CLA  | C3B-C4B-NB  | -2.82 | 108.01      | 110.53   |
| 14  | B     | 838  | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 14  | a     | 808  | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 14  | G     | 802  | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 14  | N     | 838  | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 14  | a     | 823  | CLA  | O2D-CGD-O1D | -2.82 | 118.36      | 123.85   |
| 14  | n     | 811  | CLA  | C3B-C4B-NB  | -2.82 | 108.02      | 110.53   |
| 17  | n     | 843  | BCR  | C28-C27-C26 | -2.82 | 109.03      | 114.06   |
| 14  | a     | 838  | CLA  | O2D-CGD-O1D | -2.82 | 118.37      | 123.85   |
| 14  | n     | 836  | CLA  | C3B-C4B-NB  | -2.82 | 108.02      | 110.53   |
| 14  | a     | 838  | CLA  | C3B-C4B-NB  | -2.82 | 108.02      | 110.53   |
| 14  | G     | 820  | CLA  | O2D-CGD-O1D | -2.82 | 118.37      | 123.85   |
| 15  | b     | 842  | PQN  | C11-C3-C2   | -2.82 | 120.06      | 124.89   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | a     | 844  | BCR  | C23-C24-C25 | -2.82 | 119.48      | 127.00   |
| 14  | A     | 817  | CLA  | C3B-C4B-NB  | -2.82 | 108.02      | 110.53   |
| 19  | g     | 851  | CL0  | CMD-C2D-C3D | 2.81  | 130.31      | 124.68   |
| 14  | A     | 831  | CLA  | O2D-CGD-O1D | -2.81 | 118.37      | 123.85   |
| 14  | A     | 836  | CLA  | O2D-CGD-O1D | -2.81 | 118.37      | 123.85   |
| 14  | N     | 806  | CLA  | O2D-CGD-O1D | -2.81 | 118.37      | 123.85   |
| 17  | N     | 846  | BCR  | C33-C5-C4   | 2.81  | 119.59      | 113.60   |
| 17  | A     | 847  | BCR  | C15-C16-C17 | -2.81 | 117.76      | 123.52   |
| 14  | A     | 823  | CLA  | O2D-CGD-O1D | -2.81 | 118.37      | 123.85   |
| 17  | N     | 848  | BCR  | C8-C7-C6    | -2.81 | 119.48      | 127.00   |
| 14  | G     | 822  | CLA  | O2D-CGD-O1D | -2.81 | 118.38      | 123.85   |
| 14  | a     | 813  | CLA  | O2D-CGD-O1D | -2.81 | 118.38      | 123.85   |
| 14  | g     | 802  | CLA  | C3B-C4B-NB  | -2.81 | 108.02      | 110.53   |
| 14  | g     | 812  | CLA  | O2D-CGD-O1D | -2.81 | 118.38      | 123.85   |
| 14  | b     | 828  | CLA  | O2D-CGD-O1D | -2.81 | 118.38      | 123.85   |
| 17  | l     | 206  | BCR  | C8-C7-C6    | -2.81 | 119.50      | 127.00   |
| 14  | G     | 819  | CLA  | C3B-C4B-NB  | -2.81 | 108.02      | 110.53   |
| 14  | A     | 854  | CLA  | C3B-C4B-NB  | -2.81 | 108.02      | 110.53   |
| 14  | B     | 838  | CLA  | C3B-C4B-NB  | -2.81 | 108.02      | 110.53   |
| 14  | G     | 834  | CLA  | O2D-CGD-O1D | -2.81 | 118.38      | 123.85   |
| 14  | N     | 822  | CLA  | C3B-C4B-NB  | -2.81 | 108.03      | 110.53   |
| 14  | g     | 833  | CLA  | C3B-C4B-NB  | -2.81 | 108.03      | 110.53   |
| 14  | b     | 816  | CLA  | O2D-CGD-O1D | -2.81 | 118.39      | 123.85   |
| 14  | B     | 835  | CLA  | O2D-CGD-O1D | -2.80 | 118.39      | 123.85   |
| 14  | h     | 1701 | CLA  | O2D-CGD-O1D | -2.80 | 118.39      | 123.85   |
| 14  | G     | 825  | CLA  | O2D-CGD-O1D | -2.80 | 118.39      | 123.85   |
| 17  | N     | 847  | BCR  | C28-C27-C26 | -2.80 | 109.06      | 114.06   |
| 17  | B     | 844  | BCR  | C33-C5-C4   | 2.80  | 119.57      | 113.60   |
| 17  | b     | 850  | BCR  | C11-C12-C13 | -2.80 | 118.68      | 126.36   |
| 14  | A     | 833  | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 17  | B     | 852  | BCR  | C2-C1-C6    | 2.80  | 114.51      | 110.44   |
| 14  | W     | 204  | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 14  | B     | 806  | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 14  | a     | 828  | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 20  | l     | 201  | SQD  | O9-S-C6     | 2.80  | 110.93      | 106.76   |
| 17  | G     | 848  | BCR  | C34-C9-C10  | -2.80 | 118.28      | 122.82   |
| 14  | K     | 101  | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 14  | g     | 809  | CLA  | O2D-CGD-O1D | -2.80 | 118.40      | 123.85   |
| 17  | S     | 204  | BCR  | C23-C24-C25 | -2.80 | 119.53      | 127.00   |
| 14  | A     | 814  | CLA  | O2D-CGD-O1D | -2.80 | 118.41      | 123.85   |
| 14  | g     | 838  | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 14  | n     | 830  | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | B     | 814 | CLA  | C3B-C4B-NB  | -2.80 | 108.03      | 110.53   |
| 14  | F     | 201 | CLA  | O2D-CGD-O1D | -2.80 | 118.41      | 123.85   |
| 14  | b     | 821 | CLA  | O2D-CGD-O1D | -2.80 | 118.41      | 123.85   |
| 17  | w     | 207 | BCR  | C8-C7-C6    | -2.80 | 119.53      | 127.00   |
| 17  | w     | 207 | BCR  | C23-C24-C25 | -2.79 | 119.53      | 127.00   |
| 17  | a     | 846 | BCR  | C33-C5-C6   | -2.79 | 121.44      | 124.48   |
| 17  | I     | 103 | BCR  | C16-C15-C14 | -2.79 | 117.80      | 123.52   |
| 14  | n     | 820 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 14  | A     | 831 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 17  | A     | 856 | BCR  | C16-C15-C14 | -2.79 | 117.81      | 123.52   |
| 14  | g     | 833 | CLA  | O2D-CGD-O1D | -2.79 | 118.41      | 123.85   |
| 17  | b     | 846 | BCR  | C33-C5-C4   | 2.79  | 119.55      | 113.60   |
| 14  | b     | 822 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 14  | B     | 810 | CLA  | O2D-CGD-O1D | -2.79 | 118.42      | 123.85   |
| 14  | a     | 833 | CLA  | O2D-CGD-O1D | -2.79 | 118.42      | 123.85   |
| 14  | a     | 833 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 14  | n     | 837 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 14  | G     | 853 | CLA  | O2D-CGD-O1D | -2.79 | 118.42      | 123.85   |
| 14  | b     | 835 | CLA  | O2D-CGD-O1D | -2.79 | 118.42      | 123.85   |
| 14  | G     | 834 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 14  | N     | 828 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 14  | g     | 822 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 17  | K     | 102 | BCR  | C23-C24-C25 | -2.79 | 119.55      | 127.00   |
| 14  | G     | 832 | CLA  | C1-C2-C3    | -2.79 | 121.63      | 126.20   |
| 14  | a     | 810 | CLA  | C3B-C4B-NB  | -2.79 | 108.04      | 110.53   |
| 17  | m     | 102 | BCR  | C20-C19-C18 | -2.79 | 118.73      | 126.36   |
| 14  | N     | 832 | CLA  | O2D-CGD-O1D | -2.78 | 118.43      | 123.85   |
| 14  | B     | 804 | CLA  | O2D-CGD-O1D | -2.78 | 118.43      | 123.85   |
| 14  | A     | 827 | CLA  | O2D-CGD-O1D | -2.78 | 118.43      | 123.85   |
| 14  | g     | 826 | CLA  | O2D-CGD-O1D | -2.78 | 118.44      | 123.85   |
| 14  | a     | 826 | CLA  | O2D-CGD-O1D | -2.78 | 118.44      | 123.85   |
| 17  | w     | 207 | BCR  | C28-C27-C26 | -2.78 | 109.10      | 114.06   |
| 14  | J     | 102 | CLA  | C3B-C4B-NB  | -2.78 | 108.05      | 110.53   |
| 19  | g     | 851 | CL0  | O2D-CGD-CBD | 2.78  | 114.00      | 110.95   |
| 14  | N     | 815 | CLA  | C1-C2-C3    | -2.78 | 121.64      | 126.20   |
| 17  | t     | 104 | BCR  | C16-C15-C14 | -2.78 | 117.84      | 123.52   |
| 14  | N     | 811 | CLA  | O2D-CGD-O1D | -2.78 | 118.44      | 123.85   |
| 17  | Y     | 101 | BCR  | C10-C11-C12 | -2.78 | 115.16      | 123.20   |
| 14  | G     | 807 | CLA  | C3B-C4B-NB  | -2.78 | 108.05      | 110.53   |
| 14  | G     | 815 | CLA  | C3B-C4B-NB  | -2.78 | 108.05      | 110.53   |
| 14  | n     | 805 | CLA  | C3B-C4B-NB  | -2.78 | 108.05      | 110.53   |
| 14  | B     | 823 | CLA  | O2D-CGD-O1D | -2.78 | 118.44      | 123.85   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | B     | 816  | CLA  | C3B-C4B-NB  | -2.77 | 108.05      | 110.53   |
| 19  | a     | 851  | CL0  | O2D-CGD-CBD | 2.77  | 114.00      | 110.95   |
| 20  | B     | 801  | SQD  | O48-C23-C24 | 2.77  | 120.29      | 111.83   |
| 17  | T     | 104  | BCR  | C16-C15-C14 | -2.77 | 117.85      | 123.52   |
| 14  | g     | 818  | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 14  | a     | 840  | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 14  | b     | 829  | CLA  | O2D-CGD-O1D | -2.77 | 118.45      | 123.85   |
| 14  | N     | 839  | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 14  | B     | 831  | CLA  | O2D-CGD-O1D | -2.77 | 118.46      | 123.85   |
| 14  | a     | 839  | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 14  | a     | 815  | CLA  | O2D-CGD-O1D | -2.77 | 118.46      | 123.85   |
| 20  | w     | 202  | SQD  | O48-C23-C24 | 2.77  | 120.28      | 111.83   |
| 17  | b     | 846  | BCR  | C38-C26-C25 | -2.77 | 121.46      | 124.48   |
| 17  | B     | 843  | BCR  | C7-C8-C9    | -2.77 | 122.14      | 126.23   |
| 14  | a     | 837  | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 14  | b     | 853  | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 14  | B     | 839  | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 14  | w     | 205  | CLA  | C3B-C4B-NB  | -2.77 | 108.06      | 110.53   |
| 14  | G     | 852  | CLA  | O2D-CGD-O1D | -2.77 | 118.47      | 123.85   |
| 14  | G     | 809  | CLA  | O2D-CGD-O1D | -2.76 | 118.47      | 123.85   |
| 17  | g     | 845  | BCR  | C24-C23-C22 | -2.76 | 122.14      | 126.23   |
| 17  | B     | 844  | BCR  | C30-C25-C26 | -2.76 | 118.86      | 122.64   |
| 14  | n     | 852  | CLA  | C3B-C4B-NB  | -2.76 | 108.06      | 110.53   |
| 17  | v     | 101  | BCR  | C2-C1-C6    | 2.76  | 114.45      | 110.44   |
| 14  | n     | 815  | CLA  | C3B-C4B-NB  | -2.76 | 108.06      | 110.53   |
| 17  | B     | 851  | BCR  | C16-C15-C14 | -2.76 | 117.87      | 123.52   |
| 17  | n     | 843  | BCR  | C24-C23-C22 | -2.76 | 122.15      | 126.23   |
| 14  | G     | 821  | CLA  | C3B-C4B-NB  | -2.76 | 108.06      | 110.53   |
| 14  | A     | 810  | CLA  | C3B-C4B-NB  | -2.76 | 108.06      | 110.53   |
| 17  | i     | 102  | BCR  | C12-C13-C14 | -2.76 | 114.67      | 119.01   |
| 14  | A     | 834  | CLA  | O2D-CGD-O1D | -2.76 | 118.47      | 123.85   |
| 14  | X     | 1701 | CLA  | C3B-C4B-NB  | -2.76 | 108.07      | 110.53   |
| 17  | A     | 847  | BCR  | C33-C5-C6   | -2.76 | 121.47      | 124.48   |
| 17  | a     | 846  | BCR  | C8-C7-C6    | -2.76 | 119.63      | 127.00   |
| 14  | B     | 831  | CLA  | C3B-C4B-NB  | -2.76 | 108.07      | 110.53   |
| 14  | N     | 808  | CLA  | C3B-C4B-NB  | -2.76 | 108.07      | 110.53   |
| 14  | w     | 203  | CLA  | C3B-C4B-NB  | -2.76 | 108.07      | 110.53   |
| 14  | B     | 805  | CLA  | C3B-C4B-NB  | -2.76 | 108.07      | 110.53   |
| 14  | N     | 821  | CLA  | O2D-CGD-O1D | -2.76 | 118.48      | 123.85   |
| 14  | a     | 829  | CLA  | O2D-CGD-O1D | -2.76 | 118.48      | 123.85   |
| 14  | S     | 201  | CLA  | O2D-CGD-O1D | -2.75 | 118.49      | 123.85   |
| 14  | a     | 818  | CLA  | C3B-C4B-NB  | -2.75 | 108.07      | 110.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 19  | G     | 851  | CL0  | O2D-CGD-O1D | -2.75 | 118.49      | 123.85   |
| 14  | A     | 803  | CLA  | C3B-C4B-NB  | -2.75 | 108.07      | 110.53   |
| 14  | N     | 810  | CLA  | C3B-C4B-NB  | -2.75 | 108.08      | 110.53   |
| 14  | g     | 837  | CLA  | C3B-C4B-NB  | -2.75 | 108.08      | 110.53   |
| 17  | I     | 101  | BCR  | C4-C5-C6    | -2.75 | 118.99      | 122.70   |
| 17  | b     | 848  | BCR  | C38-C26-C25 | -2.74 | 121.49      | 124.48   |
| 14  | B     | 827  | CLA  | C3B-C4B-NB  | -2.74 | 108.08      | 110.53   |
| 14  | b     | 837  | CLA  | O2D-CGD-O1D | -2.74 | 118.51      | 123.85   |
| 17  | A     | 848  | BCR  | C27-C26-C25 | -2.74 | 119.00      | 122.70   |
| 14  | s     | 201  | CLA  | O2D-CGD-O1D | -2.74 | 118.51      | 123.85   |
| 14  | B     | 840  | CLA  | O2D-CGD-O1D | -2.74 | 118.51      | 123.85   |
| 14  | G     | 832  | CLA  | O2D-CGD-O1D | -2.74 | 118.52      | 123.85   |
| 14  | N     | 804  | CLA  | C3B-C4B-NB  | -2.74 | 108.09      | 110.53   |
| 14  | f     | 202  | CLA  | C3B-C4B-NB  | -2.74 | 108.09      | 110.53   |
| 17  | G     | 848  | BCR  | C10-C11-C12 | -2.74 | 115.27      | 123.20   |
| 14  | n     | 850  | CLA  | C3B-C4B-NB  | -2.74 | 108.09      | 110.53   |
| 18  | A     | 850  | LHG  | O8-C23-C24  | 2.74  | 120.18      | 111.83   |
| 17  | w     | 207  | BCR  | C38-C26-C27 | 2.74  | 119.43      | 113.60   |
| 14  | n     | 804  | CLA  | O2D-CGD-O1D | -2.73 | 118.53      | 123.85   |
| 15  | N     | 843  | PQN  | C2M-C2-C3   | -2.73 | 119.95      | 124.45   |
| 15  | B     | 842  | PQN  | C14-C13-C15 | 2.73  | 119.97      | 115.23   |
| 14  | B     | 814  | CLA  | C1-C2-C3    | -2.73 | 121.72      | 126.20   |
| 14  | a     | 813  | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 14  | G     | 809  | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 14  | N     | 826  | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 14  | b     | 825  | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 17  | B     | 846  | BCR  | C27-C26-C25 | -2.73 | 119.02      | 122.70   |
| 14  | N     | 825  | CLA  | C3B-C4B-NB  | -2.73 | 108.09      | 110.53   |
| 17  | A     | 846  | BCR  | C28-C27-C26 | -2.73 | 109.19      | 114.06   |
| 17  | g     | 844  | BCR  | C23-C24-C25 | -2.73 | 119.71      | 127.00   |
| 17  | a     | 848  | BCR  | C8-C9-C10   | 2.73  | 123.30      | 119.01   |
| 14  | a     | 814  | CLA  | C3B-C4B-NB  | -2.73 | 108.10      | 110.53   |
| 14  | W     | 202  | CLA  | CHB-C4A-NA  | 2.73  | 128.33      | 124.40   |
| 17  | j     | 104  | BCR  | C8-C7-C6    | -2.73 | 119.72      | 127.00   |
| 17  | b     | 844  | BCR  | C38-C26-C27 | 2.72  | 119.40      | 113.60   |
| 17  | s     | 203  | BCR  | C28-C27-C26 | -2.72 | 109.20      | 114.06   |
| 20  | h     | 1702 | SQD  | O48-C23-C24 | 2.72  | 120.14      | 111.83   |
| 17  | N     | 847  | BCR  | C33-C5-C4   | 2.72  | 119.40      | 113.60   |
| 17  | b     | 852  | BCR  | C28-C27-C26 | -2.72 | 109.20      | 114.06   |
| 17  | f     | 203  | BCR  | C3-C4-C5    | -2.72 | 109.20      | 114.06   |
| 14  | N     | 817  | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 14  | N     | 823  | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | A     | 802  | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 14  | G     | 814  | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 17  | N     | 852  | BCR  | C15-C16-C17 | -2.72 | 117.95      | 123.52   |
| 14  | G     | 810  | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 14  | G     | 830  | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 17  | j     | 104  | BCR  | C7-C8-C9    | -2.72 | 122.21      | 126.23   |
| 14  | g     | 838  | CLA  | O2D-CGD-O1D | -2.72 | 118.56      | 123.85   |
| 14  | N     | 813  | CLA  | C3B-C4B-NB  | -2.72 | 108.10      | 110.53   |
| 20  | H     | 1702 | SQD  | O48-C23-C24 | 2.71  | 120.11      | 111.83   |
| 17  | b     | 846  | BCR  | C21-C20-C19 | -2.71 | 115.33      | 123.20   |
| 14  | a     | 812  | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 17  | B     | 847  | BCR  | C15-C16-C17 | -2.71 | 117.97      | 123.52   |
| 17  | s     | 203  | BCR  | C3-C4-C5    | -2.71 | 109.22      | 114.06   |
| 14  | a     | 802  | CLA  | CHB-C4A-NA  | 2.71  | 128.31      | 124.40   |
| 14  | N     | 806  | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 14  | B     | 823  | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 14  | B     | 834  | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 14  | t     | 101  | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 14  | B     | 804  | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 17  | B     | 846  | BCR  | C33-C5-C4   | 2.71  | 119.38      | 113.60   |
| 14  | N     | 827  | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 14  | g     | 821  | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 14  | a     | 808  | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 14  | b     | 827  | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 18  | A     | 851  | LHG  | O8-C23-C24  | 2.71  | 120.10      | 111.83   |
| 17  | I     | 103  | BCR  | C24-C23-C22 | -2.71 | 122.23      | 126.23   |
| 18  | G     | 849  | LHG  | O8-C23-C24  | 2.71  | 120.09      | 111.83   |
| 14  | a     | 823  | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 19  | a     | 851  | CL0  | O2A-CGA-O1A | -2.71 | 116.85      | 123.63   |
| 18  | S     | 202  | LHG  | O8-C23-C24  | 2.71  | 120.09      | 111.83   |
| 17  | a     | 848  | BCR  | C10-C11-C12 | -2.71 | 115.35      | 123.20   |
| 14  | g     | 814  | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 14  | b     | 834  | CLA  | C3B-C4B-NB  | -2.71 | 108.11      | 110.53   |
| 14  | a     | 807  | CLA  | O2D-CGD-O1D | -2.71 | 118.58      | 123.85   |
| 17  | N     | 849  | BCR  | C3-C4-C5    | -2.71 | 109.23      | 114.06   |
| 17  | g     | 848  | BCR  | C8-C9-C10   | 2.71  | 123.27      | 119.01   |
| 14  | n     | 814  | CLA  | C1-C2-C3    | -2.70 | 122.39      | 126.76   |
| 14  | N     | 831  | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 14  | g     | 808  | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 17  | G     | 845  | BCR  | C28-C27-C26 | -2.70 | 109.24      | 114.06   |
| 17  | a     | 843  | BCR  | C3-C4-C5    | -2.70 | 109.24      | 114.06   |
| 14  | b     | 805  | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | a     | 845 | BCR  | C23-C24-C25 | -2.70 | 119.79      | 127.00   |
| 14  | a     | 830 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 14  | A     | 826 | CLA  | CHB-C4A-NA  | 2.70  | 128.30      | 124.40   |
| 14  | A     | 831 | CLA  | CMB-C2B-C1B | -2.70 | 121.31      | 125.42   |
| 17  | G     | 846 | BCR  | C4-C5-C6    | -2.70 | 119.06      | 122.70   |
| 17  | G     | 846 | BCR  | C33-C5-C4   | 2.70  | 119.35      | 113.60   |
| 14  | B     | 826 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 18  | v     | 102 | LHG  | O8-C23-C24  | 2.70  | 120.05      | 111.83   |
| 14  | N     | 809 | CLA  | C1-C2-C3    | -2.70 | 121.78      | 126.20   |
| 14  | b     | 816 | CLA  | C3B-C4B-NB  | -2.70 | 108.12      | 110.53   |
| 14  | g     | 831 | CLA  | C1-C2-C3    | -2.69 | 121.78      | 126.20   |
| 17  | G     | 848 | BCR  | C33-C5-C4   | 2.69  | 119.34      | 113.60   |
| 14  | G     | 823 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 14  | g     | 806 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 17  | b     | 847 | BCR  | C15-C16-C17 | -2.69 | 118.01      | 123.52   |
| 14  | S     | 203 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 14  | n     | 826 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 14  | G     | 804 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 14  | g     | 830 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 14  | G     | 824 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 14  | N     | 804 | CLA  | O2D-CGD-CBD | 2.69  | 115.93      | 111.23   |
| 14  | G     | 831 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 14  | A     | 809 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 14  | a     | 820 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 17  | g     | 845 | BCR  | C28-C27-C26 | -2.69 | 109.27      | 114.06   |
| 14  | g     | 812 | CLA  | C3B-C4B-NB  | -2.69 | 108.13      | 110.53   |
| 17  | W     | 205 | BCR  | C24-C23-C22 | -2.68 | 122.27      | 126.23   |
| 17  | B     | 844 | BCR  | C38-C26-C25 | -2.68 | 121.56      | 124.48   |
| 17  | a     | 846 | BCR  | C20-C21-C22 | -2.68 | 123.52      | 127.28   |
| 14  | g     | 818 | CLA  | CHB-C4A-NA  | 2.68  | 128.27      | 124.40   |
| 15  | N     | 843 | PQN  | C11-C3-C2   | -2.68 | 120.30      | 124.89   |
| 15  | g     | 841 | PQN  | C11-C3-C2   | -2.68 | 120.30      | 124.89   |
| 17  | B     | 846 | BCR  | C38-C26-C27 | 2.68  | 119.31      | 113.60   |
| 20  | l     | 201 | SQD  | O48-C23-C24 | 2.68  | 120.00      | 111.83   |
| 20  | b     | 801 | SQD  | O7-S-C6     | 2.68  | 110.75      | 106.76   |
| 14  | g     | 827 | CLA  | C3B-C4B-NB  | -2.68 | 108.14      | 110.53   |
| 14  | A     | 825 | CLA  | C3B-C4B-NB  | -2.67 | 108.14      | 110.53   |
| 14  | a     | 804 | CLA  | C3B-C4B-NB  | -2.67 | 108.14      | 110.53   |
| 17  | B     | 851 | BCR  | C3-C4-C5    | -2.67 | 109.29      | 114.06   |
| 14  | n     | 833 | CLA  | C3B-C4B-NB  | -2.67 | 108.15      | 110.53   |
| 14  | b     | 810 | CLA  | C3B-C4B-NB  | -2.67 | 108.15      | 110.53   |
| 14  | j     | 102 | CLA  | C3B-C4B-NB  | -2.67 | 108.15      | 110.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | B     | 852  | BCR  | C33-C5-C6   | -2.67 | 121.57      | 124.48   |
| 14  | b     | 807  | CLA  | C3B-C4B-NB  | -2.67 | 108.15      | 110.53   |
| 17  | v     | 101  | BCR  | C16-C15-C14 | -2.67 | 118.06      | 123.52   |
| 17  | A     | 847  | BCR  | C38-C26-C27 | 2.67  | 119.28      | 113.60   |
| 17  | G     | 848  | BCR  | C20-C19-C18 | -2.67 | 119.05      | 126.36   |
| 17  | G     | 845  | BCR  | C23-C24-C25 | -2.67 | 119.88      | 127.00   |
| 14  | B     | 822  | CLA  | C3B-C4B-NB  | -2.66 | 108.15      | 110.53   |
| 17  | B     | 843  | BCR  | C2-C1-C6    | 2.66  | 114.31      | 110.44   |
| 15  | g     | 841  | PQN  | C2M-C2-C3   | -2.66 | 120.07      | 124.45   |
| 14  | A     | 814  | CLA  | C3B-C4B-NB  | -2.66 | 108.15      | 110.53   |
| 14  | b     | 814  | CLA  | C3B-C4B-NB  | -2.66 | 108.15      | 110.53   |
| 17  | B     | 848  | BCR  | C10-C11-C12 | -2.66 | 115.48      | 123.20   |
| 17  | B     | 844  | BCR  | C38-C26-C27 | 2.66  | 119.27      | 113.60   |
| 18  | m     | 101  | LHG  | O8-C23-C24  | 2.66  | 119.95      | 111.83   |
| 14  | g     | 824  | CLA  | C3B-C4B-NB  | -2.66 | 108.15      | 110.53   |
| 14  | B     | 809  | CLA  | C3B-C4B-NB  | -2.66 | 108.15      | 110.53   |
| 17  | a     | 843  | BCR  | C29-C30-C25 | 2.66  | 114.31      | 110.44   |
| 14  | A     | 819  | CLA  | CHB-C4A-NA  | 2.66  | 128.24      | 124.40   |
| 17  | n     | 847  | BCR  | C11-C10-C9  | -2.66 | 123.55      | 127.28   |
| 17  | W     | 206  | BCR  | C33-C5-C4   | 2.66  | 119.26      | 113.60   |
| 14  | u     | 102  | CLA  | C3B-C4B-NB  | -2.66 | 108.16      | 110.53   |
| 14  | N     | 803  | CLA  | O2D-CGD-O1D | -2.66 | 118.68      | 123.85   |
| 14  | A     | 818  | CLA  | C3B-C4B-NB  | -2.65 | 108.16      | 110.53   |
| 14  | b     | 817  | CLA  | C3B-C4B-NB  | -2.65 | 108.16      | 110.53   |
| 14  | B     | 830  | CLA  | C3B-C4B-NB  | -2.65 | 108.16      | 110.53   |
| 18  | a     | 850  | LHG  | O8-C23-C24  | 2.65  | 119.92      | 111.83   |
| 17  | n     | 847  | BCR  | C16-C15-C14 | -2.65 | 118.09      | 123.52   |
| 17  | w     | 201  | BCR  | C28-C27-C26 | -2.65 | 109.33      | 114.06   |
| 14  | g     | 836  | CLA  | C3B-C4B-NB  | -2.65 | 108.16      | 110.53   |
| 14  | b     | 826  | CLA  | C3B-C4B-NB  | -2.65 | 108.16      | 110.53   |
| 17  | g     | 848  | BCR  | C20-C19-C18 | -2.65 | 119.10      | 126.36   |
| 14  | b     | 834  | CLA  | CHB-C4A-NA  | 2.65  | 128.22      | 124.40   |
| 17  | G     | 846  | BCR  | C33-C5-C6   | -2.65 | 121.59      | 124.48   |
| 14  | A     | 826  | CLA  | C1-C2-C3    | -2.65 | 121.86      | 126.20   |
| 14  | A     | 823  | CLA  | C3B-C4B-NB  | -2.65 | 108.17      | 110.53   |
| 17  | b     | 848  | BCR  | C3-C4-C5    | -2.65 | 109.34      | 114.06   |
| 14  | n     | 824  | CLA  | C3B-C4B-NB  | -2.65 | 108.17      | 110.53   |
| 20  | x     | 1702 | SQD  | O48-C23-C24 | 2.65  | 119.90      | 111.83   |
| 15  | g     | 841  | PQN  | C11-C12-C13 | -2.65 | 122.27      | 126.83   |
| 14  | A     | 805  | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 14  | B     | 824  | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 17  | n     | 842  | BCR  | C30-C25-C26 | -2.64 | 119.03      | 122.64   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | i     | 102  | BCR  | C35-C13-C12 | 2.64  | 122.12      | 118.09   |
| 17  | a     | 843  | BCR  | C11-C12-C13 | -2.64 | 119.12      | 126.36   |
| 14  | n     | 822  | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 14  | l     | 202  | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 20  | n     | 801  | SQD  | O48-C23-C24 | 2.64  | 119.88      | 111.83   |
| 17  | B     | 845  | BCR  | C28-C27-C26 | -2.64 | 109.35      | 114.06   |
| 14  | G     | 813  | CLA  | C3B-C4B-NB  | -2.64 | 108.17      | 110.53   |
| 15  | N     | 843  | PQN  | C14-C13-C15 | 2.64  | 119.81      | 115.23   |
| 14  | a     | 815  | CLA  | CHB-C4A-NA  | 2.64  | 128.21      | 124.40   |
| 17  | b     | 843  | BCR  | C38-C26-C25 | -2.64 | 121.61      | 124.48   |
| 17  | B     | 844  | BCR  | C15-C14-C13 | -2.64 | 123.58      | 127.28   |
| 14  | g     | 852  | CLA  | CMB-C2B-C1B | -2.64 | 121.40      | 125.42   |
| 17  | L     | 1504 | BCR  | C33-C5-C4   | 2.64  | 119.22      | 113.60   |
| 18  | g     | 849  | LHG  | O8-C23-C24  | 2.64  | 119.87      | 111.83   |
| 14  | n     | 818  | CLA  | C3B-C4B-NB  | -2.63 | 108.18      | 110.53   |
| 17  | B     | 846  | BCR  | C30-C25-C26 | -2.63 | 119.04      | 122.64   |
| 17  | A     | 847  | BCR  | C28-C27-C26 | -2.63 | 109.36      | 114.06   |
| 19  | A     | 852  | CL0  | C1B-CHB-C4A | 2.63  | 123.02      | 121.32   |
| 14  | g     | 811  | CLA  | O2D-CGD-O1D | -2.63 | 118.73      | 123.85   |
| 14  | W     | 203  | CLA  | CHB-C4A-NA  | 2.63  | 128.20      | 124.40   |
| 14  | g     | 819  | CLA  | CHB-C4A-NA  | 2.63  | 128.20      | 124.40   |
| 18  | G     | 850  | LHG  | O8-C23-C24  | 2.63  | 119.85      | 111.83   |
| 14  | n     | 807  | CLA  | C1-C2-C3    | -2.63 | 121.89      | 126.20   |
| 14  | N     | 824  | CLA  | C3B-C4B-NB  | -2.63 | 108.18      | 110.53   |
| 14  | g     | 820  | CLA  | C3B-C4B-NB  | -2.63 | 108.18      | 110.53   |
| 17  | A     | 844  | BCR  | C16-C15-C14 | -2.63 | 118.14      | 123.52   |
| 14  | N     | 833  | CLA  | C3B-C4B-NB  | -2.63 | 108.19      | 110.53   |
| 17  | a     | 848  | BCR  | C34-C9-C10  | -2.62 | 118.56      | 122.82   |
| 17  | B     | 846  | BCR  | C20-C19-C18 | -2.62 | 119.17      | 126.36   |
| 15  | A     | 842  | PQN  | C14-C13-C15 | 2.62  | 119.78      | 115.23   |
| 14  | n     | 808  | CLA  | O2A-CGA-O1A | -2.62 | 117.06      | 123.63   |
| 17  | g     | 847  | BCR  | C38-C26-C25 | -2.62 | 121.62      | 124.48   |
| 15  | a     | 841  | PQN  | C2M-C2-C3   | -2.62 | 120.14      | 124.45   |
| 17  | A     | 848  | BCR  | C30-C25-C26 | -2.62 | 119.05      | 122.64   |
| 17  | B     | 844  | BCR  | C27-C26-C25 | -2.62 | 119.16      | 122.70   |
| 17  | g     | 848  | BCR  | C34-C9-C10  | -2.62 | 118.57      | 122.82   |
| 14  | B     | 812  | CLA  | O2D-CGD-CBD | 2.62  | 115.81      | 111.23   |
| 19  | A     | 852  | CL0  | C4D-CHA-CBD | -2.62 | 106.33      | 108.97   |
| 17  | g     | 847  | BCR  | C27-C26-C25 | -2.62 | 119.17      | 122.70   |
| 17  | n     | 844  | BCR  | C28-C27-C26 | -2.62 | 109.39      | 114.06   |
| 14  | A     | 807  | CLA  | CHB-C4A-NA  | 2.62  | 128.18      | 124.40   |
| 14  | A     | 838  | CLA  | C3B-C4B-NB  | -2.62 | 108.19      | 110.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | A     | 856  | BCR  | C7-C8-C9    | -2.62 | 122.36      | 126.23   |
| 17  | i     | 101  | BCR  | C28-C27-C26 | -2.62 | 109.39      | 114.06   |
| 15  | n     | 841  | PQN  | C2M-C2-C3   | -2.62 | 120.15      | 124.45   |
| 17  | n     | 847  | BCR  | C10-C11-C12 | -2.62 | 115.62      | 123.20   |
| 17  | M     | 101  | BCR  | C3-C4-C5    | -2.61 | 109.39      | 114.06   |
| 14  | N     | 834  | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 14  | b     | 804  | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 17  | a     | 845  | BCR  | C2-C1-C6    | 2.61  | 114.24      | 110.44   |
| 14  | H     | 1701 | CLA  | CHB-C4A-NA  | 2.61  | 128.17      | 124.40   |
| 14  | n     | 838  | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 17  | g     | 847  | BCR  | C38-C26-C27 | 2.61  | 119.17      | 113.60   |
| 15  | n     | 841  | PQN  | C11-C3-C2   | -2.61 | 120.41      | 124.89   |
| 17  | n     | 851  | BCR  | C28-C27-C26 | -2.61 | 109.40      | 114.06   |
| 14  | A     | 819  | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 14  | b     | 813  | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 14  | J     | 102  | CLA  | CAA-C2A-C3A | -2.61 | 110.25      | 116.23   |
| 14  | x     | 1701 | CLA  | CHB-C4A-NA  | 2.61  | 128.17      | 124.40   |
| 17  | G     | 846  | BCR  | C24-C23-C22 | -2.61 | 122.38      | 126.23   |
| 17  | N     | 852  | BCR  | C7-C8-C9    | -2.61 | 122.38      | 126.23   |
| 14  | a     | 832  | CLA  | C3B-C4B-NB  | -2.61 | 108.20      | 110.53   |
| 20  | b     | 801  | SQD  | O48-C23-C24 | 2.61  | 119.79      | 111.83   |
| 14  | N     | 831  | CLA  | CHB-C4A-NA  | 2.61  | 128.16      | 124.40   |
| 17  | N     | 848  | BCR  | C11-C12-C13 | -2.61 | 119.22      | 126.36   |
| 14  | n     | 828  | CLA  | C3B-C4B-NB  | -2.60 | 108.20      | 110.53   |
| 17  | W     | 201  | BCR  | C38-C26-C27 | 2.60  | 119.15      | 113.60   |
| 17  | B     | 846  | BCR  | C38-C26-C25 | -2.60 | 121.64      | 124.48   |
| 17  | a     | 847  | BCR  | C38-C26-C27 | 2.60  | 119.14      | 113.60   |
| 17  | a     | 848  | BCR  | C16-C15-C14 | -2.60 | 118.19      | 123.52   |
| 17  | t     | 104  | BCR  | C28-C27-C26 | -2.60 | 109.42      | 114.06   |
| 14  | g     | 854  | CLA  | C3B-C4B-NB  | -2.60 | 108.21      | 110.53   |
| 17  | G     | 847  | BCR  | C38-C26-C27 | 2.60  | 119.14      | 113.60   |
| 14  | n     | 832  | CLA  | C1-C2-C3    | -2.60 | 121.94      | 126.20   |
| 17  | A     | 848  | BCR  | C38-C26-C27 | 2.60  | 119.14      | 113.60   |
| 17  | B     | 843  | BCR  | C28-C27-C26 | -2.60 | 109.42      | 114.06   |
| 14  | b     | 829  | CLA  | C3B-C4B-NB  | -2.60 | 108.21      | 110.53   |
| 17  | j     | 104  | BCR  | C28-C27-C26 | -2.60 | 109.42      | 114.06   |
| 17  | Y     | 101  | BCR  | C16-C15-C14 | -2.60 | 118.21      | 123.52   |
| 17  | i     | 102  | BCR  | C36-C18-C19 | 2.60  | 122.05      | 118.09   |
| 17  | K     | 102  | BCR  | C38-C26-C27 | 2.60  | 119.13      | 113.60   |
| 14  | g     | 831  | CLA  | C3B-C4B-NB  | -2.60 | 108.21      | 110.53   |
| 14  | A     | 855  | CLA  | O2D-CGD-O1D | -2.59 | 118.80      | 123.85   |
| 17  | n     | 846  | BCR  | C23-C24-C25 | -2.59 | 120.07      | 127.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | y     | 101  | BCR  | C38-C26-C27 | 2.59  | 119.13      | 113.60   |
| 17  | v     | 101  | BCR  | C20-C19-C18 | -2.59 | 119.25      | 126.36   |
| 14  | N     | 839  | CLA  | C1-C2-C3    | -2.59 | 121.95      | 126.20   |
| 17  | n     | 847  | BCR  | C8-C7-C6    | -2.59 | 120.07      | 127.00   |
| 17  | B     | 848  | BCR  | C8-C7-C6    | -2.59 | 120.07      | 127.00   |
| 17  | B     | 847  | BCR  | C11-C12-C13 | -2.59 | 119.25      | 126.36   |
| 17  | B     | 846  | BCR  | C8-C7-C6    | -2.59 | 120.08      | 127.00   |
| 14  | n     | 804  | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 14  | n     | 809  | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 14  | b     | 831  | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 14  | N     | 835  | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 14  | n     | 803  | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 14  | n     | 806  | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 14  | g     | 827  | CLA  | C1-C2-C3    | -2.59 | 121.96      | 126.20   |
| 18  | a     | 849  | LHG  | O8-C23-C24  | 2.59  | 119.72      | 111.83   |
| 14  | G     | 825  | CLA  | C3B-C4B-NB  | -2.59 | 108.22      | 110.53   |
| 14  | B     | 809  | CLA  | CHB-C4A-NA  | 2.58  | 128.13      | 124.40   |
| 14  | a     | 806  | CLA  | CHB-C4A-NA  | 2.58  | 128.13      | 124.40   |
| 14  | B     | 834  | CLA  | CHB-C4A-NA  | 2.58  | 128.13      | 124.40   |
| 14  | B     | 815  | CLA  | CHB-C4A-NA  | 2.58  | 128.13      | 124.40   |
| 17  | i     | 101  | BCR  | C38-C26-C25 | -2.58 | 121.67      | 124.48   |
| 14  | a     | 801  | CLA  | C3B-C4B-NB  | -2.58 | 108.23      | 110.53   |
| 17  | W     | 201  | BCR  | C37-C22-C21 | -2.58 | 118.64      | 122.82   |
| 14  | n     | 829  | CLA  | CHB-C4A-NA  | 2.58  | 128.12      | 124.40   |
| 18  | X     | 1702 | LHG  | O8-C23-C24  | 2.58  | 119.69      | 111.83   |
| 14  | b     | 835  | CLA  | CMB-C2B-C1B | -2.58 | 121.50      | 125.42   |
| 14  | A     | 840  | CLA  | C3B-C4B-NB  | -2.58 | 108.23      | 110.53   |
| 14  | a     | 807  | CLA  | C3B-C4B-NB  | -2.58 | 108.23      | 110.53   |
| 17  | i     | 102  | BCR  | C28-C27-C26 | -2.57 | 109.46      | 114.06   |
| 17  | w     | 206  | BCR  | C40-C30-C25 | -2.57 | 106.21      | 110.24   |
| 14  | G     | 808  | CLA  | C3B-C4B-NB  | -2.57 | 108.23      | 110.53   |
| 15  | a     | 841  | PQN  | C11-C3-C2   | -2.57 | 120.48      | 124.89   |
| 14  | B     | 812  | CLA  | C3B-C4B-NB  | -2.57 | 108.23      | 110.53   |
| 17  | s     | 203  | BCR  | C23-C24-C25 | -2.57 | 120.13      | 127.00   |
| 14  | G     | 838  | CLA  | C3B-C4B-NB  | -2.57 | 108.23      | 110.53   |
| 17  | B     | 848  | BCR  | C38-C26-C25 | -2.57 | 121.68      | 124.48   |
| 14  | b     | 803  | CLA  | C3B-C4B-NB  | -2.57 | 108.24      | 110.53   |
| 14  | B     | 817  | CLA  | CHB-C4A-NA  | 2.57  | 128.11      | 124.40   |
| 14  | G     | 819  | CLA  | CHB-C4A-NA  | 2.57  | 128.11      | 124.40   |
| 14  | N     | 818  | CLA  | C3B-C4B-NB  | -2.57 | 108.24      | 110.53   |
| 14  | n     | 807  | CLA  | C3B-C4B-NB  | -2.57 | 108.24      | 110.53   |
| 14  | a     | 826  | CLA  | C1-C2-C3    | -2.57 | 121.99      | 126.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | g     | 852  | CLA  | O2D-CGD-O1D | -2.56 | 118.86      | 123.85   |
| 17  | B     | 851  | BCR  | C20-C19-C18 | -2.56 | 119.33      | 126.36   |
| 14  | A     | 832  | CLA  | C3B-C4B-NB  | -2.56 | 108.24      | 110.53   |
| 14  | b     | 830  | CLA  | C1-C2-C3    | -2.56 | 122.00      | 126.20   |
| 14  | g     | 840  | CLA  | C1-C2-C3    | -2.56 | 122.62      | 126.76   |
| 14  | L     | 1501 | CLA  | C3B-C4B-NB  | -2.56 | 108.24      | 110.53   |
| 14  | b     | 802  | CLA  | C3B-C4B-NB  | -2.56 | 108.24      | 110.53   |
| 14  | X     | 1701 | CLA  | CHB-C4A-NA  | 2.56  | 128.10      | 124.40   |
| 17  | G     | 846  | BCR  | C23-C24-C25 | -2.56 | 120.16      | 127.00   |
| 14  | h     | 1701 | CLA  | CHB-C4A-NA  | 2.56  | 128.09      | 124.40   |
| 14  | B     | 830  | CLA  | CHB-C4A-NA  | 2.56  | 128.09      | 124.40   |
| 17  | a     | 843  | BCR  | C33-C5-C4   | 2.56  | 119.05      | 113.60   |
| 14  | A     | 821  | CLA  | C3B-C4B-NB  | -2.56 | 108.25      | 110.53   |
| 17  | W     | 201  | BCR  | C34-C9-C8   | 2.56  | 121.99      | 118.09   |
| 14  | B     | 807  | CLA  | C3B-C4B-NB  | -2.56 | 108.25      | 110.53   |
| 17  | b     | 844  | BCR  | C38-C26-C25 | -2.56 | 121.69      | 124.48   |
| 14  | B     | 805  | CLA  | CHB-C4A-NA  | 2.56  | 128.09      | 124.40   |
| 17  | a     | 846  | BCR  | C33-C5-C4   | 2.56  | 119.04      | 113.60   |
| 17  | b     | 844  | BCR  | C24-C23-C22 | -2.55 | 122.46      | 126.23   |
| 14  | A     | 828  | CLA  | C1-C2-C3    | -2.55 | 122.01      | 126.20   |
| 14  | a     | 819  | CLA  | CHB-C4A-NA  | 2.55  | 128.09      | 124.40   |
| 14  | b     | 808  | CLA  | C3B-C4B-NB  | -2.55 | 108.25      | 110.53   |
| 17  | k     | 102  | BCR  | C8-C7-C6    | -2.55 | 120.18      | 127.00   |
| 17  | N     | 849  | BCR  | C15-C16-C17 | -2.55 | 118.30      | 123.52   |
| 17  | b     | 843  | BCR  | C28-C27-C26 | -2.55 | 109.50      | 114.06   |
| 14  | B     | 810  | CLA  | C3B-C4B-NB  | -2.55 | 108.25      | 110.53   |
| 17  | v     | 101  | BCR  | C10-C11-C12 | -2.55 | 115.81      | 123.20   |
| 14  | B     | 816  | CLA  | CHB-C4A-NA  | 2.55  | 128.08      | 124.40   |
| 14  | b     | 815  | CLA  | CHB-C4A-NA  | 2.55  | 128.08      | 124.40   |
| 14  | N     | 827  | CLA  | O2D-CGD-CBD | 2.55  | 115.69      | 111.23   |
| 15  | G     | 841  | PQN  | C14-C13-C15 | 2.55  | 119.65      | 115.23   |
| 14  | N     | 851  | CLA  | C1-C2-C3    | -2.55 | 122.02      | 126.20   |
| 17  | W     | 205  | BCR  | C20-C21-C22 | -2.55 | 123.71      | 127.28   |
| 17  | S     | 204  | BCR  | C15-C16-C17 | -2.55 | 118.31      | 123.52   |
| 14  | N     | 840  | CLA  | C3B-C4B-NB  | -2.55 | 108.26      | 110.53   |
| 14  | g     | 823  | CLA  | C3B-C4B-NB  | -2.55 | 108.26      | 110.53   |
| 17  | g     | 848  | BCR  | C10-C11-C12 | -2.54 | 115.83      | 123.20   |
| 17  | I     | 101  | BCR  | C28-C27-C26 | -2.54 | 109.52      | 114.06   |
| 17  | B     | 845  | BCR  | C33-C5-C4   | 2.54  | 119.01      | 113.60   |
| 14  | g     | 801  | CLA  | CHB-C4A-NA  | 2.54  | 128.07      | 124.40   |
| 14  | a     | 811  | CLA  | CHB-C4A-NA  | 2.54  | 128.07      | 124.40   |
| 14  | B     | 828  | CLA  | C3B-C4B-NB  | -2.54 | 108.26      | 110.53   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | N     | 819 | CLA  | CHB-C4A-NA  | 2.54  | 128.07      | 124.40   |
| 14  | N     | 829 | CLA  | C1-C2-C3    | -2.54 | 122.03      | 126.20   |
| 17  | y     | 101 | BCR  | C20-C19-C18 | -2.54 | 119.40      | 126.36   |
| 14  | w     | 204 | CLA  | CHB-C4A-NA  | 2.54  | 128.06      | 124.40   |
| 19  | A     | 852 | CL0  | C3D-C4D-CHA | 2.54  | 112.40      | 108.54   |
| 17  | w     | 207 | BCR  | C2-C1-C6    | 2.54  | 114.13      | 110.44   |
| 15  | A     | 842 | PQN  | C11-C3-C2   | -2.54 | 120.54      | 124.89   |
| 14  | n     | 803 | CLA  | C1-C2-C3    | -2.54 | 122.04      | 126.20   |
| 14  | A     | 818 | CLA  | C1-C2-C3    | -2.54 | 122.04      | 126.20   |
| 14  | n     | 814 | CLA  | CHB-C4A-NA  | 2.53  | 128.06      | 124.40   |
| 14  | A     | 816 | CLA  | CHB-C4A-NA  | 2.53  | 128.06      | 124.40   |
| 17  | b     | 847 | BCR  | C11-C12-C13 | -2.53 | 119.41      | 126.36   |
| 17  | S     | 204 | BCR  | C11-C12-C13 | -2.53 | 119.41      | 126.36   |
| 17  | g     | 845 | BCR  | C38-C26-C27 | 2.53  | 119.00      | 113.60   |
| 17  | A     | 846 | BCR  | C15-C16-C17 | -2.53 | 118.33      | 123.52   |
| 17  | n     | 851 | BCR  | C33-C5-C6   | -2.53 | 121.72      | 124.48   |
| 14  | N     | 810 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 14  | a     | 807 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 14  | N     | 820 | CLA  | C3B-C4B-NB  | -2.53 | 108.27      | 110.53   |
| 14  | b     | 806 | CLA  | C3B-C4B-NB  | -2.53 | 108.27      | 110.53   |
| 14  | a     | 830 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 14  | b     | 813 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 17  | F     | 203 | BCR  | C3-C4-C5    | -2.53 | 109.54      | 114.06   |
| 15  | B     | 842 | PQN  | C11-C3-C2   | -2.53 | 120.55      | 124.89   |
| 14  | t     | 101 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 14  | B     | 807 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 17  | g     | 843 | BCR  | C3-C4-C5    | -2.53 | 109.55      | 114.06   |
| 14  | g     | 806 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 14  | A     | 857 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 14  | b     | 825 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 17  | A     | 856 | BCR  | C38-C26-C27 | 2.53  | 118.99      | 113.60   |
| 18  | g     | 850 | LHG  | O8-C23-C24  | 2.53  | 119.54      | 111.83   |
| 17  | b     | 850 | BCR  | C33-C5-C6   | -2.53 | 121.73      | 124.48   |
| 14  | G     | 831 | CLA  | CMB-C2B-C1B | -2.53 | 121.57      | 125.42   |
| 17  | N     | 848 | BCR  | C23-C24-C25 | -2.53 | 120.25      | 127.00   |
| 14  | N     | 816 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 14  | B     | 838 | CLA  | CHB-C4A-NA  | 2.53  | 128.05      | 124.40   |
| 14  | A     | 803 | CLA  | CHB-C4A-NA  | 2.53  | 128.04      | 124.40   |
| 14  | a     | 852 | CLA  | O2D-CGD-O1D | -2.53 | 118.93      | 123.85   |
| 14  | b     | 815 | CLA  | C1-C2-C3    | -2.53 | 122.68      | 126.76   |
| 14  | G     | 812 | CLA  | CHB-C4A-NA  | 2.53  | 128.04      | 124.40   |
| 14  | N     | 828 | CLA  | CHB-C4A-NA  | 2.53  | 128.04      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | A     | 814 | CLA  | CHB-C4A-NA  | 2.53  | 128.04      | 124.40   |
| 14  | g     | 817 | CLA  | C1-C2-C3    | -2.52 | 122.06      | 126.20   |
| 14  | G     | 853 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 17  | n     | 846 | BCR  | C11-C12-C13 | -2.52 | 119.44      | 126.36   |
| 17  | U     | 103 | BCR  | C8-C7-C6    | -2.52 | 120.26      | 127.00   |
| 14  | b     | 832 | CLA  | C3B-C4B-NB  | -2.52 | 108.28      | 110.53   |
| 14  | A     | 854 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 14  | n     | 834 | CLA  | C3B-C4B-NB  | -2.52 | 108.28      | 110.53   |
| 17  | Y     | 101 | BCR  | C20-C19-C18 | -2.52 | 119.45      | 126.36   |
| 19  | a     | 851 | CL0  | C1B-CHB-C4A | 2.52  | 122.94      | 121.32   |
| 14  | g     | 802 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 14  | n     | 816 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 17  | N     | 847 | BCR  | C38-C26-C25 | -2.52 | 121.73      | 124.48   |
| 14  | G     | 817 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 14  | A     | 804 | CLA  | CHB-C4A-NA  | 2.52  | 128.04      | 124.40   |
| 14  | a     | 827 | CLA  | C3B-C4B-NB  | -2.52 | 108.28      | 110.53   |
| 14  | b     | 809 | CLA  | O2A-CGA-O1A | -2.52 | 117.33      | 123.63   |
| 14  | g     | 801 | CLA  | C3B-C4B-NB  | -2.52 | 108.28      | 110.53   |
| 17  | W     | 205 | BCR  | C23-C24-C25 | -2.52 | 120.27      | 127.00   |
| 17  | I     | 103 | BCR  | C3-C4-C5    | -2.52 | 109.57      | 114.06   |
| 19  | A     | 852 | CL0  | C1C-CHC-C4B | 2.52  | 125.08      | 116.07   |
| 15  | B     | 842 | PQN  | C2M-C2-C3   | -2.52 | 120.31      | 124.45   |
| 17  | a     | 845 | BCR  | C28-C27-C26 | -2.52 | 109.57      | 114.06   |
| 14  | G     | 820 | CLA  | CMB-C2B-C1B | -2.51 | 121.59      | 125.42   |
| 17  | N     | 846 | BCR  | C28-C27-C26 | -2.51 | 109.57      | 114.06   |
| 14  | N     | 813 | CLA  | O2D-CGD-CBD | 2.51  | 115.62      | 111.23   |
| 14  | a     | 831 | CLA  | C1-C2-C3    | -2.51 | 122.08      | 126.20   |
| 17  | m     | 102 | BCR  | C23-C24-C25 | -2.51 | 120.29      | 127.00   |
| 14  | N     | 810 | CLA  | O2A-CGA-O1A | -2.51 | 117.34      | 123.63   |
| 14  | G     | 822 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 14  | G     | 823 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 19  | a     | 851 | CL0  | C1C-CHC-C4B | 2.51  | 125.05      | 116.07   |
| 17  | u     | 103 | BCR  | C16-C15-C14 | -2.51 | 118.38      | 123.52   |
| 17  | g     | 847 | BCR  | C28-C27-C26 | -2.51 | 109.58      | 114.06   |
| 15  | G     | 841 | PQN  | C2M-C2-C3   | -2.51 | 120.33      | 124.45   |
| 14  | G     | 833 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 14  | A     | 825 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 14  | G     | 811 | CLA  | CHB-C4A-NA  | 2.51  | 128.02      | 124.40   |
| 19  | G     | 851 | CL0  | C3D-C4D-CHA | 2.51  | 112.35      | 108.54   |
| 19  | a     | 851 | CL0  | C4D-CHA-CBD | -2.51 | 106.44      | 108.97   |
| 14  | G     | 814 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 14  | G     | 821 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | A     | 845  | BCR  | C8-C7-C6    | -2.50 | 120.31      | 127.00   |
| 14  | G     | 839  | CLA  | C1-C2-C3    | -2.50 | 122.09      | 126.20   |
| 17  | i     | 101  | BCR  | C15-C16-C17 | -2.50 | 118.40      | 123.52   |
| 14  | T     | 102  | CLA  | C3B-C4B-NB  | -2.50 | 108.30      | 110.53   |
| 17  | f     | 203  | BCR  | C23-C24-C25 | -2.50 | 120.31      | 127.00   |
| 14  | N     | 813  | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 14  | g     | 816  | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 17  | g     | 845  | BCR  | C1-C6-C5    | -2.50 | 119.22      | 122.64   |
| 17  | b     | 843  | BCR  | C38-C26-C27 | 2.50  | 118.93      | 113.60   |
| 14  | G     | 816  | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 14  | B     | 840  | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 14  | f     | 201  | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 14  | g     | 828  | CLA  | C3B-C4B-NB  | -2.50 | 108.30      | 110.53   |
| 17  | V     | 101  | BCR  | C11-C12-C13 | -2.50 | 119.51      | 126.36   |
| 14  | L     | 1501 | CLA  | CHB-C4A-NA  | 2.50  | 128.01      | 124.40   |
| 17  | M     | 101  | BCR  | C38-C26-C27 | 2.50  | 118.92      | 113.60   |
| 14  | b     | 838  | CLA  | C3B-C4B-NB  | -2.50 | 108.30      | 110.53   |
| 17  | I     | 102  | BCR  | C20-C21-C22 | -2.50 | 123.78      | 127.28   |
| 14  | G     | 827  | CLA  | C1-C2-C3    | -2.50 | 122.11      | 126.20   |
| 14  | a     | 812  | CLA  | CHB-C4A-NA  | 2.50  | 128.00      | 124.40   |
| 14  | a     | 838  | CLA  | CHB-C4A-NA  | 2.50  | 128.00      | 124.40   |
| 14  | b     | 816  | CLA  | CHB-C4A-NA  | 2.50  | 128.00      | 124.40   |
| 14  | G     | 803  | CLA  | CHB-C4A-NA  | 2.49  | 128.00      | 124.40   |
| 14  | b     | 851  | CLA  | CHB-C4A-NA  | 2.49  | 128.00      | 124.40   |
| 17  | A     | 848  | BCR  | C8-C7-C6    | -2.49 | 120.33      | 127.00   |
| 17  | V     | 101  | BCR  | C15-C16-C17 | -2.49 | 118.42      | 123.52   |
| 14  | g     | 813  | CLA  | CHB-C4A-NA  | 2.49  | 128.00      | 124.40   |
| 17  | g     | 843  | BCR  | C24-C23-C22 | -2.49 | 122.55      | 126.23   |
| 20  | l     | 201  | SQD  | O5-C5-C4    | 2.49  | 114.19      | 109.70   |
| 17  | T     | 103  | BCR  | C8-C7-C6    | -2.49 | 120.34      | 127.00   |
| 14  | a     | 818  | CLA  | CHB-C4A-NA  | 2.49  | 128.00      | 124.40   |
| 14  | A     | 832  | CLA  | C1-C2-C3    | -2.49 | 122.11      | 126.20   |
| 17  | g     | 848  | BCR  | C1-C6-C7    | 2.49  | 122.41      | 115.65   |
| 17  | t     | 104  | BCR  | C38-C26-C27 | 2.49  | 118.91      | 113.60   |
| 14  | U     | 102  | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 14  | B     | 812  | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 14  | G     | 836  | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 17  | A     | 847  | BCR  | C11-C12-C13 | -2.49 | 119.54      | 126.36   |
| 14  | n     | 813  | CLA  | C3B-C4B-NB  | -2.49 | 108.31      | 110.53   |
| 14  | b     | 836  | CLA  | C3B-C4B-NB  | -2.49 | 108.31      | 110.53   |
| 14  | g     | 805  | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 14  | n     | 840  | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | B     | 813 | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 15  | A     | 842 | PQN  | C2M-C2-C3   | -2.49 | 120.36      | 124.45   |
| 15  | b     | 842 | PQN  | C14-C13-C15 | 2.49  | 119.54      | 115.23   |
| 14  | B     | 836 | CLA  | C3B-C4B-NB  | -2.49 | 108.31      | 110.53   |
| 14  | U     | 101 | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 14  | n     | 825 | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 14  | a     | 820 | CLA  | CHB-C4A-NA  | 2.49  | 127.99      | 124.40   |
| 17  | I     | 102 | BCR  | C38-C26-C25 | -2.49 | 121.77      | 124.48   |
| 14  | g     | 838 | CLA  | CHB-C4A-NA  | 2.48  | 127.99      | 124.40   |
| 14  | n     | 833 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 17  | N     | 852 | BCR  | C23-C24-C25 | -2.48 | 120.36      | 127.00   |
| 14  | t     | 102 | CLA  | C3B-C4B-NB  | -2.48 | 108.31      | 110.53   |
| 14  | g     | 830 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 14  | n     | 806 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 14  | b     | 807 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 14  | S     | 203 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 14  | B     | 803 | CLA  | C3B-C4B-NB  | -2.48 | 108.31      | 110.53   |
| 14  | n     | 824 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 14  | J     | 101 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 14  | a     | 839 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 14  | G     | 827 | CLA  | C3B-C4B-NB  | -2.48 | 108.32      | 110.53   |
| 17  | B     | 851 | BCR  | C1-C6-C5    | -2.48 | 119.25      | 122.64   |
| 14  | G     | 824 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 14  | N     | 835 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 14  | n     | 830 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 17  | a     | 846 | BCR  | C36-C18-C17 | -2.48 | 118.80      | 122.82   |
| 19  | a     | 851 | CL0  | C3D-C4D-CHA | 2.48  | 112.31      | 108.54   |
| 14  | g     | 835 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 14  | a     | 810 | CLA  | CHB-C4A-NA  | 2.48  | 127.98      | 124.40   |
| 14  | g     | 817 | CLA  | C3B-C4B-NB  | -2.48 | 108.32      | 110.53   |
| 14  | g     | 823 | CLA  | CHB-C4A-NA  | 2.48  | 127.97      | 124.40   |
| 14  | b     | 830 | CLA  | CMB-C2B-C1B | -2.48 | 121.65      | 125.42   |
| 14  | B     | 827 | CLA  | CHB-C4A-NA  | 2.48  | 127.97      | 124.40   |
| 14  | a     | 822 | CLA  | CHB-C4A-NA  | 2.48  | 127.97      | 124.40   |
| 14  | G     | 808 | CLA  | C1-C2-C3    | -2.48 | 122.14      | 126.20   |
| 14  | g     | 825 | CLA  | CHB-C4A-NA  | 2.48  | 127.97      | 124.40   |
| 14  | b     | 822 | CLA  | CHB-C4A-NA  | 2.48  | 127.97      | 124.40   |
| 14  | A     | 808 | CLA  | C1-C2-C3    | -2.47 | 122.14      | 126.20   |
| 14  | N     | 823 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 14  | b     | 835 | CLA  | C3B-C4B-NB  | -2.47 | 108.32      | 110.53   |
| 14  | A     | 824 | CLA  | CMB-C2B-C1B | -2.47 | 121.65      | 125.42   |
| 17  | g     | 843 | BCR  | C29-C30-C25 | 2.47  | 114.03      | 110.44   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | I     | 103 | BCR  | C1-C6-C5    | -2.47 | 119.26      | 122.64   |
| 14  | A     | 806 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 14  | G     | 828 | CLA  | C3B-C4B-NB  | -2.47 | 108.32      | 110.53   |
| 17  | b     | 848 | BCR  | C33-C5-C4   | 2.47  | 118.87      | 113.60   |
| 14  | t     | 102 | CLA  | CAA-C2A-C3A | -2.47 | 110.56      | 116.23   |
| 14  | n     | 808 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 17  | N     | 849 | BCR  | C21-C20-C19 | -2.47 | 116.04      | 123.20   |
| 14  | n     | 840 | CLA  | C3B-C4B-NB  | -2.47 | 108.32      | 110.53   |
| 14  | B     | 819 | CLA  | C3B-C4B-NB  | -2.47 | 108.32      | 110.53   |
| 14  | A     | 841 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 14  | A     | 823 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 14  | B     | 821 | CLA  | CHB-C4A-NA  | 2.47  | 127.97      | 124.40   |
| 14  | b     | 809 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 17  | M     | 101 | BCR  | C15-C16-C17 | -2.47 | 118.47      | 123.52   |
| 14  | A     | 802 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 14  | B     | 809 | CLA  | O2A-CGA-O1A | -2.47 | 117.45      | 123.63   |
| 17  | F     | 203 | BCR  | C11-C12-C13 | -2.47 | 119.59      | 126.36   |
| 14  | N     | 834 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 14  | a     | 833 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 14  | n     | 819 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 17  | I     | 103 | BCR  | C23-C24-C25 | -2.47 | 120.41      | 127.00   |
| 14  | G     | 806 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 14  | N     | 811 | CLA  | C3B-C4B-NB  | -2.47 | 108.33      | 110.53   |
| 14  | g     | 822 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 17  | Y     | 101 | BCR  | C23-C24-C25 | -2.47 | 120.41      | 127.00   |
| 14  | N     | 814 | CLA  | CHB-C4A-NA  | 2.47  | 127.96      | 124.40   |
| 17  | l     | 205 | BCR  | C3-C4-C5    | -2.46 | 109.66      | 114.06   |
| 14  | n     | 803 | CLA  | O2D-CGD-O1D | -2.46 | 119.05      | 123.85   |
| 14  | b     | 806 | CLA  | CHB-C4A-NA  | 2.46  | 127.96      | 124.40   |
| 14  | b     | 821 | CLA  | CHB-C4A-NA  | 2.46  | 127.96      | 124.40   |
| 14  | b     | 837 | CLA  | C3B-C4B-NB  | -2.46 | 108.33      | 110.53   |
| 14  | A     | 813 | CLA  | CHB-C4A-NA  | 2.46  | 127.96      | 124.40   |
| 14  | J     | 102 | CLA  | CHB-C4A-NA  | 2.46  | 127.96      | 124.40   |
| 14  | g     | 828 | CLA  | C1-C2-C3    | -2.46 | 122.16      | 126.20   |
| 14  | N     | 826 | CLA  | C1-C2-C3    | -2.46 | 122.16      | 126.20   |
| 14  | G     | 807 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 14  | G     | 804 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 17  | i     | 102 | BCR  | C33-C5-C4   | 2.46  | 118.84      | 113.60   |
| 14  | g     | 814 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 14  | B     | 822 | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 14  | B     | 808 | CLA  | C3B-C4B-NB  | -2.46 | 108.33      | 110.53   |
| 19  | G     | 851 | CL0  | C1C-CHC-C4B | 2.46  | 124.87      | 116.07   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | g     | 812  | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 14  | n     | 812  | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 14  | F     | 202  | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 17  | k     | 102  | BCR  | C38-C26-C27 | 2.46  | 118.84      | 113.60   |
| 14  | T     | 101  | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 14  | n     | 836  | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 14  | b     | 817  | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 14  | T     | 102  | CLA  | CAA-C2A-C3A | -2.46 | 110.59      | 116.23   |
| 14  | w     | 203  | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 14  | N     | 810  | CLA  | O2D-CGD-CBD | 2.46  | 115.53      | 111.23   |
| 14  | G     | 805  | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 14  | k     | 101  | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 14  | G     | 813  | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 14  | N     | 827  | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 14  | b     | 826  | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 14  | l     | 202  | CLA  | CHB-C4A-NA  | 2.46  | 127.95      | 124.40   |
| 14  | j     | 102  | CLA  | CAA-C2A-C3A | -2.46 | 110.60      | 116.23   |
| 14  | A     | 825  | CLA  | C1-C2-C3    | -2.46 | 122.17      | 126.20   |
| 17  | N     | 848  | BCR  | C33-C5-C4   | 2.46  | 118.83      | 113.60   |
| 14  | g     | 815  | CLA  | CHB-C4A-NA  | 2.46  | 127.94      | 124.40   |
| 14  | A     | 811  | CLA  | CHB-C4A-NA  | 2.46  | 127.94      | 124.40   |
| 14  | A     | 829  | CLA  | O2D-CGD-CBD | 2.45  | 115.52      | 111.23   |
| 14  | a     | 835  | CLA  | CHB-C4A-NA  | 2.45  | 127.94      | 124.40   |
| 17  | n     | 843  | BCR  | C21-C20-C19 | -2.45 | 116.09      | 123.20   |
| 14  | G     | 802  | CLA  | CHB-C4A-NA  | 2.45  | 127.94      | 124.40   |
| 14  | L     | 1502 | CLA  | CHB-C4A-NA  | 2.45  | 127.94      | 124.40   |
| 17  | W     | 205  | BCR  | C15-C14-C13 | -2.45 | 123.84      | 127.28   |
| 17  | M     | 101  | BCR  | C20-C19-C18 | -2.45 | 119.64      | 126.36   |
| 14  | a     | 828  | CLA  | CHB-C4A-NA  | 2.45  | 127.94      | 124.40   |
| 17  | B     | 848  | BCR  | C3-C4-C5    | -2.45 | 109.68      | 114.06   |
| 14  | A     | 829  | CLA  | CMB-C2B-C1B | -2.45 | 121.69      | 125.42   |
| 14  | n     | 810  | CLA  | CHB-C4A-NA  | 2.45  | 127.94      | 124.40   |
| 14  | n     | 831  | CLA  | C3B-C4B-NB  | -2.45 | 108.34      | 110.53   |
| 14  | u     | 101  | CLA  | CHB-C4A-NA  | 2.45  | 127.94      | 124.40   |
| 17  | b     | 848  | BCR  | C10-C11-C12 | -2.45 | 116.10      | 123.20   |
| 14  | s     | 202  | CLA  | CHB-C4A-NA  | 2.45  | 127.94      | 124.40   |
| 14  | l     | 203  | CLA  | CHB-C4A-NA  | 2.45  | 127.93      | 124.40   |
| 14  | b     | 830  | CLA  | C3B-C4B-NB  | -2.45 | 108.34      | 110.53   |
| 14  | G     | 818  | CLA  | C3B-C4B-NB  | -2.45 | 108.34      | 110.53   |
| 14  | A     | 824  | CLA  | CHB-C4A-NA  | 2.45  | 127.93      | 124.40   |
| 14  | K     | 101  | CLA  | CHB-C4A-NA  | 2.45  | 127.93      | 124.40   |
| 17  | T     | 103  | BCR  | C23-C24-C25 | -2.45 | 120.46      | 127.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | G     | 824 | CLA  | C1-C2-C3    | -2.45 | 122.19      | 126.20   |
| 14  | a     | 801 | CLA  | CHB-C4A-NA  | 2.45  | 127.93      | 124.40   |
| 14  | a     | 804 | CLA  | CHB-C4A-NA  | 2.45  | 127.93      | 124.40   |
| 15  | g     | 841 | PQN  | C12-C11-C3  | -2.45 | 106.06      | 112.08   |
| 14  | a     | 825 | CLA  | CHB-C4A-NA  | 2.45  | 127.93      | 124.40   |
| 14  | b     | 814 | CLA  | CHB-C4A-NA  | 2.45  | 127.93      | 124.40   |
| 14  | a     | 807 | CLA  | C1-C2-C3    | -2.45 | 122.19      | 126.20   |
| 17  | B     | 844 | BCR  | C1-C6-C7    | 2.44  | 122.28      | 115.65   |
| 17  | f     | 203 | BCR  | C33-C5-C4   | 2.44  | 118.81      | 113.60   |
| 17  | m     | 102 | BCR  | C38-C26-C27 | 2.44  | 118.81      | 113.60   |
| 14  | a     | 813 | CLA  | CHB-C4A-NA  | 2.44  | 127.93      | 124.40   |
| 17  | A     | 856 | BCR  | C8-C7-C6    | -2.44 | 120.47      | 127.00   |
| 14  | B     | 833 | CLA  | C3B-C4B-NB  | -2.44 | 108.35      | 110.53   |
| 14  | n     | 821 | CLA  | CHB-C4A-NA  | 2.44  | 127.93      | 124.40   |
| 14  | F     | 201 | CLA  | C1-C2-C3    | -2.44 | 122.20      | 126.20   |
| 17  | B     | 845 | BCR  | C3-C4-C5    | -2.44 | 109.70      | 114.06   |
| 14  | a     | 852 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 14  | a     | 801 | CLA  | C1-C2-C3    | -2.44 | 122.20      | 126.20   |
| 17  | N     | 849 | BCR  | C7-C8-C9    | -2.44 | 122.63      | 126.23   |
| 14  | g     | 804 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 14  | n     | 805 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 14  | B     | 814 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 17  | b     | 843 | BCR  | C27-C26-C25 | -2.44 | 119.41      | 122.70   |
| 14  | N     | 817 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 14  | n     | 815 | CLA  | CHB-C4A-NA  | 2.44  | 127.92      | 124.40   |
| 14  | n     | 817 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 14  | a     | 840 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 14  | b     | 832 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 14  | N     | 808 | CLA  | C1-C2-C3    | -2.43 | 122.21      | 126.20   |
| 14  | n     | 804 | CLA  | C1-C2-C3    | -2.43 | 122.21      | 126.20   |
| 14  | B     | 807 | CLA  | O2A-CGA-O1A | -2.43 | 117.54      | 123.63   |
| 14  | G     | 809 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 14  | b     | 823 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 14  | b     | 837 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 14  | a     | 805 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 14  | A     | 815 | CLA  | C3B-C4B-NB  | -2.43 | 108.36      | 110.53   |
| 14  | A     | 833 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 14  | b     | 827 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 17  | n     | 845 | BCR  | C8-C7-C6    | -2.43 | 120.50      | 127.00   |
| 14  | N     | 851 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 14  | n     | 802 | CLA  | C3B-C4B-NB  | -2.43 | 108.36      | 110.53   |
| 14  | n     | 832 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | n     | 850 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 14  | N     | 815 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 19  | G     | 851 | CL0  | C4C-C3C-C2C | -2.43 | 103.78      | 113.37   |
| 17  | S     | 204 | BCR  | C3-C4-C5    | -2.43 | 109.72      | 114.06   |
| 14  | a     | 824 | CLA  | CHB-C4A-NA  | 2.43  | 127.91      | 124.40   |
| 14  | A     | 808 | CLA  | C3B-C4B-NB  | -2.43 | 108.36      | 110.53   |
| 17  | U     | 103 | BCR  | C38-C26-C27 | 2.43  | 118.77      | 113.60   |
| 14  | G     | 839 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 14  | a     | 809 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 14  | b     | 833 | CLA  | C1-C2-C3    | -2.43 | 122.22      | 126.20   |
| 17  | A     | 848 | BCR  | C38-C26-C25 | -2.43 | 121.83      | 124.48   |
| 17  | i     | 101 | BCR  | C33-C5-C4   | 2.43  | 118.77      | 113.60   |
| 14  | F     | 201 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 14  | b     | 840 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 17  | s     | 203 | BCR  | C33-C5-C4   | 2.43  | 118.77      | 113.60   |
| 17  | j     | 104 | BCR  | C11-C12-C13 | -2.43 | 119.71      | 126.36   |
| 14  | a     | 823 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 14  | b     | 841 | CLA  | C3B-C4B-NB  | -2.43 | 108.36      | 110.53   |
| 19  | G     | 851 | CL0  | O2A-CGA-O1A | -2.43 | 117.56      | 123.63   |
| 17  | U     | 103 | BCR  | C23-C24-C25 | -2.43 | 120.52      | 127.00   |
| 14  | N     | 826 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 14  | a     | 814 | CLA  | CHB-C4A-NA  | 2.43  | 127.90      | 124.40   |
| 14  | j     | 101 | CLA  | CHB-C4A-NA  | 2.42  | 127.90      | 124.40   |
| 14  | G     | 826 | CLA  | CHB-C4A-NA  | 2.42  | 127.90      | 124.40   |
| 14  | N     | 822 | CLA  | CHB-C4A-NA  | 2.42  | 127.90      | 124.40   |
| 14  | n     | 820 | CLA  | CHB-C4A-NA  | 2.42  | 127.90      | 124.40   |
| 17  | A     | 844 | BCR  | C29-C30-C25 | 2.42  | 113.96      | 110.44   |
| 14  | g     | 852 | CLA  | CHB-C4A-NA  | 2.42  | 127.90      | 124.40   |
| 14  | a     | 804 | CLA  | C1-C2-C3    | -2.42 | 122.23      | 126.20   |
| 14  | g     | 840 | CLA  | C3B-C4B-NB  | -2.42 | 108.37      | 110.53   |
| 14  | g     | 810 | CLA  | CHB-C4A-NA  | 2.42  | 127.90      | 124.40   |
| 17  | n     | 843 | BCR  | C20-C21-C22 | -2.42 | 123.88      | 127.28   |
| 14  | G     | 829 | CLA  | C3B-C4B-NB  | -2.42 | 108.37      | 110.53   |
| 14  | g     | 811 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 17  | w     | 206 | BCR  | C3-C4-C5    | -2.42 | 109.74      | 114.06   |
| 17  | t     | 103 | BCR  | C33-C5-C4   | 2.42  | 118.76      | 113.60   |
| 17  | T     | 104 | BCR  | C3-C4-C5    | -2.42 | 109.74      | 114.06   |
| 14  | B     | 825 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 14  | N     | 830 | CLA  | CMB-C2B-C1B | -2.42 | 121.73      | 125.42   |
| 14  | u     | 102 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 14  | A     | 812 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 14  | a     | 832 | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | b     | 831  | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 14  | b     | 837  | CLA  | C1-C2-C3    | -2.42 | 122.23      | 126.20   |
| 17  | A     | 844  | BCR  | C21-C20-C19 | -2.42 | 116.19      | 123.20   |
| 14  | s     | 201  | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 17  | A     | 846  | BCR  | C23-C24-C25 | -2.42 | 120.53      | 127.00   |
| 17  | u     | 103  | BCR  | C38-C26-C27 | 2.42  | 118.75      | 113.60   |
| 17  | b     | 845  | BCR  | C28-C27-C26 | -2.42 | 109.74      | 114.06   |
| 14  | B     | 850  | CLA  | C1-C2-C3    | -2.42 | 122.24      | 126.20   |
| 14  | B     | 833  | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 14  | n     | 839  | CLA  | CHB-C4A-NA  | 2.42  | 127.89      | 124.40   |
| 19  | A     | 852  | CL0  | C4C-C3C-C2C | -2.42 | 103.83      | 113.37   |
| 14  | N     | 818  | CLA  | CHB-C4A-NA  | 2.41  | 127.89      | 124.40   |
| 14  | N     | 803  | CLA  | CAA-CBA-CGA | -2.41 | 106.35      | 113.21   |
| 14  | g     | 840  | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 14  | b     | 839  | CLA  | C3B-C4B-NB  | -2.41 | 108.38      | 110.53   |
| 14  | a     | 817  | CLA  | C1-C2-C3    | -2.41 | 122.24      | 126.20   |
| 14  | N     | 824  | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 14  | A     | 810  | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 14  | B     | 832  | CLA  | C3B-C4B-NB  | -2.41 | 108.38      | 110.53   |
| 17  | A     | 846  | BCR  | C33-C5-C4   | 2.41  | 118.74      | 113.60   |
| 14  | w     | 205  | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 19  | a     | 851  | CL0  | C4C-C3C-C2C | -2.41 | 103.85      | 113.37   |
| 14  | g     | 832  | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 14  | A     | 839  | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 17  | f     | 203  | BCR  | C38-C26-C27 | 2.41  | 118.74      | 113.60   |
| 15  | b     | 842  | PQN  | C2M-C2-C3   | -2.41 | 120.49      | 124.45   |
| 14  | G     | 808  | CLA  | O2A-CGA-O1A | -2.41 | 117.60      | 123.63   |
| 14  | G     | 818  | CLA  | C1-C2-C3    | -2.41 | 122.25      | 126.20   |
| 14  | B     | 818  | CLA  | CHB-C4A-NA  | 2.41  | 127.88      | 124.40   |
| 17  | L     | 1504 | BCR  | C23-C24-C25 | -2.41 | 120.56      | 127.00   |
| 14  | B     | 805  | CLA  | CAA-C2A-C3A | -2.41 | 106.49      | 113.00   |
| 14  | a     | 837  | CLA  | CHB-C4A-NA  | 2.41  | 127.87      | 124.40   |
| 14  | b     | 853  | CLA  | CHB-C4A-NA  | 2.41  | 127.87      | 124.40   |
| 14  | B     | 829  | CLA  | CMB-C2B-C1B | -2.41 | 121.75      | 125.42   |
| 17  | b     | 846  | BCR  | C28-C27-C26 | -2.41 | 109.77      | 114.06   |
| 14  | g     | 826  | CLA  | C1-C2-C3    | -2.41 | 122.26      | 126.20   |
| 14  | n     | 804  | CLA  | CHB-C4A-NA  | 2.41  | 127.87      | 124.40   |
| 14  | G     | 834  | CLA  | CHB-C4A-NA  | 2.40  | 127.87      | 124.40   |
| 14  | a     | 816  | CLA  | CHB-C4A-NA  | 2.40  | 127.87      | 124.40   |
| 14  | b     | 806  | CLA  | CMB-C2B-C1B | -2.40 | 121.76      | 125.42   |
| 14  | b     | 811  | CLA  | CHB-C4A-NA  | 2.40  | 127.87      | 124.40   |
| 14  | G     | 820  | CLA  | CHB-C4A-NA  | 2.40  | 127.87      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | N     | 844 | BCR  | C8-C7-C6    | -2.40 | 120.58      | 127.00   |
| 14  | n     | 831 | CLA  | CHB-C4A-NA  | 2.40  | 127.87      | 124.40   |
| 14  | N     | 827 | CLA  | CMB-C2B-C1B | -2.40 | 121.76      | 125.42   |
| 17  | N     | 848 | BCR  | C38-C26-C27 | 2.40  | 118.72      | 113.60   |
| 14  | A     | 822 | CLA  | C3B-C4B-NB  | -2.40 | 108.39      | 110.53   |
| 17  | B     | 845 | BCR  | C37-C22-C21 | -2.40 | 118.92      | 122.82   |
| 14  | B     | 837 | CLA  | CMB-C2B-C1B | -2.40 | 121.76      | 125.42   |
| 14  | A     | 817 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 14  | A     | 822 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 14  | b     | 820 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 14  | b     | 805 | CLA  | C1-C2-C3    | -2.40 | 122.26      | 126.20   |
| 14  | A     | 834 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 14  | N     | 841 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 14  | n     | 822 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 14  | B     | 831 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 17  | B     | 846 | BCR  | C16-C15-C14 | -2.40 | 118.61      | 123.52   |
| 14  | N     | 840 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 14  | A     | 829 | CLA  | C3B-C4B-NB  | -2.40 | 108.39      | 110.53   |
| 14  | g     | 833 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 14  | A     | 809 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 14  | l     | 204 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 14  | g     | 807 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 14  | B     | 823 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 19  | g     | 851 | CL0  | C1C-CHC-C4B | 2.40  | 124.64      | 116.07   |
| 17  | G     | 848 | BCR  | C16-C15-C14 | -2.40 | 118.62      | 123.52   |
| 14  | N     | 839 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 14  | g     | 834 | CLA  | CHB-C4A-NA  | 2.40  | 127.86      | 124.40   |
| 14  | n     | 835 | CLA  | C3B-C4B-NB  | -2.39 | 108.39      | 110.53   |
| 14  | G     | 837 | CLA  | CHB-C4A-NA  | 2.39  | 127.86      | 124.40   |
| 17  | j     | 104 | BCR  | C38-C26-C27 | 2.39  | 118.70      | 113.60   |
| 17  | k     | 102 | BCR  | C23-C24-C25 | -2.39 | 120.60      | 127.00   |
| 14  | N     | 832 | CLA  | CHB-C4A-NA  | 2.39  | 127.86      | 124.40   |
| 14  | B     | 811 | CLA  | CHB-C4A-NA  | 2.39  | 127.86      | 124.40   |
| 17  | b     | 844 | BCR  | C23-C24-C25 | -2.39 | 120.60      | 127.00   |
| 14  | g     | 808 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 14  | A     | 815 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 14  | A     | 828 | CLA  | C3B-C4B-NB  | -2.39 | 108.39      | 110.53   |
| 14  | G     | 852 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 17  | A     | 849 | BCR  | C16-C15-C14 | -2.39 | 118.63      | 123.52   |
| 14  | B     | 806 | CLA  | CMB-C2B-C1B | -2.39 | 121.78      | 125.42   |
| 17  | B     | 848 | BCR  | C33-C5-C4   | 2.39  | 118.69      | 113.60   |
| 14  | N     | 808 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | g     | 828 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 14  | b     | 829 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 14  | A     | 818 | CLA  | CMB-C2B-C1B | -2.39 | 121.78      | 125.42   |
| 14  | B     | 826 | CLA  | CHB-C4A-NA  | 2.39  | 127.85      | 124.40   |
| 14  | b     | 807 | CLA  | C1-C2-C3    | -2.39 | 122.28      | 126.20   |
| 17  | a     | 843 | BCR  | C21-C20-C19 | -2.39 | 116.28      | 123.20   |
| 14  | A     | 838 | CLA  | CHB-C4A-NA  | 2.39  | 127.84      | 124.40   |
| 17  | I     | 101 | BCR  | C2-C1-C6    | 2.39  | 113.91      | 110.44   |
| 14  | b     | 810 | CLA  | CHB-C4A-NA  | 2.39  | 127.84      | 124.40   |
| 14  | S     | 201 | CLA  | C1-C2-C3    | -2.39 | 122.29      | 126.20   |
| 19  | g     | 851 | CL0  | C3D-C4D-CHA | 2.39  | 112.17      | 108.54   |
| 14  | N     | 829 | CLA  | C3B-C4B-NB  | -2.39 | 108.40      | 110.53   |
| 17  | b     | 850 | BCR  | C3-C4-C5    | -2.39 | 109.80      | 114.06   |
| 19  | g     | 851 | CL0  | O2A-CGA-O1A | -2.39 | 117.66      | 123.63   |
| 14  | g     | 807 | CLA  | C3B-C4B-NB  | -2.38 | 108.40      | 110.53   |
| 20  | l     | 201 | SQD  | O8-S-C6     | 2.38  | 110.58      | 105.97   |
| 14  | n     | 813 | CLA  | CHB-C4A-NA  | 2.38  | 127.84      | 124.40   |
| 14  | N     | 821 | CLA  | CHB-C4A-NA  | 2.38  | 127.84      | 124.40   |
| 17  | t     | 103 | BCR  | C8-C7-C6    | -2.38 | 120.63      | 127.00   |
| 14  | A     | 820 | CLA  | CHB-C4A-NA  | 2.38  | 127.84      | 124.40   |
| 14  | g     | 820 | CLA  | CHB-C4A-NA  | 2.38  | 127.84      | 124.40   |
| 17  | J     | 103 | BCR  | C23-C24-C25 | -2.38 | 120.64      | 127.00   |
| 14  | G     | 838 | CLA  | CHB-C4A-NA  | 2.38  | 127.84      | 124.40   |
| 14  | g     | 802 | CLA  | C1-C2-C3    | -2.38 | 122.30      | 126.20   |
| 14  | b     | 838 | CLA  | C1-C2-C3    | -2.38 | 122.30      | 126.20   |
| 14  | a     | 854 | CLA  | CHB-C4A-NA  | 2.38  | 127.84      | 124.40   |
| 14  | b     | 830 | CLA  | CHB-C4A-NA  | 2.38  | 127.84      | 124.40   |
| 17  | A     | 856 | BCR  | C24-C23-C22 | -2.38 | 122.71      | 126.23   |
| 14  | G     | 830 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 14  | a     | 834 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 17  | N     | 847 | BCR  | C11-C12-C13 | -2.38 | 119.84      | 126.36   |
| 14  | g     | 803 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 14  | A     | 829 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 14  | b     | 804 | CLA  | C1-C2-C3    | -2.38 | 122.30      | 126.20   |
| 14  | n     | 837 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 17  | a     | 847 | BCR  | C15-C16-C17 | -2.38 | 118.65      | 123.52   |
| 17  | J     | 103 | BCR  | C8-C7-C6    | -2.38 | 120.65      | 127.00   |
| 14  | f     | 201 | CLA  | C1-C2-C3    | -2.38 | 122.30      | 126.20   |
| 17  | n     | 843 | BCR  | C38-C26-C25 | -2.38 | 121.89      | 124.48   |
| 14  | G     | 835 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |
| 17  | N     | 853 | BCR  | C28-C27-C26 | -2.38 | 109.82      | 114.06   |
| 14  | B     | 808 | CLA  | CHB-C4A-NA  | 2.38  | 127.83      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | b     | 819 | CLA  | C3B-C4B-NB  | -2.38 | 108.41      | 110.53   |
| 17  | A     | 847 | BCR  | C23-C24-C25 | -2.38 | 120.65      | 127.00   |
| 17  | l     | 205 | BCR  | C28-C27-C26 | -2.37 | 109.82      | 114.06   |
| 17  | A     | 848 | BCR  | C23-C24-C25 | -2.37 | 120.66      | 127.00   |
| 14  | b     | 802 | CLA  | C1-C2-C3    | -2.37 | 122.31      | 126.20   |
| 14  | n     | 826 | CLA  | CHB-C4A-NA  | 2.37  | 127.83      | 124.40   |
| 14  | A     | 835 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 14  | a     | 803 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 14  | b     | 835 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 14  | b     | 828 | CLA  | C1-C2-C3    | -2.37 | 122.31      | 126.20   |
| 14  | N     | 803 | CLA  | C3B-C4B-NB  | -2.37 | 108.41      | 110.53   |
| 14  | B     | 806 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 17  | i     | 102 | BCR  | C37-C22-C23 | 2.37  | 121.71      | 118.09   |
| 14  | b     | 828 | CLA  | C3B-C4B-NB  | -2.37 | 108.41      | 110.53   |
| 14  | g     | 837 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 14  | n     | 814 | CLA  | CAA-C2A-C3A | -2.37 | 106.60      | 113.00   |
| 14  | A     | 830 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 17  | b     | 848 | BCR  | C16-C15-C14 | -2.37 | 118.67      | 123.52   |
| 14  | B     | 809 | CLA  | O2D-CGD-CBD | 2.37  | 115.37      | 111.23   |
| 14  | G     | 810 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 14  | A     | 853 | CLA  | C1-C2-C3    | -2.37 | 122.32      | 126.20   |
| 14  | G     | 822 | CLA  | C3B-C4B-NB  | -2.37 | 108.42      | 110.53   |
| 14  | b     | 824 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 14  | B     | 820 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 14  | B     | 837 | CLA  | CHB-C4A-NA  | 2.37  | 127.82      | 124.40   |
| 14  | N     | 841 | CLA  | O2A-CGA-O1A | -2.37 | 117.71      | 123.63   |
| 14  | N     | 811 | CLA  | CHB-C4A-NA  | 2.37  | 127.81      | 124.40   |
| 17  | W     | 206 | BCR  | C10-C11-C12 | -2.37 | 116.34      | 123.20   |
| 14  | G     | 818 | CLA  | CHB-C4A-NA  | 2.37  | 127.81      | 124.40   |
| 14  | n     | 811 | CLA  | CHB-C4A-NA  | 2.37  | 127.81      | 124.40   |
| 14  | n     | 836 | CLA  | CMB-C2B-C1B | -2.37 | 121.82      | 125.42   |
| 17  | v     | 101 | BCR  | C29-C30-C25 | 2.37  | 113.88      | 110.44   |
| 17  | n     | 842 | BCR  | C38-C26-C27 | 2.36  | 118.64      | 113.60   |
| 17  | a     | 846 | BCR  | C4-C5-C6    | -2.36 | 119.51      | 122.70   |
| 14  | G     | 802 | CLA  | C1-C2-C3    | -2.36 | 122.33      | 126.20   |
| 14  | g     | 809 | CLA  | CHB-C4A-NA  | 2.36  | 127.81      | 124.40   |
| 14  | g     | 821 | CLA  | CHB-C4A-NA  | 2.36  | 127.81      | 124.40   |
| 17  | B     | 847 | BCR  | C8-C7-C6    | -2.36 | 120.69      | 127.00   |
| 14  | G     | 825 | CLA  | CHB-C4A-NA  | 2.36  | 127.81      | 124.40   |
| 14  | g     | 839 | CLA  | CHB-C4A-NA  | 2.36  | 127.81      | 124.40   |
| 14  | b     | 838 | CLA  | CHB-C4A-NA  | 2.36  | 127.81      | 124.40   |
| 14  | a     | 817 | CLA  | C3B-C4B-NB  | -2.36 | 108.42      | 110.53   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | b     | 843  | BCR  | C3-C4-C5    | -2.36 | 109.84      | 114.06   |
| 17  | b     | 852  | BCR  | C33-C5-C6   | -2.36 | 121.91      | 124.48   |
| 14  | B     | 813  | CLA  | C1-C2-C3    | -2.36 | 122.33      | 126.20   |
| 14  | b     | 832  | CLA  | CMB-C2B-C1B | -2.36 | 121.83      | 125.42   |
| 17  | B     | 848  | BCR  | C20-C19-C18 | -2.36 | 119.89      | 126.36   |
| 17  | L     | 1504 | BCR  | C38-C26-C27 | 2.36  | 118.63      | 113.60   |
| 17  | T     | 103  | BCR  | C33-C5-C4   | 2.36  | 118.63      | 113.60   |
| 14  | W     | 203  | CLA  | O2D-CGD-CBD | 2.36  | 115.35      | 111.23   |
| 14  | b     | 833  | CLA  | CHB-C4A-NA  | 2.36  | 127.80      | 124.40   |
| 17  | N     | 846  | BCR  | C8-C7-C6    | -2.36 | 120.70      | 127.00   |
| 17  | a     | 844  | BCR  | C20-C19-C18 | -2.36 | 119.90      | 126.36   |
| 14  | A     | 831  | CLA  | CHB-C4A-NA  | 2.36  | 127.80      | 124.40   |
| 14  | N     | 805  | CLA  | CHB-C4A-NA  | 2.36  | 127.80      | 124.40   |
| 14  | N     | 833  | CLA  | CHB-C4A-NA  | 2.36  | 127.80      | 124.40   |
| 17  | n     | 849  | BCR  | C8-C7-C6    | -2.36 | 120.70      | 127.00   |
| 14  | B     | 835  | CLA  | CHB-C4A-NA  | 2.36  | 127.80      | 124.40   |
| 17  | J     | 103  | BCR  | C33-C5-C4   | 2.36  | 118.62      | 113.60   |
| 17  | I     | 101  | BCR  | C33-C5-C4   | 2.36  | 118.62      | 113.60   |
| 17  | n     | 843  | BCR  | C27-C26-C25 | -2.36 | 119.52      | 122.70   |
| 14  | G     | 831  | CLA  | CHB-C4A-NA  | 2.36  | 127.80      | 124.40   |
| 14  | A     | 855  | CLA  | CHB-C4A-NA  | 2.36  | 127.80      | 124.40   |
| 14  | N     | 805  | CLA  | CAC-C3C-C4C | 2.36  | 127.86      | 124.79   |
| 17  | N     | 852  | BCR  | C33-C5-C4   | 2.36  | 118.62      | 113.60   |
| 17  | u     | 103  | BCR  | C8-C7-C6    | -2.36 | 120.70      | 127.00   |
| 14  | G     | 830  | CLA  | C1-C2-C3    | -2.36 | 122.34      | 126.20   |
| 17  | G     | 847  | BCR  | C16-C15-C14 | -2.35 | 118.70      | 123.52   |
| 14  | n     | 809  | CLA  | CHB-C4A-NA  | 2.35  | 127.80      | 124.40   |
| 14  | A     | 832  | CLA  | CHB-C4A-NA  | 2.35  | 127.80      | 124.40   |
| 14  | j     | 102  | CLA  | CHB-C4A-NA  | 2.35  | 127.80      | 124.40   |
| 14  | G     | 853  | CLA  | O2A-CGA-O1A | -2.35 | 117.74      | 123.63   |
| 14  | g     | 840  | CLA  | CMB-C2B-C1B | -2.35 | 121.83      | 125.42   |
| 14  | B     | 819  | CLA  | CHB-C4A-NA  | 2.35  | 127.80      | 124.40   |
| 14  | G     | 805  | CLA  | C3B-C4B-NB  | -2.35 | 108.43      | 110.53   |
| 14  | N     | 851  | CLA  | O2A-CGA-O1A | -2.35 | 117.75      | 123.63   |
| 14  | N     | 838  | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 17  | n     | 846  | BCR  | C38-C26-C27 | 2.35  | 118.61      | 113.60   |
| 17  | K     | 102  | BCR  | C8-C7-C6    | -2.35 | 120.72      | 127.00   |
| 14  | n     | 834  | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 17  | a     | 843  | BCR  | C16-C15-C14 | -2.35 | 118.71      | 123.52   |
| 14  | N     | 836  | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 14  | a     | 808  | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 14  | G     | 821  | CLA  | CMB-C2B-C1B | -2.35 | 121.84      | 125.42   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | N     | 836 | CLA  | C3B-C4B-NB  | -2.35 | 108.43      | 110.53   |
| 14  | a     | 829 | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 17  | n     | 842 | BCR  | C8-C7-C6    | -2.35 | 120.72      | 127.00   |
| 17  | B     | 851 | BCR  | C30-C25-C26 | -2.35 | 119.43      | 122.64   |
| 17  | g     | 843 | BCR  | C33-C5-C4   | 2.35  | 118.60      | 113.60   |
| 14  | n     | 835 | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 17  | G     | 847 | BCR  | C10-C11-C12 | -2.35 | 116.40      | 123.20   |
| 17  | A     | 849 | BCR  | C1-C6-C7    | 2.35  | 122.02      | 115.65   |
| 17  | W     | 205 | BCR  | C21-C20-C19 | -2.35 | 116.40      | 123.20   |
| 14  | A     | 818 | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 14  | n     | 828 | CLA  | CHB-C4A-NA  | 2.35  | 127.79      | 124.40   |
| 14  | N     | 842 | CLA  | C3B-C4B-NB  | -2.35 | 108.44      | 110.53   |
| 14  | T     | 102 | CLA  | CHB-C4A-NA  | 2.35  | 127.78      | 124.40   |
| 14  | G     | 832 | CLA  | C3B-C4B-NB  | -2.34 | 108.44      | 110.53   |
| 14  | g     | 806 | CLA  | C1-C2-C3    | -2.34 | 122.36      | 126.20   |
| 14  | G     | 840 | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 14  | b     | 841 | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 17  | i     | 102 | BCR  | C38-C26-C27 | 2.34  | 118.59      | 113.60   |
| 17  | M     | 101 | BCR  | C11-C10-C9  | -2.34 | 123.99      | 127.28   |
| 14  | N     | 807 | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 17  | G     | 845 | BCR  | C1-C6-C5    | -2.34 | 119.44      | 122.64   |
| 14  | N     | 809 | CLA  | CMB-C2B-C1B | -2.34 | 121.85      | 125.42   |
| 14  | b     | 818 | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 17  | N     | 853 | BCR  | C38-C26-C27 | 2.34  | 118.59      | 113.60   |
| 14  | G     | 829 | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 19  | G     | 851 | CL0  | O1D-CGD-CBD | 2.34  | 128.27      | 124.72   |
| 17  | N     | 847 | BCR  | C38-C26-C27 | 2.34  | 118.58      | 113.60   |
| 17  | N     | 849 | BCR  | C34-C9-C8   | 2.34  | 121.66      | 118.09   |
| 17  | B     | 844 | BCR  | C19-C18-C17 | 2.34  | 122.69      | 119.01   |
| 19  | g     | 851 | CL0  | C1-C2-C3    | -2.34 | 122.36      | 126.20   |
| 14  | a     | 836 | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 17  | u     | 103 | BCR  | C23-C24-C25 | -2.34 | 120.75      | 127.00   |
| 14  | N     | 812 | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 14  | A     | 836 | CLA  | CHB-C4A-NA  | 2.34  | 127.78      | 124.40   |
| 14  | n     | 804 | CLA  | CAC-C3C-C4C | 2.34  | 127.83      | 124.79   |
| 14  | N     | 829 | CLA  | O2A-CGA-O1A | -2.34 | 117.78      | 123.63   |
| 14  | B     | 820 | CLA  | CMB-C2B-C1B | -2.34 | 121.86      | 125.42   |
| 17  | m     | 102 | BCR  | C10-C11-C12 | -2.34 | 116.43      | 123.20   |
| 14  | G     | 827 | CLA  | CHB-C4A-NA  | 2.34  | 127.77      | 124.40   |
| 14  | b     | 802 | CLA  | CHB-C4A-NA  | 2.34  | 127.77      | 124.40   |
| 17  | g     | 845 | BCR  | C2-C1-C6    | 2.34  | 113.83      | 110.44   |
| 14  | t     | 102 | CLA  | CHB-C4A-NA  | 2.33  | 127.77      | 124.40   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | y     | 101 | BCR  | C10-C11-C12 | -2.33 | 116.44      | 123.20   |
| 14  | W     | 202 | CLA  | C3B-C4B-NB  | -2.33 | 108.45      | 110.53   |
| 17  | b     | 843 | BCR  | C33-C5-C4   | 2.33  | 118.57      | 113.60   |
| 14  | b     | 836 | CLA  | CHB-C4A-NA  | 2.33  | 127.77      | 124.40   |
| 17  | n     | 851 | BCR  | C33-C5-C4   | 2.33  | 118.57      | 113.60   |
| 14  | b     | 808 | CLA  | CHB-C4A-NA  | 2.33  | 127.77      | 124.40   |
| 14  | n     | 838 | CLA  | CHB-C4A-NA  | 2.33  | 127.76      | 124.40   |
| 14  | a     | 838 | CLA  | C1-C2-C3    | -2.33 | 122.38      | 126.20   |
| 14  | A     | 837 | CLA  | CHB-C4A-NA  | 2.33  | 127.76      | 124.40   |
| 17  | l     | 206 | BCR  | C2-C1-C6    | 2.33  | 113.82      | 110.44   |
| 17  | A     | 848 | BCR  | C21-C20-C19 | -2.33 | 116.46      | 123.20   |
| 14  | g     | 838 | CLA  | C1-C2-C3    | -2.33 | 122.39      | 126.20   |
| 17  | n     | 843 | BCR  | C38-C26-C27 | 2.33  | 118.56      | 113.60   |
| 17  | b     | 852 | BCR  | C38-C26-C27 | 2.33  | 118.56      | 113.60   |
| 14  | N     | 825 | CLA  | CHB-C4A-NA  | 2.33  | 127.76      | 124.40   |
| 14  | A     | 808 | CLA  | CHB-C4A-NA  | 2.33  | 127.76      | 124.40   |
| 14  | b     | 827 | CLA  | CMB-C2B-C1B | -2.32 | 121.88      | 125.42   |
| 14  | g     | 829 | CLA  | CHB-C4A-NA  | 2.32  | 127.75      | 124.40   |
| 14  | b     | 839 | CLA  | CHB-C4A-NA  | 2.32  | 127.75      | 124.40   |
| 14  | N     | 837 | CLA  | CHB-C4A-NA  | 2.32  | 127.75      | 124.40   |
| 20  | b     | 801 | SQD  | O5-C5-C4    | 2.32  | 113.88      | 109.70   |
| 14  | N     | 809 | CLA  | C3B-C4B-NB  | -2.32 | 108.46      | 110.53   |
| 14  | N     | 806 | CLA  | CHB-C4A-NA  | 2.32  | 127.75      | 124.40   |
| 14  | a     | 831 | CLA  | C3B-C4B-NB  | -2.32 | 108.46      | 110.53   |
| 14  | B     | 815 | CLA  | C1-C2-C3    | -2.32 | 123.01      | 126.76   |
| 17  | B     | 848 | BCR  | C29-C30-C25 | 2.32  | 113.81      | 110.44   |
| 14  | s     | 201 | CLA  | C1-C2-C3    | -2.32 | 122.40      | 126.20   |
| 14  | n     | 834 | CLA  | CMB-C2B-C1B | -2.32 | 121.89      | 125.42   |
| 17  | B     | 843 | BCR  | C33-C5-C6   | -2.31 | 121.96      | 124.48   |
| 17  | I     | 102 | BCR  | C31-C1-C6   | -2.31 | 106.61      | 110.24   |
| 17  | n     | 845 | BCR  | C15-C16-C17 | -2.31 | 118.78      | 123.52   |
| 14  | S     | 201 | CLA  | CHB-C4A-NA  | 2.31  | 127.74      | 124.40   |
| 14  | g     | 836 | CLA  | CMB-C2B-C1B | -2.31 | 121.90      | 125.42   |
| 14  | A     | 827 | CLA  | CMB-C2B-C1B | -2.31 | 121.90      | 125.42   |
| 14  | B     | 832 | CLA  | CHB-C4A-NA  | 2.31  | 127.74      | 124.40   |
| 14  | B     | 850 | CLA  | CHB-C4A-NA  | 2.31  | 127.73      | 124.40   |
| 14  | G     | 835 | CLA  | C3B-C4B-NB  | -2.31 | 108.47      | 110.53   |
| 17  | N     | 853 | BCR  | C20-C19-C18 | -2.31 | 120.03      | 126.36   |
| 19  | g     | 851 | CL0  | C4C-C3C-C2C | -2.31 | 104.25      | 113.37   |
| 14  | B     | 841 | CLA  | CHB-C4A-NA  | 2.31  | 127.73      | 124.40   |
| 17  | w     | 206 | BCR  | C28-C27-C26 | -2.31 | 109.94      | 114.06   |
| 14  | n     | 807 | CLA  | CHB-C4A-NA  | 2.31  | 127.73      | 124.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | g     | 848  | BCR  | C33-C5-C4   | 2.31  | 118.52      | 113.60   |
| 14  | L     | 1503 | CLA  | CHB-C4A-NA  | 2.31  | 127.73      | 124.40   |
| 14  | B     | 850  | CLA  | O2A-CGA-O1A | -2.31 | 117.85      | 123.63   |
| 14  | G     | 808  | CLA  | CHB-C4A-NA  | 2.31  | 127.73      | 124.40   |
| 17  | a     | 845  | BCR  | C1-C6-C5    | -2.31 | 119.48      | 122.64   |
| 14  | G     | 807  | CLA  | C1-C2-C3    | -2.31 | 122.42      | 126.20   |
| 14  | g     | 836  | CLA  | CHB-C4A-NA  | 2.31  | 127.73      | 124.40   |
| 14  | B     | 807  | CLA  | C1-C2-C3    | -2.31 | 122.42      | 126.20   |
| 14  | a     | 827  | CLA  | C1-C2-C3    | -2.31 | 122.42      | 126.20   |
| 17  | a     | 848  | BCR  | C23-C24-C25 | -2.31 | 120.84      | 127.00   |
| 14  | B     | 836  | CLA  | CHB-C4A-NA  | 2.30  | 127.72      | 124.40   |
| 14  | n     | 832  | CLA  | O2A-CGA-O1A | -2.30 | 117.86      | 123.63   |
| 17  | m     | 102  | BCR  | C7-C8-C9    | -2.30 | 122.83      | 126.23   |
| 17  | F     | 203  | BCR  | C15-C16-C17 | -2.30 | 118.81      | 123.52   |
| 17  | g     | 843  | BCR  | C21-C20-C19 | -2.30 | 116.53      | 123.20   |
| 14  | N     | 820  | CLA  | CHB-C4A-NA  | 2.30  | 127.72      | 124.40   |
| 17  | n     | 842  | BCR  | C33-C5-C4   | 2.30  | 118.50      | 113.60   |
| 14  | g     | 827  | CLA  | CHB-C4A-NA  | 2.30  | 127.72      | 124.40   |
| 14  | G     | 853  | CLA  | C1-C2-C3    | -2.30 | 122.43      | 126.20   |
| 17  | A     | 848  | BCR  | C10-C11-C12 | -2.30 | 116.53      | 123.20   |
| 17  | b     | 845  | BCR  | C37-C22-C21 | -2.30 | 119.09      | 122.82   |
| 14  | A     | 802  | CLA  | C1-C2-C3    | -2.30 | 122.43      | 126.20   |
| 14  | a     | 834  | CLA  | C3B-C4B-NB  | -2.30 | 108.48      | 110.53   |
| 14  | g     | 831  | CLA  | CHB-C4A-NA  | 2.30  | 127.72      | 124.40   |
| 17  | l     | 206  | BCR  | C15-C16-C17 | -2.30 | 118.82      | 123.52   |
| 14  | B     | 834  | CLA  | O2A-CGA-O1A | -2.30 | 117.88      | 123.63   |
| 14  | g     | 823  | CLA  | CMB-C2B-C1B | -2.30 | 121.92      | 125.42   |
| 17  | N     | 846  | BCR  | C11-C12-C13 | -2.30 | 120.07      | 126.36   |
| 17  | i     | 101  | BCR  | C21-C20-C19 | -2.30 | 116.55      | 123.20   |
| 17  | G     | 845  | BCR  | C15-C16-C17 | -2.30 | 118.82      | 123.52   |
| 15  | a     | 841  | PQN  | C11-C12-C13 | -2.30 | 122.88      | 126.83   |
| 14  | N     | 842  | CLA  | CHB-C4A-NA  | 2.29  | 127.71      | 124.40   |
| 14  | G     | 828  | CLA  | C1-C2-C3    | -2.29 | 122.44      | 126.20   |
| 17  | A     | 848  | BCR  | C16-C15-C14 | -2.29 | 118.83      | 123.52   |
| 15  | n     | 841  | PQN  | C14-C13-C15 | 2.29  | 119.21      | 115.23   |
| 14  | G     | 805  | CLA  | C1-C2-C3    | -2.29 | 122.44      | 126.20   |
| 14  | g     | 824  | CLA  | CHB-C4A-NA  | 2.29  | 127.71      | 124.40   |
| 14  | b     | 812  | CLA  | CHB-C4A-NA  | 2.29  | 127.71      | 124.40   |
| 14  | b     | 803  | CLA  | CHB-C4A-NA  | 2.29  | 127.71      | 124.40   |
| 14  | B     | 829  | CLA  | C3B-C4B-NB  | -2.29 | 108.48      | 110.53   |
| 17  | N     | 847  | BCR  | C30-C25-C26 | -2.29 | 119.50      | 122.64   |
| 17  | G     | 847  | BCR  | C8-C7-C6    | -2.29 | 120.88      | 127.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | b     | 847 | BCR  | C38-C26-C27 | 2.29  | 118.48      | 113.60   |
| 17  | w     | 206 | BCR  | C38-C26-C27 | 2.29  | 118.48      | 113.60   |
| 14  | A     | 853 | CLA  | CHB-C4A-NA  | 2.29  | 127.70      | 124.40   |
| 14  | a     | 821 | CLA  | CHB-C4A-NA  | 2.29  | 127.70      | 124.40   |
| 14  | g     | 834 | CLA  | C3B-C4B-NB  | -2.29 | 108.49      | 110.53   |
| 14  | G     | 832 | CLA  | CHB-C4A-NA  | 2.29  | 127.70      | 124.40   |
| 17  | A     | 849 | BCR  | C23-C24-C25 | -2.29 | 120.89      | 127.00   |
| 17  | n     | 843 | BCR  | C33-C5-C4   | 2.29  | 118.47      | 113.60   |
| 14  | n     | 814 | CLA  | O2A-CGA-O1A | -2.29 | 117.91      | 123.63   |
| 17  | j     | 103 | BCR  | C23-C24-C25 | -2.28 | 120.89      | 127.00   |
| 14  | A     | 805 | CLA  | CHB-C4A-NA  | 2.28  | 127.70      | 124.40   |
| 14  | A     | 854 | CLA  | C1-C2-C3    | -2.28 | 122.45      | 126.20   |
| 17  | G     | 844 | BCR  | C30-C25-C26 | -2.28 | 119.52      | 122.64   |
| 17  | a     | 846 | BCR  | C2-C1-C6    | 2.28  | 113.75      | 110.44   |
| 17  | A     | 844 | BCR  | C33-C5-C4   | 2.28  | 118.46      | 113.60   |
| 17  | I     | 102 | BCR  | C2-C1-C6    | 2.28  | 113.75      | 110.44   |
| 17  | w     | 201 | BCR  | C33-C5-C4   | 2.28  | 118.46      | 113.60   |
| 14  | B     | 839 | CLA  | CHB-C4A-NA  | 2.28  | 127.69      | 124.40   |
| 14  | b     | 810 | CLA  | O2A-CGA-O1A | -2.28 | 117.92      | 123.63   |
| 17  | Y     | 101 | BCR  | C7-C8-C9    | -2.28 | 122.86      | 126.23   |
| 14  | A     | 821 | CLA  | CHB-C4A-NA  | 2.28  | 127.69      | 124.40   |
| 14  | N     | 816 | CLA  | C1-C2-C3    | -2.28 | 123.07      | 126.76   |
| 14  | A     | 808 | CLA  | CMB-C2B-C1B | -2.28 | 121.95      | 125.42   |
| 17  | G     | 843 | BCR  | C28-C27-C26 | -2.28 | 109.99      | 114.06   |
| 14  | b     | 805 | CLA  | CHB-C4A-NA  | 2.28  | 127.69      | 124.40   |
| 14  | b     | 814 | CLA  | CMB-C2B-C1B | -2.28 | 121.95      | 125.42   |
| 14  | a     | 807 | CLA  | O2A-CGA-O1A | -2.28 | 117.93      | 123.63   |
| 20  | b     | 801 | SQD  | O8-S-C6     | 2.28  | 110.37      | 105.97   |
| 14  | a     | 853 | CLA  | C1-C2-C3    | -2.28 | 122.47      | 126.20   |
| 14  | n     | 852 | CLA  | CHB-C4A-NA  | 2.28  | 127.68      | 124.40   |
| 14  | N     | 827 | CLA  | C1-C2-C3    | -2.27 | 122.47      | 126.20   |
| 14  | g     | 823 | CLA  | C1-C2-C3    | -2.27 | 122.47      | 126.20   |
| 14  | N     | 811 | CLA  | CMB-C2B-C1B | -2.27 | 121.96      | 125.42   |
| 14  | N     | 814 | CLA  | C1-C2-C3    | -2.27 | 122.47      | 126.20   |
| 17  | b     | 847 | BCR  | C8-C7-C6    | -2.27 | 120.92      | 127.00   |
| 17  | U     | 103 | BCR  | C33-C5-C4   | 2.27  | 118.44      | 113.60   |
| 14  | N     | 809 | CLA  | CHB-C4A-NA  | 2.27  | 127.68      | 124.40   |
| 14  | b     | 829 | CLA  | CMB-C2B-C1B | -2.27 | 121.96      | 125.42   |
| 17  | N     | 849 | BCR  | C38-C26-C25 | -2.27 | 122.01      | 124.48   |
| 17  | l     | 206 | BCR  | C23-C24-C25 | -2.27 | 120.93      | 127.00   |
| 14  | b     | 809 | CLA  | O2D-CGD-CBD | 2.27  | 115.20      | 111.23   |
| 17  | M     | 101 | BCR  | C34-C9-C8   | 2.27  | 121.56      | 118.09   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | b     | 809 | CLA  | C1-C2-C3    | -2.27 | 122.48      | 126.20   |
| 14  | a     | 831 | CLA  | CMB-C2B-C1B | -2.27 | 121.96      | 125.42   |
| 17  | k     | 102 | BCR  | C20-C19-C18 | -2.27 | 120.14      | 126.36   |
| 14  | W     | 203 | CLA  | O2A-CGA-O1A | -2.27 | 117.95      | 123.63   |
| 17  | l     | 205 | BCR  | C40-C30-C25 | -2.27 | 106.69      | 110.24   |
| 17  | W     | 205 | BCR  | C3-C4-C5    | -2.27 | 110.01      | 114.06   |
| 14  | n     | 823 | CLA  | CHB-C4A-NA  | 2.27  | 127.67      | 124.40   |
| 17  | a     | 847 | BCR  | C23-C24-C25 | -2.27 | 120.94      | 127.00   |
| 14  | f     | 202 | CLA  | CHB-C4A-NA  | 2.27  | 127.67      | 124.40   |
| 14  | A     | 831 | CLA  | CMB-C2B-C3B | 2.27  | 131.88      | 126.55   |
| 14  | N     | 829 | CLA  | CHB-C4A-NA  | 2.27  | 127.67      | 124.40   |
| 17  | A     | 846 | BCR  | C38-C26-C27 | 2.27  | 118.43      | 113.60   |
| 17  | n     | 849 | BCR  | C16-C15-C14 | -2.27 | 118.88      | 123.52   |
| 17  | a     | 844 | BCR  | C16-C15-C14 | -2.27 | 118.88      | 123.52   |
| 14  | g     | 826 | CLA  | CMB-C2B-C1B | -2.27 | 121.97      | 125.42   |
| 14  | A     | 811 | CLA  | C1-C2-C3    | -2.26 | 122.49      | 126.20   |
| 14  | b     | 840 | CLA  | O2A-CGA-O1A | -2.26 | 117.97      | 123.63   |
| 17  | t     | 103 | BCR  | C23-C24-C25 | -2.26 | 120.95      | 127.00   |
| 14  | b     | 828 | CLA  | O2A-CGA-O1A | -2.26 | 117.97      | 123.63   |
| 14  | G     | 805 | CLA  | CMB-C2B-C1B | -2.26 | 121.97      | 125.42   |
| 17  | i     | 101 | BCR  | C31-C1-C6   | -2.26 | 106.69      | 110.24   |
| 14  | B     | 841 | CLA  | C1-C2-C3    | -2.26 | 122.49      | 126.20   |
| 14  | n     | 818 | CLA  | CHB-C4A-NA  | 2.26  | 127.66      | 124.40   |
| 14  | n     | 819 | CLA  | C1-C2-C3    | -2.26 | 122.49      | 126.20   |
| 14  | n     | 803 | CLA  | CHB-C4A-NA  | 2.26  | 127.66      | 124.40   |
| 17  | Y     | 101 | BCR  | C38-C26-C27 | 2.26  | 118.41      | 113.60   |
| 17  | b     | 847 | BCR  | C23-C24-C25 | -2.26 | 120.96      | 127.00   |
| 17  | a     | 845 | BCR  | C38-C26-C27 | 2.26  | 118.41      | 113.60   |
| 17  | a     | 848 | BCR  | C1-C6-C7    | 2.26  | 121.77      | 115.65   |
| 17  | a     | 846 | BCR  | C35-C13-C12 | 2.26  | 121.54      | 118.09   |
| 14  | B     | 834 | CLA  | C1-C2-C3    | -2.26 | 122.50      | 126.20   |
| 14  | n     | 827 | CLA  | C3B-C4B-NB  | -2.26 | 108.52      | 110.53   |
| 17  | l     | 205 | BCR  | C38-C26-C27 | 2.26  | 118.41      | 113.60   |
| 17  | N     | 853 | BCR  | C33-C5-C6   | -2.26 | 122.02      | 124.48   |
| 17  | g     | 843 | BCR  | C37-C22-C23 | 2.25  | 121.53      | 118.09   |
| 17  | a     | 847 | BCR  | C38-C26-C25 | -2.25 | 122.03      | 124.48   |
| 14  | N     | 801 | CLA  | CHB-C4A-NA  | 2.25  | 127.65      | 124.40   |
| 14  | g     | 817 | CLA  | CHB-C4A-NA  | 2.25  | 127.65      | 124.40   |
| 14  | B     | 827 | CLA  | C1-C2-C3    | -2.25 | 122.51      | 126.20   |
| 14  | A     | 830 | CLA  | O2A-CGA-O1A | -2.25 | 117.99      | 123.63   |
| 14  | a     | 819 | CLA  | CMB-C2B-C1B | -2.25 | 121.99      | 125.42   |
| 14  | B     | 828 | CLA  | CHB-C4A-NA  | 2.25  | 127.65      | 124.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 824  | CLA  | O2A-CGA-O1A | -2.25 | 118.00      | 123.63   |
| 17  | N     | 847  | BCR  | C27-C26-C25 | -2.25 | 119.66      | 122.70   |
| 14  | W     | 204  | CLA  | CHB-C4A-NA  | 2.25  | 127.65      | 124.40   |
| 14  | a     | 817  | CLA  | CHB-C4A-NA  | 2.25  | 127.65      | 124.40   |
| 17  | a     | 848  | BCR  | C4-C5-C6    | -2.25 | 119.66      | 122.70   |
| 14  | N     | 841  | CLA  | C1-C2-C3    | -2.25 | 122.51      | 126.20   |
| 14  | B     | 835  | CLA  | C3B-C4B-NB  | -2.25 | 108.52      | 110.53   |
| 14  | a     | 826  | CLA  | CHB-C4A-NA  | 2.25  | 127.65      | 124.40   |
| 20  | H     | 1702 | SQD  | O5-C5-C4    | 2.25  | 113.75      | 109.70   |
| 14  | G     | 822  | CLA  | C1-C2-C3    | -2.25 | 122.51      | 126.20   |
| 17  | b     | 845  | BCR  | C33-C5-C4   | 2.25  | 118.39      | 113.60   |
| 14  | g     | 801  | CLA  | CMB-C2B-C1B | -2.25 | 122.00      | 125.42   |
| 17  | V     | 101  | BCR  | C28-C27-C26 | -2.25 | 110.05      | 114.06   |
| 17  | A     | 856  | BCR  | C33-C5-C4   | 2.25  | 118.39      | 113.60   |
| 17  | J     | 103  | BCR  | C15-C16-C17 | -2.25 | 118.92      | 123.52   |
| 14  | A     | 825  | CLA  | O2A-CGA-O1A | -2.25 | 118.01      | 123.63   |
| 14  | A     | 854  | CLA  | O2A-CGA-O1A | -2.25 | 118.01      | 123.63   |
| 14  | a     | 801  | CLA  | CMB-C2B-C1B | -2.25 | 122.00      | 125.42   |
| 17  | g     | 843  | BCR  | C8-C7-C6    | -2.25 | 121.00      | 127.00   |
| 14  | n     | 852  | CLA  | O2A-CGA-O1A | -2.25 | 118.01      | 123.63   |
| 14  | g     | 830  | CLA  | O2A-CGA-O1A | -2.25 | 118.01      | 123.63   |
| 14  | G     | 815  | CLA  | CHB-C4A-NA  | 2.25  | 127.64      | 124.40   |
| 14  | b     | 826  | CLA  | CMB-C2B-C1B | -2.25 | 122.00      | 125.42   |
| 17  | T     | 104  | BCR  | C8-C7-C6    | -2.25 | 121.00      | 127.00   |
| 14  | G     | 806  | CLA  | O2A-CGA-O1A | -2.25 | 118.01      | 123.63   |
| 14  | B     | 810  | CLA  | CHB-C4A-NA  | 2.24  | 127.64      | 124.40   |
| 17  | g     | 844  | BCR  | C33-C5-C4   | 2.24  | 118.38      | 113.60   |
| 17  | W     | 201  | BCR  | C8-C9-C10   | -2.24 | 115.48      | 119.01   |
| 14  | b     | 819  | CLA  | CHB-C4A-NA  | 2.24  | 127.64      | 124.40   |
| 14  | g     | 830  | CLA  | CMB-C2B-C1B | -2.24 | 122.01      | 125.42   |
| 14  | N     | 809  | CLA  | O2A-CGA-O1A | -2.24 | 118.02      | 123.63   |
| 17  | G     | 848  | BCR  | C32-C1-C6   | -2.24 | 106.73      | 110.24   |
| 14  | A     | 812  | CLA  | C1-C2-C3    | -2.24 | 122.53      | 126.20   |
| 17  | G     | 848  | BCR  | C1-C6-C7    | 2.24  | 121.72      | 115.65   |
| 14  | n     | 808  | CLA  | O2D-CGD-CBD | 2.24  | 115.14      | 111.23   |
| 17  | b     | 848  | BCR  | C21-C20-C19 | -2.24 | 116.72      | 123.20   |
| 14  | a     | 830  | CLA  | O2A-CGA-O1A | -2.24 | 118.03      | 123.63   |
| 17  | b     | 843  | BCR  | C8-C7-C6    | -2.24 | 121.02      | 127.00   |
| 14  | G     | 819  | CLA  | O2A-CGA-O1A | -2.24 | 118.03      | 123.63   |
| 14  | A     | 822  | CLA  | C1-C2-C3    | -2.24 | 122.53      | 126.20   |
| 17  | T     | 104  | BCR  | C20-C19-C18 | -2.24 | 120.23      | 126.36   |
| 17  | N     | 852  | BCR  | C27-C26-C25 | -2.23 | 119.68      | 122.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | A     | 847  | BCR  | C8-C7-C6    | -2.23 | 121.03      | 127.00   |
| 14  | A     | 839  | CLA  | C1-C2-C3    | -2.23 | 122.54      | 126.20   |
| 14  | G     | 822  | CLA  | CMB-C2B-C1B | -2.23 | 122.02      | 125.42   |
| 14  | g     | 820  | CLA  | CMB-C2B-C1B | -2.23 | 122.02      | 125.42   |
| 14  | G     | 801  | CLA  | CMB-C2B-C1B | -2.23 | 122.02      | 125.42   |
| 14  | B     | 838  | CLA  | O2A-CGA-O1A | -2.23 | 118.04      | 123.63   |
| 17  | n     | 851  | BCR  | C38-C26-C25 | -2.23 | 122.05      | 124.48   |
| 14  | A     | 801  | CLA  | C1-C2-C3    | -2.23 | 122.54      | 126.20   |
| 17  | g     | 847  | BCR  | C23-C24-C25 | -2.23 | 121.04      | 127.00   |
| 14  | N     | 830  | CLA  | CHB-C4A-NA  | 2.23  | 127.61      | 124.40   |
| 17  | b     | 846  | BCR  | C23-C24-C25 | -2.23 | 121.05      | 127.00   |
| 14  | n     | 826  | CLA  | C1-C2-C3    | -2.23 | 122.55      | 126.20   |
| 14  | A     | 804  | CLA  | O2A-CGA-O1A | -2.23 | 118.06      | 123.63   |
| 14  | B     | 838  | CLA  | C1-C2-C3    | -2.23 | 122.55      | 126.20   |
| 14  | b     | 828  | CLA  | CHB-C4A-NA  | 2.23  | 127.61      | 124.40   |
| 14  | b     | 813  | CLA  | CMB-C2B-C1B | -2.23 | 122.03      | 125.42   |
| 17  | L     | 1504 | BCR  | C4-C5-C6    | -2.22 | 119.70      | 122.70   |
| 17  | A     | 846  | BCR  | C2-C1-C6    | 2.22  | 113.67      | 110.44   |
| 14  | N     | 813  | CLA  | C1-C2-C3    | -2.22 | 122.55      | 126.20   |
| 17  | S     | 204  | BCR  | C38-C26-C27 | 2.22  | 118.34      | 113.60   |
| 14  | G     | 829  | CLA  | CMB-C2B-C1B | -2.22 | 122.03      | 125.42   |
| 17  | g     | 843  | BCR  | C23-C24-C25 | -2.22 | 121.06      | 127.00   |
| 14  | n     | 832  | CLA  | O2D-CGD-CBD | 2.22  | 115.12      | 111.23   |
| 14  | n     | 813  | CLA  | CMB-C2B-C1B | -2.22 | 122.03      | 125.42   |
| 14  | b     | 827  | CLA  | C1-C2-C3    | -2.22 | 122.56      | 126.20   |
| 14  | b     | 840  | CLA  | C1-C2-C3    | -2.22 | 122.56      | 126.20   |
| 17  | G     | 845  | BCR  | C38-C26-C27 | 2.22  | 118.33      | 113.60   |
| 19  | a     | 851  | CL0  | O1D-CGD-CBD | 2.22  | 128.09      | 124.72   |
| 17  | a     | 844  | BCR  | C8-C7-C6    | -2.22 | 121.06      | 127.00   |
| 14  | b     | 814  | CLA  | O2A-CGA-O1A | -2.22 | 118.07      | 123.63   |
| 17  | t     | 104  | BCR  | C33-C5-C4   | 2.22  | 118.33      | 113.60   |
| 17  | a     | 848  | BCR  | C38-C26-C27 | 2.22  | 118.33      | 113.60   |
| 17  | n     | 844  | BCR  | C33-C5-C4   | 2.22  | 118.33      | 113.60   |
| 14  | b     | 837  | CLA  | CMB-C2B-C1B | -2.22 | 122.04      | 125.42   |
| 17  | n     | 842  | BCR  | C20-C19-C18 | -2.22 | 120.28      | 126.36   |
| 14  | b     | 838  | CLA  | O2A-CGA-O1A | -2.22 | 118.08      | 123.63   |
| 14  | G     | 828  | CLA  | CHB-C4A-NA  | 2.22  | 127.60      | 124.40   |
| 14  | n     | 839  | CLA  | C1-C2-C3    | -2.22 | 122.56      | 126.20   |
| 14  | N     | 834  | CLA  | O2A-CGA-O1A | -2.22 | 118.08      | 123.63   |
| 14  | n     | 837  | CLA  | O2A-CGA-O1A | -2.22 | 118.08      | 123.63   |
| 17  | G     | 844  | BCR  | C8-C7-C6    | -2.22 | 121.08      | 127.00   |
| 14  | A     | 827  | CLA  | CHB-C4A-NA  | 2.22  | 127.60      | 124.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | a     | 831  | CLA  | CHB-C4A-NA  | 2.22  | 127.60      | 124.40   |
| 17  | n     | 851  | BCR  | C4-C5-C6    | -2.22 | 119.71      | 122.70   |
| 14  | B     | 824  | CLA  | CHB-C4A-NA  | 2.22  | 127.60      | 124.40   |
| 17  | S     | 204  | BCR  | C33-C5-C4   | 2.22  | 118.32      | 113.60   |
| 17  | I     | 103  | BCR  | C21-C20-C19 | -2.22 | 116.78      | 123.20   |
| 17  | N     | 849  | BCR  | C33-C5-C4   | 2.22  | 118.32      | 113.60   |
| 14  | B     | 826  | CLA  | O2A-CGA-O1A | -2.22 | 118.09      | 123.63   |
| 14  | A     | 824  | CLA  | C3B-C4B-NB  | -2.21 | 108.55      | 110.53   |
| 17  | t     | 104  | BCR  | C8-C7-C6    | -2.21 | 121.08      | 127.00   |
| 14  | g     | 806  | CLA  | O2D-CGD-CBD | 2.21  | 115.10      | 111.23   |
| 17  | n     | 842  | BCR  | C3-C4-C5    | -2.21 | 110.11      | 114.06   |
| 17  | k     | 102  | BCR  | C16-C15-C14 | -2.21 | 118.99      | 123.52   |
| 17  | s     | 203  | BCR  | C38-C26-C27 | 2.21  | 118.31      | 113.60   |
| 17  | g     | 844  | BCR  | C8-C7-C6    | -2.21 | 121.09      | 127.00   |
| 14  | a     | 826  | CLA  | C3B-C4B-NB  | -2.21 | 108.56      | 110.53   |
| 17  | G     | 843  | BCR  | C16-C15-C14 | -2.21 | 119.00      | 123.52   |
| 17  | G     | 843  | BCR  | C21-C20-C19 | -2.21 | 116.80      | 123.20   |
| 14  | B     | 828  | CLA  | O2A-CGA-O1A | -2.21 | 118.10      | 123.63   |
| 17  | B     | 852  | BCR  | C28-C27-C26 | -2.21 | 110.12      | 114.06   |
| 17  | G     | 843  | BCR  | C33-C5-C4   | 2.21  | 118.30      | 113.60   |
| 17  | B     | 845  | BCR  | C34-C9-C10  | -2.21 | 119.24      | 122.82   |
| 14  | n     | 850  | CLA  | O2A-CGA-O1A | -2.21 | 118.11      | 123.63   |
| 14  | B     | 833  | CLA  | O2A-CGA-O1A | -2.21 | 118.11      | 123.63   |
| 14  | g     | 804  | CLA  | O2A-CGA-O1A | -2.21 | 118.11      | 123.63   |
| 14  | g     | 811  | CLA  | C1-C2-C3    | -2.21 | 122.58      | 126.20   |
| 14  | N     | 808  | CLA  | O2A-CGA-O1A | -2.21 | 118.11      | 123.63   |
| 17  | b     | 846  | BCR  | C37-C22-C23 | 2.21  | 121.46      | 118.09   |
| 14  | g     | 824  | CLA  | O2A-CGA-O1A | -2.21 | 118.11      | 123.63   |
| 14  | A     | 834  | CLA  | O2A-CGA-O1A | -2.20 | 118.11      | 123.63   |
| 17  | G     | 847  | BCR  | C38-C26-C25 | -2.20 | 122.08      | 124.48   |
| 14  | a     | 838  | CLA  | O2A-CGA-O1A | -2.20 | 118.12      | 123.63   |
| 17  | n     | 844  | BCR  | C37-C22-C21 | -2.20 | 119.25      | 122.82   |
| 14  | g     | 832  | CLA  | C1-C2-C3    | -2.20 | 122.59      | 126.20   |
| 17  | w     | 206  | BCR  | C15-C16-C17 | -2.20 | 119.01      | 123.52   |
| 14  | B     | 804  | CLA  | CHB-C4A-NA  | 2.20  | 127.58      | 124.40   |
| 20  | x     | 1702 | SQD  | O8-S-C6     | 2.20  | 110.22      | 105.97   |
| 14  | N     | 804  | CLA  | CHB-C4A-NA  | 2.20  | 127.58      | 124.40   |
| 14  | g     | 804  | CLA  | C1-C2-C3    | -2.20 | 122.59      | 126.20   |
| 18  | v     | 102  | LHG  | C26-C25-C24 | 2.20  | 121.21      | 113.13   |
| 15  | a     | 841  | PQN  | C12-C11-C3  | -2.20 | 106.66      | 112.08   |
| 17  | g     | 843  | BCR  | C16-C15-C14 | -2.20 | 119.02      | 123.52   |
| 17  | S     | 204  | BCR  | C21-C20-C19 | -2.20 | 116.83      | 123.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | b     | 844  | BCR  | C21-C20-C19 | -2.20 | 116.84      | 123.20   |
| 17  | A     | 847  | BCR  | C20-C19-C18 | -2.20 | 120.34      | 126.36   |
| 14  | a     | 853  | CLA  | C3B-C4B-NB  | -2.20 | 108.57      | 110.53   |
| 17  | N     | 845  | BCR  | C4-C5-C6    | -2.19 | 119.74      | 122.70   |
| 17  | B     | 844  | BCR  | C36-C18-C17 | -2.19 | 119.26      | 122.82   |
| 14  | B     | 811  | CLA  | C1-C2-C3    | -2.19 | 122.60      | 126.20   |
| 14  | B     | 840  | CLA  | O2A-CGA-O1A | -2.19 | 118.15      | 123.63   |
| 14  | n     | 808  | CLA  | C1-C2-C3    | -2.19 | 122.61      | 126.20   |
| 17  | K     | 102  | BCR  | C10-C11-C12 | -2.19 | 116.85      | 123.20   |
| 14  | a     | 823  | CLA  | C1-C2-C3    | -2.19 | 122.61      | 126.20   |
| 17  | g     | 848  | BCR  | C16-C15-C14 | -2.19 | 119.04      | 123.52   |
| 14  | A     | 826  | CLA  | CHD-C1D-ND  | -2.19 | 121.72      | 124.80   |
| 14  | A     | 808  | CLA  | O2A-CGA-O1A | -2.19 | 118.15      | 123.63   |
| 14  | g     | 806  | CLA  | O2A-CGA-O1A | -2.19 | 118.15      | 123.63   |
| 14  | g     | 854  | CLA  | CHB-C4A-NA  | 2.19  | 127.56      | 124.40   |
| 14  | B     | 827  | CLA  | CMB-C2B-C1B | -2.19 | 122.09      | 125.42   |
| 17  | G     | 846  | BCR  | C21-C20-C19 | -2.19 | 116.86      | 123.20   |
| 17  | t     | 104  | BCR  | C10-C11-C12 | -2.19 | 116.86      | 123.20   |
| 14  | A     | 818  | CLA  | O2A-CGA-O1A | -2.19 | 118.16      | 123.63   |
| 14  | b     | 825  | CLA  | C1-C2-C3    | -2.19 | 122.61      | 126.20   |
| 17  | k     | 102  | BCR  | C33-C5-C4   | 2.19  | 118.26      | 113.60   |
| 14  | L     | 1501 | CLA  | O2D-CGD-CBD | 2.19  | 115.05      | 111.23   |
| 17  | A     | 845  | BCR  | C33-C5-C4   | 2.19  | 118.26      | 113.60   |
| 20  | B     | 801  | SQD  | O8-S-C6     | 2.18  | 110.19      | 105.97   |
| 14  | a     | 806  | CLA  | O2D-CGD-CBD | 2.18  | 115.05      | 111.23   |
| 14  | L     | 1501 | CLA  | C1-C2-C3    | -2.18 | 122.62      | 126.20   |
| 20  | w     | 202  | SQD  | O8-S-C6     | 2.18  | 110.19      | 105.97   |
| 14  | B     | 841  | CLA  | C3B-C4B-NB  | -2.18 | 108.58      | 110.53   |
| 14  | G     | 818  | CLA  | O2A-CGA-O1A | -2.18 | 118.16      | 123.63   |
| 14  | B     | 814  | CLA  | O2A-CGA-O1A | -2.18 | 118.16      | 123.63   |
| 14  | n     | 833  | CLA  | O2D-CGD-CBD | 2.18  | 115.05      | 111.23   |
| 17  | W     | 205  | BCR  | C33-C5-C6   | -2.18 | 122.10      | 124.48   |
| 17  | g     | 847  | BCR  | C16-C15-C14 | -2.18 | 119.05      | 123.52   |
| 14  | l     | 202  | CLA  | O2D-CGD-CBD | 2.18  | 115.04      | 111.23   |
| 14  | A     | 833  | CLA  | C1-C2-C3    | -2.18 | 122.62      | 126.20   |
| 14  | B     | 808  | CLA  | CMB-C2B-C1B | -2.18 | 122.10      | 125.42   |
| 17  | G     | 844  | BCR  | C27-C26-C25 | -2.18 | 119.76      | 122.70   |
| 14  | N     | 827  | CLA  | O2A-CGA-O1A | -2.18 | 118.18      | 123.63   |
| 14  | G     | 836  | CLA  | C1-C2-C3    | -2.18 | 122.63      | 126.20   |
| 17  | a     | 844  | BCR  | C33-C5-C4   | 2.18  | 118.24      | 113.60   |
| 17  | a     | 847  | BCR  | C21-C20-C19 | -2.18 | 116.89      | 123.20   |
| 14  | n     | 811  | CLA  | C1-C2-C3    | -2.18 | 122.63      | 126.20   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | G     | 830 | CLA  | O2A-CGA-O1A | -2.18 | 118.19      | 123.63   |
| 14  | G     | 813 | CLA  | O2A-CGA-O1A | -2.17 | 118.19      | 123.63   |
| 14  | N     | 814 | CLA  | O2A-CGA-O1A | -2.17 | 118.19      | 123.63   |
| 14  | a     | 811 | CLA  | O2A-CGA-O1A | -2.17 | 118.19      | 123.63   |
| 14  | a     | 827 | CLA  | CHB-C4A-NA  | 2.17  | 127.54      | 124.40   |
| 17  | g     | 847 | BCR  | C33-C5-C4   | 2.17  | 118.23      | 113.60   |
| 14  | n     | 836 | CLA  | CMB-C2B-C3B | 2.17  | 131.66      | 126.55   |
| 14  | N     | 835 | CLA  | O2A-CGA-O1A | -2.17 | 118.19      | 123.63   |
| 17  | y     | 101 | BCR  | C7-C8-C9    | -2.17 | 123.02      | 126.23   |
| 14  | B     | 819 | CLA  | C1-C2-C3    | -2.17 | 122.64      | 126.20   |
| 14  | b     | 820 | CLA  | C1-C2-C3    | -2.17 | 122.64      | 126.20   |
| 14  | G     | 837 | CLA  | O2D-CGD-CBD | 2.17  | 115.03      | 111.23   |
| 17  | B     | 848 | BCR  | C35-C13-C12 | 2.17  | 121.41      | 118.09   |
| 14  | b     | 835 | CLA  | CMB-C2B-C3B | 2.17  | 131.66      | 126.55   |
| 14  | B     | 836 | CLA  | CMB-C2B-C1B | -2.17 | 122.11      | 125.42   |
| 17  | w     | 201 | BCR  | C10-C11-C12 | -2.17 | 116.91      | 123.20   |
| 14  | a     | 825 | CLA  | C1-C2-C3    | -2.17 | 122.64      | 126.20   |
| 14  | n     | 824 | CLA  | O2A-CGA-O1A | -2.17 | 118.20      | 123.63   |
| 14  | B     | 831 | CLA  | C1-C2-C3    | -2.17 | 122.64      | 126.20   |
| 14  | g     | 826 | CLA  | CHB-C4A-NA  | 2.17  | 127.53      | 124.40   |
| 14  | g     | 834 | CLA  | CMB-C2B-C1B | -2.17 | 122.12      | 125.42   |
| 14  | a     | 812 | CLA  | O2A-CGA-O1A | -2.17 | 118.20      | 123.63   |
| 17  | N     | 853 | BCR  | C23-C24-C25 | -2.17 | 121.21      | 127.00   |
| 14  | g     | 854 | CLA  | C1-C2-C3    | -2.17 | 122.65      | 126.20   |
| 17  | u     | 103 | BCR  | C33-C5-C4   | 2.17  | 118.22      | 113.60   |
| 14  | A     | 830 | CLA  | C1-C2-C3    | -2.17 | 122.65      | 126.20   |
| 17  | A     | 856 | BCR  | C21-C20-C19 | -2.17 | 116.92      | 123.20   |
| 14  | b     | 834 | CLA  | O2D-CGD-CBD | 2.17  | 115.02      | 111.23   |
| 17  | B     | 843 | BCR  | C20-C19-C18 | -2.17 | 120.42      | 126.36   |
| 17  | a     | 845 | BCR  | C21-C20-C19 | -2.16 | 116.93      | 123.20   |
| 17  | a     | 845 | BCR  | C15-C16-C17 | -2.16 | 119.09      | 123.52   |
| 17  | w     | 201 | BCR  | C37-C22-C21 | -2.16 | 119.31      | 122.82   |
| 14  | B     | 815 | CLA  | O2A-CGA-O1A | -2.16 | 118.22      | 123.63   |
| 17  | T     | 103 | BCR  | C21-C20-C19 | -2.16 | 116.93      | 123.20   |
| 14  | A     | 815 | CLA  | CMB-C2B-C1B | -2.16 | 122.13      | 125.42   |
| 14  | n     | 837 | CLA  | C1-C2-C3    | -2.16 | 122.65      | 126.20   |
| 17  | N     | 844 | BCR  | C33-C5-C4   | 2.16  | 118.20      | 113.60   |
| 17  | W     | 206 | BCR  | C4-C5-C6    | -2.16 | 119.78      | 122.70   |
| 14  | N     | 827 | CLA  | CMB-C2B-C3B | 2.16  | 131.63      | 126.55   |
| 17  | N     | 852 | BCR  | C10-C11-C12 | -2.16 | 116.94      | 123.20   |
| 17  | b     | 846 | BCR  | C8-C7-C6    | -2.16 | 121.23      | 127.00   |
| 17  | F     | 203 | BCR  | C38-C26-C27 | 2.16  | 118.20      | 113.60   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 801  | CLA  | CMB-C2B-C3B | 2.16  | 131.63      | 126.55   |
| 17  | K     | 102  | BCR  | C2-C1-C6    | 2.16  | 113.58      | 110.44   |
| 14  | N     | 811  | CLA  | C1-C2-C3    | -2.16 | 122.66      | 126.20   |
| 14  | g     | 853  | CLA  | C1-C2-C3    | -2.16 | 122.66      | 126.20   |
| 17  | n     | 851  | BCR  | C27-C26-C25 | -2.16 | 119.79      | 122.70   |
| 14  | B     | 841  | CLA  | O2A-CGA-O1A | -2.16 | 118.23      | 123.63   |
| 17  | j     | 104  | BCR  | C4-C5-C6    | -2.16 | 119.79      | 122.70   |
| 14  | n     | 805  | CLA  | O2A-CGA-O1A | -2.16 | 118.23      | 123.63   |
| 14  | b     | 820  | CLA  | O2A-CGA-O1A | -2.16 | 118.23      | 123.63   |
| 17  | y     | 101  | BCR  | C15-C16-C17 | -2.16 | 119.11      | 123.52   |
| 17  | j     | 103  | BCR  | C38-C26-C27 | 2.16  | 118.19      | 113.60   |
| 14  | G     | 816  | CLA  | O2A-CGA-O1A | -2.15 | 118.24      | 123.63   |
| 17  | a     | 847  | BCR  | C16-C15-C14 | -2.15 | 119.11      | 123.52   |
| 17  | L     | 1504 | BCR  | C10-C11-C12 | -2.15 | 116.96      | 123.20   |
| 14  | b     | 812  | CLA  | O2D-CGD-CBD | 2.15  | 115.00      | 111.23   |
| 14  | g     | 807  | CLA  | O2A-CGA-O1A | -2.15 | 118.24      | 123.63   |
| 14  | B     | 806  | CLA  | CMB-C2B-C3B | 2.15  | 131.62      | 126.55   |
| 14  | B     | 810  | CLA  | C1-C2-C3    | -2.15 | 122.67      | 126.20   |
| 17  | T     | 104  | BCR  | C33-C5-C4   | 2.15  | 118.19      | 113.60   |
| 14  | s     | 201  | CLA  | O2A-CGA-O1A | -2.15 | 118.24      | 123.63   |
| 17  | I     | 101  | BCR  | C20-C19-C18 | -2.15 | 120.46      | 126.36   |
| 14  | G     | 839  | CLA  | O2A-CGA-O1A | -2.15 | 118.24      | 123.63   |
| 14  | n     | 825  | CLA  | O2A-CGA-O1A | -2.15 | 118.24      | 123.63   |
| 14  | A     | 827  | CLA  | CMB-C2B-C3B | 2.15  | 131.61      | 126.55   |
| 17  | A     | 849  | BCR  | C38-C26-C27 | 2.15  | 118.18      | 113.60   |
| 14  | A     | 840  | CLA  | C1-C2-C3    | -2.15 | 122.67      | 126.20   |
| 14  | G     | 807  | CLA  | CMB-C2B-C1B | -2.15 | 122.14      | 125.42   |
| 14  | N     | 830  | CLA  | C3B-C4B-NB  | -2.15 | 108.61      | 110.53   |
| 14  | b     | 834  | CLA  | O2A-CGA-O1A | -2.15 | 118.25      | 123.63   |
| 14  | g     | 801  | CLA  | C1-C2-C3    | -2.15 | 122.68      | 126.20   |
| 14  | b     | 832  | CLA  | C1-C2-C3    | -2.15 | 122.68      | 126.20   |
| 14  | n     | 827  | CLA  | O2A-CGA-O1A | -2.15 | 118.25      | 123.63   |
| 14  | n     | 829  | CLA  | C1-C2-C3    | -2.15 | 122.68      | 126.20   |
| 14  | n     | 827  | CLA  | CHB-C4A-NA  | 2.15  | 127.50      | 124.40   |
| 14  | G     | 805  | CLA  | O2A-CGA-O1A | -2.15 | 118.26      | 123.63   |
| 14  | a     | 832  | CLA  | O2D-CGD-CBD | 2.15  | 114.98      | 111.23   |
| 14  | G     | 807  | CLA  | O2A-CGA-O1A | -2.15 | 118.26      | 123.63   |
| 14  | U     | 102  | CLA  | O2A-CGA-O1A | -2.15 | 118.26      | 123.63   |
| 17  | G     | 847  | BCR  | C21-C20-C19 | -2.14 | 116.98      | 123.20   |
| 17  | n     | 843  | BCR  | C34-C9-C10  | -2.14 | 119.34      | 122.82   |
| 14  | g     | 805  | CLA  | C1-C2-C3    | -2.14 | 122.68      | 126.20   |
| 14  | b     | 830  | CLA  | O2A-CGA-O1A | -2.14 | 118.27      | 123.63   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | g     | 824  | CLA  | C1-C2-C3    | -2.14 | 122.69      | 126.20   |
| 17  | a     | 847  | BCR  | C10-C11-C12 | -2.14 | 116.99      | 123.20   |
| 17  | W     | 206  | BCR  | C38-C26-C27 | 2.14  | 118.16      | 113.60   |
| 14  | N     | 828  | CLA  | C1-C2-C3    | -2.14 | 122.69      | 126.20   |
| 17  | j     | 104  | BCR  | C16-C15-C14 | -2.14 | 119.14      | 123.52   |
| 17  | g     | 847  | BCR  | C15-C16-C17 | -2.14 | 119.14      | 123.52   |
| 14  | A     | 853  | CLA  | O1D-CGD-CBD | 2.14  | 128.74      | 124.52   |
| 17  | f     | 203  | BCR  | C11-C12-C13 | -2.14 | 120.50      | 126.36   |
| 14  | A     | 826  | CLA  | O2A-CGA-O1A | -2.14 | 118.28      | 123.63   |
| 14  | g     | 803  | CLA  | O2A-CGA-O1A | -2.14 | 118.28      | 123.63   |
| 19  | g     | 851  | CL0  | O1D-CGD-CBD | 2.14  | 127.97      | 124.72   |
| 17  | N     | 849  | BCR  | C11-C10-C9  | -2.14 | 124.28      | 127.28   |
| 14  | b     | 807  | CLA  | CMB-C2B-C1B | -2.14 | 122.16      | 125.42   |
| 17  | b     | 846  | BCR  | C38-C26-C27 | 2.14  | 118.15      | 113.60   |
| 17  | G     | 844  | BCR  | C16-C15-C14 | -2.14 | 119.14      | 123.52   |
| 14  | G     | 831  | CLA  | CMB-C2B-C3B | 2.14  | 131.58      | 126.55   |
| 17  | b     | 850  | BCR  | C20-C19-C18 | -2.14 | 120.50      | 126.36   |
| 14  | G     | 820  | CLA  | C1-C2-C3    | -2.14 | 122.69      | 126.20   |
| 14  | G     | 820  | CLA  | CMB-C2B-C3B | 2.14  | 131.58      | 126.55   |
| 17  | B     | 847  | BCR  | C21-C20-C19 | -2.14 | 117.01      | 123.20   |
| 14  | G     | 831  | CLA  | O2A-CGA-O1A | -2.14 | 118.28      | 123.63   |
| 14  | N     | 842  | CLA  | C1-C2-C3    | -2.14 | 122.70      | 126.20   |
| 17  | f     | 203  | BCR  | C15-C16-C17 | -2.14 | 119.15      | 123.52   |
| 14  | a     | 829  | CLA  | C1-C2-C3    | -2.14 | 122.70      | 126.20   |
| 14  | g     | 837  | CLA  | O2A-CGA-O1A | -2.14 | 118.29      | 123.63   |
| 14  | A     | 832  | CLA  | O2A-CGA-O1A | -2.14 | 118.29      | 123.63   |
| 14  | g     | 832  | CLA  | O2D-CGD-CBD | 2.14  | 114.96      | 111.23   |
| 17  | n     | 849  | BCR  | C10-C11-C12 | -2.14 | 117.01      | 123.20   |
| 17  | l     | 205  | BCR  | C15-C16-C17 | -2.14 | 119.15      | 123.52   |
| 17  | b     | 844  | BCR  | C33-C5-C4   | 2.13  | 118.15      | 113.60   |
| 14  | N     | 817  | CLA  | O2A-CGA-O1A | -2.13 | 118.29      | 123.63   |
| 17  | J     | 103  | BCR  | C38-C26-C27 | 2.13  | 118.15      | 113.60   |
| 17  | F     | 203  | BCR  | C21-C20-C19 | -2.13 | 117.02      | 123.20   |
| 14  | g     | 825  | CLA  | C1-C2-C3    | -2.13 | 122.70      | 126.20   |
| 17  | G     | 846  | BCR  | C38-C26-C27 | 2.13  | 118.14      | 113.60   |
| 17  | n     | 851  | BCR  | C38-C26-C27 | 2.13  | 118.14      | 113.60   |
| 14  | G     | 829  | CLA  | O2D-CGD-CBD | 2.13  | 114.96      | 111.23   |
| 17  | A     | 844  | BCR  | C3-C4-C5    | -2.13 | 110.25      | 114.06   |
| 20  | h     | 1702 | SQD  | O8-S-C6     | 2.13  | 110.09      | 105.97   |
| 17  | l     | 206  | BCR  | C38-C26-C27 | 2.13  | 118.14      | 113.60   |
| 14  | A     | 828  | CLA  | CHB-C4A-NA  | 2.13  | 127.48      | 124.40   |
| 17  | a     | 848  | BCR  | C28-C27-C26 | -2.13 | 110.25      | 114.06   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | a     | 817 | CLA  | O2A-CGA-O1A | -2.13 | 118.30      | 123.63   |
| 14  | G     | 812 | CLA  | C1-C2-C3    | -2.13 | 122.71      | 126.20   |
| 14  | b     | 834 | CLA  | C1-C2-C3    | -2.13 | 122.71      | 126.20   |
| 14  | G     | 801 | CLA  | C1-C2-C3    | -2.13 | 122.71      | 126.20   |
| 14  | B     | 824 | CLA  | C1-C2-C3    | -2.13 | 122.71      | 126.20   |
| 14  | G     | 826 | CLA  | O2A-CGA-O1A | -2.13 | 118.30      | 123.63   |
| 14  | l     | 202 | CLA  | CMB-C2B-C1B | -2.13 | 122.18      | 125.42   |
| 14  | B     | 829 | CLA  | O2A-CGA-O1A | -2.13 | 118.30      | 123.63   |
| 14  | N     | 806 | CLA  | C1-C2-C3    | -2.13 | 122.71      | 126.20   |
| 17  | B     | 843 | BCR  | C8-C7-C6    | -2.13 | 121.32      | 127.00   |
| 14  | G     | 810 | CLA  | O2A-CGA-O1A | -2.13 | 118.31      | 123.63   |
| 14  | A     | 838 | CLA  | C1-C2-C3    | -2.13 | 122.71      | 126.20   |
| 14  | b     | 826 | CLA  | O2A-CGA-O1A | -2.12 | 118.31      | 123.63   |
| 14  | G     | 834 | CLA  | O2A-CGA-O1A | -2.12 | 118.32      | 123.63   |
| 17  | W     | 205 | BCR  | C10-C11-C12 | -2.12 | 117.05      | 123.20   |
| 14  | g     | 852 | CLA  | CMB-C2B-C3B | 2.12  | 131.54      | 126.55   |
| 14  | S     | 201 | CLA  | O2A-CGA-O1A | -2.12 | 118.32      | 123.63   |
| 14  | A     | 835 | CLA  | C3B-C4B-NB  | -2.12 | 108.64      | 110.53   |
| 14  | n     | 836 | CLA  | O2A-CGA-O1A | -2.12 | 118.32      | 123.63   |
| 14  | g     | 833 | CLA  | O2A-CGA-O1A | -2.12 | 118.32      | 123.63   |
| 14  | b     | 806 | CLA  | CMB-C2B-C3B | 2.12  | 131.54      | 126.55   |
| 14  | A     | 816 | CLA  | O2A-CGA-O1A | -2.12 | 118.33      | 123.63   |
| 14  | G     | 802 | CLA  | O2A-CGA-O1A | -2.12 | 118.33      | 123.63   |
| 14  | b     | 825 | CLA  | O2A-CGA-O1A | -2.12 | 118.33      | 123.63   |
| 14  | a     | 827 | CLA  | CMB-C2B-C1B | -2.12 | 122.19      | 125.42   |
| 17  | b     | 852 | BCR  | C20-C19-C18 | -2.12 | 120.55      | 126.36   |
| 17  | G     | 846 | BCR  | C10-C11-C12 | -2.12 | 117.06      | 123.20   |
| 14  | B     | 820 | CLA  | C1-C2-C3    | -2.12 | 122.73      | 126.20   |
| 14  | N     | 807 | CLA  | CMB-C2B-C1B | -2.12 | 122.20      | 125.42   |
| 14  | A     | 824 | CLA  | CMB-C2B-C3B | 2.12  | 131.53      | 126.55   |
| 17  | m     | 102 | BCR  | C33-C5-C4   | 2.12  | 118.11      | 113.60   |
| 17  | A     | 849 | BCR  | C32-C1-C6   | -2.12 | 106.92      | 110.24   |
| 17  | b     | 847 | BCR  | C33-C5-C4   | 2.12  | 118.11      | 113.60   |
| 14  | B     | 837 | CLA  | CMB-C2B-C3B | 2.12  | 131.53      | 126.55   |
| 14  | G     | 826 | CLA  | C1-C2-C3    | -2.12 | 122.73      | 126.20   |
| 17  | B     | 847 | BCR  | C38-C26-C27 | 2.12  | 118.11      | 113.60   |
| 17  | J     | 103 | BCR  | C21-C20-C19 | -2.11 | 117.07      | 123.20   |
| 14  | B     | 808 | CLA  | O2A-CGA-O1A | -2.11 | 118.34      | 123.63   |
| 14  | B     | 829 | CLA  | CMB-C2B-C3B | 2.11  | 131.52      | 126.55   |
| 14  | B     | 825 | CLA  | C1-C2-C3    | -2.11 | 122.73      | 126.20   |
| 17  | g     | 846 | BCR  | C33-C5-C4   | 2.11  | 118.10      | 113.60   |
| 17  | g     | 844 | BCR  | C20-C19-C18 | -2.11 | 120.57      | 126.36   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | G     | 844 | BCR  | C33-C5-C4   | 2.11  | 118.10      | 113.60   |
| 14  | G     | 803 | CLA  | O2A-CGA-O1A | -2.11 | 118.34      | 123.63   |
| 14  | n     | 839 | CLA  | O2A-CGA-O1A | -2.11 | 118.34      | 123.63   |
| 17  | u     | 103 | BCR  | C20-C19-C18 | -2.11 | 120.57      | 126.36   |
| 14  | G     | 804 | CLA  | O2A-CGA-O1A | -2.11 | 118.34      | 123.63   |
| 17  | a     | 843 | BCR  | C8-C7-C6    | -2.11 | 121.36      | 127.00   |
| 14  | A     | 855 | CLA  | O2A-CGA-O1A | -2.11 | 117.90      | 123.33   |
| 14  | a     | 805 | CLA  | O2A-CGA-O1A | -2.11 | 118.35      | 123.63   |
| 17  | N     | 845 | BCR  | C38-C26-C25 | -2.11 | 122.18      | 124.48   |
| 18  | m     | 101 | LHG  | C26-C25-C24 | 2.11  | 120.89      | 113.13   |
| 14  | A     | 827 | CLA  | C3B-C4B-NB  | -2.11 | 108.65      | 110.53   |
| 14  | A     | 810 | CLA  | O2A-CGA-O1A | -2.11 | 118.35      | 123.63   |
| 17  | s     | 203 | BCR  | C8-C7-C6    | -2.11 | 121.36      | 127.00   |
| 17  | N     | 845 | BCR  | C1-C6-C5    | -2.11 | 119.75      | 122.64   |
| 17  | w     | 201 | BCR  | C38-C26-C27 | 2.11  | 118.09      | 113.60   |
| 17  | y     | 101 | BCR  | C33-C5-C4   | 2.11  | 118.09      | 113.60   |
| 14  | B     | 835 | CLA  | CMB-C2B-C1B | -2.11 | 122.21      | 125.42   |
| 14  | b     | 831 | CLA  | O2A-CGA-O1A | -2.11 | 118.36      | 123.63   |
| 17  | B     | 844 | BCR  | C8-C7-C6    | -2.11 | 121.37      | 127.00   |
| 17  | w     | 201 | BCR  | C21-C20-C19 | -2.11 | 117.09      | 123.20   |
| 14  | B     | 834 | CLA  | O2D-CGD-CBD | 2.11  | 114.91      | 111.23   |
| 17  | G     | 845 | BCR  | C21-C20-C19 | -2.11 | 117.10      | 123.20   |
| 14  | A     | 805 | CLA  | O2A-CGA-O1A | -2.11 | 118.36      | 123.63   |
| 14  | b     | 826 | CLA  | C1-C2-C3    | -2.11 | 122.75      | 126.20   |
| 14  | g     | 817 | CLA  | O2A-CGA-O1A | -2.11 | 118.36      | 123.63   |
| 14  | N     | 804 | CLA  | C1-C2-C3    | -2.11 | 122.75      | 126.20   |
| 14  | g     | 812 | CLA  | C1-C2-C3    | -2.11 | 122.75      | 126.20   |
| 14  | g     | 853 | CLA  | CMB-C2B-C1B | -2.10 | 122.21      | 125.42   |
| 20  | n     | 801 | SQD  | O8-S-C6     | 2.10  | 110.04      | 105.97   |
| 14  | b     | 841 | CLA  | O2A-CGA-O1A | -2.10 | 118.36      | 123.63   |
| 14  | n     | 807 | CLA  | O2A-CGA-O1A | -2.10 | 118.36      | 123.63   |
| 14  | n     | 840 | CLA  | O2A-CGA-O1A | -2.10 | 118.36      | 123.63   |
| 14  | b     | 807 | CLA  | O2A-CGA-O1A | -2.10 | 118.36      | 123.63   |
| 17  | B     | 852 | BCR  | C38-C26-C27 | 2.10  | 118.08      | 113.60   |
| 17  | I     | 101 | BCR  | C10-C11-C12 | -2.10 | 117.10      | 123.20   |
| 14  | g     | 852 | CLA  | CAA-CBA-CGA | -2.10 | 107.24      | 113.21   |
| 14  | b     | 803 | CLA  | O2D-CGD-CBD | 2.10  | 114.91      | 111.23   |
| 14  | a     | 833 | CLA  | O2A-CGA-O1A | -2.10 | 118.37      | 123.63   |
| 14  | a     | 839 | CLA  | O2A-CGA-O1A | -2.10 | 118.37      | 123.63   |
| 14  | g     | 826 | CLA  | CMB-C2B-C3B | 2.10  | 131.50      | 126.55   |
| 14  | N     | 816 | CLA  | O2A-CGA-O1A | -2.10 | 118.37      | 123.63   |
| 14  | G     | 836 | CLA  | CMB-C2B-C1B | -2.10 | 122.22      | 125.42   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | N     | 836  | CLA  | CMB-C2B-C1B | -2.10 | 122.22      | 125.42   |
| 14  | A     | 813  | CLA  | C1-C2-C3    | -2.10 | 122.75      | 126.20   |
| 14  | G     | 825  | CLA  | O2A-CGA-O1A | -2.10 | 118.37      | 123.63   |
| 14  | n     | 815  | CLA  | O2A-CGA-O1A | -2.10 | 118.37      | 123.63   |
| 14  | a     | 831  | CLA  | CMB-C2B-C3B | 2.10  | 131.49      | 126.55   |
| 14  | G     | 832  | CLA  | O2A-CGA-O1A | -2.10 | 118.37      | 123.63   |
| 14  | n     | 806  | CLA  | O2A-CGA-O1A | -2.10 | 118.37      | 123.63   |
| 14  | n     | 831  | CLA  | O2A-CGA-O1A | -2.10 | 118.37      | 123.63   |
| 14  | N     | 831  | CLA  | O2A-CGA-O1A | -2.10 | 118.38      | 123.63   |
| 17  | n     | 847  | BCR  | C33-C5-C4   | 2.10  | 118.07      | 113.60   |
| 14  | n     | 805  | CLA  | CMB-C2B-C1B | -2.10 | 122.22      | 125.42   |
| 14  | N     | 812  | CLA  | O2A-CGA-O1A | -2.10 | 118.38      | 123.63   |
| 14  | n     | 828  | CLA  | CMB-C2B-C1B | -2.10 | 122.22      | 125.42   |
| 14  | n     | 819  | CLA  | O2A-CGA-O1A | -2.10 | 118.38      | 123.63   |
| 17  | A     | 846  | BCR  | C11-C12-C13 | -2.10 | 120.61      | 126.36   |
| 14  | g     | 832  | CLA  | O2A-CGA-O1A | -2.10 | 118.38      | 123.63   |
| 17  | j     | 103  | BCR  | C8-C7-C6    | -2.10 | 121.40      | 127.00   |
| 14  | A     | 802  | CLA  | O2A-CGA-O1A | -2.10 | 118.39      | 123.63   |
| 14  | u     | 102  | CLA  | O2D-CGD-CBD | 2.10  | 114.89      | 111.23   |
| 17  | g     | 845  | BCR  | C15-C16-C17 | -2.10 | 119.23      | 123.52   |
| 14  | A     | 838  | CLA  | O2A-CGA-O1A | -2.10 | 118.39      | 123.63   |
| 19  | a     | 851  | CL0  | CED-O2D-CGD | 2.10  | 120.67      | 115.92   |
| 17  | G     | 848  | BCR  | C23-C24-C25 | -2.10 | 121.40      | 127.00   |
| 17  | G     | 845  | BCR  | C2-C1-C6    | 2.09  | 113.48      | 110.44   |
| 17  | N     | 849  | BCR  | C16-C15-C14 | -2.09 | 119.24      | 123.52   |
| 17  | g     | 847  | BCR  | C10-C11-C12 | -2.09 | 117.14      | 123.20   |
| 17  | n     | 847  | BCR  | C28-C27-C26 | -2.09 | 110.32      | 114.06   |
| 14  | A     | 828  | CLA  | O2A-CGA-O1A | -2.09 | 118.39      | 123.63   |
| 17  | B     | 851  | BCR  | C4-C5-C6    | -2.09 | 119.88      | 122.70   |
| 14  | g     | 839  | CLA  | O2A-CGA-O1A | -2.09 | 118.39      | 123.63   |
| 17  | W     | 205  | BCR  | C35-C13-C12 | 2.09  | 121.28      | 118.09   |
| 17  | t     | 104  | BCR  | C2-C1-C6    | 2.09  | 113.48      | 110.44   |
| 14  | N     | 809  | CLA  | O2D-CGD-CBD | 2.09  | 114.89      | 111.23   |
| 17  | g     | 846  | BCR  | C3-C4-C5    | -2.09 | 110.33      | 114.06   |
| 14  | B     | 829  | CLA  | CHB-C4A-NA  | 2.09  | 127.42      | 124.40   |
| 17  | L     | 1504 | BCR  | C1-C6-C5    | -2.09 | 119.78      | 122.64   |
| 14  | a     | 803  | CLA  | C1-C2-C3    | -2.09 | 122.77      | 126.20   |
| 14  | N     | 839  | CLA  | O2A-CGA-O1A | -2.09 | 118.40      | 123.63   |
| 14  | B     | 830  | CLA  | O2A-CGA-O1A | -2.09 | 118.40      | 123.63   |
| 14  | N     | 825  | CLA  | CMB-C2B-C1B | -2.09 | 122.24      | 125.42   |
| 14  | A     | 857  | CLA  | O2A-CGA-O1A | -2.09 | 118.40      | 123.63   |
| 14  | A     | 813  | CLA  | O2A-CGA-O1A | -2.09 | 118.40      | 123.63   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | t     | 103  | BCR  | C38-C26-C27 | 2.09  | 118.05      | 113.60   |
| 17  | V     | 101  | BCR  | C21-C20-C19 | -2.09 | 117.15      | 123.20   |
| 14  | b     | 812  | CLA  | C1-C2-C3    | -2.09 | 122.78      | 126.20   |
| 14  | g     | 821  | CLA  | O2A-CGA-O1A | -2.09 | 118.40      | 123.63   |
| 17  | B     | 843  | BCR  | C16-C15-C14 | -2.09 | 119.25      | 123.52   |
| 14  | N     | 842  | CLA  | O2A-CGA-O1A | -2.09 | 118.41      | 123.63   |
| 17  | F     | 203  | BCR  | C33-C5-C4   | 2.09  | 118.05      | 113.60   |
| 14  | W     | 202  | CLA  | C1-C2-C3    | -2.09 | 122.78      | 126.20   |
| 17  | i     | 102  | BCR  | C8-C7-C6    | -2.09 | 121.42      | 127.00   |
| 14  | N     | 809  | CLA  | CMB-C2B-C3B | 2.09  | 131.46      | 126.55   |
| 14  | b     | 802  | CLA  | O2A-CGA-O1A | -2.09 | 118.41      | 123.63   |
| 17  | n     | 849  | BCR  | C15-C16-C17 | -2.09 | 119.25      | 123.52   |
| 14  | b     | 831  | CLA  | C1-C2-C3    | -2.09 | 122.78      | 126.20   |
| 14  | g     | 826  | CLA  | C3B-C4B-NB  | -2.09 | 108.67      | 110.53   |
| 14  | n     | 803  | CLA  | O2A-CGA-O1A | -2.09 | 118.41      | 123.63   |
| 14  | a     | 810  | CLA  | O2A-CGA-O1A | -2.09 | 118.41      | 123.63   |
| 14  | n     | 824  | CLA  | C1-C2-C3    | -2.08 | 122.78      | 126.20   |
| 17  | k     | 102  | BCR  | C10-C11-C12 | -2.08 | 117.16      | 123.20   |
| 17  | N     | 852  | BCR  | C34-C9-C8   | 2.08  | 121.27      | 118.09   |
| 14  | u     | 102  | CLA  | O2A-CGA-O1A | -2.08 | 118.42      | 123.63   |
| 14  | a     | 853  | CLA  | O2A-CGA-O1A | -2.08 | 118.42      | 123.63   |
| 14  | b     | 837  | CLA  | O2A-CGA-O1A | -2.08 | 118.42      | 123.63   |
| 17  | j     | 104  | BCR  | C34-C9-C10  | -2.08 | 119.44      | 122.82   |
| 14  | A     | 804  | CLA  | C1-C2-C3    | -2.08 | 122.78      | 126.20   |
| 14  | n     | 823  | CLA  | O2D-CGD-CBD | 2.08  | 114.87      | 111.23   |
| 14  | b     | 813  | CLA  | O2A-CGA-O1A | -2.08 | 118.42      | 123.63   |
| 14  | b     | 832  | CLA  | O2A-CGA-O1A | -2.08 | 118.42      | 123.63   |
| 17  | n     | 849  | BCR  | C33-C5-C4   | 2.08  | 118.03      | 113.60   |
| 14  | A     | 839  | CLA  | O2A-CGA-O1A | -2.08 | 118.42      | 123.63   |
| 17  | L     | 1504 | BCR  | C11-C10-C9  | -2.08 | 124.36      | 127.28   |
| 14  | N     | 831  | CLA  | C1-C2-C3    | -2.08 | 122.79      | 126.20   |
| 19  | G     | 851  | CL0  | O2D-CGD-CBD | 2.08  | 113.23      | 110.95   |
| 14  | b     | 815  | CLA  | CMB-C2B-C1B | -2.08 | 122.25      | 125.42   |
| 14  | A     | 840  | CLA  | CHB-C4A-NA  | 2.08  | 127.40      | 124.40   |
| 14  | A     | 806  | CLA  | O2A-CGA-O1A | -2.08 | 118.42      | 123.63   |
| 14  | a     | 801  | CLA  | O2A-CGA-O1A | -2.08 | 118.42      | 123.63   |
| 14  | b     | 815  | CLA  | O2A-CGA-O1A | -2.08 | 118.42      | 123.63   |
| 14  | g     | 815  | CLA  | O2A-CGA-O1A | -2.08 | 118.42      | 123.63   |
| 17  | n     | 849  | BCR  | C38-C26-C25 | -2.08 | 122.21      | 124.48   |
| 14  | N     | 830  | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 17  | g     | 848  | BCR  | C38-C26-C27 | 2.08  | 118.03      | 113.60   |
| 14  | N     | 830  | CLA  | CMB-C2B-C3B | 2.08  | 131.44      | 126.55   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | A     | 845 | BCR  | C15-C16-C17 | -2.08 | 119.27      | 123.52   |
| 14  | g     | 840 | CLA  | CMB-C2B-C3B | 2.08  | 131.44      | 126.55   |
| 14  | a     | 828 | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 14  | b     | 804 | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 14  | a     | 810 | CLA  | C1-C2-C3    | -2.08 | 122.79      | 126.20   |
| 17  | G     | 843 | BCR  | C8-C7-C6    | -2.08 | 121.45      | 127.00   |
| 14  | B     | 820 | CLA  | CHB-C1B-NB  | 2.08  | 127.17      | 124.05   |
| 17  | a     | 846 | BCR  | C37-C22-C23 | 2.08  | 121.26      | 118.09   |
| 14  | A     | 821 | CLA  | O2D-CGD-CBD | 2.08  | 114.86      | 111.23   |
| 17  | n     | 846 | BCR  | C28-C27-C26 | -2.08 | 110.35      | 114.06   |
| 17  | N     | 849 | BCR  | C35-C13-C12 | 2.08  | 121.26      | 118.09   |
| 14  | b     | 824 | CLA  | O2D-CGD-CBD | 2.08  | 114.86      | 111.23   |
| 14  | G     | 828 | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 17  | n     | 846 | BCR  | C8-C7-C6    | -2.08 | 121.45      | 127.00   |
| 14  | g     | 812 | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 14  | g     | 840 | CLA  | O2A-CGA-O1A | -2.08 | 118.43      | 123.63   |
| 14  | b     | 838 | CLA  | O2D-CGD-CBD | 2.08  | 114.86      | 111.23   |
| 17  | g     | 846 | BCR  | C36-C18-C17 | -2.08 | 119.45      | 122.82   |
| 14  | a     | 823 | CLA  | O2A-CGA-O1A | -2.07 | 118.44      | 123.63   |
| 14  | n     | 817 | CLA  | O2A-CGA-O1A | -2.07 | 118.44      | 123.63   |
| 14  | G     | 810 | CLA  | CMB-C2B-C1B | -2.07 | 122.26      | 125.42   |
| 14  | g     | 809 | CLA  | O2A-CGA-O1A | -2.07 | 118.44      | 123.63   |
| 17  | n     | 849 | BCR  | C27-C26-C25 | -2.07 | 119.90      | 122.70   |
| 14  | a     | 835 | CLA  | C1-C2-C3    | -2.07 | 122.80      | 126.20   |
| 14  | G     | 818 | CLA  | CMB-C2B-C1B | -2.07 | 122.26      | 125.42   |
| 14  | g     | 819 | CLA  | O2A-CGA-O1A | -2.07 | 118.44      | 123.63   |
| 17  | a     | 847 | BCR  | C33-C5-C4   | 2.07  | 118.02      | 113.60   |
| 14  | B     | 816 | CLA  | O2A-CGA-O1A | -2.07 | 118.44      | 123.63   |
| 14  | g     | 810 | CLA  | O2A-CGA-O1A | -2.07 | 118.44      | 123.63   |
| 17  | B     | 848 | BCR  | C39-C30-C25 | -2.07 | 106.99      | 110.24   |
| 14  | B     | 837 | CLA  | O2A-CGA-O1A | -2.07 | 118.45      | 123.63   |
| 17  | V     | 101 | BCR  | C33-C5-C4   | 2.07  | 118.01      | 113.60   |
| 14  | g     | 823 | CLA  | O2A-CGA-O1A | -2.07 | 118.45      | 123.63   |
| 17  | n     | 843 | BCR  | C15-C16-C17 | -2.07 | 119.28      | 123.52   |
| 14  | n     | 812 | CLA  | O2A-CGA-O1A | -2.07 | 118.45      | 123.63   |
| 14  | n     | 829 | CLA  | O2A-CGA-O1A | -2.07 | 118.45      | 123.63   |
| 14  | B     | 823 | CLA  | O2A-CGA-O1A | -2.07 | 118.45      | 123.63   |
| 17  | w     | 207 | BCR  | C20-C19-C18 | -2.07 | 120.69      | 126.36   |
| 17  | A     | 845 | BCR  | C27-C26-C25 | -2.07 | 119.91      | 122.70   |
| 14  | N     | 810 | CLA  | C1-C2-C3    | -2.07 | 122.81      | 126.20   |
| 14  | a     | 819 | CLA  | C1-C2-C3    | -2.07 | 122.81      | 126.20   |
| 14  | b     | 837 | CLA  | CMB-C2B-C3B | 2.07  | 131.41      | 126.55   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | G     | 826  | CLA  | CMB-C2B-C1B | -2.07 | 122.27      | 125.42   |
| 14  | B     | 825  | CLA  | O2A-CGA-O1A | -2.07 | 118.45      | 123.63   |
| 14  | n     | 805  | CLA  | C1-C2-C3    | -2.07 | 122.81      | 126.20   |
| 14  | a     | 819  | CLA  | O2A-CGA-O1A | -2.07 | 118.46      | 123.63   |
| 14  | b     | 811  | CLA  | O2A-CGA-O1A | -2.07 | 118.46      | 123.63   |
| 17  | v     | 101  | BCR  | C8-C7-C6    | -2.07 | 121.47      | 127.00   |
| 14  | N     | 821  | CLA  | C1-C2-C3    | -2.07 | 122.81      | 126.20   |
| 14  | n     | 822  | CLA  | O2A-CGA-O1A | -2.07 | 118.46      | 123.63   |
| 14  | G     | 805  | CLA  | CMB-C2B-C3B | 2.07  | 131.41      | 126.55   |
| 14  | G     | 812  | CLA  | O2A-CGA-O1A | -2.07 | 118.46      | 123.63   |
| 14  | G     | 820  | CLA  | O2A-CGA-O1A | -2.07 | 118.46      | 123.63   |
| 14  | g     | 811  | CLA  | O2A-CGA-O1A | -2.07 | 118.46      | 123.63   |
| 14  | G     | 829  | CLA  | O2A-CGA-O1A | -2.07 | 118.46      | 123.63   |
| 14  | G     | 822  | CLA  | O2A-CGA-O1A | -2.07 | 118.46      | 123.63   |
| 14  | b     | 832  | CLA  | CMB-C2B-C3B | 2.07  | 131.41      | 126.55   |
| 17  | j     | 104  | BCR  | C2-C1-C6    | 2.07  | 113.44      | 110.44   |
| 14  | b     | 805  | CLA  | O2A-CGA-O1A | -2.06 | 118.47      | 123.63   |
| 17  | K     | 102  | BCR  | C15-C16-C17 | -2.06 | 119.30      | 123.52   |
| 17  | I     | 102  | BCR  | C33-C5-C4   | 2.06  | 118.00      | 113.60   |
| 14  | N     | 828  | CLA  | CMB-C2B-C1B | -2.06 | 122.28      | 125.42   |
| 14  | L     | 1502 | CLA  | O2D-CGD-CBD | 2.06  | 114.83      | 111.23   |
| 14  | g     | 831  | CLA  | O2A-CGA-O1A | -2.06 | 118.47      | 123.63   |
| 14  | n     | 838  | CLA  | O2A-CGA-O1A | -2.06 | 118.47      | 123.63   |
| 14  | a     | 815  | CLA  | O2A-CGA-O1A | -2.06 | 118.47      | 123.63   |
| 17  | g     | 846  | BCR  | C35-C13-C14 | -2.06 | 119.48      | 122.82   |
| 17  | n     | 845  | BCR  | C1-C6-C5    | -2.06 | 119.82      | 122.64   |
| 14  | A     | 805  | CLA  | C1-C2-C3    | -2.06 | 122.82      | 126.20   |
| 17  | b     | 844  | BCR  | C34-C9-C10  | -2.06 | 119.48      | 122.82   |
| 17  | W     | 206  | BCR  | C15-C16-C17 | -2.06 | 119.30      | 123.52   |
| 14  | N     | 811  | CLA  | O2A-CGA-O1A | -2.06 | 118.47      | 123.63   |
| 17  | B     | 847  | BCR  | C33-C5-C4   | 2.06  | 117.99      | 113.60   |
| 17  | B     | 852  | BCR  | C32-C1-C6   | -2.06 | 107.01      | 110.24   |
| 17  | A     | 845  | BCR  | C20-C19-C18 | -2.06 | 120.72      | 126.36   |
| 14  | A     | 819  | CLA  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 14  | N     | 826  | CLA  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 17  | b     | 843  | BCR  | C16-C15-C14 | -2.06 | 119.31      | 123.52   |
| 14  | A     | 812  | CLA  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 14  | f     | 201  | CLA  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 14  | a     | 802  | CLA  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 14  | n     | 822  | CLA  | C1-C2-C3    | -2.06 | 122.83      | 126.20   |
| 17  | N     | 846  | BCR  | C4-C5-C6    | -2.06 | 119.92      | 122.70   |
| 14  | g     | 802  | CLA  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 14  | g     | 805 | CLA  | O2A-CGA-O1A | -2.06 | 118.48      | 123.63   |
| 17  | B     | 844 | BCR  | C1-C6-C5    | -2.06 | 119.83      | 122.64   |
| 17  | w     | 207 | BCR  | C15-C16-C17 | -2.06 | 119.31      | 123.52   |
| 14  | A     | 827 | CLA  | O2A-CGA-O1A | -2.06 | 118.49      | 123.63   |
| 14  | g     | 835 | CLA  | O2A-CGA-O1A | -2.05 | 118.49      | 123.63   |
| 14  | a     | 809 | CLA  | O2A-CGA-O1A | -2.05 | 118.49      | 123.63   |
| 14  | B     | 830 | CLA  | CMB-C2B-C3B | 2.05  | 131.38      | 126.55   |
| 14  | g     | 853 | CLA  | O2A-CGA-O1A | -2.05 | 118.49      | 123.63   |
| 14  | n     | 812 | CLA  | C1-C2-C3    | -2.05 | 122.83      | 126.20   |
| 14  | a     | 829 | CLA  | CMB-C2B-C1B | -2.05 | 122.29      | 125.42   |
| 17  | b     | 852 | BCR  | C23-C24-C25 | -2.05 | 121.51      | 127.00   |
| 14  | A     | 829 | CLA  | O2A-CGA-O1A | -2.05 | 118.49      | 123.63   |
| 17  | s     | 203 | BCR  | C15-C16-C17 | -2.05 | 119.32      | 123.52   |
| 17  | G     | 844 | BCR  | C20-C19-C18 | -2.05 | 120.73      | 126.36   |
| 14  | N     | 805 | CLA  | C1-C2-C3    | -2.05 | 122.83      | 126.20   |
| 14  | S     | 203 | CLA  | CMB-C2B-C1B | -2.05 | 122.29      | 125.42   |
| 17  | n     | 847 | BCR  | C34-C9-C8   | 2.05  | 121.22      | 118.09   |
| 14  | N     | 840 | CLA  | O2A-CGA-O1A | -2.05 | 118.49      | 123.63   |
| 17  | N     | 846 | BCR  | C37-C22-C21 | -2.05 | 119.49      | 122.82   |
| 14  | n     | 813 | CLA  | O2A-CGA-O1A | -2.05 | 118.50      | 123.63   |
| 17  | K     | 102 | BCR  | C33-C5-C4   | 2.05  | 117.97      | 113.60   |
| 17  | s     | 203 | BCR  | C11-C12-C13 | -2.05 | 120.74      | 126.36   |
| 17  | g     | 848 | BCR  | C23-C24-C25 | -2.05 | 121.52      | 127.00   |
| 14  | B     | 809 | CLA  | C1-C2-C3    | -2.05 | 122.84      | 126.20   |
| 14  | a     | 831 | CLA  | O2A-CGA-O1A | -2.05 | 118.50      | 123.63   |
| 14  | b     | 829 | CLA  | O2A-CGA-O1A | -2.05 | 118.50      | 123.63   |
| 17  | n     | 842 | BCR  | C27-C26-C25 | -2.05 | 119.93      | 122.70   |
| 17  | U     | 103 | BCR  | C10-C11-C12 | -2.05 | 117.26      | 123.20   |
| 14  | N     | 806 | CLA  | O2A-CGA-O1A | -2.05 | 118.50      | 123.63   |
| 14  | g     | 838 | CLA  | O2A-CGA-O1A | -2.05 | 118.50      | 123.63   |
| 14  | a     | 803 | CLA  | CMB-C2B-C1B | -2.05 | 122.30      | 125.42   |
| 17  | J     | 103 | BCR  | C11-C12-C13 | -2.05 | 120.75      | 126.36   |
| 17  | I     | 103 | BCR  | C4-C5-C6    | -2.05 | 119.94      | 122.70   |
| 17  | B     | 843 | BCR  | C10-C11-C12 | -2.05 | 117.27      | 123.20   |
| 14  | n     | 828 | CLA  | O2A-CGA-O1A | -2.05 | 118.51      | 123.63   |
| 14  | A     | 820 | CLA  | O2A-CGA-O1A | -2.05 | 118.51      | 123.63   |
| 14  | b     | 824 | CLA  | C1-C2-C3    | -2.05 | 122.84      | 126.20   |
| 14  | a     | 818 | CLA  | O2A-CGA-O1A | -2.05 | 118.51      | 123.63   |
| 17  | l     | 206 | BCR  | C21-C20-C19 | -2.05 | 117.27      | 123.20   |
| 14  | A     | 833 | CLA  | O2A-CGA-O1A | -2.05 | 118.51      | 123.63   |
| 14  | N     | 820 | CLA  | O2A-CGA-O1A | -2.04 | 118.51      | 123.63   |
| 14  | G     | 814 | CLA  | CMB-C2B-C1B | -2.04 | 122.31      | 125.42   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 17  | B     | 844  | BCR  | C23-C24-C25 | -2.04 | 121.54      | 127.00   |
| 14  | b     | 823  | CLA  | O2A-CGA-O1A | -2.04 | 118.52      | 123.63   |
| 14  | B     | 808  | CLA  | O2D-CGD-CBD | 2.04  | 114.80      | 111.23   |
| 17  | g     | 843  | BCR  | C38-C26-C25 | -2.04 | 122.25      | 124.48   |
| 14  | B     | 811  | CLA  | O2A-CGA-O1A | -2.04 | 118.52      | 123.63   |
| 14  | G     | 824  | CLA  | CMB-C2B-C1B | -2.04 | 122.31      | 125.42   |
| 14  | b     | 853  | CLA  | C1-C2-C3    | -2.04 | 122.85      | 126.20   |
| 17  | i     | 102  | BCR  | C3-C4-C5    | -2.04 | 110.41      | 114.06   |
| 14  | g     | 829  | CLA  | O2A-CGA-O1A | -2.04 | 118.52      | 123.63   |
| 17  | A     | 849  | BCR  | C35-C13-C12 | 2.04  | 121.21      | 118.09   |
| 14  | b     | 824  | CLA  | O2A-CGA-O1A | -2.04 | 118.52      | 123.63   |
| 14  | b     | 806  | CLA  | O2A-CGA-O1A | -2.04 | 118.52      | 123.63   |
| 14  | b     | 816  | CLA  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |
| 17  | W     | 206  | BCR  | C16-C15-C14 | -2.04 | 119.34      | 123.52   |
| 14  | g     | 835  | CLA  | C1-C2-C3    | -2.04 | 122.86      | 126.20   |
| 14  | N     | 838  | CLA  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |
| 14  | b     | 829  | CLA  | CMB-C2B-C3B | 2.04  | 131.35      | 126.55   |
| 14  | b     | 833  | CLA  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |
| 17  | N     | 847  | BCR  | C1-C6-C7    | 2.04  | 121.18      | 115.65   |
| 14  | b     | 826  | CLA  | CMB-C2B-C3B | 2.04  | 131.35      | 126.55   |
| 14  | a     | 816  | CLA  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |
| 17  | B     | 843  | BCR  | C15-C16-C17 | -2.04 | 119.35      | 123.52   |
| 14  | b     | 808  | CLA  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |
| 14  | g     | 853  | CLA  | CMB-C2B-C3B | 2.04  | 131.34      | 126.55   |
| 14  | A     | 808  | CLA  | CMB-C2B-C3B | 2.04  | 131.34      | 126.55   |
| 14  | N     | 801  | CLA  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |
| 14  | A     | 811  | CLA  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |
| 14  | b     | 827  | CLA  | CMB-C2B-C3B | 2.04  | 131.34      | 126.55   |
| 17  | v     | 101  | BCR  | C35-C13-C12 | 2.04  | 121.20      | 118.09   |
| 14  | g     | 827  | CLA  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |
| 14  | h     | 1701 | CLA  | O2A-CGA-O1A | -2.04 | 118.53      | 123.63   |
| 17  | a     | 845  | BCR  | C8-C7-C6    | -2.04 | 121.56      | 127.00   |
| 17  | j     | 103  | BCR  | C15-C16-C17 | -2.04 | 119.35      | 123.52   |
| 14  | b     | 831  | CLA  | CMB-C2B-C1B | -2.04 | 122.32      | 125.42   |
| 14  | x     | 1701 | CLA  | O2A-CGA-O1A | -2.04 | 118.54      | 123.63   |
| 17  | T     | 103  | BCR  | C11-C12-C13 | -2.04 | 120.78      | 126.36   |
| 17  | n     | 844  | BCR  | C15-C16-C17 | -2.04 | 119.36      | 123.52   |
| 14  | G     | 821  | CLA  | CMB-C2B-C3B | 2.03  | 131.34      | 126.55   |
| 14  | g     | 821  | CLA  | C1-C2-C3    | -2.03 | 122.86      | 126.20   |
| 17  | b     | 850  | BCR  | C27-C26-C25 | -2.03 | 119.96      | 122.70   |
| 14  | a     | 833  | CLA  | C1-C2-C3    | -2.03 | 122.87      | 126.20   |
| 14  | n     | 810  | CLA  | O2A-CGA-O1A | -2.03 | 118.55      | 123.63   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | g     | 828  | CLA  | CMB-C2B-C1B | -2.03 | 122.33      | 125.42   |
| 14  | A     | 818  | CLA  | CMB-C2B-C3B | 2.03  | 131.33      | 126.55   |
| 14  | n     | 818  | CLA  | O2A-CGA-O1A | -2.03 | 118.55      | 123.63   |
| 17  | W     | 206  | BCR  | C23-C24-C25 | -2.03 | 121.57      | 127.00   |
| 14  | a     | 826  | CLA  | CMB-C2B-C1B | -2.03 | 122.33      | 125.42   |
| 14  | n     | 830  | CLA  | C1-C2-C3    | -2.03 | 122.87      | 126.20   |
| 14  | N     | 813  | CLA  | O2A-CGA-O1A | -2.03 | 118.55      | 123.63   |
| 14  | a     | 804  | CLA  | O2A-CGA-O1A | -2.03 | 118.55      | 123.63   |
| 14  | G     | 838  | CLA  | O2A-CGA-O1A | -2.03 | 118.55      | 123.63   |
| 14  | B     | 820  | CLA  | CMB-C2B-C3B | 2.03  | 131.32      | 126.55   |
| 14  | b     | 820  | CLA  | CMB-C2B-C1B | -2.03 | 122.33      | 125.42   |
| 14  | b     | 814  | CLA  | CMB-C2B-C3B | 2.03  | 131.32      | 126.55   |
| 14  | A     | 840  | CLA  | O2A-CGA-O1A | -2.03 | 118.55      | 123.63   |
| 14  | a     | 801  | CLA  | CMB-C2B-C3B | 2.03  | 131.32      | 126.55   |
| 14  | A     | 836  | CLA  | O2A-CGA-O1A | -2.03 | 118.55      | 123.63   |
| 14  | a     | 825  | CLA  | O2A-CGA-O1A | -2.03 | 118.55      | 123.63   |
| 17  | T     | 103  | BCR  | C38-C26-C27 | 2.03  | 117.92      | 113.60   |
| 17  | j     | 103  | BCR  | C16-C15-C14 | -2.03 | 119.37      | 123.52   |
| 14  | N     | 824  | CLA  | O2A-CGA-O1A | -2.03 | 118.56      | 123.63   |
| 14  | g     | 828  | CLA  | O2D-CGD-CBD | 2.03  | 114.77      | 111.23   |
| 14  | n     | 809  | CLA  | C1-C2-C3    | -2.03 | 122.88      | 126.20   |
| 17  | N     | 846  | BCR  | C15-C16-C17 | -2.03 | 119.37      | 123.52   |
| 14  | n     | 826  | CLA  | CMB-C2B-C1B | -2.03 | 122.33      | 125.42   |
| 14  | g     | 825  | CLA  | O2A-CGA-O1A | -2.03 | 118.56      | 123.63   |
| 14  | B     | 812  | CLA  | O2A-CGA-O1A | -2.03 | 118.56      | 123.63   |
| 14  | a     | 806  | CLA  | O2A-CGA-O1A | -2.02 | 118.56      | 123.63   |
| 14  | b     | 838  | CLA  | CMB-C2B-C1B | -2.02 | 122.34      | 125.42   |
| 17  | N     | 853  | BCR  | C32-C1-C6   | -2.02 | 107.07      | 110.24   |
| 17  | n     | 851  | BCR  | C30-C25-C26 | -2.02 | 119.87      | 122.64   |
| 14  | N     | 803  | CLA  | CMB-C2B-C3B | 2.02  | 131.31      | 126.55   |
| 14  | G     | 836  | CLA  | O2A-CGA-O1A | -2.02 | 118.57      | 123.63   |
| 14  | B     | 824  | CLA  | O2A-CGA-O1A | -2.02 | 118.57      | 123.63   |
| 14  | n     | 852  | CLA  | C1-C2-C3    | -2.02 | 122.88      | 126.20   |
| 14  | B     | 827  | CLA  | O2A-CGA-O1A | -2.02 | 118.57      | 123.63   |
| 17  | I     | 102  | BCR  | C15-C16-C17 | 2.02  | 127.66      | 123.52   |
| 14  | G     | 838  | CLA  | C1-C2-C3    | -2.02 | 122.88      | 126.20   |
| 14  | n     | 813  | CLA  | C1-C2-C3    | -2.02 | 122.88      | 126.20   |
| 17  | I     | 101  | BCR  | C38-C26-C27 | 2.02  | 117.91      | 113.60   |
| 14  | G     | 837  | CLA  | O2A-CGA-O1A | -2.02 | 118.57      | 123.63   |
| 14  | a     | 835  | CLA  | O2A-CGA-O1A | -2.02 | 118.57      | 123.63   |
| 17  | b     | 848  | BCR  | C34-C9-C8   | 2.02  | 121.17      | 118.09   |
| 14  | X     | 1701 | CLA  | O2A-CGA-O1A | -2.02 | 118.57      | 123.63   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 14  | g     | 852  | CLA  | CHB-C1B-NB  | 2.02  | 127.08      | 124.05   |
| 14  | g     | 836  | CLA  | C1-C2-C3    | -2.02 | 122.89      | 126.20   |
| 14  | G     | 811  | CLA  | O2A-CGA-O1A | -2.02 | 118.58      | 123.63   |
| 14  | B     | 819  | CLA  | O2A-CGA-O1A | -2.02 | 118.58      | 123.63   |
| 14  | B     | 810  | CLA  | O2A-CGA-O1A | -2.02 | 118.58      | 123.63   |
| 17  | w     | 201  | BCR  | C8-C7-C6    | -2.02 | 121.61      | 127.00   |
| 14  | g     | 801  | CLA  | O2A-CGA-O1A | -2.02 | 118.58      | 123.63   |
| 17  | n     | 847  | BCR  | C38-C26-C27 | 2.02  | 117.90      | 113.60   |
| 14  | a     | 821  | CLA  | O2A-CGA-O1A | -2.02 | 118.58      | 123.63   |
| 14  | N     | 819  | CLA  | O2A-CGA-O1A | -2.02 | 118.58      | 123.63   |
| 14  | a     | 819  | CLA  | CMB-C2B-C3B | 2.02  | 131.29      | 126.55   |
| 14  | N     | 834  | CLA  | C1-C2-C3    | -2.02 | 122.89      | 126.20   |
| 17  | t     | 103  | BCR  | C15-C16-C17 | -2.02 | 119.39      | 123.52   |
| 14  | A     | 807  | CLA  | C1-C2-C3    | -2.02 | 122.89      | 126.20   |
| 17  | G     | 848  | BCR  | C35-C13-C12 | 2.02  | 121.17      | 118.09   |
| 17  | w     | 201  | BCR  | C15-C16-C17 | -2.02 | 119.39      | 123.52   |
| 17  | M     | 101  | BCR  | C33-C5-C4   | 2.02  | 117.89      | 113.60   |
| 14  | b     | 819  | CLA  | O2A-CGA-O1A | -2.02 | 118.59      | 123.63   |
| 17  | j     | 103  | BCR  | C21-C20-C19 | -2.02 | 117.36      | 123.20   |
| 14  | a     | 806  | CLA  | C1-C2-C3    | -2.01 | 122.90      | 126.20   |
| 14  | a     | 803  | CLA  | O2A-CGA-O1A | -2.01 | 118.59      | 123.63   |
| 14  | A     | 834  | CLA  | C1-C2-C3    | -2.01 | 122.90      | 126.20   |
| 14  | b     | 813  | CLA  | CMB-C2B-C3B | 2.01  | 131.29      | 126.55   |
| 17  | g     | 844  | BCR  | C16-C15-C14 | -2.01 | 119.40      | 123.52   |
| 14  | B     | 808  | CLA  | CMB-C2B-C3B | 2.01  | 131.29      | 126.55   |
| 14  | b     | 810  | CLA  | C1-C2-C3    | -2.01 | 122.90      | 126.20   |
| 14  | N     | 805  | CLA  | O2A-CGA-O1A | -2.01 | 118.59      | 123.63   |
| 14  | n     | 803  | CLA  | CED-O2D-CGD | 2.01  | 120.48      | 115.92   |
| 14  | N     | 832  | CLA  | O2A-CGA-O1A | -2.01 | 118.60      | 123.63   |
| 14  | g     | 828  | CLA  | O2A-CGA-O1A | -2.01 | 118.60      | 123.63   |
| 17  | U     | 103  | BCR  | C20-C19-C18 | -2.01 | 120.85      | 126.36   |
| 14  | b     | 841  | CLA  | C1-C2-C3    | -2.01 | 122.90      | 126.20   |
| 14  | L     | 1502 | CLA  | O2A-CGA-O1A | -2.01 | 118.60      | 123.63   |
| 17  | A     | 848  | BCR  | C37-C22-C23 | 2.01  | 121.16      | 118.09   |
| 17  | T     | 103  | BCR  | C15-C16-C17 | -2.01 | 119.41      | 123.52   |
| 17  | N     | 844  | BCR  | C11-C12-C13 | -2.01 | 120.85      | 126.36   |
| 17  | j     | 103  | BCR  | C11-C12-C13 | -2.01 | 120.85      | 126.36   |
| 17  | b     | 847  | BCR  | C21-C20-C19 | -2.01 | 117.38      | 123.20   |
| 14  | N     | 815  | CLA  | O2A-CGA-O1A | -2.01 | 118.60      | 123.63   |
| 17  | I     | 103  | BCR  | C10-C11-C12 | -2.01 | 117.38      | 123.20   |
| 17  | g     | 844  | BCR  | C30-C25-C26 | -2.01 | 119.89      | 122.64   |
| 17  | A     | 844  | BCR  | C8-C7-C6    | -2.01 | 121.63      | 127.00   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 17  | n     | 849 | BCR  | C38-C26-C27 | 2.01  | 117.88      | 113.60   |
| 14  | a     | 837 | CLA  | O2A-CGA-O1A | -2.01 | 118.61      | 123.63   |
| 14  | a     | 854 | CLA  | O2A-CGA-O1A | -2.01 | 118.61      | 123.63   |
| 14  | g     | 825 | CLA  | CMB-C2B-C1B | -2.01 | 122.36      | 125.42   |
| 14  | N     | 825 | CLA  | C1-C2-C3    | -2.01 | 122.91      | 126.20   |
| 14  | a     | 812 | CLA  | C1-C2-C3    | -2.01 | 122.91      | 126.20   |
| 14  | B     | 806 | CLA  | O2A-CGA-O1A | -2.01 | 118.61      | 123.63   |
| 17  | n     | 849 | BCR  | C3-C4-C5    | -2.01 | 110.48      | 114.06   |
| 14  | N     | 801 | CLA  | C1-C2-C3    | -2.01 | 122.91      | 126.20   |
| 17  | n     | 851 | BCR  | C20-C19-C18 | -2.01 | 120.86      | 126.36   |
| 14  | g     | 836 | CLA  | O2A-CGA-O1A | -2.00 | 118.61      | 123.63   |
| 17  | b     | 848 | BCR  | C15-C16-C17 | -2.00 | 119.42      | 123.52   |
| 14  | A     | 837 | CLA  | O2A-CGA-O1A | -2.00 | 118.61      | 123.63   |
| 14  | W     | 203 | CLA  | C1-C2-C3    | -2.00 | 122.91      | 126.20   |
| 14  | N     | 803 | CLA  | CMB-C2B-C1B | -2.00 | 122.37      | 125.42   |
| 14  | G     | 801 | CLA  | O2A-CGA-O1A | -2.00 | 118.62      | 123.63   |
| 14  | B     | 826 | CLA  | O2D-CGD-CBD | 2.00  | 114.73      | 111.23   |
| 14  | g     | 806 | CLA  | CMB-C2B-C1B | -2.00 | 122.37      | 125.42   |
| 14  | G     | 817 | CLA  | O2A-CGA-O1A | -2.00 | 118.62      | 123.63   |
| 14  | b     | 830 | CLA  | CMB-C2B-C3B | 2.00  | 131.26      | 126.55   |
| 14  | a     | 824 | CLA  | C1-C2-C3    | -2.00 | 122.92      | 126.20   |
| 14  | g     | 816 | CLA  | O2A-CGA-O1A | -2.00 | 118.62      | 123.63   |
| 14  | n     | 830 | CLA  | O2A-CGA-O1A | -2.00 | 118.62      | 123.63   |
| 14  | B     | 823 | CLA  | C1-C2-C3    | -2.00 | 122.92      | 126.20   |
| 14  | A     | 807 | CLA  | O2A-CGA-O1A | -2.00 | 118.62      | 123.63   |
| 14  | b     | 853 | CLA  | O2A-CGA-O1A | -2.00 | 118.62      | 123.63   |

All (388) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | G     | 801 | CLA  | ND   |
| 14  | G     | 802 | CLA  | ND   |
| 14  | G     | 803 | CLA  | ND   |
| 14  | G     | 804 | CLA  | ND   |
| 14  | G     | 805 | CLA  | ND   |
| 14  | G     | 806 | CLA  | ND   |
| 14  | G     | 807 | CLA  | ND   |
| 14  | G     | 808 | CLA  | ND   |
| 14  | G     | 809 | CLA  | ND   |
| 14  | G     | 810 | CLA  | ND   |
| 14  | G     | 811 | CLA  | ND   |
| 14  | G     | 812 | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | G     | 813  | CLA  | ND   |
| 14  | G     | 814  | CLA  | ND   |
| 14  | G     | 815  | CLA  | ND   |
| 14  | G     | 816  | CLA  | ND   |
| 14  | G     | 817  | CLA  | ND   |
| 14  | G     | 818  | CLA  | ND   |
| 14  | G     | 819  | CLA  | ND   |
| 14  | G     | 820  | CLA  | ND   |
| 14  | G     | 821  | CLA  | ND   |
| 14  | G     | 822  | CLA  | ND   |
| 14  | G     | 823  | CLA  | ND   |
| 14  | G     | 824  | CLA  | ND   |
| 14  | G     | 825  | CLA  | ND   |
| 14  | G     | 826  | CLA  | ND   |
| 14  | G     | 827  | CLA  | ND   |
| 14  | G     | 828  | CLA  | ND   |
| 14  | G     | 829  | CLA  | ND   |
| 14  | G     | 830  | CLA  | ND   |
| 14  | G     | 831  | CLA  | ND   |
| 14  | G     | 832  | CLA  | ND   |
| 14  | G     | 833  | CLA  | ND   |
| 14  | G     | 834  | CLA  | ND   |
| 14  | G     | 835  | CLA  | ND   |
| 14  | G     | 836  | CLA  | ND   |
| 14  | G     | 837  | CLA  | ND   |
| 14  | G     | 838  | CLA  | ND   |
| 14  | G     | 839  | CLA  | ND   |
| 14  | G     | 840  | CLA  | ND   |
| 14  | G     | 852  | CLA  | ND   |
| 14  | G     | 853  | CLA  | ND   |
| 14  | H     | 1701 | CLA  | ND   |
| 14  | N     | 801  | CLA  | ND   |
| 14  | N     | 803  | CLA  | ND   |
| 14  | N     | 804  | CLA  | ND   |
| 14  | N     | 805  | CLA  | ND   |
| 14  | N     | 806  | CLA  | ND   |
| 14  | N     | 807  | CLA  | ND   |
| 14  | N     | 808  | CLA  | ND   |
| 14  | N     | 809  | CLA  | ND   |
| 14  | N     | 810  | CLA  | ND   |
| 14  | N     | 811  | CLA  | ND   |
| 14  | N     | 812  | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | N     | 813 | CLA  | ND   |
| 14  | N     | 814 | CLA  | ND   |
| 14  | N     | 815 | CLA  | ND   |
| 14  | N     | 816 | CLA  | ND   |
| 14  | N     | 817 | CLA  | ND   |
| 14  | N     | 818 | CLA  | ND   |
| 14  | N     | 819 | CLA  | ND   |
| 14  | N     | 820 | CLA  | ND   |
| 14  | N     | 821 | CLA  | ND   |
| 14  | N     | 822 | CLA  | ND   |
| 14  | N     | 823 | CLA  | ND   |
| 14  | N     | 824 | CLA  | ND   |
| 14  | N     | 825 | CLA  | ND   |
| 14  | N     | 826 | CLA  | ND   |
| 14  | N     | 827 | CLA  | ND   |
| 14  | N     | 828 | CLA  | ND   |
| 14  | N     | 829 | CLA  | ND   |
| 14  | N     | 830 | CLA  | ND   |
| 14  | N     | 831 | CLA  | ND   |
| 14  | N     | 832 | CLA  | ND   |
| 14  | N     | 833 | CLA  | ND   |
| 14  | N     | 834 | CLA  | ND   |
| 14  | N     | 835 | CLA  | ND   |
| 14  | N     | 836 | CLA  | ND   |
| 14  | N     | 837 | CLA  | ND   |
| 14  | N     | 838 | CLA  | ND   |
| 14  | N     | 839 | CLA  | ND   |
| 14  | N     | 840 | CLA  | ND   |
| 14  | N     | 841 | CLA  | ND   |
| 14  | N     | 842 | CLA  | ND   |
| 14  | N     | 851 | CLA  | ND   |
| 14  | S     | 201 | CLA  | ND   |
| 14  | S     | 203 | CLA  | ND   |
| 14  | T     | 101 | CLA  | ND   |
| 14  | T     | 102 | CLA  | ND   |
| 14  | U     | 101 | CLA  | ND   |
| 14  | U     | 102 | CLA  | ND   |
| 14  | W     | 202 | CLA  | ND   |
| 14  | W     | 203 | CLA  | ND   |
| 14  | W     | 204 | CLA  | ND   |
| 14  | g     | 801 | CLA  | ND   |
| 14  | g     | 802 | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | g     | 803  | CLA  | ND   |
| 14  | g     | 804  | CLA  | ND   |
| 14  | g     | 805  | CLA  | ND   |
| 14  | g     | 806  | CLA  | ND   |
| 14  | g     | 807  | CLA  | ND   |
| 14  | g     | 808  | CLA  | ND   |
| 14  | g     | 809  | CLA  | ND   |
| 14  | g     | 810  | CLA  | ND   |
| 14  | g     | 811  | CLA  | ND   |
| 14  | g     | 812  | CLA  | ND   |
| 14  | g     | 813  | CLA  | ND   |
| 14  | g     | 814  | CLA  | ND   |
| 14  | g     | 815  | CLA  | ND   |
| 14  | g     | 816  | CLA  | ND   |
| 14  | g     | 817  | CLA  | ND   |
| 14  | g     | 818  | CLA  | ND   |
| 14  | g     | 819  | CLA  | ND   |
| 14  | g     | 820  | CLA  | ND   |
| 14  | g     | 821  | CLA  | ND   |
| 14  | g     | 822  | CLA  | ND   |
| 14  | g     | 823  | CLA  | ND   |
| 14  | g     | 824  | CLA  | ND   |
| 14  | g     | 825  | CLA  | ND   |
| 14  | g     | 826  | CLA  | ND   |
| 14  | g     | 827  | CLA  | ND   |
| 14  | g     | 828  | CLA  | ND   |
| 14  | g     | 829  | CLA  | ND   |
| 14  | g     | 830  | CLA  | ND   |
| 14  | g     | 831  | CLA  | ND   |
| 14  | g     | 832  | CLA  | ND   |
| 14  | g     | 833  | CLA  | ND   |
| 14  | g     | 834  | CLA  | ND   |
| 14  | g     | 835  | CLA  | ND   |
| 14  | g     | 836  | CLA  | ND   |
| 14  | g     | 837  | CLA  | ND   |
| 14  | g     | 838  | CLA  | ND   |
| 14  | g     | 839  | CLA  | ND   |
| 14  | g     | 840  | CLA  | ND   |
| 14  | g     | 852  | CLA  | ND   |
| 14  | g     | 853  | CLA  | ND   |
| 14  | g     | 854  | CLA  | ND   |
| 14  | h     | 1701 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | n     | 802 | CLA  | ND   |
| 14  | n     | 803 | CLA  | ND   |
| 14  | n     | 804 | CLA  | ND   |
| 14  | n     | 805 | CLA  | ND   |
| 14  | n     | 806 | CLA  | ND   |
| 14  | n     | 807 | CLA  | ND   |
| 14  | n     | 808 | CLA  | ND   |
| 14  | n     | 809 | CLA  | ND   |
| 14  | n     | 810 | CLA  | ND   |
| 14  | n     | 811 | CLA  | ND   |
| 14  | n     | 812 | CLA  | ND   |
| 14  | n     | 813 | CLA  | ND   |
| 14  | n     | 814 | CLA  | ND   |
| 14  | n     | 815 | CLA  | ND   |
| 14  | n     | 816 | CLA  | ND   |
| 14  | n     | 817 | CLA  | ND   |
| 14  | n     | 818 | CLA  | ND   |
| 14  | n     | 819 | CLA  | ND   |
| 14  | n     | 820 | CLA  | ND   |
| 14  | n     | 821 | CLA  | ND   |
| 14  | n     | 822 | CLA  | ND   |
| 14  | n     | 823 | CLA  | ND   |
| 14  | n     | 824 | CLA  | ND   |
| 14  | n     | 825 | CLA  | ND   |
| 14  | n     | 826 | CLA  | ND   |
| 14  | n     | 827 | CLA  | ND   |
| 14  | n     | 828 | CLA  | ND   |
| 14  | n     | 829 | CLA  | ND   |
| 14  | n     | 830 | CLA  | ND   |
| 14  | n     | 831 | CLA  | ND   |
| 14  | n     | 832 | CLA  | ND   |
| 14  | n     | 833 | CLA  | ND   |
| 14  | n     | 834 | CLA  | ND   |
| 14  | n     | 835 | CLA  | ND   |
| 14  | n     | 836 | CLA  | ND   |
| 14  | n     | 837 | CLA  | ND   |
| 14  | n     | 838 | CLA  | ND   |
| 14  | n     | 839 | CLA  | ND   |
| 14  | n     | 840 | CLA  | ND   |
| 14  | n     | 850 | CLA  | ND   |
| 14  | n     | 852 | CLA  | ND   |
| 14  | s     | 201 | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | s     | 202 | CLA  | ND   |
| 14  | t     | 101 | CLA  | ND   |
| 14  | t     | 102 | CLA  | ND   |
| 14  | u     | 101 | CLA  | ND   |
| 14  | u     | 102 | CLA  | ND   |
| 14  | w     | 203 | CLA  | ND   |
| 14  | w     | 204 | CLA  | ND   |
| 14  | w     | 205 | CLA  | ND   |
| 14  | A     | 801 | CLA  | ND   |
| 14  | A     | 802 | CLA  | ND   |
| 14  | A     | 803 | CLA  | ND   |
| 14  | A     | 804 | CLA  | ND   |
| 14  | A     | 805 | CLA  | ND   |
| 14  | A     | 806 | CLA  | ND   |
| 14  | A     | 807 | CLA  | ND   |
| 14  | A     | 808 | CLA  | ND   |
| 14  | A     | 809 | CLA  | ND   |
| 14  | A     | 810 | CLA  | ND   |
| 14  | A     | 811 | CLA  | ND   |
| 14  | A     | 812 | CLA  | ND   |
| 14  | A     | 813 | CLA  | ND   |
| 14  | A     | 814 | CLA  | ND   |
| 14  | A     | 815 | CLA  | ND   |
| 14  | A     | 816 | CLA  | ND   |
| 14  | A     | 817 | CLA  | ND   |
| 14  | A     | 818 | CLA  | ND   |
| 14  | A     | 819 | CLA  | ND   |
| 14  | A     | 820 | CLA  | ND   |
| 14  | A     | 821 | CLA  | ND   |
| 14  | A     | 822 | CLA  | ND   |
| 14  | A     | 823 | CLA  | ND   |
| 14  | A     | 824 | CLA  | ND   |
| 14  | A     | 825 | CLA  | ND   |
| 14  | A     | 826 | CLA  | ND   |
| 14  | A     | 827 | CLA  | ND   |
| 14  | A     | 828 | CLA  | ND   |
| 14  | A     | 829 | CLA  | ND   |
| 14  | A     | 830 | CLA  | ND   |
| 14  | A     | 831 | CLA  | ND   |
| 14  | A     | 832 | CLA  | ND   |
| 14  | A     | 833 | CLA  | ND   |
| 14  | A     | 834 | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | A     | 835  | CLA  | ND   |
| 14  | A     | 836  | CLA  | ND   |
| 14  | A     | 837  | CLA  | ND   |
| 14  | A     | 838  | CLA  | ND   |
| 14  | A     | 839  | CLA  | ND   |
| 14  | A     | 840  | CLA  | ND   |
| 14  | A     | 841  | CLA  | ND   |
| 14  | A     | 853  | CLA  | ND   |
| 14  | A     | 854  | CLA  | ND   |
| 14  | A     | 855  | CLA  | ND   |
| 14  | A     | 857  | CLA  | ND   |
| 14  | X     | 1701 | CLA  | ND   |
| 14  | B     | 803  | CLA  | ND   |
| 14  | B     | 804  | CLA  | ND   |
| 14  | B     | 805  | CLA  | ND   |
| 14  | B     | 806  | CLA  | ND   |
| 14  | B     | 807  | CLA  | ND   |
| 14  | B     | 808  | CLA  | ND   |
| 14  | B     | 809  | CLA  | ND   |
| 14  | B     | 810  | CLA  | ND   |
| 14  | B     | 811  | CLA  | ND   |
| 14  | B     | 812  | CLA  | ND   |
| 14  | B     | 813  | CLA  | ND   |
| 14  | B     | 814  | CLA  | ND   |
| 14  | B     | 815  | CLA  | ND   |
| 14  | B     | 816  | CLA  | ND   |
| 14  | B     | 817  | CLA  | ND   |
| 14  | B     | 818  | CLA  | ND   |
| 14  | B     | 819  | CLA  | ND   |
| 14  | B     | 820  | CLA  | ND   |
| 14  | B     | 821  | CLA  | ND   |
| 14  | B     | 822  | CLA  | ND   |
| 14  | B     | 823  | CLA  | ND   |
| 14  | B     | 824  | CLA  | ND   |
| 14  | B     | 825  | CLA  | ND   |
| 14  | B     | 826  | CLA  | ND   |
| 14  | B     | 827  | CLA  | ND   |
| 14  | B     | 828  | CLA  | ND   |
| 14  | B     | 829  | CLA  | ND   |
| 14  | B     | 830  | CLA  | ND   |
| 14  | B     | 831  | CLA  | ND   |
| 14  | B     | 832  | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | B     | 833  | CLA  | ND   |
| 14  | B     | 834  | CLA  | ND   |
| 14  | B     | 835  | CLA  | ND   |
| 14  | B     | 836  | CLA  | ND   |
| 14  | B     | 837  | CLA  | ND   |
| 14  | B     | 838  | CLA  | ND   |
| 14  | B     | 839  | CLA  | ND   |
| 14  | B     | 840  | CLA  | ND   |
| 14  | B     | 841  | CLA  | ND   |
| 14  | B     | 850  | CLA  | ND   |
| 14  | F     | 201  | CLA  | ND   |
| 14  | F     | 202  | CLA  | ND   |
| 14  | J     | 101  | CLA  | ND   |
| 14  | J     | 102  | CLA  | ND   |
| 14  | K     | 101  | CLA  | ND   |
| 14  | L     | 1501 | CLA  | ND   |
| 14  | L     | 1502 | CLA  | ND   |
| 14  | L     | 1503 | CLA  | ND   |
| 14  | a     | 801  | CLA  | ND   |
| 14  | a     | 802  | CLA  | ND   |
| 14  | a     | 803  | CLA  | ND   |
| 14  | a     | 804  | CLA  | ND   |
| 14  | a     | 805  | CLA  | ND   |
| 14  | a     | 806  | CLA  | ND   |
| 14  | a     | 807  | CLA  | ND   |
| 14  | a     | 808  | CLA  | ND   |
| 14  | a     | 809  | CLA  | ND   |
| 14  | a     | 810  | CLA  | ND   |
| 14  | a     | 811  | CLA  | ND   |
| 14  | a     | 812  | CLA  | ND   |
| 14  | a     | 813  | CLA  | ND   |
| 14  | a     | 814  | CLA  | ND   |
| 14  | a     | 815  | CLA  | ND   |
| 14  | a     | 816  | CLA  | ND   |
| 14  | a     | 817  | CLA  | ND   |
| 14  | a     | 818  | CLA  | ND   |
| 14  | a     | 819  | CLA  | ND   |
| 14  | a     | 820  | CLA  | ND   |
| 14  | a     | 821  | CLA  | ND   |
| 14  | a     | 822  | CLA  | ND   |
| 14  | a     | 823  | CLA  | ND   |
| 14  | a     | 824  | CLA  | ND   |

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| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 14  | a     | 825  | CLA  | ND   |
| 14  | a     | 826  | CLA  | ND   |
| 14  | a     | 827  | CLA  | ND   |
| 14  | a     | 828  | CLA  | ND   |
| 14  | a     | 829  | CLA  | ND   |
| 14  | a     | 830  | CLA  | ND   |
| 14  | a     | 831  | CLA  | ND   |
| 14  | a     | 832  | CLA  | ND   |
| 14  | a     | 833  | CLA  | ND   |
| 14  | a     | 834  | CLA  | ND   |
| 14  | a     | 835  | CLA  | ND   |
| 14  | a     | 836  | CLA  | ND   |
| 14  | a     | 837  | CLA  | ND   |
| 14  | a     | 838  | CLA  | ND   |
| 14  | a     | 839  | CLA  | ND   |
| 14  | a     | 840  | CLA  | ND   |
| 14  | a     | 852  | CLA  | ND   |
| 14  | a     | 853  | CLA  | ND   |
| 14  | a     | 854  | CLA  | ND   |
| 14  | x     | 1701 | CLA  | ND   |
| 14  | b     | 802  | CLA  | ND   |
| 14  | b     | 803  | CLA  | ND   |
| 14  | b     | 804  | CLA  | ND   |
| 14  | b     | 805  | CLA  | ND   |
| 14  | b     | 806  | CLA  | ND   |
| 14  | b     | 807  | CLA  | ND   |
| 14  | b     | 808  | CLA  | ND   |
| 14  | b     | 809  | CLA  | ND   |
| 14  | b     | 810  | CLA  | ND   |
| 14  | b     | 811  | CLA  | ND   |
| 14  | b     | 812  | CLA  | ND   |
| 14  | b     | 813  | CLA  | ND   |
| 14  | b     | 814  | CLA  | ND   |
| 14  | b     | 815  | CLA  | ND   |
| 14  | b     | 816  | CLA  | ND   |
| 14  | b     | 817  | CLA  | ND   |
| 14  | b     | 818  | CLA  | ND   |
| 14  | b     | 819  | CLA  | ND   |
| 14  | b     | 820  | CLA  | ND   |
| 14  | b     | 821  | CLA  | ND   |
| 14  | b     | 822  | CLA  | ND   |
| 14  | b     | 823  | CLA  | ND   |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 14  | b     | 824 | CLA  | ND   |
| 14  | b     | 825 | CLA  | ND   |
| 14  | b     | 826 | CLA  | ND   |
| 14  | b     | 827 | CLA  | ND   |
| 14  | b     | 828 | CLA  | ND   |
| 14  | b     | 829 | CLA  | ND   |
| 14  | b     | 830 | CLA  | ND   |
| 14  | b     | 831 | CLA  | ND   |
| 14  | b     | 832 | CLA  | ND   |
| 14  | b     | 833 | CLA  | ND   |
| 14  | b     | 834 | CLA  | ND   |
| 14  | b     | 835 | CLA  | ND   |
| 14  | b     | 836 | CLA  | ND   |
| 14  | b     | 837 | CLA  | ND   |
| 14  | b     | 838 | CLA  | ND   |
| 14  | b     | 839 | CLA  | ND   |
| 14  | b     | 840 | CLA  | ND   |
| 14  | b     | 841 | CLA  | ND   |
| 14  | b     | 851 | CLA  | ND   |
| 14  | b     | 853 | CLA  | ND   |
| 14  | f     | 201 | CLA  | ND   |
| 14  | f     | 202 | CLA  | ND   |
| 14  | j     | 101 | CLA  | ND   |
| 14  | j     | 102 | CLA  | ND   |
| 14  | k     | 101 | CLA  | ND   |
| 14  | l     | 202 | CLA  | ND   |
| 14  | l     | 203 | CLA  | ND   |
| 14  | l     | 204 | CLA  | ND   |
| 19  | G     | 851 | CL0  | ND   |
| 19  | G     | 851 | CL0  | NC   |
| 19  | G     | 851 | CL0  | NA   |
| 19  | g     | 851 | CL0  | ND   |
| 19  | g     | 851 | CL0  | NC   |
| 19  | g     | 851 | CL0  | NA   |
| 19  | A     | 852 | CL0  | ND   |
| 19  | A     | 852 | CL0  | NC   |
| 19  | A     | 852 | CL0  | NA   |
| 19  | a     | 851 | CL0  | ND   |
| 19  | a     | 851 | CL0  | NC   |
| 19  | a     | 851 | CL0  | NA   |

All (4424) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 803  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 803  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 803  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 804  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 805  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 805  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 805  | CLA  | C11-C10-C8-C9   |
| 14  | G     | 807  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 807  | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 807  | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 810  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 814  | CLA  | CAD-CBD-CGD-O1D |
| 14  | G     | 814  | CLA  | CAD-CBD-CGD-O2D |
| 14  | G     | 817  | CLA  | C4B-C3B-CAB-CBB |
| 14  | G     | 818  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 818  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 819  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 819  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 821  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 821  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 821  | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 821  | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 822  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 822  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 823  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 823  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 824  | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 824  | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 827  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 829  | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 829  | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 832  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 833  | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 833  | CLA  | CHA-CBD-CGD-O2D |
| 14  | G     | 837  | CLA  | CAD-CBD-CGD-O1D |
| 14  | G     | 837  | CLA  | CAD-CBD-CGD-O2D |
| 14  | G     | 840  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 840  | CLA  | CAD-CBD-CGD-O1D |
| 14  | G     | 840  | CLA  | CAD-CBD-CGD-O2D |
| 14  | G     | 852  | CLA  | C2B-C3B-CAB-CBB |
| 14  | G     | 852  | CLA  | C4B-C3B-CAB-CBB |
| 14  | H     | 1701 | CLA  | C1A-C2A-CAA-CBA |
| 14  | H     | 1701 | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | N     | 803 | CLA  | CAD-CBD-CGD-O1D |
| 14  | N     | 803 | CLA  | CAD-CBD-CGD-O2D |
| 14  | N     | 804 | CLA  | C2B-C3B-CAB-CBB |
| 14  | N     | 804 | CLA  | C4B-C3B-CAB-CBB |
| 14  | N     | 804 | CLA  | CHA-CBD-CGD-O1D |
| 14  | N     | 804 | CLA  | CHA-CBD-CGD-O2D |
| 14  | N     | 804 | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 804 | CLA  | C4-C3-C5-C6     |
| 14  | N     | 805 | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 806 | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 806 | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 807 | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 808 | CLA  | C2B-C3B-CAB-CBB |
| 14  | N     | 808 | CLA  | C4B-C3B-CAB-CBB |
| 14  | N     | 810 | CLA  | C2B-C3B-CAB-CBB |
| 14  | N     | 810 | CLA  | C4B-C3B-CAB-CBB |
| 14  | N     | 810 | CLA  | CHA-CBD-CGD-O1D |
| 14  | N     | 810 | CLA  | CHA-CBD-CGD-O2D |
| 14  | N     | 811 | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 811 | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 812 | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 812 | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 813 | CLA  | CHA-CBD-CGD-O1D |
| 14  | N     | 813 | CLA  | CHA-CBD-CGD-O2D |
| 14  | N     | 814 | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 814 | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 816 | CLA  | CHA-CBD-CGD-O1D |
| 14  | N     | 816 | CLA  | CHA-CBD-CGD-O2D |
| 14  | N     | 819 | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 819 | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 819 | CLA  | C2B-C3B-CAB-CBB |
| 14  | N     | 819 | CLA  | C4B-C3B-CAB-CBB |
| 14  | N     | 820 | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 822 | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 822 | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 823 | CLA  | CHA-CBD-CGD-O1D |
| 14  | N     | 823 | CLA  | CHA-CBD-CGD-O2D |
| 14  | N     | 824 | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 826 | CLA  | CHA-CBD-CGD-O1D |
| 14  | N     | 826 | CLA  | CHA-CBD-CGD-O2D |
| 14  | N     | 827 | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 827 | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | N     | 827 | CLA  | CHA-CBD-CGD-O2D |
| 14  | N     | 828 | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 829 | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 830 | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 830 | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 831 | CLA  | CAD-CBD-CGD-O1D |
| 14  | N     | 831 | CLA  | CAD-CBD-CGD-O2D |
| 14  | N     | 831 | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 833 | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 834 | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 835 | CLA  | CHA-CBD-CGD-O1D |
| 14  | N     | 835 | CLA  | CHA-CBD-CGD-O2D |
| 14  | N     | 835 | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 836 | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 837 | CLA  | CAD-CBD-CGD-O1D |
| 14  | N     | 837 | CLA  | CAD-CBD-CGD-O2D |
| 14  | N     | 838 | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 838 | CLA  | C2B-C3B-CAB-CBB |
| 14  | N     | 838 | CLA  | C4B-C3B-CAB-CBB |
| 14  | T     | 101 | CLA  | CAD-CBD-CGD-O1D |
| 14  | T     | 101 | CLA  | CAD-CBD-CGD-O2D |
| 14  | W     | 202 | CLA  | C1A-C2A-CAA-CBA |
| 14  | W     | 202 | CLA  | CAD-CBD-CGD-O1D |
| 14  | W     | 202 | CLA  | CAD-CBD-CGD-O2D |
| 14  | g     | 801 | CLA  | CHA-CBD-CGD-O2D |
| 14  | g     | 803 | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 805 | CLA  | CHA-CBD-CGD-O1D |
| 14  | g     | 805 | CLA  | CHA-CBD-CGD-O2D |
| 14  | g     | 806 | CLA  | C3A-C2A-CAA-CBA |
| 14  | g     | 806 | CLA  | CHA-CBD-CGD-O1D |
| 14  | g     | 806 | CLA  | CHA-CBD-CGD-O2D |
| 14  | g     | 807 | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 807 | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 808 | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 808 | CLA  | C3A-C2A-CAA-CBA |
| 14  | g     | 809 | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 817 | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 817 | CLA  | C3A-C2A-CAA-CBA |
| 14  | g     | 818 | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 14  | g     | 818 | CLA  | CHA-CBD-CGD-O1D |
| 14  | g     | 818 | CLA  | CHA-CBD-CGD-O2D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | g     | 820  | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 820  | CLA  | C3A-C2A-CAA-CBA |
| 14  | g     | 821  | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 825  | CLA  | C14-C13-C15-C16 |
| 14  | g     | 826  | CLA  | C4-C3-C5-C6     |
| 14  | g     | 828  | CLA  | CHA-CBD-CGD-O1D |
| 14  | g     | 828  | CLA  | CHA-CBD-CGD-O2D |
| 14  | g     | 830  | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 836  | CLA  | CHA-CBD-CGD-O1D |
| 14  | g     | 836  | CLA  | CHA-CBD-CGD-O2D |
| 14  | g     | 836  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 854  | CLA  | C4-C3-C5-C6     |
| 14  | g     | 854  | CLA  | C11-C10-C8-C9   |
| 14  | h     | 1701 | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 802  | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 802  | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 802  | CLA  | C6-C7-C8-C9     |
| 14  | n     | 804  | CLA  | CBD-CGD-O2D-CED |
| 14  | n     | 805  | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 805  | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 805  | CLA  | CAD-CBD-CGD-O1D |
| 14  | n     | 805  | CLA  | CAD-CBD-CGD-O2D |
| 14  | n     | 806  | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 808  | CLA  | CHA-CBD-CGD-O1D |
| 14  | n     | 808  | CLA  | CHA-CBD-CGD-O2D |
| 14  | n     | 810  | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 810  | CLA  | CAD-CBD-CGD-O1D |
| 14  | n     | 810  | CLA  | CAD-CBD-CGD-O2D |
| 14  | n     | 810  | CLA  | CBD-CGD-O2D-CED |
| 14  | n     | 810  | CLA  | C11-C10-C8-C9   |
| 14  | n     | 811  | CLA  | CHA-CBD-CGD-O1D |
| 14  | n     | 811  | CLA  | CHA-CBD-CGD-O2D |
| 14  | n     | 812  | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 812  | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 814  | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 818  | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 820  | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 820  | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 821  | CLA  | CHA-CBD-CGD-O1D |
| 14  | n     | 821  | CLA  | CHA-CBD-CGD-O2D |
| 14  | n     | 823  | CLA  | CHA-CBD-CGD-O2D |
| 14  | n     | 823  | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | n     | 825 | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 825 | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 825 | CLA  | CHA-CBD-CGD-O1D |
| 14  | n     | 825 | CLA  | CHA-CBD-CGD-O2D |
| 14  | n     | 827 | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 828 | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 829 | CLA  | CHA-CBD-CGD-O1D |
| 14  | n     | 829 | CLA  | CHA-CBD-CGD-O2D |
| 14  | n     | 833 | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 833 | CLA  | CHA-CBD-CGD-O1D |
| 14  | n     | 833 | CLA  | CHA-CBD-CGD-O2D |
| 14  | n     | 833 | CLA  | CBD-CGD-O2D-CED |
| 14  | n     | 834 | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 835 | CLA  | CAD-CBD-CGD-O1D |
| 14  | n     | 835 | CLA  | CAD-CBD-CGD-O2D |
| 14  | n     | 840 | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 840 | CLA  | CBD-CGD-O2D-CED |
| 14  | n     | 840 | CLA  | C4-C3-C5-C6     |
| 14  | n     | 850 | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 850 | CLA  | C6-C7-C8-C9     |
| 14  | s     | 201 | CLA  | C3A-C2A-CAA-CBA |
| 14  | s     | 201 | CLA  | C4B-C3B-CAB-CBB |
| 14  | s     | 201 | CLA  | CBD-CGD-O2D-CED |
| 14  | t     | 101 | CLA  | CHA-CBD-CGD-O1D |
| 14  | t     | 101 | CLA  | CHA-CBD-CGD-O2D |
| 14  | w     | 203 | CLA  | C1A-C2A-CAA-CBA |
| 14  | w     | 203 | CLA  | C3A-C2A-CAA-CBA |
| 14  | w     | 203 | CLA  | CAD-CBD-CGD-O2D |
| 14  | w     | 205 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 803 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 804 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 804 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 804 | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 804 | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 805 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 805 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 805 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 806 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 806 | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 806 | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 806 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 807 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 807  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 807  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 807  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 810  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 810  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 811  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 813  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 813  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 814  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 816  | CLA  | C2B-C3B-CAB-CBB |
| 14  | A     | 816  | CLA  | C4B-C3B-CAB-CBB |
| 14  | A     | 818  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 818  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 819  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 819  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 821  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 821  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 821  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 821  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 822  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 823  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 823  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 825  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 827  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 829  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 829  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 832  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 833  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 833  | CLA  | CHA-CBD-CGD-O2D |
| 14  | A     | 835  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 835  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 841  | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 841  | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 855  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 855  | CLA  | C2B-C3B-CAB-CBB |
| 14  | A     | 855  | CLA  | C4B-C3B-CAB-CBB |
| 14  | X     | 1701 | CLA  | C1A-C2A-CAA-CBA |
| 14  | X     | 1701 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 803  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 803  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 805  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 806  | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | B     | 807 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 807 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 809 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 809 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 810 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 810 | CLA  | C2B-C3B-CAB-CBB |
| 14  | B     | 810 | CLA  | C4B-C3B-CAB-CBB |
| 14  | B     | 810 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 810 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 811 | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 811 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 812 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 812 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 813 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 815 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 815 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 816 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 816 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 816 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 819 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 819 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 821 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 821 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 822 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 822 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 824 | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 824 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 825 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 825 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 826 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 826 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 826 | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 826 | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 828 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 828 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 829 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 829 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 830 | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 830 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 830 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 832 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 832  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 833  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 833  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 834  | CLA  | CHA-CBD-CGD-O1D |
| 14  | B     | 834  | CLA  | CHA-CBD-CGD-O2D |
| 14  | B     | 834  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 835  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 835  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 836  | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 836  | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 836  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 837  | CLA  | C1A-C2A-CAA-CBA |
| 14  | F     | 201  | CLA  | CBD-CGD-O2D-CED |
| 14  | J     | 101  | CLA  | CAD-CBD-CGD-O1D |
| 14  | J     | 101  | CLA  | CAD-CBD-CGD-O2D |
| 14  | K     | 101  | CLA  | C1A-C2A-CAA-CBA |
| 14  | K     | 101  | CLA  | C3A-C2A-CAA-CBA |
| 14  | L     | 1501 | CLA  | C1A-C2A-CAA-CBA |
| 14  | L     | 1501 | CLA  | C3A-C2A-CAA-CBA |
| 14  | L     | 1501 | CLA  | CAD-CBD-CGD-O1D |
| 14  | L     | 1501 | CLA  | CAD-CBD-CGD-O2D |
| 14  | L     | 1501 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 801  | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 801  | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 802  | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 802  | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 803  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 803  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 804  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 805  | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 805  | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 806  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 806  | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 806  | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 808  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 808  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 808  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 809  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 809  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 812  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 813  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 817  | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 817  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 818  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 818  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 820  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 820  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 820  | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 820  | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 821  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 821  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 821  | CLA  | C2-C3-C5-C6     |
| 14  | a     | 821  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 826  | CLA  | C11-C10-C8-C7   |
| 14  | a     | 828  | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 828  | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 830  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 832  | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 832  | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 834  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 840  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 840  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 840  | CLA  | C2B-C3B-CAB-CBB |
| 14  | a     | 840  | CLA  | C4B-C3B-CAB-CBB |
| 14  | a     | 852  | CLA  | C2B-C3B-CAB-CBB |
| 14  | a     | 852  | CLA  | C4B-C3B-CAB-CBB |
| 14  | a     | 852  | CLA  | CBD-CGD-O2D-CED |
| 14  | x     | 1701 | CLA  | C1A-C2A-CAA-CBA |
| 14  | x     | 1701 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 803  | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 803  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 803  | CLA  | C4-C3-C5-C6     |
| 14  | b     | 804  | CLA  | C2B-C3B-CAB-CBB |
| 14  | b     | 804  | CLA  | C4B-C3B-CAB-CBB |
| 14  | b     | 804  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 805  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 806  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 806  | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 809  | CLA  | C4B-C3B-CAB-CBB |
| 14  | b     | 809  | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 809  | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 810  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 810  | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 811  | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | b     | 812 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 812 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 813 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 813 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 813 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 814 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 814 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 818 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 818 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 819 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 819 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 821 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 821 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 826 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 826 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 826 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 826 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 828 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 828 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 829 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 829 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 831 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 831 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 832 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 832 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 834 | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 834 | CLA  | CHA-CBD-CGD-O2D |
| 14  | b     | 834 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 835 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 836 | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 836 | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 839 | CLA  | C2B-C3B-CAB-CBB |
| 14  | b     | 839 | CLA  | C4B-C3B-CAB-CBB |
| 14  | b     | 841 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 851 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 853 | CLA  | C1A-C2A-CAA-CBA |
| 14  | f     | 201 | CLA  | CBD-CGD-O2D-CED |
| 14  | j     | 101 | CLA  | C1A-C2A-CAA-CBA |
| 14  | j     | 101 | CLA  | C3A-C2A-CAA-CBA |
| 14  | j     | 101 | CLA  | CAD-CBD-CGD-O1D |
| 14  | j     | 101 | CLA  | CAD-CBD-CGD-O2D |
| 14  | l     | 202 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | l     | 202 | CLA  | C3A-C2A-CAA-CBA |
| 14  | l     | 203 | CLA  | C2B-C3B-CAB-CBB |
| 14  | l     | 203 | CLA  | C4B-C3B-CAB-CBB |
| 14  | l     | 204 | CLA  | CBD-CGD-O2D-CED |
| 17  | G     | 848 | BCR  | C1-C6-C7-C8     |
| 17  | G     | 848 | BCR  | C5-C6-C7-C8     |
| 17  | G     | 848 | BCR  | C7-C8-C9-C10    |
| 17  | G     | 848 | BCR  | C7-C8-C9-C34    |
| 17  | G     | 848 | BCR  | C21-C22-C23-C24 |
| 17  | G     | 848 | BCR  | C37-C22-C23-C24 |
| 17  | N     | 844 | BCR  | C21-C22-C23-C24 |
| 17  | N     | 844 | BCR  | C37-C22-C23-C24 |
| 17  | N     | 847 | BCR  | C1-C6-C7-C8     |
| 17  | N     | 847 | BCR  | C5-C6-C7-C8     |
| 17  | N     | 848 | BCR  | C21-C22-C23-C24 |
| 17  | N     | 852 | BCR  | C17-C18-C19-C20 |
| 17  | N     | 852 | BCR  | C36-C18-C19-C20 |
| 17  | T     | 104 | BCR  | C1-C6-C7-C8     |
| 17  | T     | 104 | BCR  | C5-C6-C7-C8     |
| 17  | T     | 104 | BCR  | C21-C22-C23-C24 |
| 17  | V     | 101 | BCR  | C7-C8-C9-C10    |
| 17  | V     | 101 | BCR  | C7-C8-C9-C34    |
| 17  | W     | 201 | BCR  | C7-C8-C9-C10    |
| 17  | W     | 201 | BCR  | C11-C12-C13-C14 |
| 17  | W     | 201 | BCR  | C11-C12-C13-C35 |
| 17  | W     | 201 | BCR  | C17-C18-C19-C20 |
| 17  | W     | 201 | BCR  | C36-C18-C19-C20 |
| 17  | W     | 205 | BCR  | C21-C22-C23-C24 |
| 17  | W     | 205 | BCR  | C37-C22-C23-C24 |
| 17  | W     | 206 | BCR  | C7-C8-C9-C10    |
| 17  | W     | 206 | BCR  | C7-C8-C9-C34    |
| 17  | g     | 843 | BCR  | C11-C12-C13-C14 |
| 17  | g     | 846 | BCR  | C17-C18-C19-C20 |
| 17  | g     | 846 | BCR  | C36-C18-C19-C20 |
| 17  | g     | 848 | BCR  | C1-C6-C7-C8     |
| 17  | g     | 848 | BCR  | C5-C6-C7-C8     |
| 17  | g     | 848 | BCR  | C21-C22-C23-C24 |
| 17  | g     | 848 | BCR  | C37-C22-C23-C24 |
| 17  | n     | 846 | BCR  | C21-C22-C23-C24 |
| 17  | n     | 846 | BCR  | C37-C22-C23-C24 |
| 17  | n     | 847 | BCR  | C21-C22-C23-C24 |
| 17  | n     | 847 | BCR  | C37-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | n     | 849 | BCR  | C17-C18-C19-C20 |
| 17  | t     | 104 | BCR  | C37-C22-C23-C24 |
| 17  | v     | 101 | BCR  | C21-C22-C23-C24 |
| 17  | v     | 101 | BCR  | C37-C22-C23-C24 |
| 17  | w     | 201 | BCR  | C7-C8-C9-C10    |
| 17  | w     | 206 | BCR  | C21-C22-C23-C24 |
| 17  | w     | 206 | BCR  | C37-C22-C23-C24 |
| 17  | y     | 101 | BCR  | C7-C8-C9-C10    |
| 17  | A     | 845 | BCR  | C21-C22-C23-C24 |
| 17  | A     | 845 | BCR  | C37-C22-C23-C24 |
| 17  | A     | 849 | BCR  | C1-C6-C7-C8     |
| 17  | A     | 849 | BCR  | C5-C6-C7-C8     |
| 17  | A     | 849 | BCR  | C7-C8-C9-C34    |
| 17  | A     | 849 | BCR  | C21-C22-C23-C24 |
| 17  | B     | 844 | BCR  | C1-C6-C7-C8     |
| 17  | B     | 844 | BCR  | C5-C6-C7-C8     |
| 17  | B     | 846 | BCR  | C17-C18-C19-C20 |
| 17  | B     | 848 | BCR  | C21-C22-C23-C24 |
| 17  | B     | 848 | BCR  | C37-C22-C23-C24 |
| 17  | I     | 102 | BCR  | C11-C12-C13-C14 |
| 17  | I     | 102 | BCR  | C37-C22-C23-C24 |
| 17  | I     | 103 | BCR  | C7-C8-C9-C10    |
| 17  | a     | 843 | BCR  | C11-C12-C13-C14 |
| 17  | a     | 844 | BCR  | C21-C22-C23-C24 |
| 17  | a     | 846 | BCR  | C11-C12-C13-C14 |
| 17  | a     | 846 | BCR  | C11-C12-C13-C35 |
| 17  | a     | 846 | BCR  | C19-C20-C21-C22 |
| 17  | a     | 846 | BCR  | C23-C24-C25-C26 |
| 17  | a     | 848 | BCR  | C1-C6-C7-C8     |
| 17  | a     | 848 | BCR  | C5-C6-C7-C8     |
| 17  | a     | 848 | BCR  | C7-C8-C9-C10    |
| 17  | a     | 848 | BCR  | C7-C8-C9-C34    |
| 17  | a     | 848 | BCR  | C21-C22-C23-C24 |
| 17  | a     | 848 | BCR  | C37-C22-C23-C24 |
| 17  | b     | 846 | BCR  | C5-C6-C7-C8     |
| 17  | b     | 846 | BCR  | C7-C8-C9-C10    |
| 17  | b     | 846 | BCR  | C7-C8-C9-C34    |
| 17  | b     | 846 | BCR  | C11-C12-C13-C14 |
| 17  | b     | 847 | BCR  | C21-C22-C23-C24 |
| 17  | b     | 850 | BCR  | C7-C8-C9-C10    |
| 17  | b     | 850 | BCR  | C7-C8-C9-C34    |
| 17  | b     | 850 | BCR  | C11-C12-C13-C14 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | j     | 104  | BCR  | C21-C22-C23-C24 |
| 17  | j     | 104  | BCR  | C37-C22-C23-C24 |
| 17  | j     | 104  | BCR  | C23-C24-C25-C26 |
| 17  | i     | 101  | BCR  | C7-C8-C9-C10    |
| 17  | i     | 102  | BCR  | C13-C14-C15-C16 |
| 17  | i     | 102  | BCR  | C21-C22-C23-C24 |
| 18  | G     | 849  | LHG  | O1-C1-C2-C3     |
| 18  | G     | 849  | LHG  | C1-C2-C3-O3     |
| 18  | G     | 849  | LHG  | O2-C2-C3-O3     |
| 18  | G     | 849  | LHG  | C3-O3-P-O4      |
| 18  | G     | 849  | LHG  | C3-O3-P-O5      |
| 18  | G     | 849  | LHG  | C3-O3-P-O6      |
| 18  | G     | 849  | LHG  | C4-O6-P-O4      |
| 18  | G     | 850  | LHG  | O1-C1-C2-C3     |
| 18  | G     | 850  | LHG  | C1-C2-C3-O3     |
| 18  | G     | 850  | LHG  | C4-O6-P-O3      |
| 18  | S     | 202  | LHG  | O1-C1-C2-C3     |
| 18  | S     | 202  | LHG  | C1-C2-C3-O3     |
| 18  | S     | 202  | LHG  | C3-O3-P-O5      |
| 18  | S     | 202  | LHG  | C3-O3-P-O6      |
| 18  | S     | 202  | LHG  | C8-C7-O7-C5     |
| 18  | g     | 849  | LHG  | O1-C1-C2-C3     |
| 18  | g     | 849  | LHG  | C4-O6-P-O3      |
| 18  | g     | 849  | LHG  | C4-O6-P-O4      |
| 18  | g     | 849  | LHG  | C4-O6-P-O5      |
| 18  | g     | 850  | LHG  | C3-O3-P-O6      |
| 18  | v     | 102  | LHG  | C3-O3-P-O5      |
| 18  | v     | 102  | LHG  | C3-O3-P-O6      |
| 18  | v     | 102  | LHG  | O6-C4-C5-O7     |
| 18  | A     | 850  | LHG  | O1-C1-C2-C3     |
| 18  | A     | 851  | LHG  | C1-C2-C3-O3     |
| 18  | A     | 851  | LHG  | O2-C2-C3-O3     |
| 18  | A     | 851  | LHG  | C3-O3-P-O6      |
| 18  | X     | 1702 | LHG  | O1-C1-C2-C3     |
| 18  | X     | 1702 | LHG  | C1-C2-C3-O3     |
| 18  | X     | 1702 | LHG  | O2-C2-C3-O3     |
| 18  | X     | 1702 | LHG  | O9-C7-O7-C5     |
| 18  | X     | 1702 | LHG  | C8-C7-O7-C5     |
| 18  | a     | 850  | LHG  | C3-O3-P-O5      |
| 18  | a     | 850  | LHG  | C8-C7-O7-C5     |
| 18  | m     | 101  | LHG  | C4-O6-P-O3      |
| 18  | m     | 101  | LHG  | C4-O6-P-O4      |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | m     | 101  | LHG  | O6-C4-C5-O7     |
| 20  | h     | 1702 | SQD  | O47-C45-C46-O48 |
| 20  | n     | 801  | SQD  | O5-C5-C6-S      |
| 20  | w     | 202  | SQD  | O5-C1-O6-C44    |
| 20  | w     | 202  | SQD  | O47-C45-C46-O48 |
| 20  | w     | 202  | SQD  | O5-C5-C6-S      |
| 20  | B     | 801  | SQD  | C5-C6-S-O7      |
| 20  | B     | 801  | SQD  | C5-C6-S-O8      |
| 20  | B     | 801  | SQD  | C5-C6-S-O9      |
| 20  | b     | 801  | SQD  | C2-C1-O6-C44    |
| 20  | l     | 201  | SQD  | O5-C1-O6-C44    |
| 21  | N     | 802  | LMG  | O6-C1-O1-C7     |
| 21  | B     | 802  | LMG  | C11-C10-O7-C8   |
| 14  | G     | 805  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 814  | CLA  | O1D-CGD-O2D-CED |
| 14  | n     | 804  | CLA  | O1D-CGD-O2D-CED |
| 14  | n     | 833  | CLA  | O1D-CGD-O2D-CED |
| 14  | n     | 834  | CLA  | O1D-CGD-O2D-CED |
| 14  | s     | 201  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 807  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 810  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 816  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 804  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 822  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 805  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 801  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 810  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 804  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 835  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 836  | CLA  | O1D-CGD-O2D-CED |
| 14  | S     | 201  | CLA  | O1D-CGD-O2D-CED |
| 14  | g     | 809  | CLA  | O1D-CGD-O2D-CED |
| 14  | g     | 836  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 805  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 806  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 834  | CLA  | O1D-CGD-O2D-CED |
| 14  | F     | 201  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 804  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 823  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 834  | CLA  | O1D-CGD-O2D-CED |
| 14  | f     | 201  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 801  | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 812  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 814  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 824  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 827  | CLA  | CBD-CGD-O2D-CED |
| 14  | H     | 1701 | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 817  | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 825  | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 829  | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 834  | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 837  | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 851  | CLA  | CBD-CGD-O2D-CED |
| 14  | S     | 201  | CLA  | CBD-CGD-O2D-CED |
| 14  | T     | 101  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 804  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 819  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 821  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 826  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 830  | CLA  | CBD-CGD-O2D-CED |
| 14  | n     | 803  | CLA  | CBD-CGD-O2D-CED |
| 14  | n     | 827  | CLA  | CBD-CGD-O2D-CED |
| 14  | n     | 834  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 809  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 812  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 816  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 820  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 841  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 855  | CLA  | CBD-CGD-O2D-CED |
| 14  | X     | 1701 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 804  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 805  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 807  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 810  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 817  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 819  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 820  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 823  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 828  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 850  | CLA  | CBD-CGD-O2D-CED |
| 14  | J     | 101  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 816  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 819  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 821  | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 822  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 826  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 831  | CLA  | CBD-CGD-O2D-CED |
| 14  | x     | 1701 | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 823  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 830  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 840  | CLA  | CBD-CGD-O2D-CED |
| 14  | j     | 101  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 804  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 818  | CLA  | O1A-CGA-O2A-C1  |
| 14  | N     | 808  | CLA  | O1A-CGA-O2A-C1  |
| 14  | N     | 812  | CLA  | O1A-CGA-O2A-C1  |
| 14  | N     | 814  | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 803  | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 802  | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 822  | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 831  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 819  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 834  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 803  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 807  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 811  | CLA  | O1A-CGA-O2A-C1  |
| 14  | N     | 805  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 821  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 805  | CLA  | C2C-C3C-CAC-CBC |
| 14  | H     | 1701 | CLA  | O1D-CGD-O2D-CED |
| 14  | g     | 804  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 809  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 820  | CLA  | O1D-CGD-O2D-CED |
| 14  | X     | 1701 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 852  | CLA  | O1D-CGD-O2D-CED |
| 14  | x     | 1701 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 804  | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 808  | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 812  | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 803  | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 818  | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 802  | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 806  | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 822  | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 831  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 834  | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | B     | 837 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 819 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 836 | CLA  | O1A-CGA-O2A-C1  |
| 14  | N     | 803 | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 802 | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 817 | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 818 | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 835 | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 812 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 818 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 820 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 836 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 803 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 813 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 823 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 804 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 811 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 817 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 818 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 835 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 832 | CLA  | O1A-CGA-O2A-C1  |
| 20  | w     | 202 | SQD  | O10-C23-O48-C46 |
| 14  | G     | 832 | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 824 | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 825 | CLA  | O1D-CGD-O2D-CED |
| 14  | n     | 827 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 814 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 804 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 817 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 835 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 811 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 851 | CLA  | O1D-CGD-O2D-CED |
| 14  | j     | 101 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 822 | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 831 | CLA  | O1D-CGD-O2D-CED |
| 14  | g     | 807 | CLA  | O1D-CGD-O2D-CED |
| 14  | n     | 840 | CLA  | O1D-CGD-O2D-CED |
| 14  | w     | 205 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 822 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 827 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 830 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 836 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 808  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 813  | CLA  | O1D-CGD-O2D-CED |
| 14  | l     | 204  | CLA  | O1D-CGD-O2D-CED |
| 14  | g     | 813  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 838  | CLA  | CBD-CGD-O2D-CED |
| 18  | a     | 850  | LHG  | O9-C7-O7-C5     |
| 20  | H     | 1702 | SQD  | O49-C7-O47-C45  |
| 20  | x     | 1702 | SQD  | O49-C7-O47-C45  |
| 21  | B     | 802  | LMG  | O9-C10-O7-C8    |
| 14  | n     | 810  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 804  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 806  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 822  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 830  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 837  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 839  | CLA  | C3-C5-C6-C7     |
| 14  | N     | 803  | CLA  | C3-C5-C6-C7     |
| 14  | N     | 811  | CLA  | C3-C5-C6-C7     |
| 14  | g     | 802  | CLA  | C3-C5-C6-C7     |
| 14  | g     | 803  | CLA  | C3-C5-C6-C7     |
| 14  | g     | 806  | CLA  | C3-C5-C6-C7     |
| 14  | g     | 816  | CLA  | C3-C5-C6-C7     |
| 14  | g     | 821  | CLA  | C3-C5-C6-C7     |
| 14  | g     | 826  | CLA  | C3-C5-C6-C7     |
| 14  | g     | 830  | CLA  | C3-C5-C6-C7     |
| 14  | n     | 833  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 808  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 819  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 822  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 837  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 853  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 854  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 803  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 824  | CLA  | C3-C5-C6-C7     |
| 14  | L     | 1502 | CLA  | C3-C5-C6-C7     |
| 14  | a     | 803  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 807  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 826  | CLA  | C3-C5-C6-C7     |
| 14  | b     | 837  | CLA  | C3-C5-C6-C7     |
| 14  | b     | 838  | CLA  | C3-C5-C6-C7     |
| 14  | f     | 201  | CLA  | C3-C5-C6-C7     |
| 19  | G     | 851  | CL0  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 19  | a     | 851 | CL0  | C3-C5-C6-C7     |
| 14  | B     | 833 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 803 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 807 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 818 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 819 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 820 | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 803 | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 814 | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 817 | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 802 | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 804 | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 806 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 810 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 805 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 819 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 803 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 804 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 817 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 830 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 807 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 811 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 813 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 832 | CLA  | CBA-CGA-O2A-C1  |
| 20  | w     | 202 | SQD  | C24-C23-O48-C46 |
| 14  | G     | 823 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 833 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 852 | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 815 | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 832 | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 814 | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 832 | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 837 | CLA  | CBD-CGD-O2D-CED |
| 14  | n     | 828 | CLA  | CBD-CGD-O2D-CED |
| 14  | n     | 835 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 813 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 823 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 833 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 836 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 812 | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 814 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 810 | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 811  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 827  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 830  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 832  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 812  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 836  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 837  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 841  | CLA  | CBD-CGD-O2D-CED |
| 20  | H     | 1702 | SQD  | C8-C7-O47-C45   |
| 20  | x     | 1702 | SQD  | C8-C7-O47-C45   |
| 14  | N     | 806  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 834  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 832  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 823  | CLA  | O1D-CGD-O2D-CED |
| 14  | J     | 101  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 812  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 835  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 842  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 802  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 819  | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 826  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 806  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 831  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 839  | CLA  | C4-C3-C5-C6     |
| 14  | n     | 822  | CLA  | C4-C3-C5-C6     |
| 14  | n     | 850  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 826  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 828  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 830  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 806  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 831  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 839  | CLA  | C2-C3-C5-C6     |
| 14  | N     | 804  | CLA  | C2-C3-C5-C6     |
| 14  | g     | 826  | CLA  | C2-C3-C5-C6     |
| 14  | g     | 854  | CLA  | C2-C3-C5-C6     |
| 14  | n     | 822  | CLA  | C2-C3-C5-C6     |
| 14  | n     | 840  | CLA  | C2-C3-C5-C6     |
| 14  | n     | 850  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 805  | CLA  | C2-C3-C5-C6     |
| 14  | a     | 826  | CLA  | C2-C3-C5-C6     |
| 14  | a     | 830  | CLA  | C2-C3-C5-C6     |
| 14  | N     | 818  | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | n     | 824 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 812 | CLA  | O1D-CGD-O2D-CED |
| 14  | g     | 819 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 831 | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 842 | CLA  | C2A-CAA-CBA-CGA |
| 14  | n     | 809 | CLA  | C2A-CAA-CBA-CGA |
| 14  | u     | 101 | CLA  | C2A-CAA-CBA-CGA |
| 14  | w     | 205 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 828 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 807 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 808 | CLA  | C3-C5-C6-C7     |
| 14  | g     | 836 | CLA  | C3-C5-C6-C7     |
| 14  | n     | 809 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 834 | CLA  | C3-C5-C6-C7     |
| 14  | a     | 806 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 811 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 831 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 851 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 836 | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 809 | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 816 | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 817 | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 835 | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 812 | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 818 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 817 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 818 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 820 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 836 | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 857 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 803 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 813 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 823 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 802 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 806 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 809 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 811 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 816 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 818 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 821 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 835 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 803 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | G     | 849  | LHG  | C24-C23-O8-C6   |
| 18  | X     | 1702 | LHG  | C24-C23-O8-C6   |
| 20  | H     | 1702 | SQD  | C24-C23-O48-C46 |
| 20  | x     | 1702 | SQD  | C24-C23-O48-C46 |
| 18  | G     | 849  | LHG  | C24-C25-C26-C27 |
| 18  | G     | 850  | LHG  | C24-C25-C26-C27 |
| 18  | v     | 102  | LHG  | C24-C25-C26-C27 |
| 18  | X     | 1702 | LHG  | C24-C25-C26-C27 |
| 18  | m     | 101  | LHG  | C24-C25-C26-C27 |
| 18  | g     | 850  | LHG  | C24-C25-C26-C27 |
| 17  | W     | 201  | BCR  | C15-C16-C17-C18 |
| 17  | W     | 201  | BCR  | C19-C20-C21-C22 |
| 17  | I     | 102  | BCR  | C19-C20-C21-C22 |
| 17  | b     | 846  | BCR  | C19-C20-C21-C22 |
| 14  | G     | 817  | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 806  | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 816  | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 830  | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 815  | CLA  | O1A-CGA-O2A-C1  |
| 14  | u     | 102  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 807  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 816  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 821  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 854  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 803  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 816  | CLA  | O1A-CGA-O2A-C1  |
| 20  | x     | 1702 | SQD  | O10-C23-O48-C46 |
| 18  | S     | 202  | LHG  | O9-C7-O7-C5     |
| 14  | A     | 855  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 820  | CLA  | O1D-CGD-O2D-CED |
| 18  | a     | 850  | LHG  | C24-C25-C26-C27 |
| 14  | N     | 829  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 851  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 812  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 826  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 830  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 806  | CLA  | C3-C5-C6-C7     |
| 14  | n     | 803  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 832  | CLA  | C3-C5-C6-C7     |
| 14  | g     | 834  | CLA  | CBD-CGD-O2D-CED |
| 14  | h     | 1701 | CLA  | CBD-CGD-O2D-CED |
| 14  | n     | 811  | CLA  | CBD-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | n     | 819  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 835  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 803  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 837  | CLA  | CBD-CGD-O2D-CED |
| 18  | S     | 202  | LHG  | O2-C2-C3-O3     |
| 14  | N     | 817  | CLA  | O1D-CGD-O2D-CED |
| 14  | T     | 101  | CLA  | O1D-CGD-O2D-CED |
| 14  | n     | 803  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 828  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 819  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 820  | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 833  | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 842  | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 821  | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 840  | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 815  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 803  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 841  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 802  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 816  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 819  | CLA  | CBA-CGA-O2A-C1  |
| 20  | l     | 201  | SQD  | C24-C23-O48-C46 |
| 18  | m     | 101  | LHG  | C15-C16-C17-C18 |
| 14  | G     | 807  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 820  | CLA  | O1A-CGA-O2A-C1  |
| 14  | N     | 817  | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 804  | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 810  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 810  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 805  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 841  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 806  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 830  | CLA  | O1A-CGA-O2A-C1  |
| 18  | X     | 1702 | LHG  | O10-C23-O8-C6   |
| 20  | l     | 201  | SQD  | O10-C23-O48-C46 |
| 14  | g     | 821  | CLA  | O1D-CGD-O2D-CED |
| 21  | N     | 802  | LMG  | O6-C5-C6-O5     |
| 14  | g     | 816  | CLA  | CBD-CGD-O2D-CED |
| 14  | n     | 815  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 816  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 840  | CLA  | O1D-CGD-O2D-CED |
| 18  | G     | 849  | LHG  | O10-C23-O8-C6   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | g     | 830  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 816  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 805  | CLA  | O1D-CGD-O2D-CED |
| 14  | g     | 807  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 811  | CLA  | C3-C5-C6-C7     |
| 14  | N     | 813  | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 833  | CLA  | CBD-CGD-O2D-CED |
| 14  | S     | 203  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 829  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 824  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 824  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 841  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 850  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 817  | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 810  | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 830  | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 810  | CLA  | CBA-CGA-O2A-C1  |
| 14  | u     | 102  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 807  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 854  | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 834  | CLA  | C4-C3-C5-C6     |
| 14  | g     | 830  | CLA  | C4-C3-C5-C6     |
| 14  | g     | 830  | CLA  | C2-C3-C5-C6     |
| 14  | N     | 820  | CLA  | O1A-CGA-O2A-C1  |
| 14  | N     | 833  | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 809  | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 821  | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 818  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 803  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 817  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 857  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 809  | CLA  | O1A-CGA-O2A-C1  |
| 20  | H     | 1702 | SQD  | O10-C23-O48-C46 |
| 14  | n     | 802  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 819  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 810  | CLA  | C2A-CAA-CBA-CGA |
| 19  | G     | 851  | CL0  | C2A-CAA-CBA-CGA |
| 14  | N     | 837  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 819  | CLA  | O1D-CGD-O2D-CED |
| 14  | g     | 810  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 802  | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 838  | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | H     | 1702 | SQD  | O5-C1-O6-C44    |
| 20  | b     | 801  | SQD  | O5-C1-O6-C44    |
| 14  | G     | 827  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 805  | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 819  | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 832  | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 819  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 839  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 831  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 809  | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 842  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 806  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 810  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 812  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 822  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 853  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 830  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 839  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 829  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 831  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 834  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 840  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 853  | CLA  | CBD-CGD-O2D-CED |
| 14  | l     | 202  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 840  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 837  | CLA  | O1D-CGD-O2D-CED |
| 14  | g     | 835  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 853  | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 818  | CLA  | CBD-CGD-O2D-CED |
| 17  | B     | 844  | BCR  | C19-C20-C21-C22 |
| 14  | G     | 805  | CLA  | O1A-CGA-O2A-C1  |
| 14  | N     | 832  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 831  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 810  | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 813  | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 827  | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 830  | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 838  | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 840  | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 850  | CLA  | CBA-CGA-O2A-C1  |
| 14  | s     | 201  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 822  | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 806  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 832  | CLA  | CBA-CGA-O2A-C1  |
| 14  | L     | 1502 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 810  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 819  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 823  | CLA  | CBA-CGA-O2A-C1  |
| 19  | a     | 851  | CL0  | CBA-CGA-O2A-C1  |
| 20  | h     | 1702 | SQD  | C24-C23-O48-C46 |
| 20  | B     | 801  | SQD  | C24-C23-O48-C46 |
| 18  | S     | 202  | LHG  | C26-C27-C28-C29 |
| 14  | G     | 835  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 838  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 801  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 820  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 828  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 831  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 841  | CLA  | CBD-CGD-O2D-CED |
| 18  | a     | 850  | LHG  | C11-C10-C9-C8   |
| 20  | h     | 1702 | SQD  | C9-C10-C11-C12  |
| 14  | g     | 813  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 838  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 834  | CLA  | C2-C3-C5-C6     |
| 14  | a     | 828  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 805  | CLA  | C4C-C3C-CAC-CBC |
| 14  | A     | 811  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 828  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 804  | CLA  | C6-C7-C8-C9     |
| 14  | G     | 853  | CLA  | C11-C12-C13-C14 |
| 14  | N     | 831  | CLA  | C14-C13-C15-C16 |
| 14  | N     | 851  | CLA  | C11-C12-C13-C14 |
| 14  | g     | 803  | CLA  | C6-C7-C8-C9     |
| 14  | g     | 805  | CLA  | C11-C10-C8-C9   |
| 14  | g     | 807  | CLA  | C11-C10-C8-C9   |
| 14  | g     | 816  | CLA  | C6-C7-C8-C9     |
| 14  | g     | 825  | CLA  | C6-C7-C8-C9     |
| 14  | g     | 825  | CLA  | C11-C12-C13-C14 |
| 14  | g     | 852  | CLA  | C11-C10-C8-C9   |
| 14  | n     | 808  | CLA  | C14-C13-C15-C16 |
| 14  | n     | 832  | CLA  | C11-C12-C13-C14 |
| 14  | n     | 837  | CLA  | C14-C13-C15-C16 |
| 14  | w     | 204  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 802  | CLA  | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | A     | 811 | CLA  | C11-C10-C8-C9   |
| 14  | A     | 826 | CLA  | C14-C13-C15-C16 |
| 14  | A     | 831 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 831 | CLA  | C14-C13-C15-C16 |
| 14  | A     | 839 | CLA  | C11-C12-C13-C14 |
| 14  | A     | 854 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 811 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 818 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 818 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 830 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 841 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 850 | CLA  | C11-C12-C13-C14 |
| 14  | b     | 803 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 807 | CLA  | C14-C13-C15-C16 |
| 14  | b     | 809 | CLA  | C14-C13-C15-C16 |
| 14  | b     | 811 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 818 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 830 | CLA  | C11-C12-C13-C14 |
| 14  | f     | 201 | CLA  | C6-C7-C8-C9     |
| 21  | N     | 802 | LMG  | C4-C5-C6-O5     |
| 14  | g     | 814 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 836 | CLA  | O1D-CGD-O2D-CED |
| 18  | G     | 850 | LHG  | O2-C2-C3-O3     |
| 18  | g     | 849 | LHG  | O2-C2-C3-O3     |
| 14  | A     | 823 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 812 | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 827 | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 840 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 810 | CLA  | O1A-CGA-O2A-C1  |
| 17  | N     | 845 | BCR  | C37-C22-C23-C24 |
| 17  | N     | 848 | BCR  | C37-C22-C23-C24 |
| 17  | T     | 104 | BCR  | C37-C22-C23-C24 |
| 17  | W     | 201 | BCR  | C7-C8-C9-C34    |
| 17  | g     | 843 | BCR  | C11-C12-C13-C35 |
| 17  | g     | 848 | BCR  | C7-C8-C9-C34    |
| 17  | n     | 845 | BCR  | C7-C8-C9-C34    |
| 17  | n     | 849 | BCR  | C36-C18-C19-C20 |
| 17  | w     | 201 | BCR  | C7-C8-C9-C34    |
| 17  | y     | 101 | BCR  | C7-C8-C9-C34    |
| 17  | A     | 849 | BCR  | C37-C22-C23-C24 |
| 17  | B     | 844 | BCR  | C7-C8-C9-C34    |
| 17  | B     | 844 | BCR  | C36-C18-C19-C20 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | B     | 844  | BCR  | C37-C22-C23-C24 |
| 17  | B     | 846  | BCR  | C36-C18-C19-C20 |
| 17  | B     | 846  | BCR  | C37-C22-C23-C24 |
| 17  | I     | 101  | BCR  | C37-C22-C23-C24 |
| 17  | I     | 102  | BCR  | C7-C8-C9-C34    |
| 17  | I     | 102  | BCR  | C11-C12-C13-C35 |
| 17  | I     | 103  | BCR  | C7-C8-C9-C34    |
| 17  | I     | 103  | BCR  | C37-C22-C23-C24 |
| 17  | L     | 1504 | BCR  | C11-C12-C13-C35 |
| 17  | a     | 843  | BCR  | C11-C12-C13-C35 |
| 17  | a     | 844  | BCR  | C37-C22-C23-C24 |
| 17  | a     | 846  | BCR  | C36-C18-C19-C20 |
| 17  | a     | 846  | BCR  | C37-C22-C23-C24 |
| 17  | b     | 846  | BCR  | C11-C12-C13-C35 |
| 17  | b     | 846  | BCR  | C36-C18-C19-C20 |
| 17  | b     | 847  | BCR  | C37-C22-C23-C24 |
| 17  | b     | 850  | BCR  | C11-C12-C13-C35 |
| 17  | j     | 104  | BCR  | C7-C8-C9-C34    |
| 17  | i     | 101  | BCR  | C7-C8-C9-C34    |
| 17  | i     | 102  | BCR  | C7-C8-C9-C34    |
| 17  | i     | 102  | BCR  | C37-C22-C23-C24 |
| 17  | l     | 205  | BCR  | C37-C22-C23-C24 |
| 17  | m     | 102  | BCR  | C7-C8-C9-C34    |
| 17  | g     | 848  | BCR  | C7-C8-C9-C10    |
| 17  | t     | 104  | BCR  | C21-C22-C23-C24 |
| 17  | A     | 846  | BCR  | C7-C8-C9-C10    |
| 17  | A     | 849  | BCR  | C7-C8-C9-C10    |
| 17  | B     | 844  | BCR  | C7-C8-C9-C10    |
| 17  | B     | 846  | BCR  | C21-C22-C23-C24 |
| 17  | I     | 102  | BCR  | C7-C8-C9-C10    |
| 17  | I     | 103  | BCR  | C21-C22-C23-C24 |
| 17  | b     | 846  | BCR  | C17-C18-C19-C20 |
| 17  | j     | 104  | BCR  | C7-C8-C9-C10    |
| 17  | i     | 102  | BCR  | C7-C8-C9-C10    |
| 17  | l     | 205  | BCR  | C21-C22-C23-C24 |
| 14  | N     | 811  | CLA  | C2A-CAA-CBA-CGA |
| 14  | n     | 803  | CLA  | C2A-CAA-CBA-CGA |
| 14  | n     | 839  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 809  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 853  | CLA  | C2A-CAA-CBA-CGA |
| 18  | S     | 202  | LHG  | C7-C8-C9-C10    |
| 14  | G     | 833  | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 812  | CLA  | O1D-CGD-O2D-CED |
| 20  | h     | 1702 | SQD  | C11-C12-C13-C14 |
| 14  | G     | 810  | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 830  | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 850  | CLA  | O1A-CGA-O2A-C1  |
| 14  | L     | 1502 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 819  | CLA  | O1A-CGA-O2A-C1  |
| 20  | B     | 801  | SQD  | O10-C23-O48-C46 |
| 14  | G     | 827  | CLA  | C10-C11-C12-C13 |
| 14  | n     | 835  | CLA  | O1D-CGD-O2D-CED |
| 14  | n     | 852  | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 850  | LHG  | O7-C5-C6-O8     |
| 18  | m     | 101  | LHG  | O7-C5-C6-O8     |
| 20  | l     | 201  | SQD  | O47-C45-C46-O48 |
| 14  | b     | 836  | CLA  | O1D-CGD-O2D-CED |
| 20  | B     | 801  | SQD  | C10-C11-C12-C13 |
| 14  | g     | 832  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 832  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 818  | CLA  | C15-C16-C17-C18 |
| 14  | g     | 801  | CLA  | C8-C10-C11-C12  |
| 14  | g     | 854  | CLA  | C13-C15-C16-C17 |
| 14  | n     | 802  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 809  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 811  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 807  | CLA  | C5-C6-C7-C8     |
| 18  | G     | 850  | LHG  | O1-C1-C2-O2     |
| 14  | G     | 817  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 838  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 833  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 811  | CLA  | C8-C10-C11-C12  |
| 14  | G     | 838  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 837  | CLA  | C11-C12-C13-C15 |
| 14  | n     | 827  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 802  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 802  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 810  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 820  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 827  | CLA  | C11-C10-C8-C7   |
| 14  | a     | 830  | CLA  | C11-C12-C13-C15 |
| 14  | a     | 836  | CLA  | C11-C12-C13-C15 |
| 14  | b     | 804  | CLA  | C6-C7-C8-C10    |
| 14  | n     | 803  | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 819  | CLA  | CBA-CGA-O2A-C1  |
| 18  | A     | 850  | LHG  | C24-C23-O8-C6   |
| 14  | A     | 822  | CLA  | C4-C3-C5-C6     |
| 17  | W     | 201  | BCR  | C13-C14-C15-C16 |
| 17  | b     | 846  | BCR  | C9-C10-C11-C12  |
| 18  | a     | 850  | LHG  | C31-C32-C33-C34 |
| 20  | x     | 1702 | SQD  | C33-C34-C35-C36 |
| 14  | a     | 811  | CLA  | C2C-C3C-CAC-CBC |
| 14  | b     | 812  | CLA  | O1D-CGD-O2D-CED |
| 18  | m     | 101  | LHG  | C9-C10-C11-C12  |
| 14  | N     | 801  | CLA  | C8-C10-C11-C12  |
| 14  | N     | 807  | CLA  | C13-C15-C16-C17 |
| 14  | N     | 815  | CLA  | C10-C11-C12-C13 |
| 14  | g     | 830  | CLA  | C8-C10-C11-C12  |
| 14  | n     | 805  | CLA  | C13-C15-C16-C17 |
| 14  | n     | 806  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 833  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 804  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 807  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 826  | CLA  | C8-C10-C11-C12  |
| 18  | v     | 102  | LHG  | C12-C13-C14-C15 |
| 14  | n     | 838  | CLA  | O1A-CGA-O2A-C1  |
| 14  | s     | 201  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 822  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 806  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 832  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 838  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 827  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 823  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 832  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 810  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 827  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 841  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 803  | CLA  | C13-C15-C16-C17 |
| 14  | N     | 804  | CLA  | C8-C10-C11-C12  |
| 14  | N     | 819  | CLA  | C8-C10-C11-C12  |
| 14  | N     | 827  | CLA  | C10-C11-C12-C13 |
| 14  | g     | 806  | CLA  | C8-C10-C11-C12  |
| 14  | g     | 826  | CLA  | C8-C10-C11-C12  |
| 14  | n     | 837  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 804  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 810  | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | A     | 811 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 817 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 820 | CLA  | C13-C15-C16-C17 |
| 14  | A     | 820 | CLA  | C15-C16-C17-C18 |
| 14  | A     | 832 | CLA  | C5-C6-C7-C8     |
| 14  | A     | 837 | CLA  | C13-C15-C16-C17 |
| 14  | B     | 806 | CLA  | C13-C15-C16-C17 |
| 14  | B     | 807 | CLA  | C13-C15-C16-C17 |
| 14  | B     | 850 | CLA  | C10-C11-C12-C13 |
| 14  | a     | 807 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 809 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 841 | CLA  | C8-C10-C11-C12  |
| 20  | l     | 201 | SQD  | C11-C12-C13-C14 |
| 14  | G     | 810 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 828 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 830 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 839 | CLA  | C2A-CAA-CBA-CGA |
| 14  | N     | 806 | CLA  | C2A-CAA-CBA-CGA |
| 14  | T     | 101 | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 807 | CLA  | C2A-CAA-CBA-CGA |
| 14  | n     | 812 | CLA  | C2A-CAA-CBA-CGA |
| 14  | n     | 820 | CLA  | C2A-CAA-CBA-CGA |
| 14  | n     | 828 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 808 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 830 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 855 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 821 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 836 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 840 | CLA  | C2A-CAA-CBA-CGA |
| 14  | J     | 101 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 827 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 834 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 810 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 813 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 840 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 814 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 830 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 801 | CLA  | C15-C16-C17-C18 |
| 14  | N     | 828 | CLA  | C8-C10-C11-C12  |
| 14  | N     | 851 | CLA  | C8-C10-C11-C12  |
| 14  | g     | 809 | CLA  | C8-C10-C11-C12  |
| 14  | g     | 817 | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | g     | 823 | CLA  | C8-C10-C11-C12  |
| 14  | g     | 852 | CLA  | C5-C6-C7-C8     |
| 14  | g     | 854 | CLA  | C8-C10-C11-C12  |
| 14  | g     | 854 | CLA  | C15-C16-C17-C18 |
| 14  | n     | 823 | CLA  | C13-C15-C16-C17 |
| 14  | n     | 828 | CLA  | C15-C16-C17-C18 |
| 14  | A     | 806 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 820 | CLA  | C5-C6-C7-C8     |
| 14  | A     | 824 | CLA  | C15-C16-C17-C18 |
| 14  | A     | 831 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 837 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 824 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 811 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 814 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 829 | CLA  | C13-C15-C16-C17 |
| 14  | b     | 829 | CLA  | C15-C16-C17-C18 |
| 18  | g     | 850 | LHG  | C23-C24-C25-C26 |
| 20  | w     | 202 | SQD  | C23-C24-C25-C26 |
| 20  | B     | 801 | SQD  | C7-C8-C9-C10    |
| 14  | G     | 852 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 813 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 823 | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 820 | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 815 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 820 | CLA  | C8-C10-C11-C12  |
| 14  | N     | 808 | CLA  | C15-C16-C17-C18 |
| 14  | N     | 826 | CLA  | C15-C16-C17-C18 |
| 14  | g     | 819 | CLA  | C13-C15-C16-C17 |
| 14  | n     | 803 | CLA  | C10-C11-C12-C13 |
| 14  | n     | 822 | CLA  | C5-C6-C7-C8     |
| 14  | n     | 850 | CLA  | C5-C6-C7-C8     |
| 14  | s     | 201 | CLA  | C5-C6-C7-C8     |
| 14  | w     | 204 | CLA  | C5-C6-C7-C8     |
| 14  | A     | 802 | CLA  | C13-C15-C16-C17 |
| 14  | A     | 840 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 854 | CLA  | C13-C15-C16-C17 |
| 14  | B     | 814 | CLA  | C10-C11-C12-C13 |
| 14  | B     | 826 | CLA  | C10-C11-C12-C13 |
| 14  | a     | 817 | CLA  | C15-C16-C17-C18 |
| 14  | a     | 819 | CLA  | C10-C11-C12-C13 |
| 14  | a     | 830 | CLA  | C8-C10-C11-C12  |
| 14  | b     | 802 | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 806  | CLA  | C13-C15-C16-C17 |
| 15  | B     | 842  | PQN  | C15-C16-C17-C18 |
| 18  | a     | 850  | LHG  | O2-C2-C3-O3     |
| 14  | n     | 828  | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 819  | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 819  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 839  | CLA  | O1A-CGA-O2A-C1  |
| 19  | a     | 851  | CL0  | O1A-CGA-O2A-C1  |
| 20  | h     | 1702 | SQD  | O10-C23-O48-C46 |
| 14  | G     | 824  | CLA  | C8-C10-C11-C12  |
| 14  | n     | 813  | CLA  | C10-C11-C12-C13 |
| 14  | n     | 829  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 854  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 837  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 824  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 826  | CLA  | C5-C6-C7-C8     |
| 14  | N     | 818  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 811  | CLA  | O1D-CGD-O2D-CED |
| 14  | n     | 831  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 829  | CLA  | C3-C5-C6-C7     |
| 14  | g     | 837  | CLA  | O1D-CGD-O2D-CED |
| 14  | n     | 811  | CLA  | O1D-CGD-O2D-CED |
| 14  | n     | 819  | CLA  | O1D-CGD-O2D-CED |
| 14  | n     | 824  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 837  | CLA  | O1D-CGD-O2D-CED |
| 14  | g     | 803  | CLA  | C15-C16-C17-C18 |
| 14  | g     | 836  | CLA  | C10-C11-C12-C13 |
| 14  | g     | 838  | CLA  | C15-C16-C17-C18 |
| 14  | n     | 808  | CLA  | C10-C11-C12-C13 |
| 14  | n     | 823  | CLA  | C5-C6-C7-C8     |
| 14  | n     | 840  | CLA  | C8-C10-C11-C12  |
| 14  | b     | 802  | CLA  | C5-C6-C7-C8     |
| 14  | g     | 808  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 832  | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 813  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 812  | CLA  | O1A-CGA-O2A-C1  |
| 14  | h     | 1701 | CLA  | O1D-CGD-O2D-CED |
| 14  | n     | 828  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 803  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 837  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 808  | CLA  | C8-C10-C11-C12  |
| 14  | n     | 840  | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 830  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 808  | CLA  | C5-C6-C7-C8     |
| 14  | N     | 801  | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 834  | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 838  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 820  | CLA  | CBA-CGA-O2A-C1  |
| 20  | h     | 1702 | SQD  | C8-C7-O47-C45   |
| 20  | B     | 801  | SQD  | C8-C7-O47-C45   |
| 14  | g     | 834  | CLA  | O1D-CGD-O2D-CED |
| 21  | b     | 849  | LMG  | C28-C29-C30-C31 |
| 14  | G     | 806  | CLA  | C8-C10-C11-C12  |
| 14  | N     | 842  | CLA  | C5-C6-C7-C8     |
| 20  | w     | 202  | SQD  | C31-C32-C33-C34 |
| 14  | n     | 852  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 839  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 813  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 801  | CLA  | C3-C5-C6-C7     |
| 17  | i     | 102  | BCR  | C15-C16-C17-C18 |
| 18  | A     | 850  | LHG  | O10-C23-O8-C6   |
| 14  | N     | 805  | CLA  | C2C-C3C-CAC-CBC |
| 14  | n     | 804  | CLA  | C2C-C3C-CAC-CBC |
| 20  | h     | 1702 | SQD  | O49-C7-O47-C45  |
| 20  | B     | 801  | SQD  | O49-C7-O47-C45  |
| 14  | N     | 841  | CLA  | C2A-CAA-CBA-CGA |
| 14  | n     | 833  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 811  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 839  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 829  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 841  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 810  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 852  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 829  | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 827  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 840  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 837  | CLA  | CBA-CGA-O2A-C1  |
| 18  | g     | 850  | LHG  | C34-C35-C36-C37 |
| 18  | A     | 850  | LHG  | C26-C27-C28-C29 |
| 14  | G     | 804  | CLA  | C13-C15-C16-C17 |
| 14  | N     | 808  | CLA  | C5-C6-C7-C8     |
| 14  | g     | 803  | CLA  | C13-C15-C16-C17 |
| 14  | g     | 819  | CLA  | C8-C10-C11-C12  |
| 14  | g     | 837  | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | n     | 806  | CLA  | C15-C16-C17-C18 |
| 14  | n     | 807  | CLA  | C13-C15-C16-C17 |
| 14  | n     | 810  | CLA  | C8-C10-C11-C12  |
| 14  | n     | 817  | CLA  | C13-C15-C16-C17 |
| 14  | n     | 825  | CLA  | C5-C6-C7-C8     |
| 14  | n     | 828  | CLA  | C13-C15-C16-C17 |
| 14  | n     | 832  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 802  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 818  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 818  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 801  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 825  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 830  | CLA  | C8-C10-C11-C12  |
| 15  | G     | 841  | PQN  | C18-C20-C21-C22 |
| 14  | G     | 829  | CLA  | CBD-CGD-O2D-CED |
| 14  | n     | 832  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 801  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 815  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 816  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 835  | CLA  | O1D-CGD-O2D-CED |
| 20  | H     | 1702 | SQD  | C7-C8-C9-C10    |
| 14  | G     | 805  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 808  | CLA  | C10-C11-C12-C13 |
| 14  | N     | 809  | CLA  | C15-C16-C17-C18 |
| 14  | n     | 806  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 804  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 826  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 818  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 829  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 807  | CLA  | C13-C15-C16-C17 |
| 14  | n     | 815  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 839  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 833  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 838  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 805  | CLA  | C15-C16-C17-C18 |
| 14  | g     | 815  | CLA  | C5-C6-C7-C8     |
| 14  | g     | 853  | CLA  | C15-C16-C17-C18 |
| 14  | n     | 831  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 854  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 814  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 824  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 819  | CLA  | C13-C15-C16-C17 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 827  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 841  | CLA  | C5-C6-C7-C8     |
| 15  | B     | 842  | PQN  | C23-C25-C26-C27 |
| 14  | g     | 836  | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 811  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 834  | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 803  | CLA  | C4-C3-C5-C6     |
| 14  | N     | 813  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 816  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 803  | CLA  | C15-C16-C17-C18 |
| 14  | N     | 842  | CLA  | C3-C5-C6-C7     |
| 14  | s     | 201  | CLA  | C3-C5-C6-C7     |
| 14  | N     | 801  | CLA  | C14-C13-C15-C16 |
| 14  | n     | 803  | CLA  | O1A-CGA-O2A-C1  |
| 20  | h     | 1702 | SQD  | C2-C1-O6-C44    |
| 20  | w     | 202  | SQD  | C2-C1-O6-C44    |
| 21  | B     | 849  | LMG  | C2-C1-O1-C7     |
| 14  | a     | 810  | CLA  | C8-C10-C11-C12  |
| 14  | N     | 807  | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 822  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 819  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 829  | CLA  | O1D-CGD-O2D-CED |
| 17  | G     | 843  | BCR  | C11-C12-C13-C35 |
| 17  | G     | 844  | BCR  | C37-C22-C23-C24 |
| 17  | N     | 847  | BCR  | C36-C18-C19-C20 |
| 17  | Y     | 101  | BCR  | C7-C8-C9-C34    |
| 17  | g     | 847  | BCR  | C7-C8-C9-C34    |
| 17  | A     | 846  | BCR  | C7-C8-C9-C34    |
| 17  | b     | 847  | BCR  | C7-C8-C9-C34    |
| 18  | v     | 102  | LHG  | C2-C3-O3-P      |
| 18  | g     | 849  | LHG  | C15-C16-C17-C18 |
| 17  | N     | 845  | BCR  | C21-C22-C23-C24 |
| 17  | n     | 845  | BCR  | C7-C8-C9-C10    |
| 17  | B     | 844  | BCR  | C17-C18-C19-C20 |
| 17  | B     | 844  | BCR  | C21-C22-C23-C24 |
| 17  | I     | 101  | BCR  | C21-C22-C23-C24 |
| 17  | I     | 102  | BCR  | C21-C22-C23-C24 |
| 17  | L     | 1504 | BCR  | C11-C12-C13-C14 |
| 17  | a     | 846  | BCR  | C17-C18-C19-C20 |
| 17  | a     | 846  | BCR  | C21-C22-C23-C24 |
| 14  | b     | 812  | CLA  | C5-C6-C7-C8     |
| 18  | S     | 202  | LHG  | C32-C33-C34-C35 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | x     | 1702 | SQD  | C10-C11-C12-C13 |
| 14  | G     | 808  | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 815  | CLA  | C2A-CAA-CBA-CGA |
| 14  | N     | 830  | CLA  | C2A-CAA-CBA-CGA |
| 14  | N     | 833  | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 808  | CLA  | C2A-CAA-CBA-CGA |
| 14  | n     | 822  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 819  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 820  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 840  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 807  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 823  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 828  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 832  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 834  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 808  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 840  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 802  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 830  | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 820  | CLA  | C15-C16-C17-C18 |
| 14  | N     | 826  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 837  | CLA  | C5-C6-C7-C8     |
| 18  | v     | 102  | LHG  | O1-C1-C2-C3     |
| 18  | a     | 849  | LHG  | O1-C1-C2-C3     |
| 18  | a     | 850  | LHG  | O1-C1-C2-C3     |
| 18  | m     | 101  | LHG  | O1-C1-C2-C3     |
| 14  | N     | 841  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 824  | CLA  | O1D-CGD-O2D-CED |
| 17  | N     | 852  | BCR  | C19-C20-C21-C22 |
| 14  | G     | 828  | CLA  | C16-C17-C18-C20 |
| 14  | N     | 804  | CLA  | C16-C17-C18-C19 |
| 14  | N     | 811  | CLA  | C16-C17-C18-C20 |
| 14  | N     | 812  | CLA  | C11-C12-C13-C15 |
| 14  | g     | 816  | CLA  | C11-C12-C13-C14 |
| 14  | g     | 819  | CLA  | C16-C17-C18-C20 |
| 14  | g     | 825  | CLA  | C16-C17-C18-C20 |
| 14  | n     | 840  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 812  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 837  | CLA  | C11-C12-C13-C15 |
| 14  | b     | 826  | CLA  | C16-C17-C18-C20 |
| 14  | b     | 829  | CLA  | C16-C17-C18-C20 |
| 18  | a     | 849  | LHG  | C28-C29-C30-C31 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | N     | 833  | CLA  | O1D-CGD-O2D-CED |
| 14  | S     | 203  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 834  | CLA  | O1A-CGA-O2A-C1  |
| 14  | N     | 825  | CLA  | C3-C5-C6-C7     |
| 14  | n     | 839  | CLA  | C3-C5-C6-C7     |
| 14  | b     | 833  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 807  | CLA  | C8-C10-C11-C12  |
| 20  | h     | 1702 | SQD  | C29-C30-C31-C32 |
| 21  | B     | 849  | LMG  | O6-C1-O1-C7     |
| 14  | N     | 825  | CLA  | C5-C6-C7-C8     |
| 20  | w     | 202  | SQD  | C10-C11-C12-C13 |
| 14  | b     | 820  | CLA  | O1A-CGA-O2A-C1  |
| 21  | B     | 849  | LMG  | O7-C8-C9-O8     |
| 14  | a     | 812  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 812  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 841  | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 820  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 828  | CLA  | C15-C16-C17-C18 |
| 14  | G     | 837  | CLA  | C8-C10-C11-C12  |
| 19  | g     | 851  | CL0  | C5-C6-C7-C8     |
| 19  | g     | 851  | CL0  | C13-C15-C16-C17 |
| 14  | A     | 802  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 824  | CLA  | C3-C5-C6-C7     |
| 14  | N     | 835  | CLA  | C2-C1-O2A-CGA   |
| 14  | N     | 810  | CLA  | C16-C17-C18-C19 |
| 14  | n     | 840  | CLA  | C16-C17-C18-C19 |
| 14  | B     | 832  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 840  | CLA  | C16-C17-C18-C20 |
| 14  | L     | 1502 | CLA  | C11-C12-C13-C14 |
| 14  | a     | 816  | CLA  | C11-C12-C13-C14 |
| 14  | b     | 806  | CLA  | C16-C17-C18-C19 |
| 14  | b     | 830  | CLA  | C16-C17-C18-C19 |
| 19  | g     | 851  | CL0  | C16-C17-C18-C19 |
| 14  | G     | 827  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 826  | CLA  | C15-C16-C17-C18 |
| 18  | S     | 202  | LHG  | C29-C30-C31-C32 |
| 14  | N     | 838  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 809  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 825  | CLA  | CBD-CGD-O2D-CED |
| 18  | G     | 850  | LHG  | C27-C28-C29-C30 |
| 18  | a     | 849  | LHG  | C13-C14-C15-C16 |
| 20  | h     | 1702 | SQD  | C33-C34-C35-C36 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | l     | 201  | SQD  | C33-C34-C35-C36 |
| 21  | b     | 849  | LMG  | C34-C35-C36-C37 |
| 14  | n     | 802  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 839  | CLA  | O1D-CGD-O2D-CED |
| 18  | G     | 849  | LHG  | C9-C10-C11-C12  |
| 18  | G     | 849  | LHG  | C13-C14-C15-C16 |
| 18  | m     | 101  | LHG  | C28-C29-C30-C31 |
| 20  | B     | 801  | SQD  | C30-C31-C32-C33 |
| 20  | b     | 801  | SQD  | C11-C10-C9-C8   |
| 14  | N     | 801  | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 828  | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 833  | CLA  | CBA-CGA-O2A-C1  |
| 18  | g     | 850  | LHG  | C10-C11-C12-C13 |
| 18  | g     | 850  | LHG  | C25-C26-C27-C28 |
| 20  | n     | 801  | SQD  | C11-C12-C13-C14 |
| 20  | B     | 801  | SQD  | C9-C10-C11-C12  |
| 18  | g     | 849  | LHG  | O1-C1-C2-O2     |
| 18  | v     | 102  | LHG  | O1-C1-C2-O2     |
| 18  | a     | 849  | LHG  | O1-C1-C2-O2     |
| 18  | m     | 101  | LHG  | O1-C1-C2-O2     |
| 14  | b     | 853  | CLA  | C3-C5-C6-C7     |
| 18  | a     | 850  | LHG  | C29-C30-C31-C32 |
| 14  | N     | 842  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 805  | CLA  | C4B-C3B-CAB-CBB |
| 14  | N     | 841  | CLA  | C4B-C3B-CAB-CBB |
| 14  | g     | 816  | CLA  | C4B-C3B-CAB-CBB |
| 14  | g     | 831  | CLA  | C4B-C3B-CAB-CBB |
| 14  | h     | 1701 | CLA  | C4B-C3B-CAB-CBB |
| 14  | n     | 804  | CLA  | C4B-C3B-CAB-CBB |
| 14  | n     | 808  | CLA  | C4B-C3B-CAB-CBB |
| 14  | n     | 838  | CLA  | C4B-C3B-CAB-CBB |
| 14  | n     | 839  | CLA  | C4B-C3B-CAB-CBB |
| 14  | n     | 850  | CLA  | C4B-C3B-CAB-CBB |
| 14  | A     | 853  | CLA  | C4B-C3B-CAB-CBB |
| 14  | b     | 824  | CLA  | C4B-C3B-CAB-CBB |
| 14  | b     | 851  | CLA  | C4B-C3B-CAB-CBB |
| 14  | j     | 101  | CLA  | C4B-C3B-CAB-CBB |
| 18  | a     | 850  | LHG  | C15-C16-C17-C18 |
| 14  | G     | 828  | CLA  | C16-C17-C18-C19 |
| 14  | N     | 811  | CLA  | C16-C17-C18-C19 |
| 14  | N     | 812  | CLA  | C11-C12-C13-C14 |
| 14  | N     | 819  | CLA  | C16-C17-C18-C20 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | N     | 833  | CLA  | C11-C12-C13-C15 |
| 14  | g     | 816  | CLA  | C11-C12-C13-C15 |
| 14  | g     | 817  | CLA  | C16-C17-C18-C19 |
| 14  | g     | 817  | CLA  | C16-C17-C18-C20 |
| 14  | g     | 825  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 812  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 807  | CLA  | C16-C17-C18-C19 |
| 14  | B     | 807  | CLA  | C16-C17-C18-C20 |
| 14  | L     | 1502 | CLA  | C11-C12-C13-C15 |
| 14  | b     | 806  | CLA  | C16-C17-C18-C20 |
| 14  | b     | 826  | CLA  | C16-C17-C18-C19 |
| 14  | b     | 829  | CLA  | C16-C17-C18-C19 |
| 14  | N     | 838  | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 836  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 835  | CLA  | C2A-CAA-CBA-CGA |
| 14  | N     | 829  | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 810  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 806  | CLA  | C2A-CAA-CBA-CGA |
| 20  | B     | 801  | SQD  | C31-C32-C33-C34 |
| 14  | G     | 801  | CLA  | C13-C15-C16-C17 |
| 14  | n     | 824  | CLA  | C15-C16-C17-C18 |
| 14  | n     | 829  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 807  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 831  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 839  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 803  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 807  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 825  | CLA  | C5-C6-C7-C8     |
| 20  | n     | 801  | SQD  | C27-C28-C29-C30 |
| 14  | G     | 807  | CLA  | C11-C12-C13-C15 |
| 14  | G     | 827  | CLA  | C11-C10-C8-C7   |
| 14  | G     | 828  | CLA  | C12-C13-C15-C16 |
| 14  | g     | 830  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 824  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 827  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 850  | CLA  | C11-C12-C13-C15 |
| 14  | a     | 803  | CLA  | C12-C13-C15-C16 |
| 14  | b     | 803  | CLA  | C11-C10-C8-C7   |
| 14  | b     | 827  | CLA  | C11-C12-C13-C15 |
| 18  | G     | 849  | LHG  | C15-C16-C17-C18 |
| 20  | l     | 201  | SQD  | C23-C24-C25-C26 |
| 14  | G     | 853  | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 804  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 818  | CLA  | C10-C11-C12-C13 |
| 18  | g     | 850  | LHG  | C26-C27-C28-C29 |
| 18  | v     | 102  | LHG  | C9-C10-C11-C12  |
| 18  | a     | 850  | LHG  | C10-C11-C12-C13 |
| 18  | m     | 101  | LHG  | C14-C15-C16-C17 |
| 20  | h     | 1702 | SQD  | C25-C26-C27-C28 |
| 21  | n     | 848  | LMG  | C17-C18-C19-C20 |
| 14  | g     | 804  | CLA  | C3-C5-C6-C7     |
| 14  | n     | 806  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 804  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 827  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 840  | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 815  | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 828  | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 838  | CLA  | C3A-C2A-CAA-CBA |
| 14  | T     | 101  | CLA  | C3A-C2A-CAA-CBA |
| 14  | W     | 202  | CLA  | C3A-C2A-CAA-CBA |
| 14  | g     | 803  | CLA  | C3A-C2A-CAA-CBA |
| 14  | g     | 804  | CLA  | C3A-C2A-CAA-CBA |
| 14  | g     | 853  | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 804  | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 809  | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 810  | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 823  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 806  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 811  | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 841  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 805  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 810  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 811  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 833  | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 837  | CLA  | C3A-C2A-CAA-CBA |
| 14  | F     | 201  | CLA  | C3A-C2A-CAA-CBA |
| 14  | J     | 101  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 804  | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 834  | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 805  | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 811  | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 824  | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 827  | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 841  | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 841  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 809  | CLA  | O1D-CGD-O2D-CED |
| 14  | g     | 812  | CLA  | O1D-CGD-O2D-CED |
| 14  | g     | 822  | CLA  | O1D-CGD-O2D-CED |
| 18  | G     | 850  | LHG  | C17-C18-C19-C20 |
| 20  | l     | 201  | SQD  | C10-C11-C12-C13 |
| 20  | w     | 202  | SQD  | C33-C34-C35-C36 |
| 14  | N     | 821  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 810  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 803  | CLA  | C10-C11-C12-C13 |
| 14  | g     | 806  | CLA  | O1D-CGD-O2D-CED |
| 14  | g     | 853  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 831  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 819  | CLA  | C16-C17-C18-C19 |
| 14  | N     | 833  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 837  | CLA  | C11-C12-C13-C14 |
| 14  | b     | 810  | CLA  | C16-C17-C18-C20 |
| 14  | b     | 823  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 841  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 834  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 840  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 837  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 829  | CLA  | O1D-CGD-O2D-CED |
| 21  | n     | 848  | LMG  | C33-C34-C35-C36 |
| 21  | B     | 849  | LMG  | C38-C39-C40-C41 |
| 14  | N     | 821  | CLA  | CBD-CGD-O2D-CED |
| 14  | n     | 831  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 815  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 829  | CLA  | C5-C6-C7-C8     |
| 18  | X     | 1702 | LHG  | C27-C28-C29-C30 |
| 20  | b     | 801  | SQD  | C30-C31-C32-C33 |
| 14  | g     | 828  | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 818  | CLA  | CBA-CGA-O2A-C1  |
| 18  | A     | 850  | LHG  | C10-C11-C12-C13 |
| 18  | a     | 849  | LHG  | C15-C16-C17-C18 |
| 20  | b     | 801  | SQD  | C10-C11-C12-C13 |
| 21  | n     | 848  | LMG  | C37-C38-C39-C40 |
| 14  | g     | 824  | CLA  | C3-C5-C6-C7     |
| 18  | v     | 102  | LHG  | C23-C24-C25-C26 |
| 20  | b     | 801  | SQD  | C23-C24-C25-C26 |
| 14  | b     | 831  | CLA  | C5-C6-C7-C8     |
| 18  | A     | 851  | LHG  | C15-C16-C17-C18 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | a     | 849  | LHG  | C32-C33-C34-C35 |
| 20  | h     | 1702 | SQD  | C14-C15-C16-C17 |
| 20  | n     | 801  | SQD  | C30-C31-C32-C33 |
| 21  | N     | 850  | LMG  | C17-C18-C19-C20 |
| 21  | B     | 802  | LMG  | C29-C30-C31-C32 |
| 14  | N     | 807  | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 811  | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 812  | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 810  | CLA  | O1D-CGD-O2D-CED |
| 20  | x     | 1702 | SQD  | C9-C10-C11-C12  |
| 20  | x     | 1702 | SQD  | C27-C28-C29-C30 |
| 14  | a     | 834  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 853  | CLA  | O1D-CGD-O2D-CED |
| 20  | H     | 1702 | SQD  | C33-C34-C35-C36 |
| 21  | B     | 802  | LMG  | C11-C12-C13-C14 |
| 14  | N     | 810  | CLA  | C16-C17-C18-C20 |
| 14  | n     | 828  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 804  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 832  | CLA  | C11-C12-C13-C15 |
| 18  | m     | 101  | LHG  | C23-C24-C25-C26 |
| 14  | G     | 817  | CLA  | C2B-C3B-CAB-CBB |
| 14  | N     | 841  | CLA  | C2B-C3B-CAB-CBB |
| 14  | g     | 816  | CLA  | C2B-C3B-CAB-CBB |
| 14  | g     | 831  | CLA  | C2B-C3B-CAB-CBB |
| 14  | h     | 1701 | CLA  | C2B-C3B-CAB-CBB |
| 14  | n     | 808  | CLA  | C2B-C3B-CAB-CBB |
| 14  | n     | 838  | CLA  | C2B-C3B-CAB-CBB |
| 14  | n     | 850  | CLA  | C2B-C3B-CAB-CBB |
| 14  | s     | 201  | CLA  | C2B-C3B-CAB-CBB |
| 14  | F     | 201  | CLA  | C2B-C3B-CAB-CBB |
| 14  | K     | 101  | CLA  | C2B-C3B-CAB-CBB |
| 14  | x     | 1701 | CLA  | C2B-C3B-CAB-CBB |
| 14  | b     | 809  | CLA  | C2B-C3B-CAB-CBB |
| 14  | b     | 824  | CLA  | C2B-C3B-CAB-CBB |
| 14  | b     | 851  | CLA  | C2B-C3B-CAB-CBB |
| 14  | j     | 101  | CLA  | C2B-C3B-CAB-CBB |
| 17  | G     | 846  | BCR  | C1-C6-C7-C8     |
| 17  | G     | 846  | BCR  | C23-C24-C25-C30 |
| 17  | G     | 847  | BCR  | C23-C24-C25-C26 |
| 17  | G     | 847  | BCR  | C23-C24-C25-C30 |
| 17  | T     | 103  | BCR  | C1-C6-C7-C8     |
| 17  | T     | 104  | BCR  | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | T     | 104 | BCR  | C23-C24-C25-C30 |
| 17  | W     | 201 | BCR  | C23-C24-C25-C26 |
| 17  | g     | 845 | BCR  | C5-C6-C7-C8     |
| 17  | t     | 103 | BCR  | C1-C6-C7-C8     |
| 17  | t     | 104 | BCR  | C1-C6-C7-C8     |
| 17  | t     | 104 | BCR  | C23-C24-C25-C26 |
| 17  | t     | 104 | BCR  | C23-C24-C25-C30 |
| 17  | w     | 206 | BCR  | C23-C24-C25-C26 |
| 17  | w     | 206 | BCR  | C23-C24-C25-C30 |
| 17  | A     | 847 | BCR  | C1-C6-C7-C8     |
| 17  | A     | 847 | BCR  | C5-C6-C7-C8     |
| 17  | A     | 856 | BCR  | C1-C6-C7-C8     |
| 17  | A     | 856 | BCR  | C5-C6-C7-C8     |
| 17  | A     | 856 | BCR  | C23-C24-C25-C26 |
| 17  | A     | 856 | BCR  | C23-C24-C25-C30 |
| 17  | B     | 851 | BCR  | C23-C24-C25-C26 |
| 17  | B     | 851 | BCR  | C23-C24-C25-C30 |
| 17  | J     | 103 | BCR  | C1-C6-C7-C8     |
| 17  | J     | 103 | BCR  | C5-C6-C7-C8     |
| 17  | I     | 102 | BCR  | C1-C6-C7-C8     |
| 17  | I     | 102 | BCR  | C5-C6-C7-C8     |
| 17  | I     | 103 | BCR  | C1-C6-C7-C8     |
| 17  | I     | 103 | BCR  | C5-C6-C7-C8     |
| 17  | I     | 103 | BCR  | C23-C24-C25-C26 |
| 17  | I     | 103 | BCR  | C23-C24-C25-C30 |
| 17  | M     | 101 | BCR  | C1-C6-C7-C8     |
| 17  | M     | 101 | BCR  | C5-C6-C7-C8     |
| 17  | a     | 846 | BCR  | C23-C24-C25-C30 |
| 17  | a     | 847 | BCR  | C23-C24-C25-C26 |
| 17  | a     | 847 | BCR  | C23-C24-C25-C30 |
| 17  | b     | 845 | BCR  | C1-C6-C7-C8     |
| 17  | b     | 846 | BCR  | C1-C6-C7-C8     |
| 17  | j     | 104 | BCR  | C1-C6-C7-C8     |
| 17  | j     | 104 | BCR  | C5-C6-C7-C8     |
| 17  | j     | 104 | BCR  | C23-C24-C25-C30 |
| 17  | l     | 205 | BCR  | C23-C24-C25-C26 |
| 17  | l     | 205 | BCR  | C23-C24-C25-C30 |
| 14  | g     | 840 | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 854 | CLA  | CBD-CGD-O2D-CED |
| 14  | n     | 837 | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 851 | LHG  | C8-C7-O7-C5     |
| 14  | N     | 840 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | g     | 837  | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 809  | CLA  | C13-C15-C16-C17 |
| 15  | G     | 841  | PQN  | C13-C15-C16-C17 |
| 18  | v     | 102  | LHG  | C26-C27-C28-C29 |
| 14  | A     | 830  | CLA  | O1D-CGD-O2D-CED |
| 18  | a     | 849  | LHG  | C10-C11-C12-C13 |
| 20  | H     | 1702 | SQD  | C31-C32-C33-C34 |
| 14  | G     | 827  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 817  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 820  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 821  | CLA  | C2A-CAA-CBA-CGA |
| 19  | a     | 851  | CL0  | C2A-CAA-CBA-CGA |
| 18  | A     | 851  | LHG  | C23-C24-C25-C26 |
| 14  | g     | 806  | CLA  | C13-C15-C16-C17 |
| 20  | H     | 1702 | SQD  | C16-C17-C18-C19 |
| 20  | n     | 801  | SQD  | C10-C11-C12-C13 |
| 20  | b     | 801  | SQD  | C25-C26-C27-C28 |
| 14  | n     | 833  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 818  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 812  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 841  | CLA  | O1A-CGA-O2A-C1  |
| 18  | v     | 102  | LHG  | C25-C26-C27-C28 |
| 20  | w     | 202  | SQD  | C11-C12-C13-C14 |
| 20  | l     | 201  | SQD  | C11-C10-C9-C8   |
| 14  | B     | 823  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 833  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 804  | CLA  | C4-C3-C5-C6     |
| 18  | a     | 849  | LHG  | C14-C15-C16-C17 |
| 20  | n     | 801  | SQD  | C9-C10-C11-C12  |
| 20  | l     | 201  | SQD  | C31-C32-C33-C34 |
| 14  | N     | 803  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 822  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 841  | CLA  | C2-C3-C5-C6     |
| 14  | N     | 804  | CLA  | C16-C17-C18-C20 |
| 18  | g     | 849  | LHG  | C26-C27-C28-C29 |
| 14  | a     | 811  | CLA  | C4C-C3C-CAC-CBC |
| 14  | N     | 835  | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 819  | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 825  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 825  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 832  | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 830  | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | n     | 829  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 801  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 805  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 805  | CLA  | C11-C10-C8-C9   |
| 20  | x     | 1702 | SQD  | C29-C30-C31-C32 |
| 14  | G     | 853  | CLA  | C15-C16-C17-C18 |
| 14  | N     | 804  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 818  | CLA  | O1D-CGD-O2D-CED |
| 20  | n     | 801  | SQD  | C11-C10-C9-C8   |
| 20  | h     | 1702 | SQD  | O5-C1-O6-C44    |
| 18  | g     | 850  | LHG  | C14-C15-C16-C17 |
| 20  | x     | 1702 | SQD  | C32-C33-C34-C35 |
| 20  | l     | 201  | SQD  | C30-C31-C32-C33 |
| 14  | n     | 836  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 834  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 802  | CLA  | C13-C15-C16-C17 |
| 14  | N     | 830  | CLA  | C8-C10-C11-C12  |
| 14  | B     | 808  | CLA  | C5-C6-C7-C8     |
| 20  | b     | 801  | SQD  | C27-C28-C29-C30 |
| 14  | l     | 202  | CLA  | O1D-CGD-O2D-CED |
| 21  | n     | 848  | LMG  | C21-C22-C23-C24 |
| 21  | B     | 849  | LMG  | C20-C21-C22-C23 |
| 21  | b     | 849  | LMG  | C17-C18-C19-C20 |
| 18  | v     | 102  | LHG  | C14-C15-C16-C17 |
| 20  | l     | 201  | SQD  | C17-C18-C19-C20 |
| 14  | g     | 852  | CLA  | C8-C10-C11-C12  |
| 14  | n     | 809  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 806  | CLA  | C15-C16-C17-C18 |
| 20  | n     | 801  | SQD  | C24-C23-O48-C46 |
| 14  | n     | 809  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 840  | CLA  | C16-C17-C18-C19 |
| 14  | b     | 830  | CLA  | C16-C17-C18-C20 |
| 18  | A     | 850  | LHG  | C11-C12-C13-C14 |
| 18  | G     | 850  | LHG  | C8-C7-O7-C5     |
| 18  | a     | 849  | LHG  | C8-C7-O7-C5     |
| 18  | v     | 102  | LHG  | C7-C8-C9-C10    |
| 14  | G     | 802  | CLA  | C15-C16-C17-C18 |
| 14  | G     | 804  | CLA  | C8-C10-C11-C12  |
| 14  | N     | 808  | CLA  | C10-C11-C12-C13 |
| 14  | a     | 823  | CLA  | C8-C10-C11-C12  |
| 18  | X     | 1702 | LHG  | C12-C13-C14-C15 |
| 18  | a     | 849  | LHG  | C17-C18-C19-C20 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 18  | a     | 850 | LHG  | C27-C28-C29-C30 |
| 18  | m     | 101 | LHG  | C12-C13-C14-C15 |
| 20  | B     | 801 | SQD  | C33-C34-C35-C36 |
| 14  | n     | 825 | CLA  | C8-C10-C11-C12  |
| 14  | B     | 841 | CLA  | C15-C16-C17-C18 |
| 17  | A     | 844 | BCR  | C11-C12-C13-C35 |
| 17  | B     | 843 | BCR  | C7-C8-C9-C34    |
| 17  | B     | 846 | BCR  | C7-C8-C9-C34    |
| 17  | a     | 847 | BCR  | C7-C8-C9-C34    |
| 20  | B     | 801 | SQD  | C13-C14-C15-C16 |
| 21  | N     | 850 | LMG  | C19-C20-C21-C22 |
| 21  | N     | 850 | LMG  | C33-C34-C35-C36 |
| 14  | N     | 804 | CLA  | C2A-CAA-CBA-CGA |
| 14  | U     | 101 | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 819 | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 833 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 804 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 810 | CLA  | C16-C17-C18-C20 |
| 14  | G     | 820 | CLA  | C16-C17-C18-C19 |
| 14  | G     | 820 | CLA  | C16-C17-C18-C20 |
| 14  | n     | 809 | CLA  | C16-C17-C18-C19 |
| 14  | n     | 822 | CLA  | C6-C7-C8-C9     |
| 14  | n     | 825 | CLA  | C16-C17-C18-C19 |
| 14  | n     | 825 | CLA  | C16-C17-C18-C20 |
| 14  | n     | 828 | CLA  | C16-C17-C18-C19 |
| 14  | A     | 804 | CLA  | C16-C17-C18-C19 |
| 14  | B     | 805 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 823 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 823 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 841 | CLA  | C16-C17-C18-C19 |
| 14  | B     | 841 | CLA  | C16-C17-C18-C20 |
| 14  | a     | 816 | CLA  | C11-C12-C13-C15 |
| 14  | b     | 807 | CLA  | C16-C17-C18-C19 |
| 14  | b     | 807 | CLA  | C16-C17-C18-C20 |
| 14  | b     | 823 | CLA  | C6-C7-C8-C10    |
| 19  | g     | 851 | CL0  | C16-C17-C18-C20 |
| 14  | A     | 840 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 833 | CLA  | C2-C3-C5-C6     |
| 18  | G     | 849 | LHG  | C14-C15-C16-C17 |
| 20  | b     | 801 | SQD  | C33-C34-C35-C36 |
| 14  | a     | 840 | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 807 | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | l     | 201  | SQD  | C26-C27-C28-C29 |
| 18  | a     | 849  | LHG  | C16-C17-C18-C19 |
| 14  | A     | 817  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 826  | CLA  | C3-C5-C6-C7     |
| 14  | N     | 804  | CLA  | C5-C6-C7-C8     |
| 21  | n     | 848  | LMG  | C16-C17-C18-C19 |
| 18  | A     | 851  | LHG  | O9-C7-O7-C5     |
| 14  | g     | 835  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 804  | CLA  | C15-C16-C17-C18 |
| 14  | g     | 819  | CLA  | C16-C17-C18-C19 |
| 14  | B     | 805  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 841  | CLA  | C16-C17-C18-C20 |
| 18  | A     | 851  | LHG  | C14-C15-C16-C17 |
| 14  | g     | 828  | CLA  | O1A-CGA-O2A-C1  |
| 20  | w     | 202  | SQD  | C13-C14-C15-C16 |
| 21  | b     | 849  | LMG  | C37-C38-C39-C40 |
| 14  | N     | 842  | CLA  | C15-C16-C17-C18 |
| 14  | n     | 804  | CLA  | C10-C11-C12-C13 |
| 14  | n     | 809  | CLA  | C5-C6-C7-C8     |
| 14  | g     | 828  | CLA  | O1D-CGD-O2D-CED |
| 18  | v     | 102  | LHG  | C15-C16-C17-C18 |
| 20  | h     | 1702 | SQD  | C16-C17-C18-C19 |
| 14  | b     | 813  | CLA  | CBD-CGD-O2D-CED |
| 18  | G     | 850  | LHG  | O7-C5-C6-O8     |
| 18  | G     | 850  | LHG  | C34-C35-C36-C37 |
| 18  | g     | 850  | LHG  | C32-C33-C34-C35 |
| 20  | n     | 801  | SQD  | C25-C26-C27-C28 |
| 14  | A     | 853  | CLA  | O1D-CGD-O2D-CED |
| 18  | a     | 850  | LHG  | C24-C23-O8-C6   |
| 14  | g     | 836  | CLA  | C8-C10-C11-C12  |
| 14  | B     | 837  | CLA  | C10-C11-C12-C13 |
| 14  | b     | 851  | CLA  | C5-C6-C7-C8     |
| 18  | A     | 850  | LHG  | C14-C15-C16-C17 |
| 14  | a     | 833  | CLA  | C5-C6-C7-C8     |
| 21  | N     | 850  | LMG  | O6-C5-C6-O5     |
| 14  | g     | 831  | CLA  | O1D-CGD-O2D-CED |
| 14  | n     | 837  | CLA  | C16-C17-C18-C20 |
| 14  | b     | 810  | CLA  | C16-C17-C18-C19 |
| 14  | l     | 203  | CLA  | C11-C12-C13-C14 |
| 18  | a     | 850  | LHG  | C11-C12-C13-C14 |
| 14  | G     | 808  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 824  | CLA  | C4-C3-C5-C6     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 15  | G     | 841 | PQN  | C14-C13-C15-C16 |
| 19  | a     | 851 | CL0  | C2-C3-C5-C6     |
| 18  | A     | 851 | LHG  | C10-C11-C12-C13 |
| 14  | G     | 807 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 817 | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 820 | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 838 | CLA  | C2A-CAA-CBA-CGA |
| 14  | n     | 807 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 821 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 835 | CLA  | C2A-CAA-CBA-CGA |
| 14  | K     | 101 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 808 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 814 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 823 | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 803 | CLA  | CBD-CGD-O2D-CED |
| 18  | v     | 102 | LHG  | C28-C29-C30-C31 |
| 18  | a     | 849 | LHG  | C9-C10-C11-C12  |
| 14  | G     | 835 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 838 | CLA  | O1D-CGD-O2D-CED |
| 14  | g     | 801 | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 841 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 851 | LHG  | C12-C13-C14-C15 |
| 18  | S     | 202 | LHG  | C11-C10-C9-C8   |
| 18  | A     | 850 | LHG  | C9-C10-C11-C12  |
| 18  | A     | 850 | LHG  | C25-C26-C27-C28 |
| 21  | B     | 849 | LMG  | O6-C5-C6-O5     |
| 14  | a     | 828 | CLA  | O1D-CGD-O2D-CED |
| 18  | A     | 850 | LHG  | O1-C1-C2-O2     |
| 18  | a     | 850 | LHG  | O1-C1-C2-O2     |
| 14  | N     | 840 | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 837 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 825 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 832 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 807 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 808 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 813 | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 830 | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 807 | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 820 | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 827 | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 829 | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 834 | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | T     | 101  | CLA  | C1A-C2A-CAA-CBA |
| 14  | W     | 203  | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 804  | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 806  | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 812  | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 834  | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 853  | CLA  | C1A-C2A-CAA-CBA |
| 14  | h     | 1701 | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 804  | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 809  | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 816  | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 818  | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 823  | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 827  | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 833  | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 850  | CLA  | C1A-C2A-CAA-CBA |
| 14  | s     | 201  | CLA  | C1A-C2A-CAA-CBA |
| 14  | t     | 101  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 803  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 805  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 814  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 815  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 817  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 825  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 830  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 841  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 855  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 806  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 811  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 817  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 818  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 822  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 831  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 834  | CLA  | C1A-C2A-CAA-CBA |
| 14  | F     | 201  | CLA  | C1A-C2A-CAA-CBA |
| 14  | J     | 101  | CLA  | C1A-C2A-CAA-CBA |
| 14  | L     | 1502 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 804  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 806  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 812  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 803  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 811  | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 817  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 822  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 827  | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 820  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 821  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 827  | CLA  | C13-C15-C16-C17 |
| 20  | h     | 1702 | SQD  | C32-C33-C34-C35 |
| 20  | x     | 1702 | SQD  | C25-C26-C27-C28 |
| 18  | g     | 850  | LHG  | C15-C16-C17-C18 |
| 14  | n     | 825  | CLA  | O1A-CGA-O2A-C1  |
| 18  | X     | 1702 | LHG  | C11-C10-C9-C8   |
| 14  | A     | 805  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 831  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 826  | CLA  | CBD-CGD-O2D-CED |
| 20  | n     | 801  | SQD  | C17-C18-C19-C20 |
| 14  | N     | 841  | CLA  | C3-C5-C6-C7     |
| 15  | A     | 842  | PQN  | C13-C15-C16-C17 |
| 14  | G     | 808  | CLA  | C11-C10-C8-C7   |
| 14  | G     | 810  | CLA  | C11-C10-C8-C7   |
| 14  | G     | 810  | CLA  | C11-C12-C13-C15 |
| 14  | G     | 818  | CLA  | C12-C13-C15-C16 |
| 14  | G     | 832  | CLA  | C12-C13-C15-C16 |
| 14  | N     | 801  | CLA  | C6-C7-C8-C10    |
| 14  | N     | 821  | CLA  | C11-C12-C13-C15 |
| 14  | N     | 851  | CLA  | C6-C7-C8-C10    |
| 14  | g     | 827  | CLA  | C12-C13-C15-C16 |
| 14  | g     | 837  | CLA  | C6-C7-C8-C10    |
| 14  | g     | 838  | CLA  | C12-C13-C15-C16 |
| 14  | g     | 852  | CLA  | C6-C7-C8-C10    |
| 14  | n     | 802  | CLA  | C6-C7-C8-C10    |
| 14  | n     | 803  | CLA  | C6-C7-C8-C10    |
| 14  | n     | 807  | CLA  | C12-C13-C15-C16 |
| 14  | n     | 818  | CLA  | C6-C7-C8-C10    |
| 14  | n     | 824  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 808  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 832  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 840  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 808  | CLA  | C12-C13-C15-C16 |
| 14  | B     | 810  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 825  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 826  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 827  | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | B     | 832 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 833 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 840 | CLA  | C11-C12-C13-C15 |
| 14  | a     | 831 | CLA  | C12-C13-C15-C16 |
| 14  | b     | 806 | CLA  | C12-C13-C15-C16 |
| 14  | b     | 818 | CLA  | C6-C7-C8-C10    |
| 14  | b     | 827 | CLA  | C12-C13-C15-C16 |
| 14  | b     | 833 | CLA  | C6-C7-C8-C10    |
| 14  | b     | 833 | CLA  | C11-C10-C8-C7   |
| 14  | G     | 812 | CLA  | C11-C12-C13-C15 |
| 14  | N     | 835 | CLA  | O1A-CGA-O2A-C1  |
| 18  | A     | 851 | LHG  | C32-C33-C34-C35 |
| 14  | t     | 101 | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 820 | CLA  | C13-C15-C16-C17 |
| 14  | a     | 816 | CLA  | C10-C11-C12-C13 |
| 14  | g     | 836 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 853 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 817 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 838 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 853 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 823 | CLA  | C2-C3-C5-C6     |
| 14  | a     | 824 | CLA  | C2-C3-C5-C6     |
| 21  | n     | 848 | LMG  | O6-C5-C6-O5     |
| 14  | N     | 805 | CLA  | C10-C11-C12-C13 |
| 14  | g     | 807 | CLA  | C5-C6-C7-C8     |
| 14  | n     | 803 | CLA  | C8-C10-C11-C12  |
| 14  | n     | 832 | CLA  | C3-C5-C6-C7     |
| 14  | b     | 840 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 821 | CLA  | C2A-CAA-CBA-CGA |
| 14  | N     | 824 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 811 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 813 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 816 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 818 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 839 | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 802 | CLA  | C11-C12-C13-C14 |
| 14  | G     | 810 | CLA  | C11-C12-C13-C14 |
| 14  | G     | 820 | CLA  | C11-C10-C8-C9   |
| 14  | G     | 831 | CLA  | C11-C12-C13-C14 |
| 14  | G     | 832 | CLA  | C14-C13-C15-C16 |
| 14  | G     | 853 | CLA  | C14-C13-C15-C16 |
| 14  | N     | 820 | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | g     | 827  | CLA  | C14-C13-C15-C16 |
| 14  | g     | 854  | CLA  | C11-C12-C13-C14 |
| 14  | n     | 807  | CLA  | C14-C13-C15-C16 |
| 14  | n     | 809  | CLA  | C11-C12-C13-C14 |
| 14  | n     | 813  | CLA  | C11-C10-C8-C9   |
| 14  | n     | 829  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 805  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 811  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 818  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 824  | CLA  | C11-C10-C8-C9   |
| 14  | B     | 810  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 810  | CLA  | C11-C10-C8-C9   |
| 14  | B     | 825  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 826  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 840  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 841  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 801  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 804  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 806  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 827  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 838  | CLA  | C11-C10-C8-C9   |
| 14  | b     | 818  | CLA  | C14-C13-C15-C16 |
| 14  | b     | 827  | CLA  | C14-C13-C15-C16 |
| 14  | l     | 203  | CLA  | C11-C10-C8-C9   |
| 14  | F     | 201  | CLA  | C10-C11-C12-C13 |
| 18  | a     | 850  | LHG  | C25-C26-C27-C28 |
| 18  | v     | 102  | LHG  | C10-C11-C12-C13 |
| 14  | G     | 837  | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 854  | CLA  | CBA-CGA-O2A-C1  |
| 14  | h     | 1701 | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 837  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 829  | CLA  | CBA-CGA-O2A-C1  |
| 19  | G     | 851  | CL0  | CBA-CGA-O2A-C1  |
| 14  | G     | 816  | CLA  | C8-C10-C11-C12  |
| 14  | n     | 808  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 838  | CLA  | C10-C11-C12-C13 |
| 14  | n     | 820  | CLA  | CBD-CGD-O2D-CED |
| 14  | n     | 830  | CLA  | CBD-CGD-O2D-CED |
| 21  | B     | 849  | LMG  | C23-C24-C25-C26 |
| 18  | a     | 849  | LHG  | O9-C7-O7-C5     |
| 18  | A     | 850  | LHG  | C4-C5-C6-O8     |
| 20  | h     | 1702 | SQD  | C44-C45-C46-O48 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | w     | 202  | SQD  | C44-C45-C46-O48 |
| 20  | l     | 201  | SQD  | C44-C45-C46-O48 |
| 20  | B     | 801  | SQD  | C25-C26-C27-C28 |
| 20  | x     | 1702 | SQD  | C11-C12-C13-C14 |
| 20  | b     | 801  | SQD  | C9-C10-C11-C12  |
| 14  | g     | 801  | CLA  | C15-C16-C17-C18 |
| 14  | n     | 803  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 806  | CLA  | C15-C16-C17-C18 |
| 18  | g     | 850  | LHG  | C11-C12-C13-C14 |
| 21  | N     | 850  | LMG  | C23-C24-C25-C26 |
| 14  | N     | 825  | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 829  | CLA  | CBA-CGA-O2A-C1  |
| 14  | X     | 1701 | CLA  | CBA-CGA-O2A-C1  |
| 20  | x     | 1702 | SQD  | C7-C8-C9-C10    |
| 21  | b     | 849  | LMG  | O6-C5-C6-O5     |
| 14  | G     | 831  | CLA  | C16-C17-C18-C20 |
| 14  | N     | 806  | CLA  | C6-C7-C8-C9     |
| 14  | N     | 821  | CLA  | C16-C17-C18-C20 |
| 14  | g     | 826  | CLA  | C16-C17-C18-C19 |
| 14  | n     | 837  | CLA  | C16-C17-C18-C19 |
| 14  | n     | 819  | CLA  | O1A-CGA-O2A-C1  |
| 20  | n     | 801  | SQD  | O10-C23-O48-C46 |
| 14  | n     | 852  | CLA  | O1D-CGD-O2D-CED |
| 18  | X     | 1702 | LHG  | C32-C33-C34-C35 |
| 14  | B     | 827  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 816  | CLA  | C3-C5-C6-C7     |
| 20  | w     | 202  | SQD  | C14-C15-C16-C17 |
| 18  | m     | 101  | LHG  | C7-C8-C9-C10    |
| 14  | G     | 822  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 817  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 838  | CLA  | C4-C3-C5-C6     |
| 19  | a     | 851  | CL0  | C4-C3-C5-C6     |
| 14  | G     | 808  | CLA  | C2-C3-C5-C6     |
| 14  | g     | 836  | CLA  | C2-C3-C5-C6     |
| 14  | B     | 838  | CLA  | C2-C3-C5-C6     |
| 15  | G     | 841  | PQN  | C12-C13-C15-C16 |
| 15  | A     | 842  | PQN  | C12-C13-C15-C16 |
| 14  | N     | 810  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 827  | CLA  | C5-C6-C7-C8     |
| 17  | N     | 847  | BCR  | C7-C8-C9-C34    |
| 17  | I     | 102  | BCR  | C36-C18-C19-C20 |
| 20  | B     | 801  | SQD  | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 20  | w     | 202 | SQD  | C32-C33-C34-C35 |
| 17  | G     | 843 | BCR  | C11-C12-C13-C14 |
| 17  | I     | 102 | BCR  | C17-C18-C19-C20 |
| 14  | G     | 837 | CLA  | O1A-CGA-O2A-C1  |
| 18  | a     | 850 | LHG  | O10-C23-O8-C6   |
| 19  | G     | 851 | CL0  | O1A-CGA-O2A-C1  |
| 14  | n     | 837 | CLA  | C5-C6-C7-C8     |
| 14  | B     | 837 | CLA  | C8-C10-C11-C12  |
| 14  | l     | 203 | CLA  | C8-C10-C11-C12  |
| 19  | G     | 851 | CL0  | C5-C6-C7-C8     |
| 14  | N     | 831 | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 826 | CLA  | C2A-CAA-CBA-CGA |
| 14  | n     | 827 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 811 | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 851 | LHG  | C27-C28-C29-C30 |
| 21  | N     | 850 | LMG  | C22-C23-C24-C25 |
| 21  | n     | 848 | LMG  | C40-C41-C42-C43 |
| 18  | A     | 851 | LHG  | O1-C1-C2-C3     |
| 14  | g     | 854 | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 817 | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 824 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 837 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 824 | CLA  | CBA-CGA-O2A-C1  |
| 18  | S     | 202 | LHG  | C24-C23-O8-C6   |
| 18  | g     | 849 | LHG  | C24-C23-O8-C6   |
| 14  | G     | 831 | CLA  | C15-C16-C17-C18 |
| 14  | g     | 804 | CLA  | C15-C16-C17-C18 |
| 14  | g     | 830 | CLA  | C10-C11-C12-C13 |
| 14  | b     | 803 | CLA  | C5-C6-C7-C8     |
| 14  | N     | 806 | CLA  | C6-C7-C8-C10    |
| 14  | g     | 826 | CLA  | C16-C17-C18-C20 |
| 18  | m     | 101 | LHG  | C17-C18-C19-C20 |
| 21  | n     | 848 | LMG  | C41-C42-C43-C44 |
| 18  | a     | 850 | LHG  | C1-C2-C3-O3     |
| 18  | g     | 849 | LHG  | O6-C4-C5-O7     |
| 14  | g     | 823 | CLA  | C13-C15-C16-C17 |
| 14  | n     | 808 | CLA  | C15-C16-C17-C18 |
| 20  | B     | 801 | SQD  | C16-C17-C18-C19 |
| 14  | N     | 831 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 840 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 823 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 825 | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 826  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 838  | CLA  | O1D-CGD-O2D-CED |
| 18  | X     | 1702 | LHG  | C28-C29-C30-C31 |
| 20  | l     | 201  | SQD  | C13-C14-C15-C16 |
| 14  | b     | 809  | CLA  | C13-C15-C16-C17 |
| 14  | n     | 802  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 838  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 815  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 837  | CLA  | C2-C3-C5-C6     |
| 18  | a     | 849  | LHG  | C31-C32-C33-C34 |
| 20  | w     | 202  | SQD  | C30-C31-C32-C33 |
| 14  | B     | 838  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 826  | CLA  | C16-C17-C18-C20 |
| 14  | N     | 821  | CLA  | C16-C17-C18-C19 |
| 14  | g     | 801  | CLA  | C16-C17-C18-C19 |
| 18  | a     | 850  | LHG  | C28-C29-C30-C31 |
| 14  | G     | 803  | CLA  | C6-C7-C8-C9     |
| 14  | n     | 830  | CLA  | C6-C7-C8-C9     |
| 14  | h     | 1701 | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 806  | CLA  | C5-C6-C7-C8     |
| 18  | A     | 851  | LHG  | C26-C27-C28-C29 |
| 21  | N     | 850  | LMG  | C20-C21-C22-C23 |
| 21  | b     | 849  | LMG  | C16-C17-C18-C19 |
| 20  | H     | 1702 | SQD  | O6-C44-C45-O47  |
| 20  | x     | 1702 | SQD  | O47-C45-C46-O48 |
| 18  | a     | 850  | LHG  | C34-C35-C36-C37 |
| 14  | G     | 830  | CLA  | C6-C7-C8-C9     |
| 20  | h     | 1702 | SQD  | C26-C27-C28-C29 |
| 14  | a     | 836  | CLA  | C10-C11-C12-C13 |
| 14  | g     | 824  | CLA  | C6-C7-C8-C9     |
| 20  | h     | 1702 | SQD  | C23-C24-C25-C26 |
| 14  | g     | 854  | CLA  | C2A-CAA-CBA-CGA |
| 14  | n     | 852  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 827  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 807  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 805  | CLA  | C3-C5-C6-C7     |
| 18  | a     | 849  | LHG  | C11-C12-C13-C14 |
| 15  | a     | 841  | PQN  | C26-C27-C28-C29 |
| 14  | b     | 827  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1701 | CLA  | CBA-CGA-O2A-C1  |
| 14  | n     | 805  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 833  | CLA  | CBA-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 806  | CLA  | CBA-CGA-O2A-C1  |
| 18  | a     | 849  | LHG  | C34-C35-C36-C37 |
| 20  | H     | 1702 | SQD  | C27-C28-C29-C30 |
| 14  | w     | 203  | CLA  | CBD-CGD-O2D-CED |
| 18  | A     | 851  | LHG  | C17-C18-C19-C20 |
| 20  | w     | 202  | SQD  | C11-C10-C9-C8   |
| 14  | g     | 828  | CLA  | C5-C6-C7-C8     |
| 18  | g     | 849  | LHG  | C34-C35-C36-C37 |
| 20  | w     | 202  | SQD  | C9-C10-C11-C12  |
| 14  | b     | 820  | CLA  | O1D-CGD-O2D-CED |
| 21  | B     | 802  | LMG  | C28-C29-C30-C31 |
| 14  | G     | 820  | CLA  | C5-C6-C7-C8     |
| 14  | g     | 819  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 804  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 831  | CLA  | C13-C15-C16-C17 |
| 14  | a     | 830  | CLA  | C10-C11-C12-C13 |
| 14  | g     | 808  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 832  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 812  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 826  | CLA  | C16-C17-C18-C19 |
| 14  | N     | 827  | CLA  | C4-C3-C5-C6     |
| 14  | g     | 827  | CLA  | C4-C3-C5-C6     |
| 14  | g     | 852  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 808  | CLA  | C4-C3-C5-C6     |
| 14  | b     | 810  | CLA  | C4-C3-C5-C6     |
| 14  | b     | 814  | CLA  | C4-C3-C5-C6     |
| 15  | A     | 842  | PQN  | C14-C13-C15-C16 |
| 14  | g     | 818  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 814  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 804  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 837  | CLA  | C5-C6-C7-C8     |
| 18  | X     | 1702 | LHG  | C26-C27-C28-C29 |
| 20  | h     | 1702 | SQD  | C31-C32-C33-C34 |
| 18  | G     | 849  | LHG  | O1-C1-C2-O2     |
| 18  | S     | 202  | LHG  | O1-C1-C2-O2     |
| 18  | X     | 1702 | LHG  | O1-C1-C2-O2     |
| 14  | G     | 802  | CLA  | C14-C13-C15-C16 |
| 14  | G     | 806  | CLA  | C6-C7-C8-C9     |
| 14  | G     | 806  | CLA  | C11-C10-C8-C9   |
| 14  | G     | 816  | CLA  | C6-C7-C8-C9     |
| 14  | G     | 818  | CLA  | C14-C13-C15-C16 |
| 14  | G     | 824  | CLA  | C14-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | G     | 828 | CLA  | C14-C13-C15-C16 |
| 14  | G     | 833 | CLA  | C14-C13-C15-C16 |
| 14  | N     | 801 | CLA  | C6-C7-C8-C9     |
| 14  | N     | 833 | CLA  | C6-C7-C8-C9     |
| 14  | N     | 851 | CLA  | C6-C7-C8-C9     |
| 14  | g     | 809 | CLA  | C6-C7-C8-C9     |
| 14  | g     | 838 | CLA  | C11-C10-C8-C9   |
| 14  | g     | 838 | CLA  | C14-C13-C15-C16 |
| 14  | n     | 806 | CLA  | C6-C7-C8-C9     |
| 14  | n     | 823 | CLA  | C14-C13-C15-C16 |
| 14  | n     | 824 | CLA  | C11-C10-C8-C9   |
| 14  | A     | 802 | CLA  | C11-C12-C13-C14 |
| 14  | A     | 808 | CLA  | C11-C12-C13-C14 |
| 14  | A     | 832 | CLA  | C14-C13-C15-C16 |
| 14  | A     | 840 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 808 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 825 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 827 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 832 | CLA  | C6-C7-C8-C9     |
| 14  | B     | 833 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 850 | CLA  | C11-C10-C8-C9   |
| 14  | a     | 803 | CLA  | C11-C10-C8-C9   |
| 14  | a     | 803 | CLA  | C14-C13-C15-C16 |
| 14  | a     | 804 | CLA  | C11-C12-C13-C14 |
| 14  | a     | 817 | CLA  | C14-C13-C15-C16 |
| 14  | a     | 819 | CLA  | C6-C7-C8-C9     |
| 14  | a     | 819 | CLA  | C11-C10-C8-C9   |
| 14  | a     | 825 | CLA  | C6-C7-C8-C9     |
| 14  | a     | 825 | CLA  | C11-C10-C8-C9   |
| 14  | a     | 831 | CLA  | C14-C13-C15-C16 |
| 14  | b     | 804 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 804 | CLA  | C11-C10-C8-C9   |
| 14  | b     | 806 | CLA  | C14-C13-C15-C16 |
| 14  | b     | 827 | CLA  | C11-C12-C13-C14 |
| 14  | b     | 833 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 833 | CLA  | C11-C10-C8-C9   |
| 14  | b     | 838 | CLA  | C14-C13-C15-C16 |
| 18  | G     | 849 | LHG  | C17-C18-C19-C20 |
| 14  | A     | 853 | CLA  | C5-C6-C7-C8     |
| 14  | a     | 805 | CLA  | C5-C6-C7-C8     |
| 18  | m     | 101 | LHG  | C2-C3-O3-P      |
| 14  | G     | 839 | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | N     | 834  | CLA  | C4B-C3B-CAB-CBB |
| 14  | S     | 201  | CLA  | C4B-C3B-CAB-CBB |
| 14  | U     | 101  | CLA  | C4B-C3B-CAB-CBB |
| 14  | W     | 203  | CLA  | C4B-C3B-CAB-CBB |
| 14  | g     | 807  | CLA  | C4B-C3B-CAB-CBB |
| 14  | g     | 821  | CLA  | C4B-C3B-CAB-CBB |
| 14  | g     | 832  | CLA  | C4B-C3B-CAB-CBB |
| 14  | g     | 854  | CLA  | C4B-C3B-CAB-CBB |
| 14  | n     | 816  | CLA  | C4B-C3B-CAB-CBB |
| 14  | n     | 823  | CLA  | C4B-C3B-CAB-CBB |
| 14  | n     | 830  | CLA  | C4B-C3B-CAB-CBB |
| 14  | u     | 101  | CLA  | C4B-C3B-CAB-CBB |
| 14  | w     | 204  | CLA  | C4B-C3B-CAB-CBB |
| 14  | A     | 807  | CLA  | C4B-C3B-CAB-CBB |
| 14  | A     | 834  | CLA  | C4B-C3B-CAB-CBB |
| 14  | F     | 201  | CLA  | C4B-C3B-CAB-CBB |
| 14  | K     | 101  | CLA  | C4B-C3B-CAB-CBB |
| 14  | a     | 823  | CLA  | C4B-C3B-CAB-CBB |
| 14  | a     | 824  | CLA  | C4B-C3B-CAB-CBB |
| 14  | x     | 1701 | CLA  | C4B-C3B-CAB-CBB |
| 14  | b     | 805  | CLA  | C4B-C3B-CAB-CBB |
| 18  | g     | 849  | LHG  | C13-C14-C15-C16 |
| 14  | s     | 201  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 832  | CLA  | C10-C11-C12-C13 |
| 14  | b     | 809  | CLA  | C8-C10-C11-C12  |
| 14  | G     | 822  | CLA  | C6-C7-C8-C9     |
| 18  | g     | 850  | LHG  | C35-C36-C37-C38 |
| 14  | G     | 826  | CLA  | C16-C17-C18-C19 |
| 14  | n     | 837  | CLA  | O1A-CGA-O2A-C1  |
| 14  | N     | 809  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 812  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 803  | CLA  | C2A-CAA-CBA-CGA |
| 20  | h     | 1702 | SQD  | C10-C11-C12-C13 |
| 14  | G     | 829  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 827  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 833  | CLA  | C10-C11-C12-C13 |
| 20  | H     | 1702 | SQD  | C13-C14-C15-C16 |
| 20  | H     | 1702 | SQD  | C30-C31-C32-C33 |
| 14  | G     | 853  | CLA  | C3-C5-C6-C7     |
| 18  | m     | 101  | LHG  | O6-C4-C5-C6     |
| 14  | g     | 802  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 802  | CLA  | C11-C12-C13-C15 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | G     | 805 | CLA  | C12-C13-C15-C16 |
| 14  | G     | 806 | CLA  | C6-C7-C8-C10    |
| 14  | G     | 816 | CLA  | C6-C7-C8-C10    |
| 14  | G     | 816 | CLA  | C11-C10-C8-C7   |
| 14  | G     | 824 | CLA  | C12-C13-C15-C16 |
| 14  | G     | 831 | CLA  | C11-C12-C13-C15 |
| 14  | G     | 833 | CLA  | C12-C13-C15-C16 |
| 14  | G     | 853 | CLA  | C12-C13-C15-C16 |
| 14  | N     | 820 | CLA  | C6-C7-C8-C10    |
| 14  | N     | 826 | CLA  | C11-C12-C13-C15 |
| 14  | N     | 827 | CLA  | C6-C7-C8-C10    |
| 14  | N     | 831 | CLA  | C12-C13-C15-C16 |
| 14  | N     | 833 | CLA  | C6-C7-C8-C10    |
| 14  | N     | 851 | CLA  | C11-C12-C13-C15 |
| 14  | g     | 807 | CLA  | C11-C12-C13-C15 |
| 14  | g     | 809 | CLA  | C6-C7-C8-C10    |
| 14  | g     | 825 | CLA  | C12-C13-C15-C16 |
| 14  | g     | 828 | CLA  | C11-C10-C8-C7   |
| 14  | g     | 838 | CLA  | C11-C10-C8-C7   |
| 14  | g     | 854 | CLA  | C11-C12-C13-C15 |
| 14  | n     | 802 | CLA  | C12-C13-C15-C16 |
| 14  | n     | 806 | CLA  | C6-C7-C8-C10    |
| 14  | n     | 809 | CLA  | C11-C12-C13-C15 |
| 14  | n     | 810 | CLA  | C11-C10-C8-C7   |
| 14  | n     | 813 | CLA  | C11-C10-C8-C7   |
| 14  | n     | 813 | CLA  | C12-C13-C15-C16 |
| 14  | n     | 823 | CLA  | C6-C7-C8-C10    |
| 14  | n     | 832 | CLA  | C11-C12-C13-C15 |
| 14  | n     | 837 | CLA  | C11-C12-C13-C15 |
| 14  | n     | 850 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 802 | CLA  | C12-C13-C15-C16 |
| 14  | A     | 805 | CLA  | C12-C13-C15-C16 |
| 14  | A     | 807 | CLA  | C11-C10-C8-C7   |
| 14  | A     | 811 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 818 | CLA  | C12-C13-C15-C16 |
| 14  | B     | 806 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 810 | CLA  | C11-C10-C8-C7   |
| 14  | B     | 818 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 818 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 825 | CLA  | C12-C13-C15-C16 |
| 14  | B     | 841 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 841 | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 850  | CLA  | C11-C10-C8-C7   |
| 14  | a     | 801  | CLA  | C11-C12-C13-C15 |
| 14  | a     | 803  | CLA  | C11-C10-C8-C7   |
| 14  | a     | 804  | CLA  | C11-C10-C8-C7   |
| 14  | a     | 804  | CLA  | C11-C12-C13-C15 |
| 14  | a     | 804  | CLA  | C12-C13-C15-C16 |
| 14  | a     | 806  | CLA  | C11-C12-C13-C15 |
| 14  | a     | 817  | CLA  | C12-C13-C15-C16 |
| 14  | a     | 825  | CLA  | C11-C10-C8-C7   |
| 14  | a     | 826  | CLA  | C12-C13-C15-C16 |
| 14  | a     | 827  | CLA  | C12-C13-C15-C16 |
| 14  | a     | 828  | CLA  | C11-C10-C8-C7   |
| 14  | a     | 838  | CLA  | C11-C10-C8-C7   |
| 14  | b     | 804  | CLA  | C11-C10-C8-C7   |
| 14  | b     | 818  | CLA  | C12-C13-C15-C16 |
| 14  | b     | 838  | CLA  | C12-C13-C15-C16 |
| 14  | l     | 203  | CLA  | C11-C10-C8-C7   |
| 19  | a     | 851  | CL0  | C11-C10-C8-C7   |
| 14  | G     | 837  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 841  | CLA  | C13-C15-C16-C17 |
| 14  | a     | 836  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 853  | CLA  | C5-C6-C7-C8     |
| 14  | X     | 1701 | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 816  | CLA  | C11-C12-C13-C14 |
| 18  | g     | 849  | LHG  | C19-C20-C21-C22 |
| 20  | B     | 801  | SQD  | C27-C28-C29-C30 |
| 20  | b     | 801  | SQD  | C7-C8-C9-C10    |
| 21  | N     | 850  | LMG  | C35-C36-C37-C38 |
| 14  | A     | 838  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 809  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 838  | CLA  | O1D-CGD-O2D-CED |
| 14  | g     | 829  | CLA  | O1A-CGA-O2A-C1  |
| 21  | B     | 849  | LMG  | C29-C30-C31-C32 |
| 14  | a     | 802  | CLA  | C6-C7-C8-C9     |
| 14  | G     | 801  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 805  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 813  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 822  | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 803  | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 806  | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 833  | CLA  | C3A-C2A-CAA-CBA |
| 14  | W     | 203  | CLA  | C3A-C2A-CAA-CBA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | g     | 807 | CLA  | C3A-C2A-CAA-CBA |
| 14  | g     | 812 | CLA  | C3A-C2A-CAA-CBA |
| 14  | g     | 821 | CLA  | C3A-C2A-CAA-CBA |
| 14  | g     | 834 | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 814 | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 817 | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 828 | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 834 | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 840 | CLA  | C3A-C2A-CAA-CBA |
| 14  | s     | 201 | CLA  | C4-C3-C5-C6     |
| 14  | w     | 205 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 803 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 813 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 814 | CLA  | C4-C3-C5-C6     |
| 14  | B     | 835 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 812 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 831 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 853 | CLA  | C3A-C2A-CAA-CBA |
| 14  | l     | 204 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 810 | CLA  | C15-C16-C17-C18 |
| 14  | A     | 828 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 815 | CLA  | O1D-CGD-O2D-CED |
| 18  | a     | 850 | LHG  | C35-C36-C37-C38 |
| 21  | B     | 802 | LMG  | O6-C1-O1-C7     |
| 14  | b     | 829 | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 810 | CLA  | C8-C10-C11-C12  |
| 14  | B     | 840 | CLA  | C15-C16-C17-C18 |
| 14  | A     | 801 | CLA  | O1D-CGD-O2D-CED |
| 20  | n     | 801 | SQD  | C31-C32-C33-C34 |
| 14  | A     | 811 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 829 | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 815 | CLA  | C11-C12-C13-C14 |
| 17  | B     | 846 | BCR  | C19-C20-C21-C22 |
| 17  | b     | 846 | BCR  | C15-C16-C17-C18 |
| 14  | G     | 837 | CLA  | C16-C17-C18-C20 |
| 17  | n     | 842 | BCR  | C37-C22-C23-C24 |
| 17  | A     | 856 | BCR  | C37-C22-C23-C24 |
| 17  | B     | 847 | BCR  | C37-C22-C23-C24 |
| 18  | A     | 851 | LHG  | C30-C31-C32-C33 |
| 14  | a     | 818 | CLA  | C6-C7-C8-C9     |
| 14  | N     | 825 | CLA  | O1A-CGA-O2A-C1  |
| 14  | a     | 837 | CLA  | O1A-CGA-O2A-C1  |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | g     | 833  | CLA  | O1D-CGD-O2D-CED |
| 14  | n     | 832  | CLA  | O1D-CGD-O2D-CED |
| 17  | g     | 847  | BCR  | C7-C8-C9-C10    |
| 17  | A     | 844  | BCR  | C11-C12-C13-C14 |
| 20  | n     | 801  | SQD  | C26-C27-C28-C29 |
| 14  | g     | 827  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 807  | CLA  | C2A-CAA-CBA-CGA |
| 21  | n     | 848  | LMG  | C11-C12-C13-C14 |
| 18  | G     | 850  | LHG  | C4-C5-C6-O8     |
| 18  | S     | 202  | LHG  | C4-C5-C6-O8     |
| 18  | a     | 850  | LHG  | C4-C5-C6-O8     |
| 18  | m     | 101  | LHG  | C4-C5-C6-O8     |
| 20  | x     | 1702 | SQD  | C44-C45-C46-O48 |
| 21  | B     | 849  | LMG  | C7-C8-C9-O8     |
| 20  | H     | 1702 | SQD  | C10-C11-C12-C13 |
| 14  | b     | 831  | CLA  | C6-C7-C8-C9     |
| 14  | N     | 828  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 806  | CLA  | C10-C11-C12-C13 |
| 18  | g     | 850  | LHG  | C12-C13-C14-C15 |
| 14  | b     | 824  | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 832  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 828  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 837  | CLA  | C4-C3-C5-C6     |
| 14  | N     | 827  | CLA  | C2-C3-C5-C6     |
| 14  | g     | 852  | CLA  | C2-C3-C5-C6     |
| 14  | N     | 831  | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 824  | CLA  | O1A-CGA-O2A-C1  |
| 18  | g     | 849  | LHG  | O10-C23-O8-C6   |
| 14  | B     | 812  | CLA  | C6-C7-C8-C9     |
| 14  | N     | 842  | CLA  | C13-C15-C16-C17 |
| 14  | N     | 839  | CLA  | O1D-CGD-O2D-CED |
| 21  | b     | 849  | LMG  | C19-C20-C21-C22 |
| 14  | N     | 842  | CLA  | C16-C17-C18-C20 |
| 14  | g     | 811  | CLA  | C11-C12-C13-C14 |
| 14  | n     | 806  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 826  | CLA  | C16-C17-C18-C20 |
| 18  | G     | 850  | LHG  | O9-C7-O7-C5     |
| 14  | b     | 826  | CLA  | C15-C16-C17-C18 |
| 18  | X     | 1702 | LHG  | O6-C4-C5-O7     |
| 14  | N     | 838  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 802  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 809  | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | g     | 829  | CLA  | C6-C7-C8-C9     |
| 14  | a     | 812  | CLA  | C6-C7-C8-C9     |
| 14  | G     | 839  | CLA  | C2B-C3B-CAB-CBB |
| 14  | g     | 821  | CLA  | C2B-C3B-CAB-CBB |
| 14  | g     | 832  | CLA  | C2B-C3B-CAB-CBB |
| 14  | n     | 816  | CLA  | C2B-C3B-CAB-CBB |
| 14  | n     | 823  | CLA  | C2B-C3B-CAB-CBB |
| 14  | A     | 807  | CLA  | C2B-C3B-CAB-CBB |
| 14  | A     | 834  | CLA  | C2B-C3B-CAB-CBB |
| 14  | b     | 840  | CLA  | C2B-C3B-CAB-CBB |
| 17  | G     | 846  | BCR  | C5-C6-C7-C8     |
| 17  | G     | 848  | BCR  | C23-C24-C25-C30 |
| 17  | W     | 201  | BCR  | C23-C24-C25-C30 |
| 17  | W     | 205  | BCR  | C23-C24-C25-C30 |
| 17  | Y     | 101  | BCR  | C1-C6-C7-C8     |
| 17  | g     | 847  | BCR  | C23-C24-C25-C26 |
| 17  | n     | 843  | BCR  | C23-C24-C25-C26 |
| 17  | n     | 844  | BCR  | C1-C6-C7-C8     |
| 17  | n     | 851  | BCR  | C23-C24-C25-C26 |
| 17  | t     | 103  | BCR  | C5-C6-C7-C8     |
| 17  | y     | 101  | BCR  | C1-C6-C7-C8     |
| 17  | A     | 848  | BCR  | C23-C24-C25-C26 |
| 17  | B     | 844  | BCR  | C23-C24-C25-C30 |
| 17  | I     | 102  | BCR  | C23-C24-C25-C30 |
| 17  | b     | 843  | BCR  | C23-C24-C25-C26 |
| 17  | b     | 844  | BCR  | C23-C24-C25-C26 |
| 17  | j     | 103  | BCR  | C1-C6-C7-C8     |
| 17  | m     | 102  | BCR  | C1-C6-C7-C8     |
| 14  | g     | 806  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 831  | CLA  | C10-C11-C12-C13 |
| 14  | N     | 832  | CLA  | C6-C7-C8-C9     |
| 20  | x     | 1702 | SQD  | C16-C17-C18-C19 |
| 14  | a     | 823  | CLA  | O1A-CGA-O2A-C1  |
| 18  | A     | 851  | LHG  | C9-C10-C11-C12  |
| 21  | B     | 849  | LMG  | C30-C31-C32-C33 |
| 14  | g     | 825  | CLA  | C10-C11-C12-C13 |
| 14  | n     | 827  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 853  | CLA  | CBD-CGD-O2D-CED |
| 20  | b     | 801  | SQD  | C15-C16-C17-C18 |
| 14  | G     | 837  | CLA  | C16-C17-C18-C19 |
| 14  | n     | 831  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 841  | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 821  | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 826  | CLA  | C10-C11-C12-C13 |
| 14  | n     | 827  | CLA  | C10-C11-C12-C13 |
| 14  | a     | 828  | CLA  | C5-C6-C7-C8     |
| 18  | v     | 102  | LHG  | O7-C5-C6-O8     |
| 18  | a     | 850  | LHG  | O7-C5-C6-O8     |
| 18  | a     | 849  | LHG  | C26-C27-C28-C29 |
| 14  | N     | 841  | CLA  | O1D-CGD-O2D-CED |
| 18  | G     | 849  | LHG  | C28-C29-C30-C31 |
| 14  | B     | 826  | CLA  | C15-C16-C17-C18 |
| 14  | n     | 831  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 825  | CLA  | C6-C7-C8-C9     |
| 18  | S     | 202  | LHG  | O10-C23-O8-C6   |
| 14  | G     | 829  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 806  | CLA  | C15-C16-C17-C18 |
| 14  | g     | 827  | CLA  | C2-C3-C5-C6     |
| 14  | s     | 201  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 808  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 814  | CLA  | C2-C3-C5-C6     |
| 14  | n     | 806  | CLA  | C16-C17-C18-C19 |
| 21  | B     | 849  | LMG  | C39-C40-C41-C42 |
| 18  | A     | 850  | LHG  | C7-C8-C9-C10    |
| 14  | n     | 817  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 828  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 803  | CLA  | C6-C7-C8-C9     |
| 14  | G     | 805  | CLA  | C14-C13-C15-C16 |
| 14  | G     | 816  | CLA  | C11-C10-C8-C9   |
| 14  | N     | 807  | CLA  | C14-C13-C15-C16 |
| 14  | W     | 203  | CLA  | C6-C7-C8-C9     |
| 14  | g     | 838  | CLA  | C6-C7-C8-C9     |
| 14  | g     | 852  | CLA  | C6-C7-C8-C9     |
| 14  | n     | 803  | CLA  | C11-C10-C8-C9   |
| 14  | n     | 818  | CLA  | C6-C7-C8-C9     |
| 14  | n     | 825  | CLA  | C11-C12-C13-C14 |
| 14  | n     | 837  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 810  | CLA  | C11-C10-C8-C9   |
| 14  | B     | 824  | CLA  | C14-C13-C15-C16 |
| 14  | L     | 1502 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 826  | CLA  | C11-C12-C13-C14 |
| 18  | S     | 202  | LHG  | C25-C26-C27-C28 |
| 14  | n     | 832  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 833  | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 18  | g     | 849  | LHG  | C31-C32-C33-C34 |
| 14  | g     | 833  | CLA  | C6-C7-C8-C9     |
| 14  | N     | 842  | CLA  | C16-C17-C18-C19 |
| 14  | l     | 203  | CLA  | C11-C12-C13-C15 |
| 14  | n     | 829  | CLA  | O1D-CGD-O2D-CED |
| 14  | B     | 825  | CLA  | O1D-CGD-O2D-CED |
| 20  | h     | 1702 | SQD  | C30-C31-C32-C33 |
| 20  | x     | 1702 | SQD  | C30-C31-C32-C33 |
| 14  | N     | 814  | CLA  | C6-C7-C8-C9     |
| 14  | n     | 815  | CLA  | O2A-C1-C2-C3    |
| 14  | u     | 102  | CLA  | O2A-C1-C2-C3    |
| 14  | A     | 857  | CLA  | O2A-C1-C2-C3    |
| 14  | a     | 854  | CLA  | O2A-C1-C2-C3    |
| 14  | b     | 816  | CLA  | O2A-C1-C2-C3    |
| 14  | A     | 854  | CLA  | CBD-CGD-O2D-CED |
| 14  | G     | 828  | CLA  | C13-C15-C16-C17 |
| 18  | G     | 850  | LHG  | C14-C15-C16-C17 |
| 14  | F     | 202  | CLA  | C2A-CAA-CBA-CGA |
| 18  | G     | 849  | LHG  | C29-C30-C31-C32 |
| 14  | b     | 825  | CLA  | C13-C15-C16-C17 |
| 15  | a     | 841  | PQN  | C25-C26-C27-C28 |
| 15  | B     | 842  | PQN  | C14-C13-C15-C16 |
| 18  | X     | 1702 | LHG  | C31-C32-C33-C34 |
| 20  | n     | 801  | SQD  | C29-C30-C31-C32 |
| 14  | a     | 804  | CLA  | C2-C3-C5-C6     |
| 18  | A     | 850  | LHG  | C15-C16-C17-C18 |
| 18  | X     | 1702 | LHG  | C10-C11-C12-C13 |
| 20  | x     | 1702 | SQD  | C26-C27-C28-C29 |
| 14  | N     | 821  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 833  | CLA  | C5-C6-C7-C8     |
| 14  | g     | 809  | CLA  | C10-C11-C12-C13 |
| 14  | g     | 854  | CLA  | C5-C6-C7-C8     |
| 14  | g     | 854  | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 803  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 820  | CLA  | C8-C10-C11-C12  |
| 21  | B     | 849  | LMG  | C13-C14-C15-C16 |
| 18  | a     | 849  | LHG  | C19-C20-C21-C22 |
| 14  | b     | 814  | CLA  | CAA-CBA-CGA-O2A |
| 14  | g     | 823  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 813  | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 815  | CLA  | C8-C10-C11-C12  |
| 14  | B     | 824  | CLA  | C10-C11-C12-C13 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | B     | 850 | CLA  | C8-C10-C11-C12  |
| 14  | b     | 805 | CLA  | C10-C11-C12-C13 |
| 18  | g     | 850 | LHG  | O6-C4-C5-C6     |
| 18  | v     | 102 | LHG  | O6-C4-C5-C6     |
| 14  | n     | 837 | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 834 | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 831 | CLA  | C16-C17-C18-C19 |
| 17  | l     | 206 | BCR  | C11-C12-C13-C35 |
| 14  | G     | 812 | CLA  | C11-C10-C8-C7   |
| 14  | G     | 820 | CLA  | C12-C13-C15-C16 |
| 14  | G     | 826 | CLA  | C11-C12-C13-C15 |
| 14  | N     | 807 | CLA  | C12-C13-C15-C16 |
| 14  | N     | 820 | CLA  | C11-C10-C8-C7   |
| 14  | g     | 804 | CLA  | C12-C13-C15-C16 |
| 14  | g     | 823 | CLA  | C12-C13-C15-C16 |
| 14  | n     | 803 | CLA  | C11-C10-C8-C7   |
| 14  | n     | 823 | CLA  | C11-C10-C8-C7   |
| 14  | n     | 825 | CLA  | C11-C12-C13-C15 |
| 14  | n     | 832 | CLA  | C6-C7-C8-C10    |
| 14  | n     | 837 | CLA  | C12-C13-C15-C16 |
| 14  | w     | 204 | CLA  | C11-C10-C8-C7   |
| 14  | A     | 810 | CLA  | C11-C12-C13-C15 |
| 14  | A     | 826 | CLA  | C12-C13-C15-C16 |
| 14  | A     | 831 | CLA  | C11-C12-C13-C15 |
| 14  | A     | 837 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 853 | CLA  | C11-C10-C8-C7   |
| 14  | A     | 854 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 854 | CLA  | C12-C13-C15-C16 |
| 14  | B     | 807 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 809 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 819 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 819 | CLA  | C11-C10-C8-C7   |
| 14  | a     | 819 | CLA  | C11-C10-C8-C7   |
| 14  | a     | 823 | CLA  | C12-C13-C15-C16 |
| 14  | a     | 839 | CLA  | C11-C10-C8-C7   |
| 14  | b     | 802 | CLA  | C11-C12-C13-C15 |
| 14  | b     | 814 | CLA  | C12-C13-C15-C16 |
| 14  | b     | 819 | CLA  | C6-C7-C8-C10    |
| 14  | b     | 826 | CLA  | C11-C12-C13-C15 |
| 14  | b     | 833 | CLA  | C11-C12-C13-C15 |
| 15  | g     | 841 | PQN  | C16-C17-C18-C20 |
| 18  | a     | 849 | LHG  | C23-C24-C25-C26 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | n     | 850  | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 827  | CLA  | C8-C10-C11-C12  |
| 14  | B     | 811  | CLA  | C10-C11-C12-C13 |
| 17  | G     | 844  | BCR  | C21-C22-C23-C24 |
| 17  | N     | 847  | BCR  | C7-C8-C9-C10    |
| 17  | N     | 847  | BCR  | C17-C18-C19-C20 |
| 17  | a     | 847  | BCR  | C7-C8-C9-C10    |
| 17  | b     | 847  | BCR  | C7-C8-C9-C10    |
| 17  | m     | 102  | BCR  | C7-C8-C9-C10    |
| 14  | A     | 839  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 833  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 829  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 825  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 826  | CLA  | O1A-CGA-O2A-C1  |
| 18  | S     | 202  | LHG  | C27-C28-C29-C30 |
| 14  | G     | 839  | CLA  | C5-C6-C7-C8     |
| 14  | g     | 837  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 833  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 810  | CLA  | C10-C11-C12-C13 |
| 14  | N     | 822  | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 815  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 814  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 829  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 853  | CLA  | C2A-CAA-CBA-CGA |
| 14  | x     | 1701 | CLA  | C2A-CAA-CBA-CGA |
| 14  | s     | 201  | CLA  | C11-C12-C13-C14 |
| 14  | G     | 802  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 820  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 817  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 840  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 804  | CLA  | C4-C3-C5-C6     |
| 14  | n     | 832  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 811  | CLA  | O1A-CGA-O2A-C1  |
| 14  | B     | 840  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 802  | CLA  | C10-C11-C12-C13 |
| 18  | A     | 850  | LHG  | C19-C20-C21-C22 |
| 14  | B     | 850  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 835  | CLA  | CBD-CGD-O2D-CED |
| 14  | b     | 834  | CLA  | CBA-CGA-O2A-C1  |
| 20  | l     | 201  | SQD  | C12-C13-C14-C15 |
| 18  | g     | 849  | LHG  | C28-C29-C30-C31 |
| 14  | b     | 804  | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 810  | CLA  | C16-C17-C18-C19 |
| 14  | B     | 815  | CLA  | O1D-CGD-O2D-CED |
| 14  | H     | 1701 | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 805  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 806  | CLA  | O1A-CGA-O2A-C1  |
| 15  | g     | 841  | PQN  | C13-C15-C16-C17 |
| 14  | G     | 838  | CLA  | C15-C16-C17-C18 |
| 14  | N     | 821  | CLA  | C13-C15-C16-C17 |
| 20  | w     | 202  | SQD  | C24-C25-C26-C27 |
| 14  | n     | 836  | CLA  | O1D-CGD-O2D-CED |
| 18  | g     | 850  | LHG  | O6-C4-C5-O7     |
| 18  | A     | 851  | LHG  | O6-C4-C5-O7     |
| 18  | G     | 850  | LHG  | C7-C8-C9-C10    |
| 14  | g     | 804  | CLA  | C10-C11-C12-C13 |
| 14  | g     | 801  | CLA  | C16-C17-C18-C20 |
| 15  | a     | 841  | PQN  | C26-C27-C28-C30 |
| 14  | G     | 816  | CLA  | C11-C12-C13-C14 |
| 14  | N     | 826  | CLA  | C13-C15-C16-C17 |
| 14  | N     | 838  | CLA  | C10-C11-C12-C13 |
| 14  | N     | 851  | CLA  | C13-C15-C16-C17 |
| 14  | A     | 840  | CLA  | C2-C3-C5-C6     |
| 15  | B     | 842  | PQN  | C12-C13-C15-C16 |
| 21  | b     | 849  | LMG  | C30-C31-C32-C33 |
| 14  | b     | 828  | CLA  | C8-C10-C11-C12  |
| 21  | N     | 850  | LMG  | C34-C35-C36-C37 |
| 14  | N     | 827  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 828  | CLA  | C3-C5-C6-C7     |
| 18  | G     | 850  | LHG  | C12-C13-C14-C15 |
| 20  | H     | 1702 | SQD  | C11-C10-C9-C8   |
| 18  | S     | 202  | LHG  | O7-C5-C6-O8     |
| 20  | x     | 1702 | SQD  | O6-C44-C45-O47  |
| 21  | B     | 802  | LMG  | O1-C7-C8-O7     |
| 18  | a     | 850  | LHG  | C19-C20-C21-C22 |
| 14  | G     | 804  | CLA  | C14-C13-C15-C16 |
| 14  | G     | 812  | CLA  | C11-C10-C8-C9   |
| 14  | G     | 837  | CLA  | C11-C10-C8-C9   |
| 14  | N     | 807  | CLA  | C6-C7-C8-C9     |
| 14  | g     | 807  | CLA  | C11-C12-C13-C14 |
| 14  | g     | 809  | CLA  | C14-C13-C15-C16 |
| 14  | g     | 830  | CLA  | C14-C13-C15-C16 |
| 14  | g     | 839  | CLA  | C11-C12-C13-C14 |
| 14  | g     | 854  | CLA  | C6-C7-C8-C9     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | n     | 829  | CLA  | C11-C10-C8-C9   |
| 14  | n     | 832  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 853  | CLA  | C11-C10-C8-C9   |
| 14  | B     | 807  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 819  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 823  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 826  | CLA  | C11-C10-C8-C9   |
| 14  | b     | 802  | CLA  | C11-C12-C13-C14 |
| 14  | b     | 811  | CLA  | C11-C10-C8-C9   |
| 14  | b     | 814  | CLA  | C14-C13-C15-C16 |
| 14  | n     | 808  | CLA  | C16-C17-C18-C20 |
| 18  | g     | 849  | LHG  | C10-C11-C12-C13 |
| 20  | w     | 202  | SQD  | C26-C27-C28-C29 |
| 14  | g     | 823  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 811  | CLA  | C11-C12-C13-C14 |
| 14  | b     | 813  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 839  | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 802  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 818  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 823  | CLA  | C13-C15-C16-C17 |
| 20  | H     | 1702 | SQD  | C11-C12-C13-C14 |
| 15  | n     | 841  | PQN  | C14-C13-C15-C16 |
| 14  | g     | 803  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 827  | CLA  | C8-C10-C11-C12  |
| 14  | G     | 805  | CLA  | C16-C17-C18-C19 |
| 14  | G     | 832  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 805  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 813  | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 822  | CLA  | C3-C5-C6-C7     |
| 14  | a     | 837  | CLA  | C3-C5-C6-C7     |
| 19  | A     | 852  | CL0  | C4C-C3C-CAC-CBC |
| 19  | a     | 851  | CL0  | C4C-C3C-CAC-CBC |
| 14  | B     | 810  | CLA  | C5-C6-C7-C8     |
| 14  | t     | 101  | CLA  | O1D-CGD-O2D-CED |
| 20  | x     | 1702 | SQD  | C17-C18-C19-C20 |
| 21  | b     | 849  | LMG  | C13-C14-C15-C16 |
| 14  | g     | 811  | CLA  | C11-C12-C13-C15 |
| 18  | A     | 850  | LHG  | C23-C24-C25-C26 |
| 14  | B     | 821  | CLA  | O1D-CGD-O2D-CED |
| 14  | G     | 801  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 811  | CLA  | C4B-C3B-CAB-CBB |
| 14  | G     | 816  | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 833  | CLA  | C4B-C3B-CAB-CBB |
| 14  | G     | 840  | CLA  | C4B-C3B-CAB-CBB |
| 14  | H     | 1701 | CLA  | C4B-C3B-CAB-CBB |
| 14  | N     | 801  | CLA  | C4B-C3B-CAB-CBB |
| 14  | N     | 803  | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 815  | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 821  | CLA  | C4B-C3B-CAB-CBB |
| 14  | N     | 822  | CLA  | C4B-C3B-CAB-CBB |
| 14  | N     | 837  | CLA  | C4B-C3B-CAB-CBB |
| 14  | N     | 840  | CLA  | C4B-C3B-CAB-CBB |
| 14  | N     | 842  | CLA  | C4B-C3B-CAB-CBB |
| 14  | T     | 101  | CLA  | C4B-C3B-CAB-CBB |
| 14  | g     | 809  | CLA  | C4B-C3B-CAB-CBB |
| 14  | g     | 837  | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 837  | CLA  | C4B-C3B-CAB-CBB |
| 14  | g     | 839  | CLA  | C4B-C3B-CAB-CBB |
| 14  | n     | 813  | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 821  | CLA  | C4B-C3B-CAB-CBB |
| 14  | n     | 840  | CLA  | C4B-C3B-CAB-CBB |
| 14  | s     | 202  | CLA  | C4B-C3B-CAB-CBB |
| 14  | w     | 205  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 805  | CLA  | C4B-C3B-CAB-CBB |
| 14  | A     | 811  | CLA  | C4B-C3B-CAB-CBB |
| 14  | A     | 833  | CLA  | C4B-C3B-CAB-CBB |
| 14  | A     | 838  | CLA  | C4B-C3B-CAB-CBB |
| 14  | A     | 839  | CLA  | C4B-C3B-CAB-CBB |
| 14  | X     | 1701 | CLA  | C4B-C3B-CAB-CBB |
| 14  | B     | 811  | CLA  | C4B-C3B-CAB-CBB |
| 14  | B     | 817  | CLA  | C4B-C3B-CAB-CBB |
| 14  | B     | 839  | CLA  | C4B-C3B-CAB-CBB |
| 14  | F     | 202  | CLA  | C4B-C3B-CAB-CBB |
| 14  | J     | 101  | CLA  | C4B-C3B-CAB-CBB |
| 14  | a     | 809  | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 809  | CLA  | C4B-C3B-CAB-CBB |
| 14  | a     | 815  | CLA  | C4B-C3B-CAB-CBB |
| 14  | a     | 816  | CLA  | C4B-C3B-CAB-CBB |
| 14  | a     | 821  | CLA  | C4B-C3B-CAB-CBB |
| 14  | a     | 832  | CLA  | C4B-C3B-CAB-CBB |
| 14  | a     | 836  | CLA  | C4B-C3B-CAB-CBB |
| 14  | b     | 805  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 812  | CLA  | C4B-C3B-CAB-CBB |
| 14  | b     | 815  | CLA  | C1A-C2A-CAA-CBA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 821  | CLA  | C4B-C3B-CAB-CBB |
| 14  | b     | 823  | CLA  | C4B-C3B-CAB-CBB |
| 14  | b     | 824  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 833  | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 840  | CLA  | C4B-C3B-CAB-CBB |
| 14  | b     | 841  | CLA  | C4B-C3B-CAB-CBB |
| 14  | f     | 202  | CLA  | C4B-C3B-CAB-CBB |
| 14  | k     | 101  | CLA  | C4B-C3B-CAB-CBB |
| 14  | l     | 204  | CLA  | C4B-C3B-CAB-CBB |
| 14  | n     | 820  | CLA  | O1D-CGD-O2D-CED |
| 14  | n     | 830  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 826  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 829  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 818  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 837  | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 829  | CLA  | C4-C3-C5-C6     |
| 14  | g     | 821  | CLA  | C4-C3-C5-C6     |
| 14  | n     | 837  | CLA  | C4-C3-C5-C6     |
| 17  | n     | 842  | BCR  | C21-C22-C23-C24 |
| 17  | B     | 847  | BCR  | C21-C22-C23-C24 |
| 21  | B     | 849  | LMG  | C18-C19-C20-C21 |
| 14  | A     | 839  | CLA  | O1A-CGA-O2A-C1  |
| 14  | g     | 839  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 807  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 839  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 831  | CLA  | C2A-CAA-CBA-CGA |
| 14  | f     | 202  | CLA  | C2A-CAA-CBA-CGA |
| 20  | w     | 202  | SQD  | C27-C28-C29-C30 |
| 20  | B     | 801  | SQD  | C12-C13-C14-C15 |
| 20  | w     | 202  | SQD  | C17-C18-C19-C20 |
| 21  | B     | 849  | LMG  | C14-C15-C16-C17 |
| 18  | g     | 849  | LHG  | O6-C4-C5-C6     |
| 18  | X     | 1702 | LHG  | O6-C4-C5-C6     |
| 18  | a     | 850  | LHG  | O6-C4-C5-C6     |
| 18  | a     | 849  | LHG  | C25-C26-C27-C28 |
| 14  | A     | 819  | CLA  | CBD-CGD-O2D-CED |
| 14  | W     | 202  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 826  | CLA  | C10-C11-C12-C13 |
| 14  | B     | 814  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 807  | CLA  | C11-C10-C8-C7   |
| 14  | G     | 810  | CLA  | C6-C7-C8-C10    |
| 14  | G     | 829  | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 839  | CLA  | C6-C7-C8-C10    |
| 14  | N     | 805  | CLA  | C12-C13-C15-C16 |
| 14  | N     | 808  | CLA  | C12-C13-C15-C16 |
| 14  | g     | 803  | CLA  | C11-C10-C8-C7   |
| 14  | g     | 819  | CLA  | C11-C10-C8-C7   |
| 14  | g     | 827  | CLA  | C11-C12-C13-C15 |
| 14  | g     | 832  | CLA  | C11-C12-C13-C15 |
| 14  | g     | 839  | CLA  | C12-C13-C15-C16 |
| 14  | g     | 852  | CLA  | C11-C10-C8-C7   |
| 14  | n     | 804  | CLA  | C12-C13-C15-C16 |
| 14  | n     | 805  | CLA  | C12-C13-C15-C16 |
| 14  | w     | 204  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 811  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 818  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 818  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 833  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 838  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 814  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 818  | CLA  | C12-C13-C15-C16 |
| 14  | B     | 830  | CLA  | C12-C13-C15-C16 |
| 14  | a     | 832  | CLA  | C11-C12-C13-C15 |
| 14  | a     | 836  | CLA  | C6-C7-C8-C10    |
| 14  | b     | 810  | CLA  | C11-C12-C13-C15 |
| 14  | b     | 811  | CLA  | C6-C7-C8-C10    |
| 14  | b     | 819  | CLA  | C11-C10-C8-C7   |
| 14  | b     | 825  | CLA  | C6-C7-C8-C10    |
| 15  | A     | 842  | PQN  | C16-C17-C18-C20 |
| 20  | H     | 1702 | SQD  | C14-C15-C16-C17 |
| 14  | G     | 805  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 820  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 831  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 831  | CLA  | C16-C17-C18-C20 |
| 14  | B     | 818  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 803  | CLA  | C10-C11-C12-C13 |
| 20  | h     | 1702 | SQD  | C18-C19-C20-C21 |
| 14  | A     | 828  | CLA  | CAA-CBA-CGA-O2A |
| 20  | h     | 1702 | SQD  | C17-C18-C19-C20 |
| 20  | b     | 801  | SQD  | C28-C29-C30-C31 |
| 14  | n     | 825  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 839  | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 810  | CLA  | C4-C3-C5-C6     |
| 14  | n     | 810  | CLA  | C11-C12-C13-C14 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 806  | CLA  | C2C-C3C-CAC-CBC |
| 14  | B     | 808  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 804  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 834  | CLA  | O1A-CGA-O2A-C1  |
| 18  | a     | 850  | LHG  | O6-C4-C5-O7     |
| 14  | B     | 840  | CLA  | C3-C5-C6-C7     |
| 20  | H     | 1702 | SQD  | C32-C33-C34-C35 |
| 14  | a     | 853  | CLA  | O1D-CGD-O2D-CED |
| 14  | g     | 816  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 816  | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 826  | CLA  | C11-C12-C13-C14 |
| 14  | N     | 811  | CLA  | C14-C13-C15-C16 |
| 14  | N     | 825  | CLA  | C11-C10-C8-C9   |
| 14  | N     | 826  | CLA  | C11-C12-C13-C14 |
| 14  | g     | 823  | CLA  | C14-C13-C15-C16 |
| 14  | g     | 828  | CLA  | C11-C10-C8-C9   |
| 14  | n     | 823  | CLA  | C11-C10-C8-C9   |
| 14  | n     | 827  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 802  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 808  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 810  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 837  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 838  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 854  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 809  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 820  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 824  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 827  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 804  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 826  | CLA  | C14-C13-C15-C16 |
| 14  | a     | 830  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 836  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 839  | CLA  | C11-C10-C8-C9   |
| 14  | b     | 819  | CLA  | C6-C7-C8-C9     |
| 19  | a     | 851  | CL0  | C11-C10-C8-C9   |
| 18  | G     | 849  | LHG  | C10-C11-C12-C13 |
| 17  | n     | 849  | BCR  | C19-C20-C21-C22 |
| 17  | j     | 104  | BCR  | C19-C20-C21-C22 |
| 17  | i     | 101  | BCR  | C9-C10-C11-C12  |
| 20  | n     | 801  | SQD  | C19-C20-C21-C22 |
| 14  | w     | 203  | CLA  | O1D-CGD-O2D-CED |
| 14  | N     | 838  | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | N     | 817  | CLA  | C1-C2-C3-C4     |
| 14  | n     | 815  | CLA  | C1-C2-C3-C4     |
| 14  | B     | 816  | CLA  | C1-C2-C3-C4     |
| 14  | b     | 816  | CLA  | C1-C2-C3-C4     |
| 20  | w     | 202  | SQD  | C25-C26-C27-C28 |
| 14  | G     | 833  | CLA  | C3-C5-C6-C7     |
| 14  | G     | 813  | CLA  | C6-C7-C8-C9     |
| 18  | G     | 849  | LHG  | C11-C10-C9-C8   |
| 14  | G     | 833  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 826  | CLA  | C8-C10-C11-C12  |
| 14  | N     | 826  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 818  | CLA  | O1A-CGA-O2A-C1  |
| 18  | a     | 849  | LHG  | O7-C5-C6-O8     |
| 20  | h     | 1702 | SQD  | O6-C44-C45-O47  |
| 20  | B     | 801  | SQD  | O6-C44-C45-O47  |
| 21  | b     | 849  | LMG  | C35-C36-C37-C38 |
| 14  | H     | 1701 | CLA  | O2A-C1-C2-C3    |
| 14  | U     | 102  | CLA  | O2A-C1-C2-C3    |
| 14  | B     | 811  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 819  | CLA  | C8-C10-C11-C12  |
| 14  | b     | 828  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 831  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 805  | CLA  | C16-C17-C18-C20 |
| 18  | g     | 849  | LHG  | C14-C15-C16-C17 |
| 18  | A     | 851  | LHG  | C11-C12-C13-C14 |
| 18  | v     | 102  | LHG  | C4-C5-C6-O8     |
| 20  | H     | 1702 | SQD  | O6-C44-C45-C46  |
| 14  | A     | 807  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 826  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 828  | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 837  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 804  | CLA  | CAD-CBD-CGD-O2D |
| 14  | N     | 812  | CLA  | CAD-CBD-CGD-O2D |
| 14  | N     | 825  | CLA  | CAD-CBD-CGD-O2D |
| 14  | N     | 828  | CLA  | CAD-CBD-CGD-O2D |
| 14  | g     | 803  | CLA  | CAD-CBD-CGD-O2D |
| 14  | g     | 812  | CLA  | CAD-CBD-CGD-O2D |
| 14  | g     | 835  | CLA  | CAD-CBD-CGD-O2D |
| 14  | n     | 820  | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 825  | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 830  | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 836  | CLA  | CAD-CBD-CGD-O2D |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | B     | 803 | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 806 | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 803 | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 813 | CLA  | CAD-CBD-CGD-O2D |
| 14  | a     | 835 | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 815 | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 823 | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 837 | CLA  | CAD-CBD-CGD-O2D |
| 14  | n     | 807 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 802 | CLA  | C8-C10-C11-C12  |
| 14  | a     | 853 | CLA  | C10-C11-C12-C13 |
| 14  | G     | 811 | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 830 | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 833 | CLA  | C8-C10-C11-C12  |
| 14  | b     | 829 | CLA  | C8-C10-C11-C12  |
| 14  | B     | 808 | CLA  | C16-C17-C18-C20 |
| 14  | a     | 819 | CLA  | C16-C17-C18-C20 |
| 14  | b     | 833 | CLA  | C16-C17-C18-C20 |
| 14  | b     | 853 | CLA  | C6-C7-C8-C10    |
| 14  | B     | 818 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 819 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 812 | CLA  | C6-C7-C8-C9     |
| 14  | a     | 829 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 804 | CLA  | CAD-CBD-CGD-O1D |
| 14  | G     | 830 | CLA  | CHA-CBD-CGD-O1D |
| 14  | G     | 830 | CLA  | CHA-CBD-CGD-O2D |
| 14  | N     | 807 | CLA  | CAD-CBD-CGD-O1D |
| 14  | N     | 812 | CLA  | CAD-CBD-CGD-O1D |
| 14  | N     | 814 | CLA  | CAD-CBD-CGD-O1D |
| 14  | N     | 818 | CLA  | CHA-CBD-CGD-O1D |
| 14  | N     | 825 | CLA  | CAD-CBD-CGD-O1D |
| 14  | N     | 828 | CLA  | CAD-CBD-CGD-O1D |
| 14  | g     | 801 | CLA  | CHA-CBD-CGD-O1D |
| 14  | g     | 803 | CLA  | CAD-CBD-CGD-O1D |
| 14  | g     | 812 | CLA  | CAD-CBD-CGD-O1D |
| 14  | g     | 835 | CLA  | CAD-CBD-CGD-O1D |
| 14  | n     | 812 | CLA  | CHA-CBD-CGD-O1D |
| 14  | n     | 820 | CLA  | CAD-CBD-CGD-O1D |
| 14  | n     | 823 | CLA  | CHA-CBD-CGD-O1D |
| 14  | n     | 830 | CLA  | CHA-CBD-CGD-O1D |
| 14  | n     | 830 | CLA  | CHA-CBD-CGD-O2D |
| 14  | n     | 839 | CLA  | CHA-CBD-CGD-O1D |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | w     | 203  | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 803  | CLA  | CHA-CBD-CGD-O1D |
| 14  | A     | 825  | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 830  | CLA  | CAD-CBD-CGD-O1D |
| 14  | A     | 836  | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 803  | CLA  | CAD-CBD-CGD-O1D |
| 14  | B     | 806  | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 803  | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 813  | CLA  | CAD-CBD-CGD-O1D |
| 14  | a     | 818  | CLA  | CHA-CBD-CGD-O1D |
| 14  | a     | 818  | CLA  | CHA-CBD-CGD-O2D |
| 14  | a     | 835  | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 803  | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 815  | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 823  | CLA  | CAD-CBD-CGD-O1D |
| 14  | b     | 831  | CLA  | CHA-CBD-CGD-O1D |
| 14  | b     | 837  | CLA  | CAD-CBD-CGD-O1D |
| 17  | t     | 104  | BCR  | C19-C20-C21-C22 |
| 17  | b     | 852  | BCR  | C15-C16-C17-C18 |
| 18  | G     | 849  | LHG  | C4-O6-P-O3      |
| 18  | G     | 849  | LHG  | C4-O6-P-O5      |
| 18  | G     | 850  | LHG  | C3-O3-P-O4      |
| 18  | G     | 850  | LHG  | C3-O3-P-O6      |
| 18  | G     | 850  | LHG  | C4-O6-P-O5      |
| 18  | g     | 850  | LHG  | C3-O3-P-O5      |
| 18  | v     | 102  | LHG  | C3-O3-P-O4      |
| 18  | A     | 850  | LHG  | C3-O3-P-O6      |
| 18  | A     | 850  | LHG  | C4-O6-P-O3      |
| 18  | A     | 850  | LHG  | C4-O6-P-O4      |
| 18  | A     | 850  | LHG  | C4-O6-P-O5      |
| 18  | A     | 851  | LHG  | C3-O3-P-O5      |
| 18  | X     | 1702 | LHG  | C4-O6-P-O5      |
| 14  | N     | 830  | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 827  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 833  | CLA  | C2B-C3B-CAB-CBB |
| 14  | N     | 805  | CLA  | C2B-C3B-CAB-CBB |
| 14  | N     | 821  | CLA  | C2B-C3B-CAB-CBB |
| 14  | N     | 822  | CLA  | C2B-C3B-CAB-CBB |
| 14  | N     | 837  | CLA  | C2B-C3B-CAB-CBB |
| 14  | T     | 101  | CLA  | C2B-C3B-CAB-CBB |
| 14  | U     | 101  | CLA  | C2B-C3B-CAB-CBB |
| 14  | g     | 854  | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | n     | 804  | CLA  | C2B-C3B-CAB-CBB |
| 14  | n     | 821  | CLA  | C2B-C3B-CAB-CBB |
| 14  | n     | 839  | CLA  | C2B-C3B-CAB-CBB |
| 14  | s     | 202  | CLA  | C2B-C3B-CAB-CBB |
| 14  | u     | 101  | CLA  | C2B-C3B-CAB-CBB |
| 14  | A     | 805  | CLA  | C2B-C3B-CAB-CBB |
| 14  | A     | 833  | CLA  | C2B-C3B-CAB-CBB |
| 14  | A     | 839  | CLA  | C2B-C3B-CAB-CBB |
| 14  | A     | 853  | CLA  | C2B-C3B-CAB-CBB |
| 14  | B     | 817  | CLA  | C2B-C3B-CAB-CBB |
| 14  | F     | 202  | CLA  | C2B-C3B-CAB-CBB |
| 14  | J     | 101  | CLA  | C2B-C3B-CAB-CBB |
| 14  | k     | 101  | CLA  | C2B-C3B-CAB-CBB |
| 17  | G     | 845  | BCR  | C5-C6-C7-C8     |
| 17  | T     | 103  | BCR  | C5-C6-C7-C8     |
| 17  | g     | 845  | BCR  | C1-C6-C7-C8     |
| 14  | b     | 812  | CLA  | CAA-CBA-CGA-O2A |
| 15  | n     | 841  | PQN  | C12-C13-C15-C16 |
| 14  | G     | 806  | CLA  | C4C-C3C-CAC-CBC |
| 14  | a     | 809  | CLA  | C10-C11-C12-C13 |
| 18  | X     | 1702 | LHG  | C2-C3-O3-P      |
| 18  | X     | 1702 | LHG  | C5-C4-O6-P      |
| 18  | m     | 101  | LHG  | C5-C4-O6-P      |
| 14  | g     | 815  | CLA  | C10-C11-C12-C13 |
| 14  | n     | 850  | CLA  | O1D-CGD-O2D-CED |
| 14  | A     | 854  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 837  | CLA  | C13-C15-C16-C17 |
| 20  | x     | 1702 | SQD  | C12-C13-C14-C15 |
| 14  | b     | 809  | CLA  | C16-C17-C18-C20 |
| 17  | B     | 843  | BCR  | C7-C8-C9-C10    |
| 17  | B     | 846  | BCR  | C7-C8-C9-C10    |
| 14  | G     | 808  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 817  | CLA  | O1D-CGD-O2D-CED |
| 14  | n     | 805  | CLA  | C15-C16-C17-C18 |
| 18  | g     | 850  | LHG  | O1-C1-C2-C3     |
| 14  | G     | 811  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 824  | CLA  | O1A-CGA-O2A-C1  |
| 20  | w     | 202  | SQD  | C19-C20-C21-C22 |
| 17  | g     | 846  | BCR  | C18-C19-C20-C21 |
| 17  | n     | 845  | BCR  | C18-C19-C20-C21 |
| 14  | N     | 838  | CLA  | C8-C10-C11-C12  |
| 14  | g     | 816  | CLA  | C5-C6-C7-C8     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | n     | 824 | CLA  | C13-C15-C16-C17 |
| 14  | B     | 832 | CLA  | C5-C6-C7-C8     |
| 14  | a     | 815 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 854 | CLA  | O1D-CGD-O2D-CED |
| 18  | G     | 850 | LHG  | C28-C29-C30-C31 |
| 14  | N     | 838 | CLA  | C11-C12-C13-C15 |
| 18  | A     | 851 | LHG  | O6-C4-C5-C6     |
| 14  | b     | 815 | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 804 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 829 | CLA  | C11-C10-C8-C9   |
| 14  | G     | 837 | CLA  | C11-C12-C13-C14 |
| 14  | N     | 804 | CLA  | C14-C13-C15-C16 |
| 14  | N     | 805 | CLA  | C14-C13-C15-C16 |
| 14  | N     | 815 | CLA  | C11-C10-C8-C9   |
| 14  | N     | 820 | CLA  | C11-C10-C8-C9   |
| 14  | N     | 827 | CLA  | C6-C7-C8-C9     |
| 14  | g     | 804 | CLA  | C14-C13-C15-C16 |
| 14  | g     | 827 | CLA  | C6-C7-C8-C9     |
| 14  | g     | 838 | CLA  | C11-C12-C13-C14 |
| 14  | n     | 802 | CLA  | C14-C13-C15-C16 |
| 14  | n     | 813 | CLA  | C14-C13-C15-C16 |
| 14  | n     | 828 | CLA  | C11-C12-C13-C14 |
| 14  | A     | 807 | CLA  | C11-C10-C8-C9   |
| 14  | A     | 817 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 818 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 826 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 831 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 803 | CLA  | C14-C13-C15-C16 |
| 14  | B     | 806 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 850 | CLA  | C6-C7-C8-C9     |
| 14  | a     | 809 | CLA  | C11-C12-C13-C14 |
| 14  | a     | 828 | CLA  | C11-C10-C8-C9   |
| 14  | b     | 825 | CLA  | C6-C7-C8-C9     |
| 14  | b     | 833 | CLA  | C11-C12-C13-C14 |
| 14  | b     | 828 | CLA  | O1D-CGD-O2D-CED |
| 14  | a     | 829 | CLA  | C6-C7-C8-C9     |
| 14  | G     | 804 | CLA  | C12-C13-C15-C16 |
| 14  | N     | 803 | CLA  | C6-C7-C8-C10    |
| 14  | N     | 804 | CLA  | C12-C13-C15-C16 |
| 14  | N     | 815 | CLA  | C11-C10-C8-C7   |
| 14  | g     | 827 | CLA  | C6-C7-C8-C10    |
| 14  | g     | 854 | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 818  | CLA  | C11-C10-C8-C7   |
| 14  | B     | 828  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 850  | CLA  | C6-C7-C8-C10    |
| 14  | a     | 809  | CLA  | C11-C12-C13-C15 |
| 18  | g     | 849  | LHG  | C1-C2-C3-O3     |
| 14  | A     | 826  | CLA  | O1D-CGD-O2D-CED |
| 18  | G     | 849  | LHG  | C18-C19-C20-C21 |
| 18  | G     | 849  | LHG  | C26-C27-C28-C29 |
| 14  | X     | 1701 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 818  | CLA  | C16-C17-C18-C19 |
| 14  | G     | 808  | CLA  | CBA-CGA-O2A-C1  |
| 18  | X     | 1702 | LHG  | C9-C10-C11-C12  |
| 14  | n     | 817  | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 831  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 832  | CLA  | C16-C17-C18-C19 |
| 18  | v     | 102  | LHG  | C5-C4-O6-P      |
| 14  | G     | 805  | CLA  | C3-C5-C6-C7     |
| 14  | A     | 824  | CLA  | CBA-CGA-O2A-C1  |
| 14  | b     | 840  | CLA  | CBA-CGA-O2A-C1  |
| 17  | W     | 206  | BCR  | C9-C10-C11-C12  |
| 17  | n     | 851  | BCR  | C15-C16-C17-C18 |
| 18  | v     | 102  | LHG  | C8-C7-O7-C5     |
| 14  | s     | 201  | CLA  | CAA-CBA-CGA-O2A |
| 18  | A     | 851  | LHG  | O8-C23-C24-C25  |
| 19  | G     | 851  | CL0  | CAA-CBA-CGA-O2A |
| 14  | W     | 203  | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 806  | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 834  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 806  | CLA  | C2A-CAA-CBA-CGA |
| 14  | L     | 1503 | CLA  | CBD-CGD-O2D-CED |
| 14  | a     | 835  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 815  | CLA  | O1A-CGA-O2A-C1  |
| 14  | h     | 1701 | CLA  | C2-C1-O2A-CGA   |
| 14  | N     | 811  | CLA  | C4-C3-C5-C6     |
| 14  | h     | 1701 | CLA  | O2A-C1-C2-C3    |
| 14  | N     | 851  | CLA  | CAA-CBA-CGA-O2A |
| 19  | a     | 851  | CL0  | CAA-CBA-CGA-O2A |
| 14  | n     | 802  | CLA  | C2-C3-C5-C6     |
| 21  | B     | 849  | LMG  | C16-C17-C18-C19 |
| 20  | h     | 1702 | SQD  | O6-C44-C45-C46  |
| 14  | n     | 832  | CLA  | C2C-C3C-CAC-CBC |
| 14  | B     | 850  | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 21  | B     | 849  | LMG  | C33-C34-C35-C36 |
| 14  | a     | 804  | CLA  | C3-C5-C6-C7     |
| 17  | Y     | 101  | BCR  | C7-C8-C9-C10    |
| 15  | A     | 842  | PQN  | C15-C16-C17-C18 |
| 14  | G     | 811  | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 816  | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 852  | CLA  | C2A-CAA-CBA-CGA |
| 14  | W     | 204  | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 853  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 854  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 831  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 815  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 819  | CLA  | O1D-CGD-O2D-CED |
| 21  | b     | 849  | LMG  | C22-C23-C24-C25 |
| 21  | N     | 850  | LMG  | C37-C38-C39-C40 |
| 14  | g     | 810  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 804  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 811  | CLA  | C11-C12-C13-C14 |
| 18  | A     | 850  | LHG  | C17-C18-C19-C20 |
| 20  | H     | 1702 | SQD  | C29-C30-C31-C32 |
| 20  | n     | 801  | SQD  | C13-C14-C15-C16 |
| 20  | w     | 202  | SQD  | C7-C8-C9-C10    |
| 18  | G     | 849  | LHG  | C27-C28-C29-C30 |
| 14  | l     | 203  | CLA  | C2C-C3C-CAC-CBC |
| 14  | b     | 826  | CLA  | C8-C10-C11-C12  |
| 18  | v     | 102  | LHG  | O9-C7-O7-C5     |
| 14  | w     | 204  | CLA  | C2C-C3C-CAC-CBC |
| 14  | G     | 839  | CLA  | C6-C7-C8-C9     |
| 14  | g     | 803  | CLA  | C11-C10-C8-C9   |
| 14  | g     | 830  | CLA  | C11-C12-C13-C14 |
| 14  | g     | 832  | CLA  | C11-C12-C13-C14 |
| 14  | g     | 839  | CLA  | C14-C13-C15-C16 |
| 14  | n     | 806  | CLA  | C14-C13-C15-C16 |
| 14  | n     | 818  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 818  | CLA  | C11-C10-C8-C9   |
| 14  | a     | 836  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 812  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 838  | CLA  | CBA-CGA-O2A-C1  |
| 14  | x     | 1701 | CLA  | CBA-CGA-O2A-C1  |
| 14  | G     | 823  | CLA  | C4B-C3B-CAB-CBB |
| 14  | G     | 832  | CLA  | C4B-C3B-CAB-CBB |
| 14  | B     | 818  | CLA  | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 821  | CLA  | C4B-C3B-CAB-CBB |
| 14  | a     | 822  | CLA  | C4B-C3B-CAB-CBB |
| 14  | a     | 837  | CLA  | C4B-C3B-CAB-CBB |
| 14  | N     | 810  | CLA  | C10-C11-C12-C13 |
| 14  | K     | 101  | CLA  | CAA-CBA-CGA-O2A |
| 14  | g     | 826  | CLA  | C5-C6-C7-C8     |
| 21  | N     | 850  | LMG  | C31-C32-C33-C34 |
| 14  | B     | 850  | CLA  | C16-C17-C18-C20 |
| 14  | b     | 833  | CLA  | C16-C17-C18-C19 |
| 14  | g     | 832  | CLA  | CBA-CGA-O2A-C1  |
| 14  | f     | 201  | CLA  | CBA-CGA-O2A-C1  |
| 14  | N     | 806  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 816  | CLA  | C5-C6-C7-C8     |
| 14  | b     | 803  | CLA  | C13-C15-C16-C17 |
| 14  | N     | 840  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 833  | CLA  | C2A-CAA-CBA-CGA |
| 18  | g     | 849  | LHG  | C17-C18-C19-C20 |
| 14  | n     | 827  | CLA  | C2-C3-C5-C6     |
| 18  | S     | 202  | LHG  | O6-C4-C5-O7     |
| 14  | X     | 1701 | CLA  | O2A-C1-C2-C3    |
| 18  | m     | 101  | LHG  | C18-C19-C20-C21 |
| 14  | N     | 822  | CLA  | CAA-CBA-CGA-O2A |
| 18  | A     | 851  | LHG  | C31-C32-C33-C34 |
| 14  | A     | 812  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 838  | CLA  | O1A-CGA-O2A-C1  |
| 14  | b     | 840  | CLA  | O1A-CGA-O2A-C1  |
| 14  | f     | 201  | CLA  | O1A-CGA-O2A-C1  |
| 14  | A     | 808  | CLA  | C5-C6-C7-C8     |
| 20  | H     | 1702 | SQD  | C9-C10-C11-C12  |
| 14  | n     | 810  | CLA  | C11-C12-C13-C15 |
| 14  | a     | 819  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 819  | CLA  | C5-C6-C7-C8     |
| 14  | G     | 832  | CLA  | C6-C7-C8-C10    |
| 14  | N     | 803  | CLA  | C12-C13-C15-C16 |
| 14  | g     | 804  | CLA  | C11-C12-C13-C15 |
| 14  | g     | 807  | CLA  | C11-C10-C8-C7   |
| 14  | g     | 816  | CLA  | C6-C7-C8-C10    |
| 14  | g     | 825  | CLA  | C11-C12-C13-C15 |
| 14  | n     | 803  | CLA  | C11-C12-C13-C15 |
| 14  | n     | 826  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 838  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 839  | CLA  | C6-C7-C8-C10    |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | a     | 817  | CLA  | C11-C10-C8-C7   |
| 14  | N     | 803  | CLA  | C5-C6-C7-C8     |
| 14  | N     | 851  | CLA  | C10-C11-C12-C13 |
| 14  | g     | 832  | CLA  | O1A-CGA-O2A-C1  |
| 21  | N     | 850  | LMG  | C16-C17-C18-C19 |
| 18  | G     | 849  | LHG  | C34-C35-C36-C37 |
| 18  | a     | 849  | LHG  | C12-C13-C14-C15 |
| 14  | G     | 813  | CLA  | CBA-CGA-O2A-C1  |
| 14  | A     | 829  | CLA  | C13-C15-C16-C17 |
| 21  | b     | 849  | LMG  | C38-C39-C40-C41 |
| 14  | B     | 808  | CLA  | C16-C17-C18-C19 |
| 20  | x     | 1702 | SQD  | C15-C16-C17-C18 |
| 14  | n     | 804  | CLA  | C4C-C3C-CAC-CBC |
| 14  | G     | 815  | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 810  | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 831  | CLA  | C3A-C2A-CAA-CBA |
| 14  | U     | 101  | CLA  | C3A-C2A-CAA-CBA |
| 14  | g     | 802  | CLA  | C3A-C2A-CAA-CBA |
| 14  | g     | 830  | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 813  | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 813  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 825  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 831  | CLA  | C3A-C2A-CAA-CBA |
| 14  | n     | 814  | CLA  | CAA-CBA-CGA-O2A |
| 14  | N     | 829  | CLA  | C2-C3-C5-C6     |
| 14  | g     | 836  | CLA  | C2A-CAA-CBA-CGA |
| 14  | x     | 1701 | CLA  | O1A-CGA-O2A-C1  |
| 18  | X     | 1702 | LHG  | C30-C31-C32-C33 |
| 20  | B     | 801  | SQD  | C28-C29-C30-C31 |
| 17  | G     | 848  | BCR  | C11-C10-C9-C34  |
| 17  | G     | 848  | BCR  | C16-C17-C18-C36 |
| 17  | N     | 846  | BCR  | C11-C10-C9-C34  |
| 17  | N     | 846  | BCR  | C20-C21-C22-C37 |
| 17  | S     | 204  | BCR  | C35-C13-C14-C15 |
| 17  | g     | 846  | BCR  | C11-C10-C9-C34  |
| 17  | g     | 846  | BCR  | C20-C21-C22-C37 |
| 17  | g     | 848  | BCR  | C11-C10-C9-C34  |
| 17  | g     | 848  | BCR  | C16-C17-C18-C36 |
| 17  | n     | 843  | BCR  | C11-C10-C9-C34  |
| 17  | n     | 844  | BCR  | C11-C10-C9-C34  |
| 17  | n     | 844  | BCR  | C20-C21-C22-C37 |
| 17  | s     | 203  | BCR  | C35-C13-C14-C15 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | w     | 201  | BCR  | C20-C21-C22-C37 |
| 17  | A     | 849  | BCR  | C11-C10-C9-C34  |
| 17  | A     | 849  | BCR  | C16-C17-C18-C36 |
| 17  | B     | 845  | BCR  | C11-C10-C9-C34  |
| 17  | B     | 845  | BCR  | C20-C21-C22-C37 |
| 17  | F     | 203  | BCR  | C35-C13-C14-C15 |
| 17  | a     | 848  | BCR  | C11-C10-C9-C34  |
| 17  | a     | 848  | BCR  | C16-C17-C18-C36 |
| 17  | b     | 844  | BCR  | C11-C10-C9-C34  |
| 17  | b     | 845  | BCR  | C11-C10-C9-C34  |
| 17  | b     | 845  | BCR  | C20-C21-C22-C37 |
| 17  | f     | 203  | BCR  | C35-C13-C14-C15 |
| 21  | b     | 849  | LMG  | C36-C37-C38-C39 |
| 18  | G     | 850  | LHG  | C30-C31-C32-C33 |
| 14  | G     | 809  | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 815  | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 830  | CLA  | C13-C15-C16-C17 |
| 20  | h     | 1702 | SQD  | C12-C13-C14-C15 |
| 14  | N     | 801  | CLA  | C2-C1-O2A-CGA   |
| 14  | S     | 201  | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 802  | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 831  | CLA  | C13-C15-C16-C17 |
| 14  | n     | 808  | CLA  | C8-C10-C11-C12  |
| 14  | A     | 838  | CLA  | C15-C16-C17-C18 |
| 14  | b     | 810  | CLA  | C15-C16-C17-C18 |
| 17  | w     | 207  | BCR  | C11-C12-C13-C35 |
| 17  | b     | 843  | BCR  | C37-C22-C23-C24 |
| 14  | U     | 101  | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 817  | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 831  | CLA  | C6-C7-C8-C9     |
| 20  | x     | 1702 | SQD  | C14-C15-C16-C17 |
| 14  | N     | 822  | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 839  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 810  | CLA  | C10-C11-C12-C13 |
| 18  | m     | 101  | LHG  | C16-C17-C18-C19 |
| 14  | N     | 815  | CLA  | C4-C3-C5-C6     |
| 14  | N     | 851  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 819  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 824  | CLA  | C4-C3-C5-C6     |
| 14  | b     | 828  | CLA  | C4-C3-C5-C6     |
| 14  | n     | 810  | CLA  | C2-C3-C5-C6     |
| 14  | n     | 837  | CLA  | C2-C3-C5-C6     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | N     | 838  | CLA  | C11-C12-C13-C14 |
| 14  | b     | 808  | CLA  | C8-C10-C11-C12  |
| 14  | G     | 801  | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 840  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 836  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 835  | CLA  | CAA-CBA-CGA-O1A |
| 14  | K     | 101  | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 822  | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 809  | CLA  | C3-C5-C6-C7     |
| 14  | L     | 1503 | CLA  | O1D-CGD-O2D-CED |
| 18  | G     | 850  | LHG  | C10-C11-C12-C13 |
| 14  | G     | 807  | CLA  | C11-C10-C8-C9   |
| 14  | G     | 808  | CLA  | C11-C12-C13-C14 |
| 14  | N     | 803  | CLA  | C14-C13-C15-C16 |
| 14  | N     | 809  | CLA  | C6-C7-C8-C9     |
| 14  | N     | 810  | CLA  | C14-C13-C15-C16 |
| 14  | N     | 812  | CLA  | C11-C10-C8-C9   |
| 14  | N     | 829  | CLA  | C11-C10-C8-C9   |
| 14  | g     | 804  | CLA  | C11-C12-C13-C14 |
| 14  | g     | 807  | CLA  | C14-C13-C15-C16 |
| 14  | g     | 819  | CLA  | C11-C12-C13-C14 |
| 14  | g     | 823  | CLA  | C6-C7-C8-C9     |
| 14  | n     | 809  | CLA  | C14-C13-C15-C16 |
| 14  | n     | 832  | CLA  | C11-C10-C8-C9   |
| 14  | n     | 840  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 840  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 829  | CLA  | C11-C12-C13-C14 |
| 14  | B     | 840  | CLA  | C6-C7-C8-C9     |
| 14  | a     | 803  | CLA  | C11-C12-C13-C14 |
| 14  | a     | 811  | CLA  | C6-C7-C8-C9     |
| 14  | a     | 836  | CLA  | C14-C13-C15-C16 |
| 14  | b     | 806  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 824  | CLA  | C11-C10-C8-C9   |
| 14  | g     | 839  | CLA  | C16-C17-C18-C20 |
| 20  | w     | 202  | SQD  | C12-C13-C14-C15 |
| 14  | G     | 804  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 831  | CLA  | C10-C11-C12-C13 |
| 14  | g     | 803  | CLA  | C10-C11-C12-C13 |
| 14  | b     | 805  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 815  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 826  | CLA  | C2C-C3C-CAC-CBC |
| 14  | A     | 805  | CLA  | C3-C5-C6-C7     |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | a     | 813 | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 811 | CLA  | C4-C3-C5-C6     |
| 18  | G     | 849 | LHG  | C23-C24-C25-C26 |
| 21  | b     | 849 | LMG  | C29-C28-O8-C9   |
| 14  | n     | 827 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 804 | CLA  | C2-C3-C5-C6     |
| 20  | b     | 801 | SQD  | C14-C15-C16-C17 |
| 14  | N     | 820 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 822 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 808 | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 828 | CLA  | C2A-CAA-CBA-CGA |
| 14  | N     | 804 | CLA  | C10-C11-C12-C13 |
| 14  | G     | 839 | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 802 | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 809 | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 817 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 801 | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 812 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 814 | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 830 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 837 | CLA  | C1A-C2A-CAA-CBA |
| 14  | a     | 853 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 837 | CLA  | C1A-C2A-CAA-CBA |
| 14  | b     | 851 | CLA  | C1A-C2A-CAA-CBA |
| 14  | l     | 204 | CLA  | C1A-C2A-CAA-CBA |
| 17  | G     | 848 | BCR  | C11-C10-C9-C8   |
| 17  | G     | 848 | BCR  | C16-C17-C18-C19 |
| 17  | N     | 846 | BCR  | C11-C10-C9-C8   |
| 17  | N     | 846 | BCR  | C20-C21-C22-C23 |
| 17  | S     | 204 | BCR  | C12-C13-C14-C15 |
| 17  | g     | 846 | BCR  | C11-C10-C9-C8   |
| 17  | g     | 846 | BCR  | C20-C21-C22-C23 |
| 17  | g     | 848 | BCR  | C11-C10-C9-C8   |
| 17  | g     | 848 | BCR  | C16-C17-C18-C19 |
| 17  | n     | 843 | BCR  | C11-C10-C9-C8   |
| 17  | n     | 844 | BCR  | C11-C10-C9-C8   |
| 17  | n     | 844 | BCR  | C20-C21-C22-C23 |
| 17  | s     | 203 | BCR  | C12-C13-C14-C15 |
| 17  | w     | 201 | BCR  | C20-C21-C22-C23 |
| 17  | A     | 849 | BCR  | C11-C10-C9-C8   |
| 17  | A     | 849 | BCR  | C16-C17-C18-C19 |
| 17  | B     | 845 | BCR  | C11-C10-C9-C8   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | B     | 845  | BCR  | C20-C21-C22-C23 |
| 17  | F     | 203  | BCR  | C12-C13-C14-C15 |
| 17  | a     | 848  | BCR  | C11-C10-C9-C8   |
| 17  | a     | 848  | BCR  | C16-C17-C18-C19 |
| 17  | b     | 844  | BCR  | C11-C10-C9-C8   |
| 17  | b     | 845  | BCR  | C11-C10-C9-C8   |
| 17  | b     | 845  | BCR  | C20-C21-C22-C23 |
| 17  | f     | 203  | BCR  | C12-C13-C14-C15 |
| 14  | N     | 831  | CLA  | C16-C17-C18-C20 |
| 14  | G     | 809  | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 821  | CLA  | CAA-CBA-CGA-O1A |
| 14  | n     | 816  | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 817  | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 822  | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 810  | CLA  | C13-C15-C16-C17 |
| 20  | n     | 801  | SQD  | C12-C13-C14-C15 |
| 14  | G     | 811  | CLA  | C2B-C3B-CAB-CBB |
| 14  | G     | 816  | CLA  | C2B-C3B-CAB-CBB |
| 14  | G     | 823  | CLA  | C2B-C3B-CAB-CBB |
| 14  | G     | 832  | CLA  | C2B-C3B-CAB-CBB |
| 14  | G     | 840  | CLA  | C2B-C3B-CAB-CBB |
| 14  | H     | 1701 | CLA  | C2B-C3B-CAB-CBB |
| 14  | N     | 801  | CLA  | C2B-C3B-CAB-CBB |
| 14  | N     | 840  | CLA  | C2B-C3B-CAB-CBB |
| 14  | N     | 842  | CLA  | C2B-C3B-CAB-CBB |
| 14  | S     | 201  | CLA  | C2B-C3B-CAB-CBB |
| 14  | W     | 203  | CLA  | C2B-C3B-CAB-CBB |
| 14  | g     | 809  | CLA  | C2B-C3B-CAB-CBB |
| 14  | g     | 837  | CLA  | C2B-C3B-CAB-CBB |
| 14  | g     | 839  | CLA  | C2B-C3B-CAB-CBB |
| 14  | n     | 811  | CLA  | C2B-C3B-CAB-CBB |
| 14  | n     | 840  | CLA  | C2B-C3B-CAB-CBB |
| 14  | w     | 204  | CLA  | C2B-C3B-CAB-CBB |
| 14  | A     | 811  | CLA  | C2B-C3B-CAB-CBB |
| 14  | A     | 817  | CLA  | C2B-C3B-CAB-CBB |
| 14  | A     | 832  | CLA  | C2B-C3B-CAB-CBB |
| 14  | A     | 838  | CLA  | C2B-C3B-CAB-CBB |
| 14  | X     | 1701 | CLA  | C2B-C3B-CAB-CBB |
| 14  | B     | 811  | CLA  | C2B-C3B-CAB-CBB |
| 14  | B     | 818  | CLA  | C2B-C3B-CAB-CBB |
| 14  | B     | 821  | CLA  | C2B-C3B-CAB-CBB |
| 14  | B     | 839  | CLA  | C2B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | a     | 809 | CLA  | C2B-C3B-CAB-CBB |
| 14  | a     | 815 | CLA  | C2B-C3B-CAB-CBB |
| 14  | a     | 816 | CLA  | C2B-C3B-CAB-CBB |
| 14  | a     | 821 | CLA  | C2B-C3B-CAB-CBB |
| 14  | a     | 823 | CLA  | C2B-C3B-CAB-CBB |
| 14  | a     | 832 | CLA  | C2B-C3B-CAB-CBB |
| 14  | a     | 836 | CLA  | C2B-C3B-CAB-CBB |
| 14  | b     | 805 | CLA  | C2B-C3B-CAB-CBB |
| 14  | b     | 812 | CLA  | C2B-C3B-CAB-CBB |
| 14  | b     | 821 | CLA  | C2B-C3B-CAB-CBB |
| 14  | b     | 823 | CLA  | C2B-C3B-CAB-CBB |
| 14  | b     | 841 | CLA  | C2B-C3B-CAB-CBB |
| 14  | f     | 202 | CLA  | C2B-C3B-CAB-CBB |
| 14  | l     | 204 | CLA  | C2B-C3B-CAB-CBB |
| 17  | G     | 846 | BCR  | C23-C24-C25-C26 |
| 17  | G     | 848 | BCR  | C23-C24-C25-C26 |
| 17  | W     | 205 | BCR  | C23-C24-C25-C26 |
| 17  | Y     | 101 | BCR  | C5-C6-C7-C8     |
| 17  | g     | 846 | BCR  | C1-C6-C7-C8     |
| 17  | g     | 848 | BCR  | C23-C24-C25-C30 |
| 17  | n     | 844 | BCR  | C5-C6-C7-C8     |
| 17  | t     | 104 | BCR  | C5-C6-C7-C8     |
| 17  | y     | 101 | BCR  | C5-C6-C7-C8     |
| 17  | B     | 844 | BCR  | C23-C24-C25-C26 |
| 17  | I     | 102 | BCR  | C23-C24-C25-C26 |
| 17  | a     | 848 | BCR  | C23-C24-C25-C30 |
| 17  | b     | 844 | BCR  | C1-C6-C7-C8     |
| 17  | b     | 845 | BCR  | C5-C6-C7-C8     |
| 17  | b     | 850 | BCR  | C1-C6-C7-C8     |
| 17  | j     | 103 | BCR  | C5-C6-C7-C8     |
| 17  | m     | 102 | BCR  | C5-C6-C7-C8     |
| 14  | N     | 837 | CLA  | CAA-CBA-CGA-O1A |
| 14  | U     | 101 | CLA  | CAA-CBA-CGA-O2A |
| 14  | g     | 808 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 821 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 808 | CLA  | CAA-CBA-CGA-O2A |
| 14  | W     | 203 | CLA  | C2C-C3C-CAC-CBC |
| 18  | G     | 850 | LHG  | C9-C10-C11-C12  |
| 18  | G     | 850 | LHG  | C29-C30-C31-C32 |
| 20  | n     | 801 | SQD  | C15-C16-C17-C18 |
| 20  | b     | 801 | SQD  | C26-C27-C28-C29 |
| 14  | A     | 821 | CLA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 819  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 808  | CLA  | C4-C3-C5-C6     |
| 15  | b     | 842  | PQN  | C14-C13-C15-C16 |
| 20  | n     | 801  | SQD  | C14-C15-C16-C17 |
| 14  | N     | 815  | CLA  | C2-C3-C5-C6     |
| 14  | n     | 813  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 825  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 828  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 828  | CLA  | C2-C3-C5-C6     |
| 14  | n     | 817  | CLA  | O1D-CGD-O2D-CED |
| 14  | b     | 841  | CLA  | C2C-C3C-CAC-CBC |
| 14  | x     | 1701 | CLA  | O2A-C1-C2-C3    |
| 14  | a     | 808  | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 820  | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 838  | CLA  | C13-C15-C16-C17 |
| 14  | G     | 804  | CLA  | C6-C7-C8-C10    |
| 14  | N     | 808  | CLA  | C6-C7-C8-C10    |
| 14  | N     | 809  | CLA  | C6-C7-C8-C10    |
| 14  | N     | 826  | CLA  | C6-C7-C8-C10    |
| 14  | N     | 828  | CLA  | C11-C12-C13-C15 |
| 14  | g     | 806  | CLA  | C11-C12-C13-C15 |
| 14  | g     | 819  | CLA  | C11-C12-C13-C15 |
| 14  | g     | 836  | CLA  | C6-C7-C8-C10    |
| 14  | n     | 808  | CLA  | C12-C13-C15-C16 |
| 14  | n     | 818  | CLA  | C11-C12-C13-C15 |
| 14  | A     | 810  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 831  | CLA  | C6-C7-C8-C10    |
| 14  | A     | 839  | CLA  | C11-C12-C13-C15 |
| 14  | B     | 803  | CLA  | C12-C13-C15-C16 |
| 14  | B     | 828  | CLA  | C6-C7-C8-C10    |
| 14  | a     | 811  | CLA  | C6-C7-C8-C10    |
| 14  | a     | 823  | CLA  | C11-C10-C8-C7   |
| 14  | b     | 807  | CLA  | C12-C13-C15-C16 |
| 14  | b     | 820  | CLA  | C11-C10-C8-C7   |
| 14  | b     | 830  | CLA  | C11-C12-C13-C15 |
| 14  | f     | 201  | CLA  | C6-C7-C8-C10    |
| 19  | G     | 851  | CL0  | C11-C10-C8-C7   |
| 14  | n     | 809  | CLA  | CBD-CGD-O2D-CED |
| 14  | N     | 801  | CLA  | C2A-CAA-CBA-CGA |
| 14  | n     | 810  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 801  | CLA  | C2A-CAA-CBA-CGA |
| 18  | A     | 851  | LHG  | C13-C14-C15-C16 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 20  | x     | 1702 | SQD  | C13-C14-C15-C16 |
| 14  | N     | 810  | CLA  | C5-C6-C7-C8     |
| 18  | g     | 849  | LHG  | O7-C5-C6-O8     |
| 20  | n     | 801  | SQD  | O47-C45-C46-O48 |
| 20  | b     | 801  | SQD  | O47-C45-C46-O48 |
| 21  | b     | 849  | LMG  | O7-C8-C9-O8     |
| 14  | G     | 821  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 835  | CLA  | CAA-CBA-CGA-O2A |
| 20  | h     | 1702 | SQD  | C28-C29-C30-C31 |
| 14  | A     | 820  | CLA  | C3-C5-C6-C7     |
| 14  | n     | 816  | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 829  | CLA  | C15-C16-C17-C18 |
| 14  | n     | 852  | CLA  | C6-C7-C8-C10    |
| 14  | a     | 801  | CLA  | C16-C17-C18-C20 |
| 21  | B     | 849  | LMG  | C28-C29-C30-C31 |
| 17  | W     | 206  | BCR  | C36-C18-C19-C20 |
| 17  | g     | 844  | BCR  | C37-C22-C23-C24 |
| 17  | B     | 843  | BCR  | C37-C22-C23-C24 |
| 17  | j     | 104  | BCR  | C36-C18-C19-C20 |
| 17  | l     | 206  | BCR  | C7-C8-C9-C34    |
| 14  | G     | 813  | CLA  | O1A-CGA-O2A-C1  |
| 14  | N     | 805  | CLA  | C4C-C3C-CAC-CBC |
| 14  | a     | 820  | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 826  | CLA  | C4-C3-C5-C6     |
| 14  | G     | 824  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 839  | CLA  | C15-C16-C17-C18 |
| 14  | a     | 830  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 819  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 804  | CLA  | C2-C3-C5-C6     |
| 14  | b     | 810  | CLA  | C2-C3-C5-C6     |
| 18  | g     | 849  | LHG  | C29-C30-C31-C32 |
| 14  | G     | 840  | CLA  | CBD-CGD-O2D-CED |
| 14  | g     | 814  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 814  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 815  | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 828  | CLA  | C16-C17-C18-C20 |
| 18  | g     | 850  | LHG  | C33-C34-C35-C36 |
| 14  | g     | 810  | CLA  | C11-C12-C13-C14 |
| 14  | n     | 852  | CLA  | C5-C6-C7-C8     |
| 14  | g     | 852  | CLA  | C2A-CAA-CBA-CGA |
| 14  | N     | 837  | CLA  | CAA-CBA-CGA-O2A |
| 14  | g     | 808  | CLA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | g     | 813 | CLA  | CAA-CBA-CGA-O2A |
| 14  | f     | 202 | CLA  | CAA-CBA-CGA-O2A |
| 14  | N     | 809 | CLA  | C14-C13-C15-C16 |
| 14  | N     | 851 | CLA  | C11-C10-C8-C9   |
| 14  | n     | 805 | CLA  | C14-C13-C15-C16 |
| 14  | n     | 817 | CLA  | C14-C13-C15-C16 |
| 14  | A     | 807 | CLA  | C5-C6-C7-C8     |
| 21  | N     | 802 | LMG  | O9-C10-O7-C8    |
| 17  | a     | 846 | BCR  | C9-C10-C11-C12  |
| 14  | G     | 828 | CLA  | C5-C6-C7-C8     |
| 14  | a     | 831 | CLA  | C13-C15-C16-C17 |
| 14  | N     | 823 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 813 | CLA  | CAA-CBA-CGA-O2A |
| 14  | k     | 101 | CLA  | CAA-CBA-CGA-O2A |
| 18  | g     | 850 | LHG  | C9-C10-C11-C12  |
| 18  | A     | 850 | LHG  | C27-C28-C29-C30 |
| 14  | b     | 803 | CLA  | C15-C16-C17-C18 |
| 14  | N     | 851 | CLA  | C2C-C3C-CAC-CBC |
| 14  | N     | 812 | CLA  | C4-C3-C5-C6     |
| 14  | W     | 204 | CLA  | CAA-CBA-CGA-O2A |
| 14  | n     | 834 | CLA  | CAA-CBA-CGA-O2A |
| 18  | a     | 849 | LHG  | C2-C3-O3-P      |
| 14  | N     | 851 | CLA  | C2-C3-C5-C6     |
| 14  | N     | 805 | CLA  | O1A-CGA-O2A-C1  |
| 21  | b     | 849 | LMG  | O10-C28-O8-C9   |
| 14  | B     | 809 | CLA  | C13-C15-C16-C17 |
| 14  | n     | 823 | CLA  | C16-C17-C18-C20 |
| 14  | G     | 824 | CLA  | CBA-CGA-O2A-C1  |
| 14  | B     | 804 | CLA  | CAA-CBA-CGA-O2A |
| 21  | N     | 802 | LMG  | C2-C1-O1-C7     |
| 14  | G     | 838 | CLA  | C10-C11-C12-C13 |
| 14  | N     | 819 | CLA  | C15-C16-C17-C18 |
| 14  | B     | 808 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 811 | CLA  | CAA-CBA-CGA-O2A |
| 20  | l     | 201 | SQD  | C19-C20-C21-C22 |
| 14  | l     | 204 | CLA  | CAA-CBA-CGA-O2A |
| 20  | b     | 801 | SQD  | C17-C18-C19-C20 |
| 14  | G     | 824 | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 837 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 803 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 836 | CLA  | C5-C6-C7-C8     |
| 14  | n     | 809 | CLA  | O1D-CGD-O2D-CED |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 21  | b     | 849 | LMG  | C11-C12-C13-C14 |
| 14  | B     | 821 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 852 | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 817 | CLA  | O1D-CGD-O2D-CED |
| 21  | b     | 849 | LMG  | C24-C25-C26-C27 |
| 14  | N     | 825 | CLA  | C4-C3-C5-C6     |
| 14  | A     | 807 | CLA  | C4-C3-C5-C6     |
| 14  | a     | 814 | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 810 | CLA  | CAA-CBA-CGA-O2A |
| 14  | n     | 833 | CLA  | C5-C6-C7-C8     |
| 18  | g     | 849 | LHG  | C25-C26-C27-C28 |
| 18  | a     | 850 | LHG  | C12-C13-C14-C15 |
| 14  | G     | 830 | CLA  | C4B-C3B-CAB-CBB |
| 14  | n     | 811 | CLA  | C4B-C3B-CAB-CBB |
| 14  | A     | 817 | CLA  | C4B-C3B-CAB-CBB |
| 14  | A     | 828 | CLA  | C4B-C3B-CAB-CBB |
| 14  | A     | 832 | CLA  | C4B-C3B-CAB-CBB |
| 14  | A     | 837 | CLA  | C4B-C3B-CAB-CBB |
| 14  | a     | 806 | CLA  | C4B-C3B-CAB-CBB |
| 18  | G     | 850 | LHG  | C26-C27-C28-C29 |
| 14  | b     | 810 | CLA  | C5-C6-C7-C8     |
| 14  | G     | 835 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 822 | CLA  | CAA-CBA-CGA-O2A |
| 14  | N     | 831 | CLA  | C16-C17-C18-C19 |
| 14  | B     | 850 | CLA  | C16-C17-C18-C19 |
| 14  | a     | 804 | CLA  | C16-C17-C18-C19 |
| 14  | F     | 201 | CLA  | C11-C12-C13-C14 |
| 14  | G     | 840 | CLA  | O1D-CGD-O2D-CED |
| 18  | m     | 101 | LHG  | C1-C2-C3-O3     |
| 18  | g     | 849 | LHG  | C30-C31-C32-C33 |
| 14  | a     | 810 | CLA  | C11-C12-C13-C14 |
| 14  | B     | 805 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 811 | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 814 | CLA  | CAA-CBA-CGA-O1A |
| 14  | n     | 820 | CLA  | CAA-CBA-CGA-O2A |
| 14  | n     | 835 | CLA  | CAA-CBA-CGA-O2A |
| 14  | s     | 202 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 814 | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 815 | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 817 | CLA  | CBD-CGD-O2D-CED |
| 14  | A     | 802 | CLA  | C16-C17-C18-C19 |
| 14  | A     | 839 | CLA  | C16-C17-C18-C20 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | b     | 826  | CLA  | C4-C3-C5-C6     |
| 15  | N     | 843  | PQN  | C14-C13-C15-C16 |
| 21  | N     | 802  | LMG  | O1-C7-C8-O7     |
| 14  | G     | 832  | CLA  | C15-C16-C17-C18 |
| 14  | N     | 815  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 818  | CLA  | C15-C16-C17-C18 |
| 14  | g     | 813  | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 809  | CLA  | CAA-CBA-CGA-O2A |
| 14  | f     | 202  | CLA  | CAA-CBA-CGA-O1A |
| 14  | k     | 101  | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 826  | CLA  | C2-C3-C5-C6     |
| 14  | n     | 832  | CLA  | C11-C10-C8-C7   |
| 14  | G     | 814  | CLA  | CAA-CBA-CGA-O2A |
| 14  | N     | 839  | CLA  | C10-C11-C12-C13 |
| 14  | n     | 824  | CLA  | C5-C6-C7-C8     |
| 14  | N     | 817  | CLA  | O2A-C1-C2-C3    |
| 17  | B     | 843  | BCR  | C19-C20-C21-C22 |
| 18  | m     | 101  | LHG  | C11-C12-C13-C14 |
| 20  | x     | 1702 | SQD  | C28-C29-C30-C31 |
| 14  | N     | 851  | CLA  | C3-C5-C6-C7     |
| 14  | B     | 823  | CLA  | C3-C5-C6-C7     |
| 14  | N     | 823  | CLA  | CAA-CBA-CGA-O1A |
| 14  | T     | 101  | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 810  | CLA  | C6-C7-C8-C9     |
| 14  | G     | 837  | CLA  | C14-C13-C15-C16 |
| 14  | N     | 805  | CLA  | C11-C12-C13-C14 |
| 14  | N     | 826  | CLA  | C11-C10-C8-C9   |
| 14  | g     | 819  | CLA  | C11-C10-C8-C9   |
| 14  | g     | 827  | CLA  | C11-C12-C13-C14 |
| 14  | n     | 817  | CLA  | C11-C12-C13-C14 |
| 14  | n     | 827  | CLA  | C6-C7-C8-C9     |
| 14  | w     | 204  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 833  | CLA  | C11-C12-C13-C14 |
| 14  | A     | 837  | CLA  | C14-C13-C15-C16 |
| 14  | B     | 807  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 827  | CLA  | C6-C7-C8-C9     |
| 14  | b     | 810  | CLA  | C11-C12-C13-C14 |
| 15  | A     | 842  | PQN  | C16-C17-C18-C19 |
| 14  | g     | 837  | CLA  | C10-C11-C12-C13 |
| 18  | a     | 849  | LHG  | C29-C30-C31-C32 |
| 20  | x     | 1702 | SQD  | C19-C20-C21-C22 |
| 14  | B     | 817  | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | B     | 821 | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 820 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 804 | CLA  | C2A-CAA-CBA-CGA |
| 14  | N     | 807 | CLA  | C2-C1-O2A-CGA   |
| 14  | N     | 828 | CLA  | C2-C1-O2A-CGA   |
| 14  | n     | 802 | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 827 | CLA  | C2-C1-O2A-CGA   |
| 14  | a     | 809 | CLA  | C16-C17-C18-C20 |
| 18  | S     | 202 | LHG  | C34-C35-C36-C37 |
| 14  | G     | 828 | CLA  | C3A-C2A-CAA-CBA |
| 14  | G     | 832 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 835 | CLA  | C3A-C2A-CAA-CBA |
| 14  | N     | 805 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 801 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 839 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 814 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 830 | CLA  | C3A-C2A-CAA-CBA |
| 14  | a     | 853 | CLA  | C3A-C2A-CAA-CBA |
| 14  | S     | 203 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 822 | CLA  | CAA-CBA-CGA-O1A |
| 14  | l     | 204 | CLA  | CAA-CBA-CGA-O1A |
| 14  | g     | 821 | CLA  | C2-C3-C5-C6     |
| 14  | B     | 826 | CLA  | C4C-C3C-CAC-CBC |
| 18  | A     | 850 | LHG  | C29-C30-C31-C32 |
| 21  | N     | 802 | LMG  | C28-C29-C30-C31 |
| 14  | n     | 802 | CLA  | C3-C5-C6-C7     |
| 14  | g     | 820 | CLA  | CAA-CBA-CGA-O2A |
| 14  | F     | 202 | CLA  | CAA-CBA-CGA-O2A |
| 14  | N     | 805 | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 803 | CLA  | O2A-C1-C2-C3    |
| 14  | u     | 101 | CLA  | CAA-CBA-CGA-O2A |
| 21  | n     | 848 | LMG  | C23-C24-C25-C26 |
| 14  | A     | 839 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 806 | CLA  | CAA-CBA-CGA-O2A |
| 14  | W     | 204 | CLA  | CAA-CBA-CGA-O1A |
| 14  | n     | 820 | CLA  | CAA-CBA-CGA-O1A |
| 14  | n     | 834 | CLA  | CAA-CBA-CGA-O1A |
| 14  | n     | 835 | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 804 | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 814 | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 824 | CLA  | C8-C10-C11-C12  |
| 14  | A     | 803 | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | B     | 831 | CLA  | C4-C3-C5-C6     |
| 14  | G     | 814 | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 822 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 824 | CLA  | CBA-CGA-O2A-C1  |
| 21  | B     | 849 | LMG  | C21-C22-C23-C24 |
| 14  | A     | 838 | CLA  | C13-C15-C16-C17 |
| 14  | b     | 830 | CLA  | C10-C11-C12-C13 |
| 14  | G     | 835 | CLA  | CAA-CBA-CGA-O1A |
| 14  | S     | 203 | CLA  | CAA-CBA-CGA-O1A |
| 14  | g     | 820 | CLA  | CAA-CBA-CGA-O1A |
| 18  | G     | 850 | LHG  | C25-C26-C27-C28 |
| 14  | a     | 824 | CLA  | O1A-CGA-O2A-C1  |
| 14  | n     | 826 | CLA  | O1D-CGD-O2D-CED |
| 21  | B     | 802 | LMG  | O6-C5-C6-O5     |
| 14  | N     | 811 | CLA  | C5-C6-C7-C8     |
| 14  | b     | 804 | CLA  | C13-C15-C16-C17 |
| 14  | A     | 855 | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 855 | CLA  | CAA-CBA-CGA-O2A |
| 21  | B     | 802 | LMG  | O1-C7-C8-C9     |
| 14  | n     | 808 | CLA  | C16-C17-C18-C19 |
| 14  | b     | 835 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 837 | CLA  | C4-C3-C5-C6     |
| 14  | N     | 816 | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 804 | CLA  | C4C-C3C-CAC-CBC |
| 14  | u     | 101 | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 817 | CLA  | CAA-CBA-CGA-O1A |
| 17  | I     | 102 | BCR  | C15-C16-C17-C18 |
| 21  | n     | 848 | LMG  | C32-C33-C34-C35 |
| 14  | b     | 828 | CLA  | C16-C17-C18-C19 |
| 18  | a     | 850 | LHG  | C14-C15-C16-C17 |
| 20  | l     | 201 | SQD  | C9-C10-C11-C12  |
| 14  | G     | 812 | CLA  | C10-C11-C12-C13 |
| 14  | A     | 805 | CLA  | C10-C11-C12-C13 |
| 14  | a     | 809 | CLA  | C13-C15-C16-C17 |
| 14  | A     | 809 | CLA  | CAA-CBA-CGA-O1A |
| 14  | F     | 202 | CLA  | CAA-CBA-CGA-O1A |
| 14  | g     | 802 | CLA  | C6-C7-C8-C9     |
| 21  | b     | 849 | LMG  | C42-C43-C44-C45 |
| 14  | A     | 830 | CLA  | O1A-CGA-O2A-C1  |
| 18  | g     | 850 | LHG  | C31-C32-C33-C34 |
| 14  | a     | 827 | CLA  | CAA-CBA-CGA-O2A |
| 18  | g     | 849 | LHG  | O7-C7-C8-C9     |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 813  | CLA  | C6-C7-C8-C9     |
| 18  | g     | 849  | LHG  | C9-C10-C11-C12  |
| 14  | n     | 826  | CLA  | CBD-CGD-O2D-CED |
| 14  | B     | 836  | CLA  | CAA-CBA-CGA-O2A |
| 14  | N     | 808  | CLA  | C6-C7-C8-C9     |
| 14  | N     | 808  | CLA  | C14-C13-C15-C16 |
| 14  | N     | 830  | CLA  | C11-C10-C8-C9   |
| 14  | A     | 833  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 814  | CLA  | C11-C10-C8-C9   |
| 14  | B     | 819  | CLA  | C6-C7-C8-C9     |
| 14  | a     | 832  | CLA  | C11-C12-C13-C14 |
| 14  | b     | 824  | CLA  | C11-C12-C13-C14 |
| 15  | G     | 841  | PQN  | C24-C23-C25-C26 |
| 14  | A     | 818  | CLA  | C16-C17-C18-C19 |
| 18  | A     | 851  | LHG  | C19-C20-C21-C22 |
| 14  | N     | 811  | CLA  | CAA-CBA-CGA-O2A |
| 14  | n     | 833  | CLA  | CAA-CBA-CGA-O2A |
| 14  | u     | 102  | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 834  | CLA  | CAA-CBA-CGA-O2A |
| 18  | S     | 202  | LHG  | O7-C7-C8-C9     |
| 18  | g     | 850  | LHG  | O8-C23-C24-C25  |
| 18  | a     | 849  | LHG  | O8-C23-C24-C25  |
| 18  | S     | 202  | LHG  | O6-C4-C5-C6     |
| 21  | B     | 849  | LMG  | C41-C42-C43-C44 |
| 20  | x     | 1702 | SQD  | C24-C25-C26-C27 |
| 18  | m     | 101  | LHG  | C10-C11-C12-C13 |
| 14  | b     | 818  | CLA  | CAA-CBA-CGA-O2A |
| 18  | g     | 849  | LHG  | O8-C23-C24-C25  |
| 14  | N     | 825  | CLA  | C16-C17-C18-C19 |
| 14  | A     | 824  | CLA  | C16-C17-C18-C20 |
| 14  | N     | 811  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 819  | CLA  | C2-C3-C5-C6     |
| 14  | s     | 202  | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 835  | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 830  | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 821  | CLA  | C2A-CAA-CBA-CGA |
| 14  | k     | 101  | CLA  | C2A-CAA-CBA-CGA |
| 14  | G     | 805  | CLA  | C11-C10-C8-C7   |
| 14  | G     | 808  | CLA  | C6-C7-C8-C10    |
| 14  | G     | 808  | CLA  | C11-C12-C13-C15 |
| 14  | G     | 853  | CLA  | C11-C12-C13-C15 |
| 14  | N     | 809  | CLA  | C12-C13-C15-C16 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | N     | 810 | CLA  | C6-C7-C8-C10    |
| 14  | N     | 826 | CLA  | C11-C10-C8-C7   |
| 14  | N     | 851 | CLA  | C11-C10-C8-C7   |
| 14  | g     | 803 | CLA  | C6-C7-C8-C10    |
| 14  | g     | 826 | CLA  | C6-C7-C8-C10    |
| 14  | g     | 854 | CLA  | C11-C10-C8-C7   |
| 14  | n     | 806 | CLA  | C11-C10-C8-C7   |
| 14  | n     | 817 | CLA  | C12-C13-C15-C16 |
| 14  | n     | 819 | CLA  | C11-C10-C8-C7   |
| 14  | n     | 827 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 805 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 807 | CLA  | C6-C7-C8-C10    |
| 14  | A     | 807 | CLA  | C11-C12-C13-C15 |
| 14  | A     | 831 | CLA  | C12-C13-C15-C16 |
| 14  | B     | 824 | CLA  | C11-C10-C8-C7   |
| 14  | a     | 836 | CLA  | C12-C13-C15-C16 |
| 14  | b     | 805 | CLA  | C12-C13-C15-C16 |
| 14  | b     | 809 | CLA  | C12-C13-C15-C16 |
| 14  | b     | 814 | CLA  | C11-C12-C13-C15 |
| 14  | B     | 833 | CLA  | C3-C5-C6-C7     |
| 14  | G     | 823 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 830 | CLA  | C2B-C3B-CAB-CBB |
| 14  | N     | 834 | CLA  | C2B-C3B-CAB-CBB |
| 14  | g     | 807 | CLA  | C2B-C3B-CAB-CBB |
| 14  | g     | 852 | CLA  | C2B-C3B-CAB-CBB |
| 14  | n     | 830 | CLA  | C2B-C3B-CAB-CBB |
| 14  | A     | 840 | CLA  | C2B-C3B-CAB-CBB |
| 14  | a     | 801 | CLA  | C2B-C3B-CAB-CBB |
| 14  | a     | 806 | CLA  | C2B-C3B-CAB-CBB |
| 14  | a     | 822 | CLA  | C2B-C3B-CAB-CBB |
| 14  | a     | 824 | CLA  | C2B-C3B-CAB-CBB |
| 14  | j     | 102 | CLA  | C2B-C3B-CAB-CBB |
| 17  | g     | 846 | BCR  | C5-C6-C7-C8     |
| 17  | g     | 848 | BCR  | C23-C24-C25-C26 |
| 17  | n     | 843 | BCR  | C5-C6-C7-C8     |
| 17  | n     | 843 | BCR  | C23-C24-C25-C30 |
| 17  | n     | 851 | BCR  | C23-C24-C25-C30 |
| 17  | A     | 849 | BCR  | C23-C24-C25-C26 |
| 17  | A     | 849 | BCR  | C23-C24-C25-C30 |
| 17  | B     | 843 | BCR  | C1-C6-C7-C8     |
| 17  | B     | 843 | BCR  | C5-C6-C7-C8     |
| 17  | I     | 101 | BCR  | C23-C24-C25-C26 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 17  | I     | 101 | BCR  | C23-C24-C25-C30 |
| 17  | a     | 848 | BCR  | C23-C24-C25-C26 |
| 17  | b     | 843 | BCR  | C23-C24-C25-C30 |
| 17  | b     | 844 | BCR  | C5-C6-C7-C8     |
| 17  | b     | 844 | BCR  | C23-C24-C25-C30 |
| 17  | b     | 850 | BCR  | C5-C6-C7-C8     |
| 18  | v     | 102 | LHG  | C27-C28-C29-C30 |
| 21  | N     | 802 | LMG  | C11-C10-O7-C8   |
| 14  | g     | 806 | CLA  | CAA-CBA-CGA-O2A |
| 18  | G     | 849 | LHG  | C25-C26-C27-C28 |
| 14  | G     | 812 | CLA  | C2-C1-O2A-CGA   |
| 14  | G     | 825 | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 804 | CLA  | C2-C1-O2A-CGA   |
| 14  | b     | 833 | CLA  | CAA-CBA-CGA-O1A |
| 20  | b     | 801 | SQD  | C32-C33-C34-C35 |
| 14  | B     | 836 | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 814 | CLA  | C5-C6-C7-C8     |
| 14  | G     | 826 | CLA  | CAA-CBA-CGA-O2A |
| 14  | T     | 101 | CLA  | CAA-CBA-CGA-O1A |
| 14  | n     | 817 | CLA  | C3-C5-C6-C7     |
| 14  | A     | 808 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 841 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 821 | CLA  | CAA-CBA-CGA-O2A |
| 14  | G     | 832 | CLA  | C2-C3-C5-C6     |
| 14  | A     | 831 | CLA  | C2-C3-C5-C6     |
| 14  | b     | 826 | CLA  | C2-C3-C5-C6     |
| 14  | G     | 832 | CLA  | C2A-CAA-CBA-CGA |
| 14  | N     | 807 | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 826 | CLA  | C13-C15-C16-C17 |
| 14  | N     | 818 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 835 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 852 | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 836 | CLA  | CAA-CBA-CGA-O2A |
| 14  | g     | 827 | CLA  | O1A-CGA-O2A-C1  |
| 14  | N     | 819 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 806 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 854 | CLA  | CAA-CBA-CGA-O2A |
| 14  | n     | 823 | CLA  | C16-C17-C18-C19 |
| 14  | G     | 818 | CLA  | C5-C6-C7-C8     |
| 14  | a     | 801 | CLA  | C8-C10-C11-C12  |
| 21  | b     | 849 | LMG  | C41-C42-C43-C44 |
| 14  | g     | 838 | CLA  | CAA-CBA-CGA-O2A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | A     | 819  | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 810  | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 824  | CLA  | CAA-CBA-CGA-O2A |
| 14  | g     | 812  | CLA  | O1A-CGA-O2A-C1  |
| 20  | w     | 202  | SQD  | C4-C5-C6-S      |
| 14  | G     | 834  | CLA  | C6-C7-C8-C9     |
| 18  | v     | 102  | LHG  | C17-C18-C19-C20 |
| 14  | N     | 814  | CLA  | C2C-C3C-CAC-CBC |
| 14  | A     | 820  | CLA  | C4-C3-C5-C6     |
| 21  | n     | 848  | LMG  | C13-C14-C15-C16 |
| 14  | G     | 807  | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 811  | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 811  | CLA  | CAA-CBA-CGA-O2A |
| 14  | N     | 839  | CLA  | C2-C3-C5-C6     |
| 14  | g     | 810  | CLA  | C2-C3-C5-C6     |
| 14  | A     | 811  | CLA  | C2-C3-C5-C6     |
| 14  | a     | 831  | CLA  | C2-C3-C5-C6     |
| 14  | g     | 812  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 822  | CLA  | CAA-CBA-CGA-O1A |
| 14  | g     | 832  | CLA  | C5-C6-C7-C8     |
| 20  | h     | 1702 | SQD  | C34-C35-C36-C37 |
| 14  | n     | 816  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 805  | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 815  | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 824  | CLA  | CAA-CBA-CGA-O2A |
| 21  | N     | 850  | LMG  | C24-C25-C26-C27 |
| 14  | b     | 814  | CLA  | CAA-CBA-CGA-O1A |
| 18  | v     | 102  | LHG  | C19-C20-C21-C22 |
| 14  | G     | 804  | CLA  | C11-C12-C13-C14 |
| 14  | G     | 826  | CLA  | C11-C10-C8-C9   |
| 14  | G     | 827  | CLA  | C11-C10-C8-C9   |
| 14  | N     | 830  | CLA  | C11-C12-C13-C14 |
| 14  | g     | 837  | CLA  | C11-C12-C13-C14 |
| 14  | n     | 804  | CLA  | C14-C13-C15-C16 |
| 14  | A     | 810  | CLA  | C6-C7-C8-C9     |
| 14  | A     | 820  | CLA  | C6-C7-C8-C9     |
| 14  | B     | 826  | CLA  | C14-C13-C15-C16 |
| 14  | b     | 819  | CLA  | C11-C10-C8-C9   |
| 19  | G     | 851  | CL0  | C11-C10-C8-C9   |
| 14  | g     | 830  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 807  | CLA  | C8-C10-C11-C12  |
| 17  | N     | 847  | BCR  | C37-C22-C23-C24 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | w     | 207  | BCR  | C7-C8-C9-C34    |
| 14  | B     | 818  | CLA  | CAA-CBA-CGA-O2A |
| 18  | A     | 850  | LHG  | O8-C23-C24-C25  |
| 20  | B     | 801  | SQD  | O6-C44-C45-C46  |
| 20  | x     | 1702 | SQD  | O6-C44-C45-C46  |
| 21  | N     | 802  | LMG  | O1-C7-C8-C9     |
| 18  | m     | 101  | LHG  | C29-C30-C31-C32 |
| 14  | G     | 810  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 817  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 825  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 831  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 833  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 835  | CLA  | C1A-C2A-CAA-CBA |
| 14  | G     | 838  | CLA  | C4B-C3B-CAB-CBB |
| 14  | N     | 805  | CLA  | C1A-C2A-CAA-CBA |
| 14  | N     | 814  | CLA  | C4B-C3B-CAB-CBB |
| 14  | U     | 101  | CLA  | C1A-C2A-CAA-CBA |
| 14  | g     | 815  | CLA  | C4B-C3B-CAB-CBB |
| 14  | n     | 826  | CLA  | C1A-C2A-CAA-CBA |
| 14  | n     | 829  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 804  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 831  | CLA  | C1A-C2A-CAA-CBA |
| 14  | A     | 840  | CLA  | C4B-C3B-CAB-CBB |
| 14  | B     | 813  | CLA  | C4B-C3B-CAB-CBB |
| 14  | B     | 827  | CLA  | C1A-C2A-CAA-CBA |
| 14  | B     | 841  | CLA  | C4B-C3B-CAB-CBB |
| 14  | b     | 811  | CLA  | C4B-C3B-CAB-CBB |
| 14  | f     | 201  | CLA  | C1A-C2A-CAA-CBA |
| 14  | j     | 102  | CLA  | C4B-C3B-CAB-CBB |
| 19  | A     | 852  | CL0  | CAA-CBA-CGA-O2A |
| 14  | a     | 833  | CLA  | C6-C7-C8-C9     |
| 14  | a     | 819  | CLA  | C4-C3-C5-C6     |
| 14  | a     | 831  | CLA  | C4-C3-C5-C6     |
| 14  | b     | 840  | CLA  | C4-C3-C5-C6     |
| 14  | A     | 829  | CLA  | C10-C11-C12-C13 |
| 14  | N     | 842  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 840  | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 839  | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 807  | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 823  | CLA  | CAA-CBA-CGA-O2A |
| 17  | N     | 847  | BCR  | C21-C22-C23-C24 |
| 17  | W     | 206  | BCR  | C17-C18-C19-C20 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 17  | y     | 101  | BCR  | C17-C18-C19-C20 |
| 17  | A     | 856  | BCR  | C11-C12-C13-C14 |
| 17  | A     | 856  | BCR  | C21-C22-C23-C24 |
| 17  | B     | 843  | BCR  | C21-C22-C23-C24 |
| 17  | b     | 843  | BCR  | C21-C22-C23-C24 |
| 17  | j     | 104  | BCR  | C17-C18-C19-C20 |
| 17  | l     | 206  | BCR  | C7-C8-C9-C10    |
| 17  | l     | 206  | BCR  | C11-C12-C13-C14 |
| 17  | T     | 104  | BCR  | C13-C14-C15-C16 |
| 17  | a     | 846  | BCR  | C15-C16-C17-C18 |
| 14  | n     | 819  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 853  | CLA  | C15-C16-C17-C18 |
| 14  | N     | 828  | CLA  | C16-C17-C18-C20 |
| 14  | g     | 831  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 828  | CLA  | C16-C17-C18-C19 |
| 14  | g     | 827  | CLA  | CBA-CGA-O2A-C1  |
| 14  | a     | 827  | CLA  | CBA-CGA-O2A-C1  |
| 14  | g     | 807  | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 814  | CLA  | CAA-CBA-CGA-O2A |
| 14  | H     | 1701 | CLA  | C2A-CAA-CBA-CGA |
| 14  | n     | 818  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 826  | CLA  | C2A-CAA-CBA-CGA |
| 14  | b     | 822  | CLA  | C2A-CAA-CBA-CGA |
| 14  | g     | 825  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 837  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 833  | CLA  | C16-C17-C18-C20 |
| 14  | a     | 823  | CLA  | C15-C16-C17-C18 |
| 14  | A     | 836  | CLA  | C2-C3-C5-C6     |
| 14  | G     | 824  | CLA  | C13-C15-C16-C17 |
| 14  | G     | 838  | CLA  | C8-C10-C11-C12  |
| 14  | N     | 839  | CLA  | C4-C3-C5-C6     |
| 14  | n     | 832  | CLA  | CAA-CBA-CGA-O1A |
| 20  | H     | 1702 | SQD  | C26-C27-C28-C29 |
| 14  | G     | 808  | CLA  | C2-C1-O2A-CGA   |
| 14  | g     | 810  | CLA  | C2-C1-O2A-CGA   |
| 14  | g     | 837  | CLA  | C2-C1-O2A-CGA   |
| 14  | s     | 201  | CLA  | C2-C1-O2A-CGA   |
| 14  | A     | 806  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 816  | CLA  | C2-C1-O2A-CGA   |
| 14  | B     | 819  | CLA  | C2-C1-O2A-CGA   |
| 19  | G     | 851  | CL0  | C2-C1-O2A-CGA   |
| 14  | G     | 804  | CLA  | C11-C10-C8-C7   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | N     | 801  | CLA  | C12-C13-C15-C16 |
| 14  | N     | 810  | CLA  | C11-C10-C8-C7   |
| 14  | N     | 821  | CLA  | C11-C10-C8-C7   |
| 14  | N     | 830  | CLA  | C11-C10-C8-C7   |
| 14  | S     | 201  | CLA  | C6-C7-C8-C10    |
| 14  | g     | 805  | CLA  | C6-C7-C8-C10    |
| 14  | g     | 823  | CLA  | C11-C10-C8-C7   |
| 14  | g     | 826  | CLA  | C11-C12-C13-C15 |
| 14  | n     | 827  | CLA  | C12-C13-C15-C16 |
| 14  | A     | 829  | CLA  | C11-C10-C8-C7   |
| 14  | A     | 837  | CLA  | C12-C13-C15-C16 |
| 14  | B     | 811  | CLA  | C6-C7-C8-C10    |
| 14  | B     | 814  | CLA  | C12-C13-C15-C16 |
| 14  | L     | 1502 | CLA  | C11-C10-C8-C7   |
| 14  | a     | 809  | CLA  | C11-C10-C8-C7   |
| 14  | a     | 826  | CLA  | C11-C12-C13-C15 |
| 14  | b     | 803  | CLA  | C6-C7-C8-C10    |
| 14  | g     | 837  | CLA  | C2-C3-C5-C6     |
| 14  | n     | 803  | CLA  | C5-C6-C7-C8     |
| 14  | A     | 802  | CLA  | C5-C6-C7-C8     |
| 14  | B     | 820  | CLA  | C8-C10-C11-C12  |
| 14  | a     | 809  | CLA  | C16-C17-C18-C19 |
| 20  | x     | 1702 | SQD  | C31-C32-C33-C34 |
| 18  | a     | 849  | LHG  | O10-C23-C24-C25 |
| 14  | b     | 841  | CLA  | C4C-C3C-CAC-CBC |
| 14  | a     | 827  | CLA  | O1A-CGA-O2A-C1  |
| 14  | G     | 852  | CLA  | CAA-CBA-CGA-O2A |
| 14  | n     | 806  | CLA  | CAA-CBA-CGA-O2A |
| 18  | X     | 1702 | LHG  | O8-C23-C24-C25  |
| 14  | g     | 816  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 818  | CLA  | C13-C15-C16-C17 |
| 14  | b     | 808  | CLA  | C10-C11-C12-C13 |
| 14  | b     | 811  | CLA  | C10-C11-C12-C13 |
| 14  | G     | 822  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 817  | CLA  | C2A-CAA-CBA-CGA |
| 14  | B     | 813  | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 825  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 826  | CLA  | C16-C17-C18-C20 |
| 20  | l     | 201  | SQD  | C14-C15-C16-C17 |
| 14  | G     | 823  | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 834  | CLA  | CAA-CBA-CGA-O1A |
| 14  | N     | 801  | CLA  | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | l     | 203 | CLA  | C5-C6-C7-C8     |
| 14  | N     | 825 | CLA  | CAA-CBA-CGA-O2A |
| 18  | S     | 202 | LHG  | O9-C7-C8-C9     |
| 14  | G     | 832 | CLA  | C13-C15-C16-C17 |
| 14  | g     | 823 | CLA  | C10-C11-C12-C13 |
| 14  | N     | 818 | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 804 | CLA  | C3A-C2A-CAA-CBA |
| 14  | A     | 812 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 817 | CLA  | C3A-C2A-CAA-CBA |
| 14  | b     | 837 | CLA  | C3A-C2A-CAA-CBA |
| 14  | B     | 810 | CLA  | CAA-CBA-CGA-O1A |
| 14  | n     | 825 | CLA  | C15-C16-C17-C18 |
| 14  | g     | 807 | CLA  | C16-C17-C18-C20 |
| 14  | A     | 812 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 824 | CLA  | C2-C3-C5-C6     |
| 21  | N     | 850 | LMG  | C36-C37-C38-C39 |
| 14  | B     | 835 | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 824 | CLA  | C15-C16-C17-C18 |
| 14  | g     | 837 | CLA  | C3-C5-C6-C7     |
| 14  | g     | 806 | CLA  | CAA-CBA-CGA-O1A |
| 14  | g     | 838 | CLA  | CAA-CBA-CGA-O1A |
| 18  | g     | 850 | LHG  | O10-C23-C24-C25 |
| 18  | A     | 850 | LHG  | O10-C23-C24-C25 |
| 14  | b     | 836 | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 807 | CLA  | CAA-CBA-CGA-O1A |
| 14  | u     | 102 | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 805 | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 834 | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 806 | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 815 | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 838 | CLA  | C2A-CAA-CBA-CGA |
| 14  | a     | 810 | CLA  | C2C-C3C-CAC-CBC |
| 14  | G     | 808 | CLA  | C11-C10-C8-C9   |
| 14  | N     | 826 | CLA  | C6-C7-C8-C9     |
| 14  | g     | 836 | CLA  | C6-C7-C8-C9     |
| 14  | g     | 837 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 805 | CLA  | C6-C7-C8-C9     |
| 14  | A     | 829 | CLA  | C11-C10-C8-C9   |
| 14  | B     | 818 | CLA  | C14-C13-C15-C16 |
| 14  | b     | 820 | CLA  | C11-C10-C8-C9   |
| 14  | a     | 836 | CLA  | CAA-CBA-CGA-O2A |
| 14  | N     | 819 | CLA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | B     | 818  | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 827  | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 826  | CLA  | C8-C10-C11-C12  |
| 21  | B     | 802  | LMG  | C30-C31-C32-C33 |
| 14  | n     | 807  | CLA  | C16-C17-C18-C20 |
| 14  | g     | 836  | CLA  | C5-C6-C7-C8     |
| 14  | a     | 825  | CLA  | C8-C10-C11-C12  |
| 14  | g     | 837  | CLA  | C4-C3-C5-C6     |
| 14  | B     | 841  | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 821  | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 854  | CLA  | CAA-CBA-CGA-O1A |
| 18  | g     | 849  | LHG  | O9-C7-C8-C9     |
| 14  | A     | 825  | CLA  | C6-C7-C8-C9     |
| 14  | g     | 815  | CLA  | C11-C12-C13-C14 |
| 14  | N     | 821  | CLA  | C8-C10-C11-C12  |
| 14  | g     | 825  | CLA  | C8-C10-C11-C12  |
| 14  | L     | 1501 | CLA  | C4-C3-C5-C6     |
| 14  | N     | 804  | CLA  | C4C-C3C-CAC-CBC |
| 14  | j     | 101  | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 807  | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 818  | CLA  | CAA-CBA-CGA-O1A |
| 14  | G     | 837  | CLA  | C5-C6-C7-C8     |
| 14  | n     | 811  | CLA  | C6-C7-C8-C9     |
| 14  | w     | 203  | CLA  | CAA-CBA-CGA-O2A |
| 17  | w     | 207  | BCR  | C11-C12-C13-C14 |
| 20  | n     | 801  | SQD  | C24-C25-C26-C27 |
| 14  | G     | 826  | CLA  | CAA-CBA-CGA-O1A |
| 14  | n     | 806  | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 808  | CLA  | CAA-CBA-CGA-O1A |
| 14  | A     | 840  | CLA  | CAA-CBA-CGA-O1A |
| 20  | H     | 1702 | SQD  | C45-C44-O6-C1   |
| 21  | B     | 802  | LMG  | C8-C7-O1-C1     |
| 14  | N     | 814  | CLA  | C4C-C3C-CAC-CBC |
| 14  | N     | 811  | CLA  | CAA-CBA-CGA-O1A |
| 14  | n     | 833  | CLA  | CAA-CBA-CGA-O1A |
| 14  | N     | 834  | CLA  | CAA-CBA-CGA-O2A |
| 14  | g     | 810  | CLA  | CAA-CBA-CGA-O2A |
| 21  | N     | 850  | LMG  | O7-C10-C11-C12  |
| 21  | B     | 849  | LMG  | O7-C10-C11-C12  |
| 14  | g     | 811  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 837  | CLA  | C2A-CAA-CBA-CGA |
| 14  | A     | 853  | CLA  | C2A-CAA-CBA-CGA |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 14  | G     | 807  | CLA  | C15-C16-C17-C18 |
| 21  | b     | 849  | LMG  | C29-C30-C31-C32 |
| 18  | a     | 849  | LHG  | C4-C5-C6-O8     |
| 14  | A     | 819  | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 839  | CLA  | CAA-CBA-CGA-O1A |
| 14  | a     | 811  | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 823  | CLA  | CAA-CBA-CGA-O1A |
| 14  | b     | 824  | CLA  | CAA-CBA-CGA-O1A |
| 18  | g     | 849  | LHG  | O10-C23-C24-C25 |
| 14  | N     | 811  | CLA  | C15-C16-C17-C18 |
| 14  | B     | 818  | CLA  | C10-C11-C12-C13 |
| 14  | A     | 822  | CLA  | CAA-CBA-CGA-O2A |
| 17  | N     | 847  | BCR  | C19-C20-C21-C22 |
| 14  | b     | 811  | CLA  | CAA-CBA-CGA-O1A |
| 14  | N     | 805  | CLA  | CAD-CBD-CGD-O2D |
| 14  | N     | 832  | CLA  | CAD-CBD-CGD-O2D |
| 14  | A     | 819  | CLA  | CAD-CBD-CGD-O2D |
| 14  | B     | 807  | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 803  | CLA  | CAD-CBD-CGD-O2D |
| 14  | b     | 822  | CLA  | CAD-CBD-CGD-O2D |
| 14  | l     | 202  | CLA  | CAD-CBD-CGD-O2D |
| 14  | G     | 827  | CLA  | CAA-CBA-CGA-O2A |
| 14  | g     | 826  | CLA  | CAA-CBA-CGA-O2A |
| 14  | g     | 854  | CLA  | CAA-CBA-CGA-O2A |
| 14  | n     | 809  | CLA  | CAA-CBA-CGA-O2A |
| 14  | b     | 821  | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 824  | CLA  | CAA-CBA-CGA-O1A |
| 14  | w     | 204  | CLA  | C2-C1-O2A-CGA   |
| 14  | j     | 101  | CLA  | CAA-CBA-CGA-O1A |
| 14  | S     | 201  | CLA  | C11-C12-C13-C14 |
| 14  | G     | 833  | CLA  | CAA-CBA-CGA-O2A |
| 14  | L     | 1501 | CLA  | CAA-CBA-CGA-O2A |
| 21  | n     | 848  | LMG  | O7-C10-C11-C12  |
| 14  | a     | 801  | CLA  | C16-C17-C18-C19 |
| 19  | A     | 852  | CL0  | CAA-CBA-CGA-O1A |
| 14  | A     | 830  | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 833  | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 810  | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 834  | CLA  | CAA-CBA-CGA-O2A |
| 14  | n     | 817  | CLA  | C16-C17-C18-C20 |
| 14  | A     | 802  | CLA  | C16-C17-C18-C20 |
| 14  | N     | 825  | CLA  | CAA-CBA-CGA-O1A |

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| Mol | Chain | Res | Type | Atoms           |
|-----|-------|-----|------|-----------------|
| 14  | G     | 811 | CLA  | C3-C5-C6-C7     |
| 14  | B     | 807 | CLA  | C3-C5-C6-C7     |
| 14  | S     | 201 | CLA  | CAA-CBA-CGA-O2A |
| 14  | g     | 825 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 816 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 837 | CLA  | CAA-CBA-CGA-O2A |
| 14  | A     | 854 | CLA  | CAA-CBA-CGA-O2A |
| 14  | B     | 813 | CLA  | CAA-CBA-CGA-O2A |
| 14  | a     | 815 | CLA  | CAA-CBA-CGA-O2A |
| 18  | G     | 850 | LHG  | O8-C23-C24-C25  |
| 14  | N     | 842 | CLA  | CAA-CBA-CGA-O1A |
| 14  | B     | 814 | CLA  | CAA-CBA-CGA-O1A |
| 18  | a     | 850 | LHG  | C17-C18-C19-C20 |

There are no ring outliers.

486 monomers are involved in 1938 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 14  | N     | 851 | CLA  | 6       | 0            |
| 14  | b     | 809 | CLA  | 8       | 0            |
| 14  | G     | 811 | CLA  | 1       | 0            |
| 14  | G     | 803 | CLA  | 5       | 0            |
| 14  | g     | 836 | CLA  | 3       | 0            |
| 17  | G     | 845 | BCR  | 5       | 0            |
| 14  | G     | 835 | CLA  | 2       | 0            |
| 14  | G     | 836 | CLA  | 1       | 0            |
| 17  | A     | 856 | BCR  | 10      | 0            |
| 14  | G     | 833 | CLA  | 6       | 0            |
| 14  | G     | 826 | CLA  | 2       | 0            |
| 18  | a     | 850 | LHG  | 9       | 0            |
| 14  | b     | 817 | CLA  | 4       | 0            |
| 14  | N     | 835 | CLA  | 2       | 0            |
| 18  | A     | 851 | LHG  | 5       | 0            |
| 14  | A     | 832 | CLA  | 4       | 0            |
| 19  | A     | 852 | CL0  | 2       | 0            |
| 14  | B     | 829 | CLA  | 4       | 0            |
| 21  | B     | 849 | LMG  | 5       | 0            |
| 14  | a     | 840 | CLA  | 2       | 0            |
| 14  | g     | 852 | CLA  | 6       | 0            |
| 14  | G     | 829 | CLA  | 6       | 0            |
| 14  | N     | 842 | CLA  | 8       | 0            |
| 14  | N     | 812 | CLA  | 2       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14  | a     | 822  | CLA  | 2       | 0            |
| 14  | a     | 839  | CLA  | 7       | 0            |
| 14  | g     | 805  | CLA  | 4       | 0            |
| 14  | b     | 808  | CLA  | 5       | 0            |
| 17  | G     | 843  | BCR  | 12      | 0            |
| 14  | b     | 837  | CLA  | 8       | 0            |
| 14  | g     | 823  | CLA  | 3       | 0            |
| 14  | b     | 802  | CLA  | 6       | 0            |
| 14  | L     | 1502 | CLA  | 6       | 0            |
| 17  | B     | 843  | BCR  | 5       | 0            |
| 15  | A     | 842  | PQN  | 5       | 0            |
| 17  | i     | 102  | BCR  | 6       | 0            |
| 14  | b     | 821  | CLA  | 2       | 0            |
| 17  | b     | 848  | BCR  | 6       | 0            |
| 14  | n     | 852  | CLA  | 2       | 0            |
| 16  | C     | 102  | SF4  | 1       | 0            |
| 14  | N     | 810  | CLA  | 5       | 0            |
| 14  | K     | 101  | CLA  | 2       | 0            |
| 14  | b     | 805  | CLA  | 12      | 0            |
| 18  | S     | 202  | LHG  | 4       | 0            |
| 17  | B     | 847  | BCR  | 7       | 0            |
| 14  | n     | 820  | CLA  | 2       | 0            |
| 14  | G     | 837  | CLA  | 5       | 0            |
| 14  | b     | 853  | CLA  | 3       | 0            |
| 14  | N     | 824  | CLA  | 2       | 0            |
| 15  | a     | 841  | PQN  | 4       | 0            |
| 14  | G     | 812  | CLA  | 9       | 0            |
| 17  | N     | 853  | BCR  | 7       | 0            |
| 14  | A     | 811  | CLA  | 6       | 0            |
| 14  | g     | 854  | CLA  | 8       | 0            |
| 17  | a     | 848  | BCR  | 11      | 0            |
| 14  | A     | 855  | CLA  | 21      | 0            |
| 14  | n     | 836  | CLA  | 2       | 0            |
| 14  | B     | 839  | CLA  | 4       | 0            |
| 14  | g     | 831  | CLA  | 6       | 0            |
| 14  | U     | 102  | CLA  | 1       | 0            |
| 14  | a     | 820  | CLA  | 2       | 0            |
| 18  | a     | 849  | LHG  | 5       | 0            |
| 20  | l     | 201  | SQD  | 4       | 0            |
| 21  | n     | 848  | LMG  | 3       | 0            |
| 14  | B     | 850  | CLA  | 5       | 0            |
| 14  | B     | 817  | CLA  | 2       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 15  | g     | 841  | PQN  | 4       | 0            |
| 14  | g     | 832  | CLA  | 9       | 0            |
| 14  | g     | 839  | CLA  | 8       | 0            |
| 14  | A     | 820  | CLA  | 7       | 0            |
| 14  | b     | 838  | CLA  | 3       | 0            |
| 14  | g     | 811  | CLA  | 5       | 0            |
| 14  | n     | 806  | CLA  | 7       | 0            |
| 17  | j     | 104  | BCR  | 3       | 0            |
| 14  | t     | 102  | CLA  | 1       | 0            |
| 17  | w     | 206  | BCR  | 5       | 0            |
| 16  | c     | 102  | SF4  | 1       | 0            |
| 17  | N     | 848  | BCR  | 6       | 0            |
| 17  | n     | 844  | BCR  | 6       | 0            |
| 14  | L     | 1501 | CLA  | 2       | 0            |
| 14  | g     | 834  | CLA  | 4       | 0            |
| 14  | N     | 801  | CLA  | 4       | 0            |
| 14  | g     | 826  | CLA  | 7       | 0            |
| 14  | n     | 823  | CLA  | 4       | 0            |
| 14  | B     | 815  | CLA  | 3       | 0            |
| 17  | A     | 848  | BCR  | 3       | 0            |
| 16  | P     | 102  | SF4  | 1       | 0            |
| 14  | A     | 804  | CLA  | 9       | 0            |
| 17  | B     | 851  | BCR  | 11      | 0            |
| 14  | A     | 805  | CLA  | 5       | 0            |
| 14  | n     | 807  | CLA  | 4       | 0            |
| 14  | A     | 819  | CLA  | 3       | 0            |
| 17  | T     | 104  | BCR  | 9       | 0            |
| 14  | A     | 801  | CLA  | 6       | 0            |
| 14  | B     | 826  | CLA  | 5       | 0            |
| 14  | n     | 824  | CLA  | 8       | 0            |
| 14  | G     | 817  | CLA  | 6       | 0            |
| 14  | a     | 838  | CLA  | 4       | 0            |
| 17  | W     | 201  | BCR  | 6       | 0            |
| 17  | w     | 201  | BCR  | 9       | 0            |
| 17  | W     | 206  | BCR  | 6       | 0            |
| 14  | G     | 822  | CLA  | 1       | 0            |
| 14  | n     | 804  | CLA  | 13      | 0            |
| 17  | A     | 844  | BCR  | 6       | 0            |
| 14  | B     | 805  | CLA  | 6       | 0            |
| 15  | b     | 842  | PQN  | 4       | 0            |
| 14  | n     | 832  | CLA  | 5       | 0            |
| 14  | a     | 832  | CLA  | 7       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 14  | B     | 808 | CLA  | 5       | 0            |
| 14  | a     | 827 | CLA  | 3       | 0            |
| 17  | Y     | 101 | BCR  | 4       | 0            |
| 19  | g     | 851 | CL0  | 7       | 0            |
| 14  | G     | 808 | CLA  | 7       | 0            |
| 14  | B     | 804 | CLA  | 6       | 0            |
| 14  | s     | 201 | CLA  | 2       | 0            |
| 14  | A     | 807 | CLA  | 5       | 0            |
| 17  | g     | 847 | BCR  | 3       | 0            |
| 14  | N     | 825 | CLA  | 2       | 0            |
| 14  | g     | 821 | CLA  | 2       | 0            |
| 14  | N     | 808 | CLA  | 2       | 0            |
| 14  | G     | 821 | CLA  | 4       | 0            |
| 17  | A     | 845 | BCR  | 7       | 0            |
| 17  | v     | 101 | BCR  | 7       | 0            |
| 17  | J     | 103 | BCR  | 6       | 0            |
| 14  | b     | 827 | CLA  | 7       | 0            |
| 18  | g     | 849 | LHG  | 1       | 0            |
| 14  | N     | 840 | CLA  | 8       | 0            |
| 14  | N     | 809 | CLA  | 2       | 0            |
| 18  | G     | 849 | LHG  | 6       | 0            |
| 14  | N     | 821 | CLA  | 3       | 0            |
| 14  | b     | 803 | CLA  | 12      | 0            |
| 14  | g     | 812 | CLA  | 4       | 0            |
| 14  | g     | 853 | CLA  | 5       | 0            |
| 14  | T     | 102 | CLA  | 1       | 0            |
| 14  | N     | 841 | CLA  | 4       | 0            |
| 17  | a     | 846 | BCR  | 7       | 0            |
| 14  | J     | 101 | CLA  | 1       | 0            |
| 14  | S     | 203 | CLA  | 3       | 0            |
| 14  | n     | 819 | CLA  | 5       | 0            |
| 17  | n     | 851 | BCR  | 6       | 0            |
| 14  | n     | 808 | CLA  | 10      | 0            |
| 14  | a     | 801 | CLA  | 11      | 0            |
| 14  | G     | 809 | CLA  | 2       | 0            |
| 14  | G     | 825 | CLA  | 3       | 0            |
| 14  | b     | 828 | CLA  | 9       | 0            |
| 14  | N     | 831 | CLA  | 8       | 0            |
| 14  | B     | 833 | CLA  | 5       | 0            |
| 18  | G     | 850 | LHG  | 4       | 0            |
| 17  | j     | 103 | BCR  | 5       | 0            |
| 14  | g     | 833 | CLA  | 5       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14  | G     | 838  | CLA  | 9       | 0            |
| 14  | G     | 840  | CLA  | 2       | 0            |
| 14  | b     | 810  | CLA  | 3       | 0            |
| 14  | A     | 837  | CLA  | 4       | 0            |
| 14  | T     | 101  | CLA  | 1       | 0            |
| 17  | b     | 846  | BCR  | 5       | 0            |
| 14  | b     | 811  | CLA  | 4       | 0            |
| 14  | B     | 838  | CLA  | 9       | 0            |
| 14  | G     | 805  | CLA  | 8       | 0            |
| 14  | a     | 813  | CLA  | 2       | 0            |
| 17  | n     | 843  | BCR  | 2       | 0            |
| 17  | b     | 845  | BCR  | 3       | 0            |
| 14  | n     | 818  | CLA  | 4       | 0            |
| 14  | A     | 833  | CLA  | 3       | 0            |
| 20  | h     | 1702 | SQD  | 7       | 0            |
| 14  | n     | 814  | CLA  | 3       | 0            |
| 14  | b     | 804  | CLA  | 6       | 0            |
| 14  | a     | 811  | CLA  | 7       | 0            |
| 20  | x     | 1702 | SQD  | 4       | 0            |
| 14  | a     | 828  | CLA  | 8       | 0            |
| 14  | g     | 817  | CLA  | 6       | 0            |
| 14  | j     | 101  | CLA  | 3       | 0            |
| 14  | B     | 831  | CLA  | 3       | 0            |
| 17  | g     | 845  | BCR  | 8       | 0            |
| 14  | b     | 841  | CLA  | 11      | 0            |
| 14  | x     | 1701 | CLA  | 2       | 0            |
| 14  | a     | 825  | CLA  | 5       | 0            |
| 14  | n     | 809  | CLA  | 4       | 0            |
| 14  | B     | 822  | CLA  | 1       | 0            |
| 14  | G     | 802  | CLA  | 10      | 0            |
| 14  | b     | 807  | CLA  | 6       | 0            |
| 14  | a     | 802  | CLA  | 4       | 0            |
| 14  | B     | 835  | CLA  | 1       | 0            |
| 17  | s     | 203  | BCR  | 4       | 0            |
| 14  | A     | 823  | CLA  | 1       | 0            |
| 14  | B     | 830  | CLA  | 7       | 0            |
| 17  | A     | 849  | BCR  | 10      | 0            |
| 14  | N     | 804  | CLA  | 10      | 0            |
| 14  | A     | 814  | CLA  | 1       | 0            |
| 14  | F     | 201  | CLA  | 1       | 0            |
| 14  | A     | 839  | CLA  | 4       | 0            |
| 14  | n     | 816  | CLA  | 5       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14  | n     | 817  | CLA  | 7       | 0            |
| 14  | A     | 831  | CLA  | 7       | 0            |
| 17  | G     | 848  | BCR  | 6       | 0            |
| 14  | n     | 811  | CLA  | 1       | 0            |
| 14  | A     | 802  | CLA  | 12      | 0            |
| 14  | h     | 1701 | CLA  | 4       | 0            |
| 14  | a     | 803  | CLA  | 5       | 0            |
| 14  | g     | 813  | CLA  | 1       | 0            |
| 17  | K     | 102  | BCR  | 3       | 0            |
| 14  | n     | 839  | CLA  | 6       | 0            |
| 14  | N     | 807  | CLA  | 5       | 0            |
| 14  | B     | 828  | CLA  | 8       | 0            |
| 17  | t     | 104  | BCR  | 7       | 0            |
| 18  | X     | 1702 | LHG  | 2       | 0            |
| 14  | g     | 824  | CLA  | 3       | 0            |
| 14  | N     | 828  | CLA  | 8       | 0            |
| 17  | n     | 845  | BCR  | 9       | 0            |
| 14  | a     | 854  | CLA  | 1       | 0            |
| 14  | n     | 802  | CLA  | 7       | 0            |
| 14  | g     | 837  | CLA  | 13      | 0            |
| 17  | I     | 102  | BCR  | 3       | 0            |
| 14  | b     | 812  | CLA  | 8       | 0            |
| 14  | B     | 814  | CLA  | 9       | 0            |
| 17  | B     | 846  | BCR  | 6       | 0            |
| 14  | n     | 826  | CLA  | 7       | 0            |
| 14  | g     | 804  | CLA  | 7       | 0            |
| 14  | A     | 854  | CLA  | 7       | 0            |
| 20  | B     | 801  | SQD  | 4       | 0            |
| 14  | b     | 806  | CLA  | 4       | 0            |
| 14  | f     | 202  | CLA  | 5       | 0            |
| 14  | a     | 852  | CLA  | 18      | 0            |
| 14  | b     | 820  | CLA  | 6       | 0            |
| 14  | B     | 809  | CLA  | 6       | 0            |
| 14  | b     | 824  | CLA  | 4       | 0            |
| 14  | a     | 807  | CLA  | 8       | 0            |
| 14  | g     | 828  | CLA  | 7       | 0            |
| 14  | n     | 805  | CLA  | 5       | 0            |
| 15  | G     | 841  | PQN  | 10      | 0            |
| 14  | G     | 828  | CLA  | 7       | 0            |
| 14  | b     | 832  | CLA  | 4       | 0            |
| 14  | g     | 838  | CLA  | 4       | 0            |
| 18  | m     | 101  | LHG  | 6       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 14  | g     | 810 | CLA  | 3       | 0            |
| 17  | f     | 203 | BCR  | 4       | 0            |
| 14  | G     | 810 | CLA  | 4       | 0            |
| 14  | A     | 826 | CLA  | 11      | 0            |
| 14  | N     | 814 | CLA  | 5       | 0            |
| 14  | g     | 803 | CLA  | 5       | 0            |
| 14  | a     | 824 | CLA  | 2       | 0            |
| 14  | n     | 837 | CLA  | 7       | 0            |
| 14  | A     | 816 | CLA  | 3       | 0            |
| 17  | n     | 847 | BCR  | 5       | 0            |
| 14  | n     | 821 | CLA  | 1       | 0            |
| 14  | B     | 825 | CLA  | 10      | 0            |
| 14  | b     | 813 | CLA  | 3       | 0            |
| 14  | A     | 829 | CLA  | 4       | 0            |
| 17  | W     | 205 | BCR  | 6       | 0            |
| 14  | B     | 840 | CLA  | 5       | 0            |
| 17  | N     | 852 | BCR  | 28      | 0            |
| 14  | n     | 812 | CLA  | 2       | 0            |
| 14  | A     | 825 | CLA  | 6       | 0            |
| 14  | a     | 809 | CLA  | 4       | 0            |
| 14  | g     | 829 | CLA  | 3       | 0            |
| 14  | b     | 818 | CLA  | 6       | 0            |
| 14  | a     | 821 | CLA  | 5       | 0            |
| 17  | g     | 848 | BCR  | 5       | 0            |
| 14  | g     | 822 | CLA  | 4       | 0            |
| 14  | B     | 834 | CLA  | 1       | 0            |
| 14  | g     | 830 | CLA  | 8       | 0            |
| 14  | A     | 840 | CLA  | 3       | 0            |
| 14  | G     | 814 | CLA  | 6       | 0            |
| 14  | g     | 816 | CLA  | 8       | 0            |
| 14  | G     | 830 | CLA  | 1       | 0            |
| 14  | n     | 850 | CLA  | 5       | 0            |
| 14  | g     | 801 | CLA  | 2       | 0            |
| 14  | A     | 821 | CLA  | 8       | 0            |
| 17  | N     | 844 | BCR  | 7       | 0            |
| 14  | t     | 101 | CLA  | 1       | 0            |
| 17  | V     | 101 | BCR  | 2       | 0            |
| 17  | n     | 849 | BCR  | 13      | 0            |
| 14  | N     | 823 | CLA  | 3       | 0            |
| 14  | N     | 830 | CLA  | 3       | 0            |
| 14  | N     | 820 | CLA  | 7       | 0            |
| 14  | a     | 836 | CLA  | 3       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 17  | b     | 850 | BCR  | 13      | 0            |
| 14  | n     | 838 | CLA  | 1       | 0            |
| 17  | t     | 103 | BCR  | 7       | 0            |
| 17  | F     | 203 | BCR  | 1       | 0            |
| 14  | A     | 812 | CLA  | 7       | 0            |
| 14  | b     | 816 | CLA  | 1       | 0            |
| 14  | b     | 829 | CLA  | 4       | 0            |
| 19  | a     | 851 | CL0  | 4       | 0            |
| 14  | l     | 204 | CLA  | 1       | 0            |
| 14  | W     | 203 | CLA  | 12      | 0            |
| 14  | W     | 204 | CLA  | 4       | 0            |
| 14  | w     | 204 | CLA  | 11      | 0            |
| 14  | A     | 827 | CLA  | 10      | 0            |
| 17  | a     | 844 | BCR  | 4       | 0            |
| 14  | A     | 835 | CLA  | 1       | 0            |
| 14  | a     | 853 | CLA  | 4       | 0            |
| 14  | j     | 102 | CLA  | 3       | 0            |
| 17  | w     | 207 | BCR  | 5       | 0            |
| 14  | g     | 806 | CLA  | 4       | 0            |
| 14  | g     | 807 | CLA  | 12      | 0            |
| 14  | n     | 831 | CLA  | 2       | 0            |
| 17  | b     | 852 | BCR  | 9       | 0            |
| 14  | G     | 806 | CLA  | 6       | 0            |
| 17  | B     | 848 | BCR  | 7       | 0            |
| 14  | a     | 829 | CLA  | 3       | 0            |
| 14  | G     | 820 | CLA  | 6       | 0            |
| 14  | n     | 822 | CLA  | 3       | 0            |
| 14  | n     | 833 | CLA  | 1       | 0            |
| 14  | G     | 801 | CLA  | 7       | 0            |
| 18  | A     | 850 | LHG  | 2       | 0            |
| 14  | N     | 815 | CLA  | 7       | 0            |
| 14  | B     | 832 | CLA  | 3       | 0            |
| 14  | N     | 806 | CLA  | 4       | 0            |
| 14  | a     | 805 | CLA  | 5       | 0            |
| 14  | B     | 813 | CLA  | 3       | 0            |
| 17  | T     | 103 | BCR  | 3       | 0            |
| 17  | y     | 101 | BCR  | 2       | 0            |
| 21  | b     | 849 | LMG  | 3       | 0            |
| 14  | f     | 201 | CLA  | 3       | 0            |
| 17  | g     | 843 | BCR  | 8       | 0            |
| 14  | g     | 809 | CLA  | 1       | 0            |
| 14  | N     | 813 | CLA  | 4       | 0            |

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| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14  | B     | 821  | CLA  | 1       | 0            |
| 17  | A     | 846  | BCR  | 5       | 0            |
| 17  | N     | 845  | BCR  | 5       | 0            |
| 14  | g     | 815  | CLA  | 5       | 0            |
| 14  | N     | 836  | CLA  | 2       | 0            |
| 14  | n     | 828  | CLA  | 6       | 0            |
| 14  | G     | 813  | CLA  | 4       | 0            |
| 14  | n     | 830  | CLA  | 3       | 0            |
| 14  | b     | 839  | CLA  | 3       | 0            |
| 14  | N     | 826  | CLA  | 7       | 0            |
| 17  | u     | 103  | BCR  | 2       | 0            |
| 18  | v     | 102  | LHG  | 3       | 0            |
| 17  | l     | 206  | BCR  | 4       | 0            |
| 17  | n     | 846  | BCR  | 9       | 0            |
| 14  | G     | 831  | CLA  | 7       | 0            |
| 14  | g     | 818  | CLA  | 1       | 0            |
| 21  | B     | 802  | LMG  | 1       | 0            |
| 14  | b     | 815  | CLA  | 4       | 0            |
| 14  | B     | 827  | CLA  | 10      | 0            |
| 14  | B     | 811  | CLA  | 3       | 0            |
| 14  | N     | 805  | CLA  | 6       | 0            |
| 14  | g     | 827  | CLA  | 8       | 0            |
| 14  | N     | 829  | CLA  | 5       | 0            |
| 17  | U     | 103  | BCR  | 2       | 0            |
| 17  | A     | 847  | BCR  | 5       | 0            |
| 14  | n     | 825  | CLA  | 5       | 0            |
| 17  | L     | 1504 | BCR  | 5       | 0            |
| 14  | a     | 810  | CLA  | 2       | 0            |
| 14  | A     | 828  | CLA  | 4       | 0            |
| 17  | N     | 846  | BCR  | 5       | 0            |
| 14  | A     | 830  | CLA  | 7       | 0            |
| 14  | N     | 827  | CLA  | 8       | 0            |
| 14  | a     | 808  | CLA  | 3       | 0            |
| 14  | G     | 853  | CLA  | 4       | 0            |
| 14  | b     | 826  | CLA  | 5       | 0            |
| 17  | S     | 204  | BCR  | 4       | 0            |
| 15  | B     | 842  | PQN  | 5       | 0            |
| 14  | X     | 1701 | CLA  | 3       | 0            |
| 14  | G     | 852  | CLA  | 27      | 0            |
| 14  | B     | 841  | CLA  | 5       | 0            |
| 14  | n     | 815  | CLA  | 3       | 0            |
| 14  | a     | 815  | CLA  | 3       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 14  | n     | 810 | CLA  | 4       | 0            |
| 17  | N     | 847 | BCR  | 2       | 0            |
| 14  | b     | 819 | CLA  | 3       | 0            |
| 17  | B     | 852 | BCR  | 8       | 0            |
| 14  | G     | 804 | CLA  | 12      | 0            |
| 14  | n     | 803 | CLA  | 10      | 0            |
| 14  | A     | 841 | CLA  | 1       | 0            |
| 14  | B     | 810 | CLA  | 5       | 0            |
| 17  | G     | 847 | BCR  | 6       | 0            |
| 17  | g     | 846 | BCR  | 8       | 0            |
| 17  | b     | 844 | BCR  | 3       | 0            |
| 14  | B     | 803 | CLA  | 7       | 0            |
| 19  | G     | 851 | CL0  | 7       | 0            |
| 14  | A     | 838 | CLA  | 7       | 0            |
| 17  | a     | 845 | BCR  | 3       | 0            |
| 14  | A     | 810 | CLA  | 4       | 0            |
| 17  | G     | 844 | BCR  | 3       | 0            |
| 14  | b     | 823 | CLA  | 2       | 0            |
| 14  | a     | 819 | CLA  | 11      | 0            |
| 14  | J     | 102 | CLA  | 2       | 0            |
| 17  | N     | 849 | BCR  | 3       | 0            |
| 14  | N     | 832 | CLA  | 5       | 0            |
| 14  | A     | 803 | CLA  | 4       | 0            |
| 21  | N     | 802 | LMG  | 2       | 0            |
| 14  | N     | 839 | CLA  | 5       | 0            |
| 21  | N     | 850 | LMG  | 6       | 0            |
| 14  | a     | 806 | CLA  | 5       | 0            |
| 14  | B     | 807 | CLA  | 5       | 0            |
| 14  | G     | 824 | CLA  | 4       | 0            |
| 15  | N     | 843 | PQN  | 6       | 0            |
| 14  | N     | 834 | CLA  | 7       | 0            |
| 14  | A     | 808 | CLA  | 9       | 0            |
| 14  | A     | 853 | CLA  | 12      | 0            |
| 14  | N     | 817 | CLA  | 5       | 0            |
| 14  | n     | 834 | CLA  | 1       | 0            |
| 14  | A     | 813 | CLA  | 2       | 0            |
| 14  | N     | 822 | CLA  | 2       | 0            |
| 14  | l     | 203 | CLA  | 9       | 0            |
| 14  | a     | 837 | CLA  | 10      | 0            |
| 14  | a     | 831 | CLA  | 10      | 0            |
| 14  | a     | 812 | CLA  | 2       | 0            |
| 17  | n     | 842 | BCR  | 3       | 0            |

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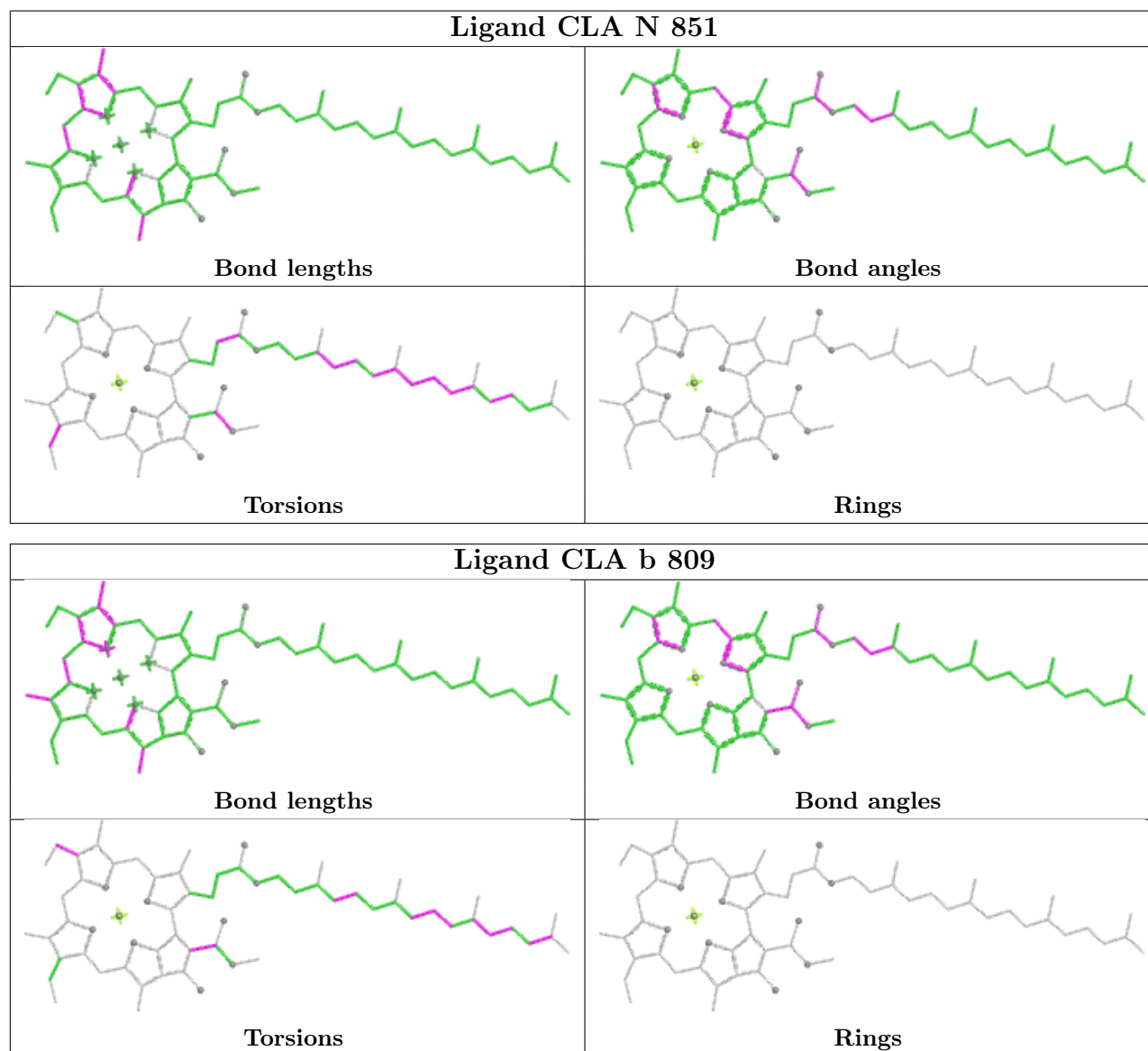
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 14  | G     | 832  | CLA  | 5       | 0            |
| 14  | a     | 826  | CLA  | 13      | 0            |
| 14  | W     | 202  | CLA  | 3       | 0            |
| 20  | w     | 202  | SQD  | 3       | 0            |
| 14  | n     | 813  | CLA  | 5       | 0            |
| 14  | a     | 816  | CLA  | 5       | 0            |
| 17  | M     | 101  | BCR  | 4       | 0            |
| 14  | s     | 202  | CLA  | 1       | 0            |
| 14  | a     | 823  | CLA  | 4       | 0            |
| 20  | H     | 1702 | SQD  | 3       | 0            |
| 14  | b     | 831  | CLA  | 5       | 0            |
| 14  | a     | 818  | CLA  | 3       | 0            |
| 14  | b     | 835  | CLA  | 1       | 0            |
| 14  | H     | 1701 | CLA  | 3       | 0            |
| 14  | A     | 834  | CLA  | 3       | 0            |
| 14  | G     | 816  | CLA  | 4       | 0            |
| 14  | B     | 837  | CLA  | 7       | 0            |
| 14  | b     | 833  | CLA  | 6       | 0            |
| 14  | n     | 840  | CLA  | 16      | 0            |
| 17  | B     | 845  | BCR  | 6       | 0            |
| 14  | b     | 834  | CLA  | 1       | 0            |
| 17  | I     | 101  | BCR  | 6       | 0            |
| 14  | A     | 809  | CLA  | 2       | 0            |
| 17  | a     | 843  | BCR  | 6       | 0            |
| 14  | g     | 819  | CLA  | 9       | 0            |
| 14  | A     | 806  | CLA  | 5       | 0            |
| 14  | N     | 816  | CLA  | 3       | 0            |
| 14  | G     | 819  | CLA  | 1       | 0            |
| 14  | B     | 819  | CLA  | 4       | 0            |
| 17  | k     | 102  | BCR  | 2       | 0            |
| 14  | G     | 807  | CLA  | 5       | 0            |
| 14  | n     | 829  | CLA  | 6       | 0            |
| 14  | A     | 817  | CLA  | 3       | 0            |
| 14  | N     | 811  | CLA  | 6       | 0            |
| 14  | N     | 819  | CLA  | 7       | 0            |
| 14  | g     | 820  | CLA  | 4       | 0            |
| 14  | A     | 818  | CLA  | 4       | 0            |
| 14  | g     | 808  | CLA  | 2       | 0            |
| 17  | g     | 844  | BCR  | 4       | 0            |
| 14  | G     | 834  | CLA  | 2       | 0            |
| 14  | A     | 836  | CLA  | 3       | 0            |
| 14  | a     | 833  | CLA  | 3       | 0            |

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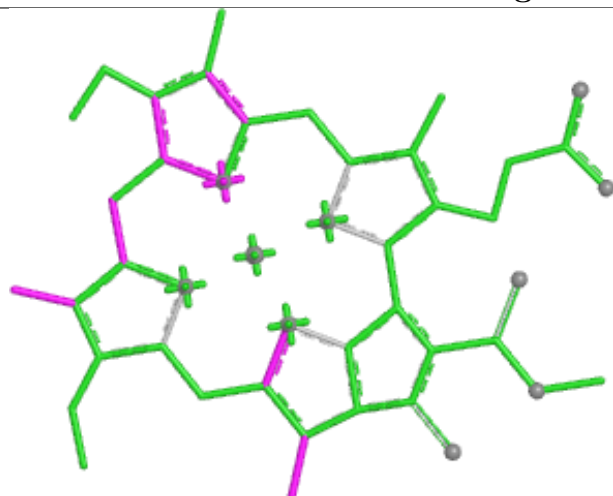
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 17  | b     | 843 | BCR  | 5       | 0            |
| 14  | a     | 830 | CLA  | 4       | 0            |
| 14  | n     | 827 | CLA  | 8       | 0            |
| 14  | A     | 824 | CLA  | 7       | 0            |
| 17  | m     | 102 | BCR  | 3       | 0            |
| 17  | B     | 844 | BCR  | 4       | 0            |
| 14  | G     | 823 | CLA  | 5       | 0            |
| 14  | b     | 814 | CLA  | 4       | 0            |
| 14  | b     | 822 | CLA  | 2       | 0            |
| 14  | B     | 823 | CLA  | 3       | 0            |
| 17  | i     | 101 | BCR  | 9       | 0            |
| 14  | N     | 838 | CLA  | 3       | 0            |
| 14  | B     | 820 | CLA  | 5       | 0            |
| 17  | b     | 847 | BCR  | 7       | 0            |
| 14  | G     | 839 | CLA  | 6       | 0            |
| 14  | B     | 818 | CLA  | 4       | 0            |
| 14  | l     | 202 | CLA  | 3       | 0            |
| 14  | G     | 818 | CLA  | 5       | 0            |
| 14  | N     | 803 | CLA  | 14      | 0            |
| 17  | a     | 847 | BCR  | 3       | 0            |
| 14  | N     | 818 | CLA  | 3       | 0            |
| 15  | n     | 841 | PQN  | 4       | 0            |
| 14  | a     | 804 | CLA  | 5       | 0            |
| 18  | g     | 850 | LHG  | 7       | 0            |
| 14  | b     | 830 | CLA  | 8       | 0            |
| 14  | g     | 825 | CLA  | 8       | 0            |
| 14  | N     | 833 | CLA  | 4       | 0            |
| 14  | B     | 812 | CLA  | 4       | 0            |
| 17  | l     | 205 | BCR  | 5       | 0            |
| 14  | g     | 840 | CLA  | 3       | 0            |
| 17  | I     | 103 | BCR  | 12      | 0            |
| 14  | B     | 806 | CLA  | 3       | 0            |
| 14  | B     | 816 | CLA  | 2       | 0            |
| 14  | B     | 824 | CLA  | 4       | 0            |
| 14  | b     | 825 | CLA  | 13      | 0            |
| 17  | G     | 846 | BCR  | 4       | 0            |
| 14  | a     | 817 | CLA  | 5       | 0            |
| 16  | p     | 102 | SF4  | 1       | 0            |
| 14  | a     | 835 | CLA  | 2       | 0            |
| 14  | G     | 827 | CLA  | 12      | 0            |
| 20  | b     | 801 | SQD  | 6       | 0            |
| 14  | b     | 840 | CLA  | 2       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

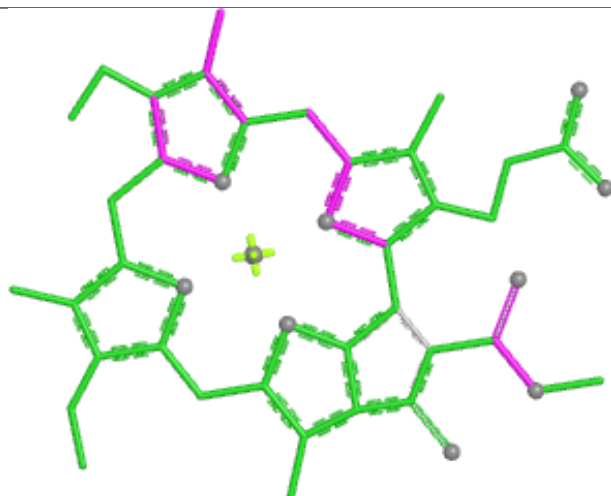




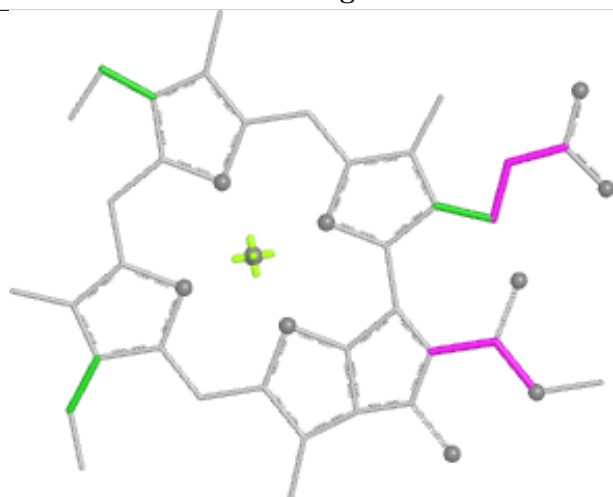
## Ligand CLA B 836



Bond lengths



Bond angles

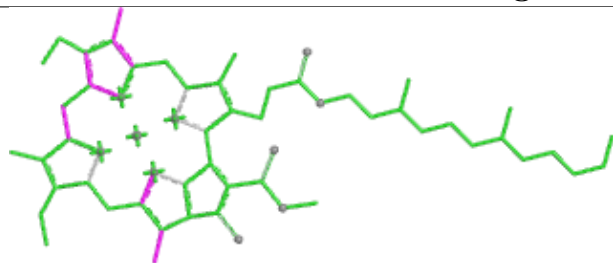


Torsions

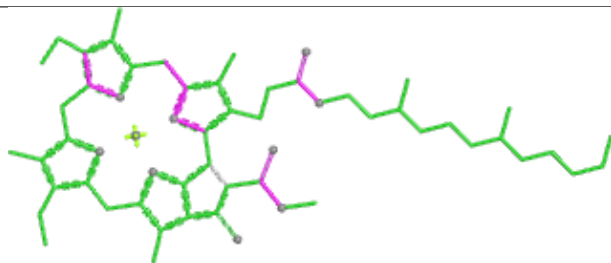


Rings

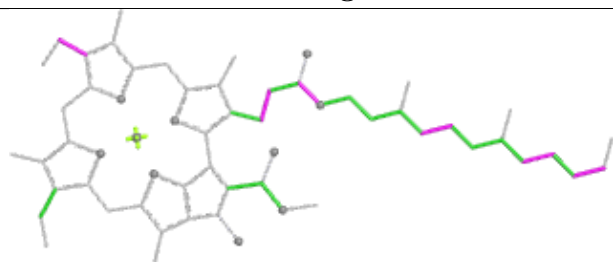
## Ligand CLA G 811



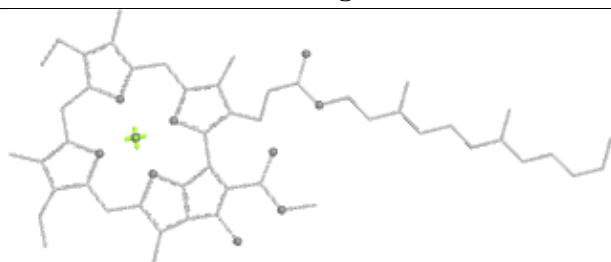
Bond lengths



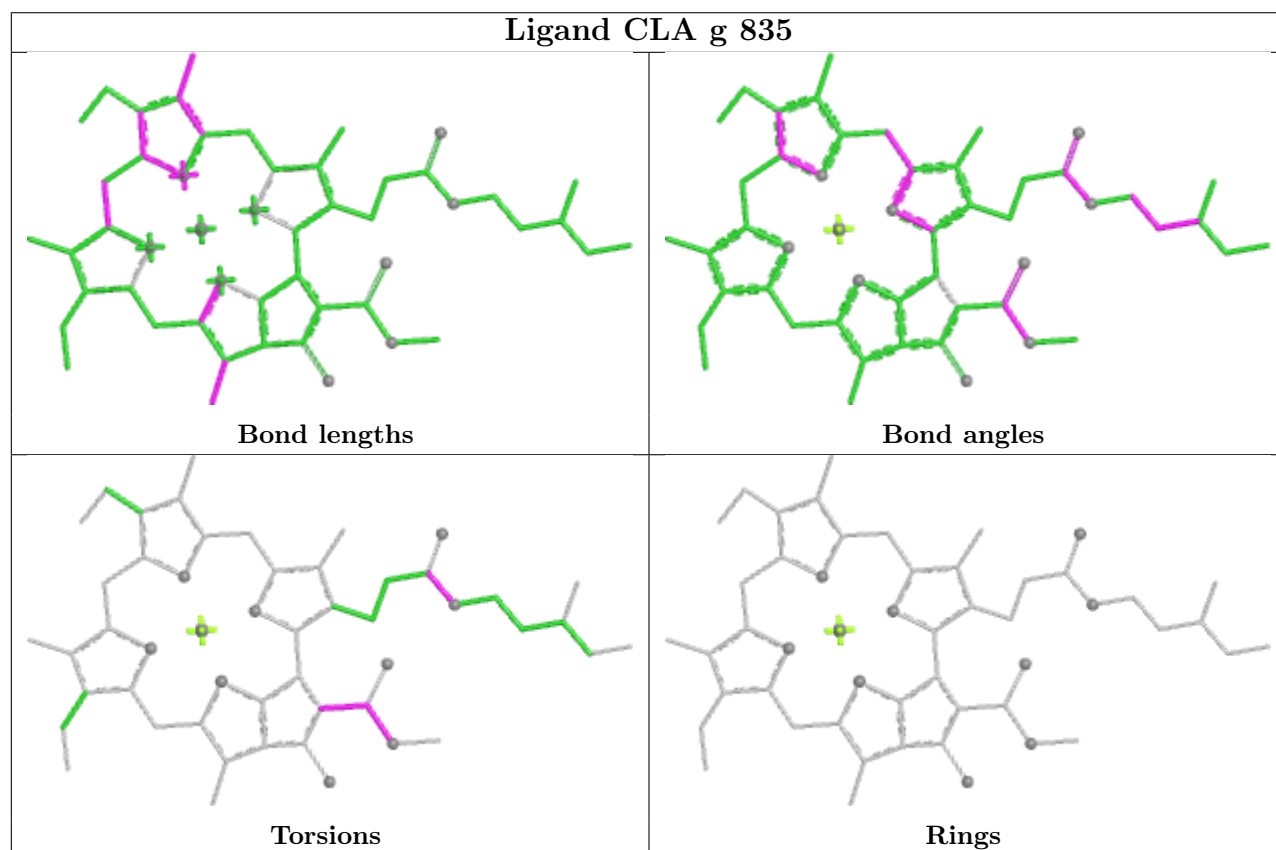
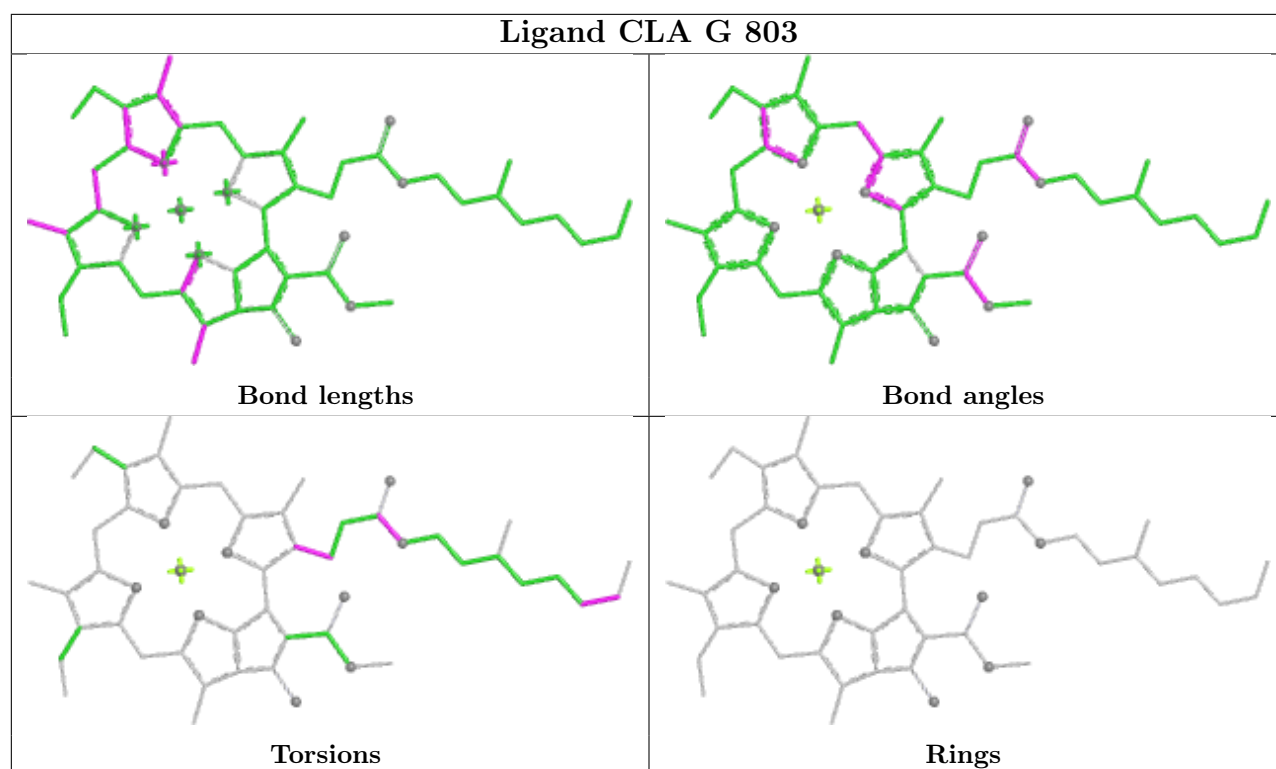
Bond angles

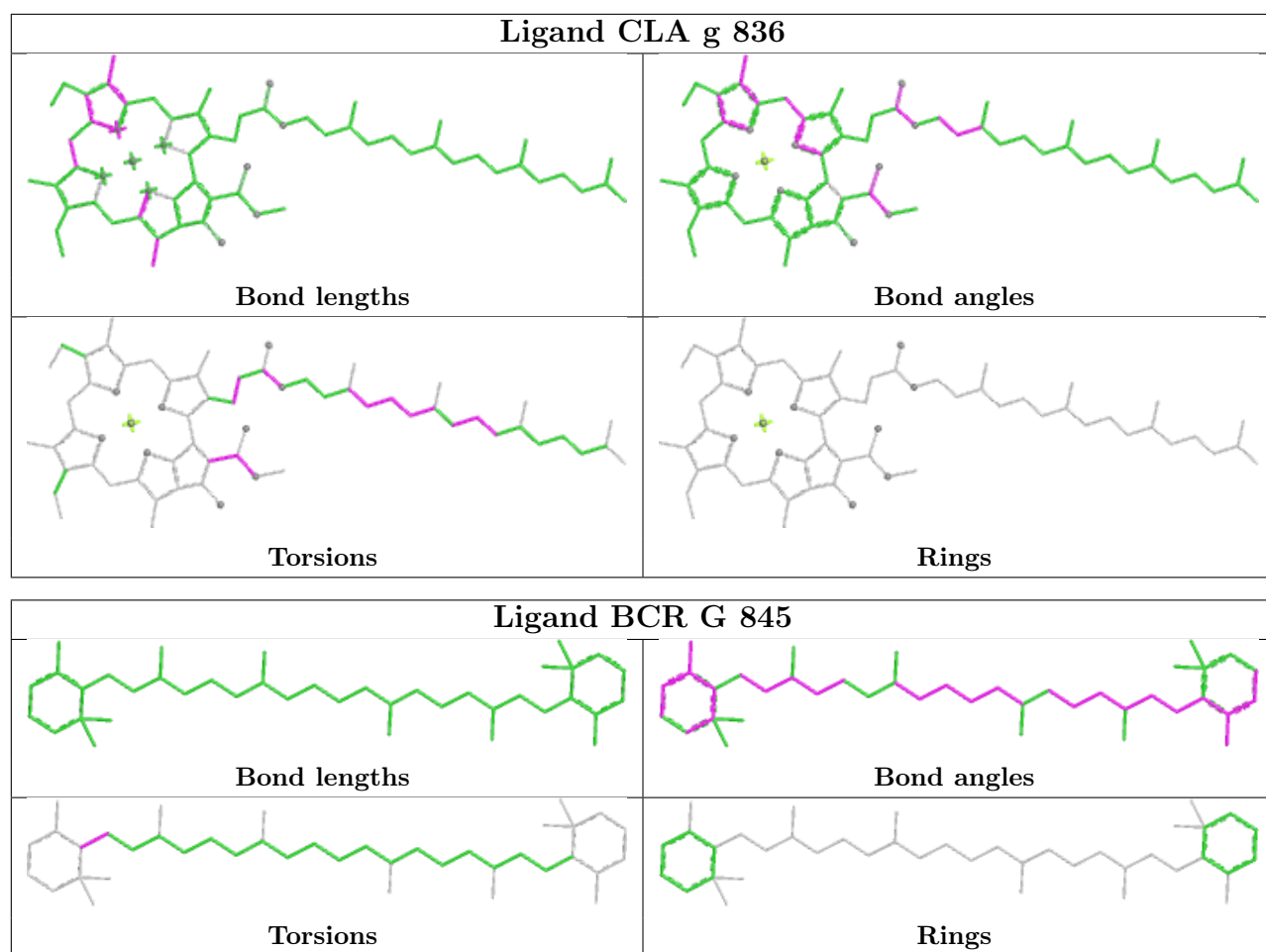


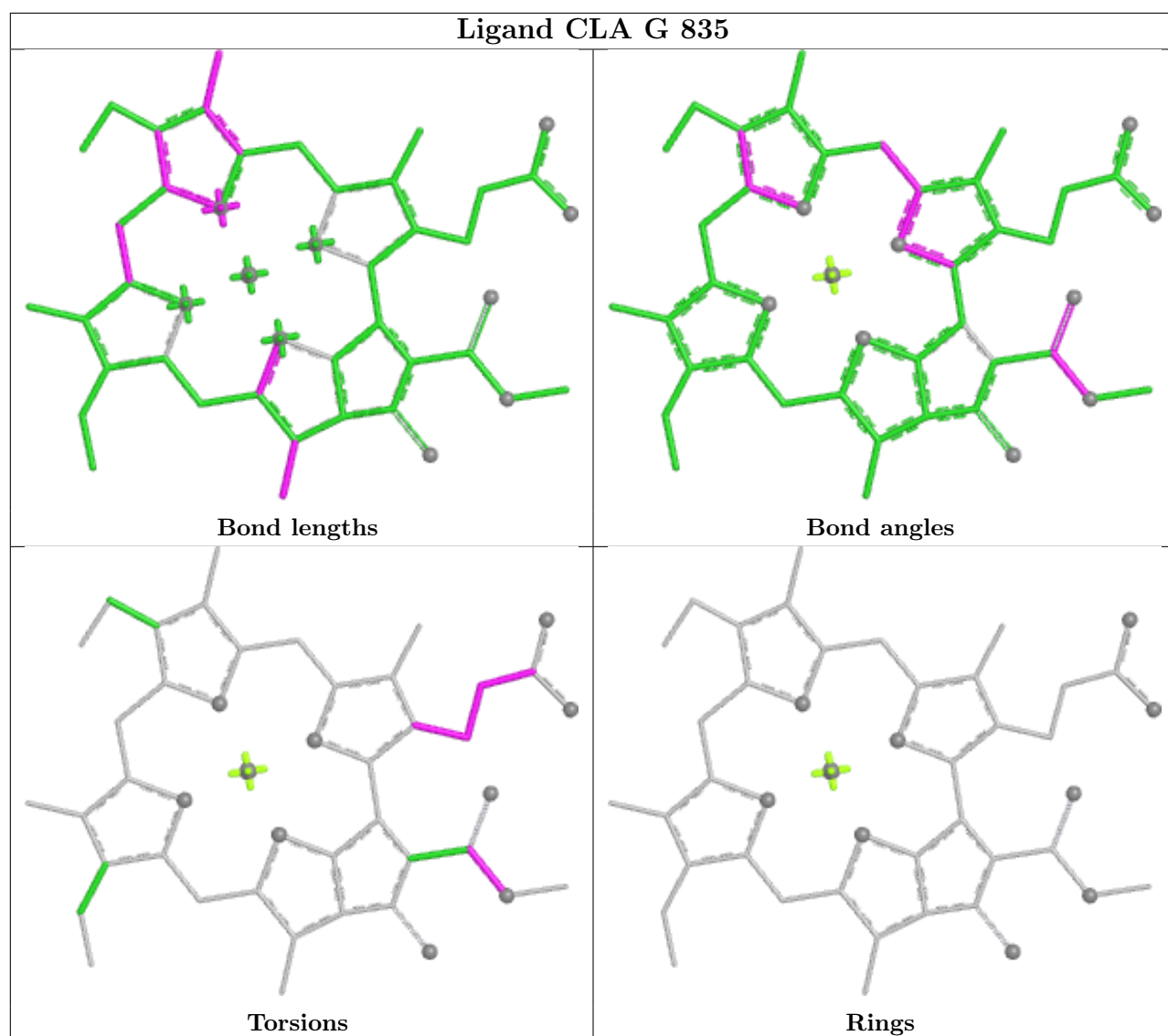
Torsions

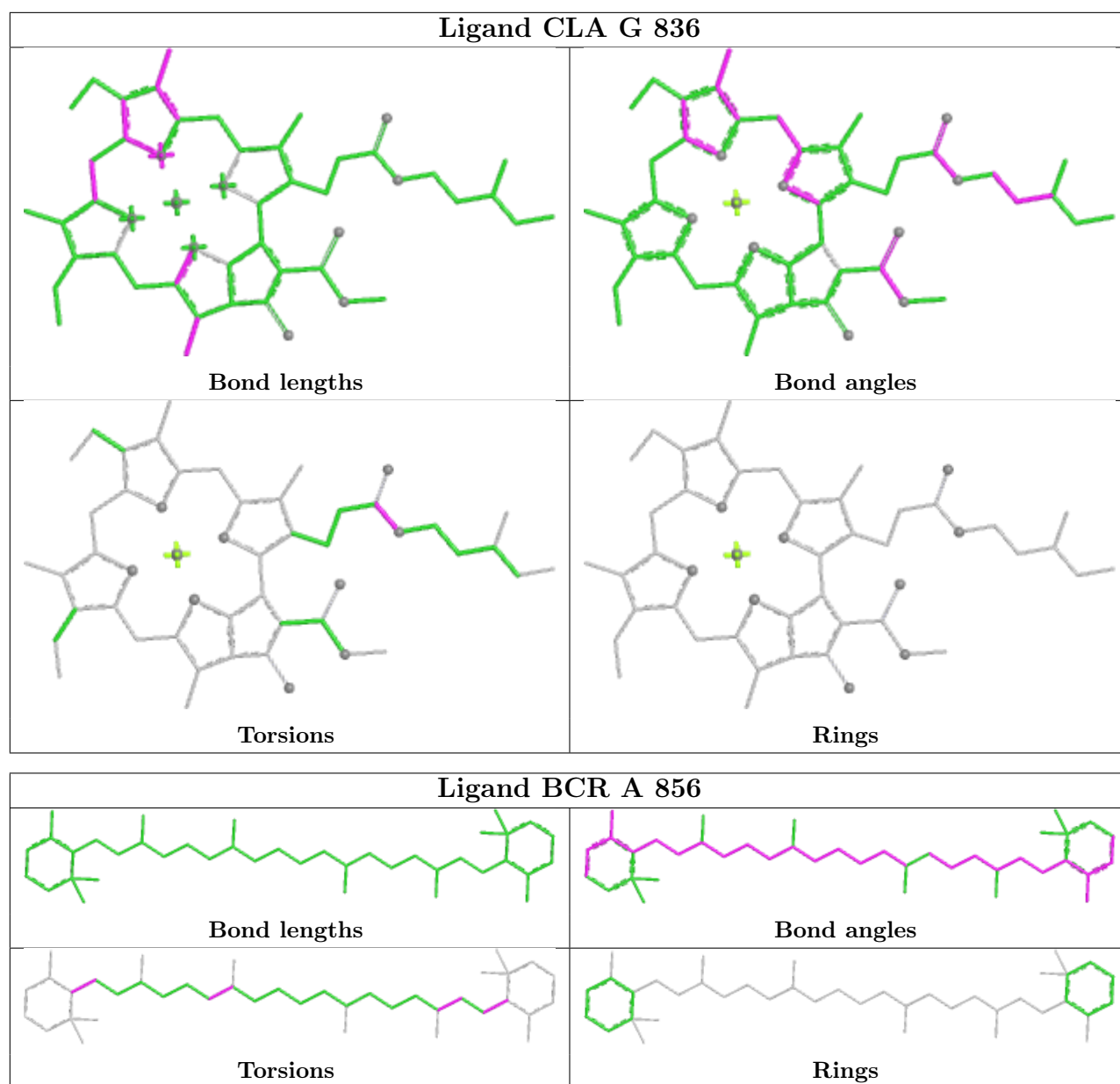


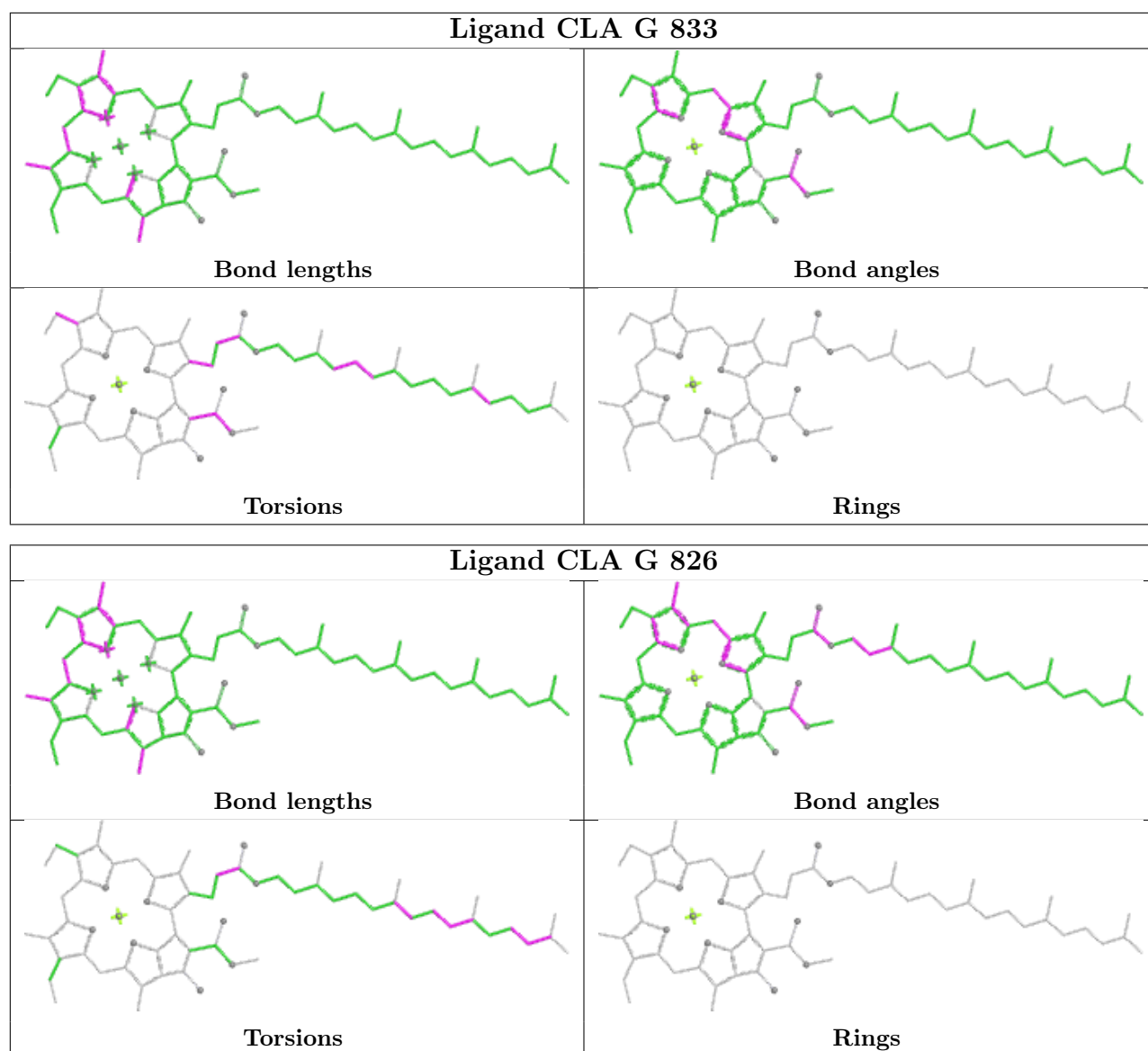
Rings

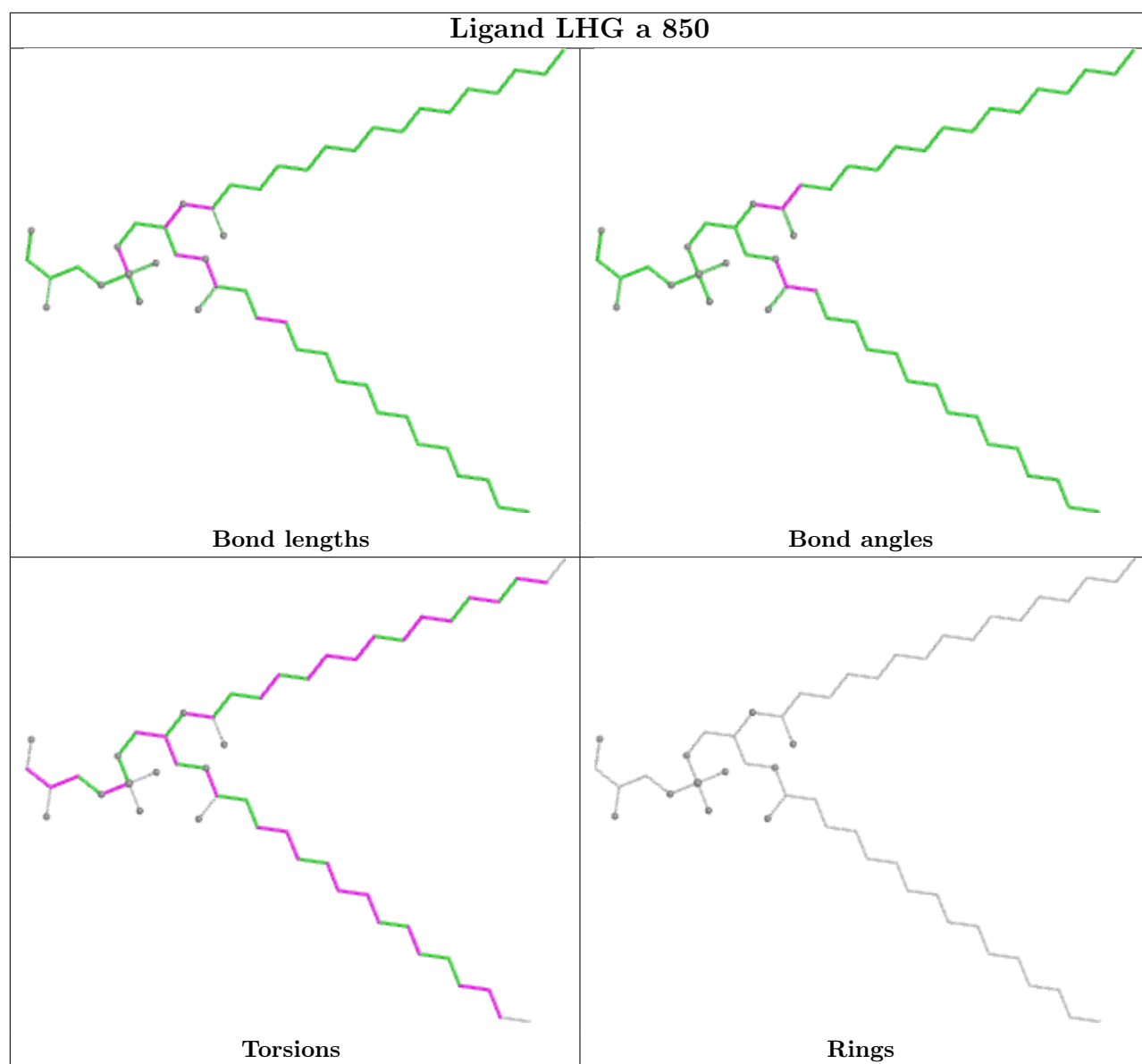




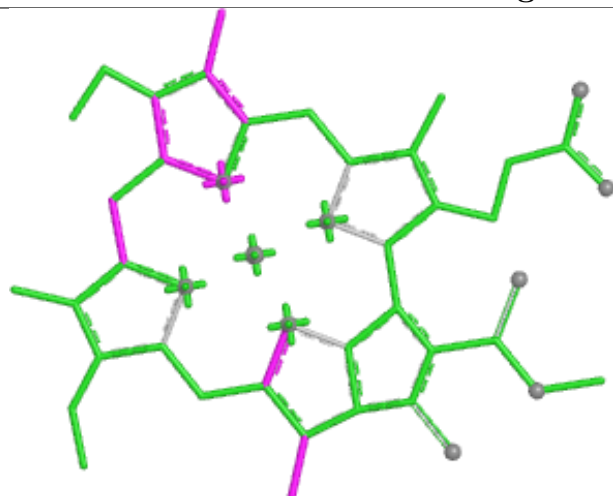








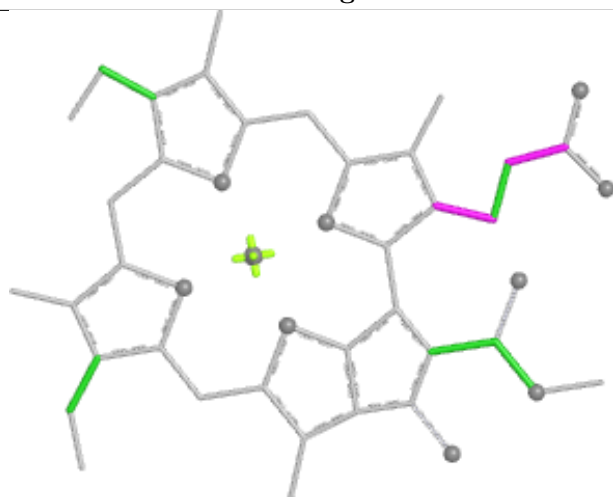
## Ligand CLA b 817



Bond lengths



Bond angles

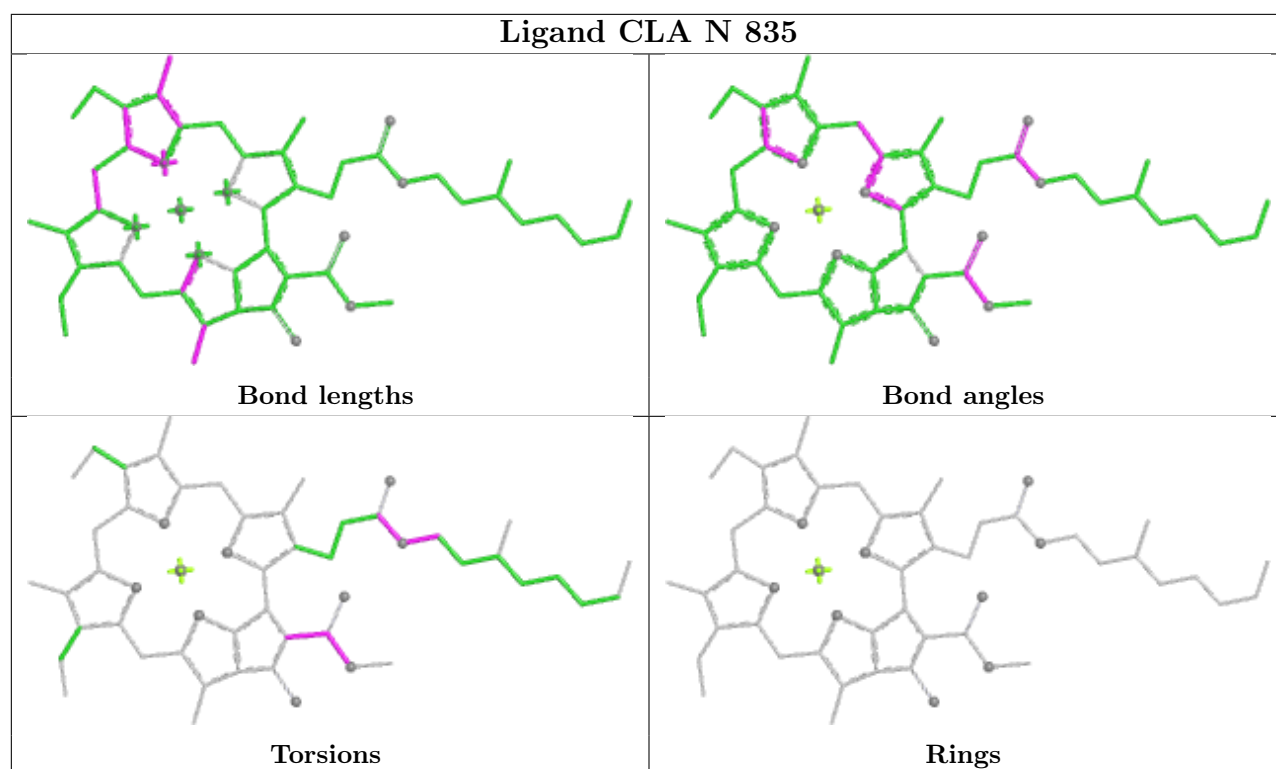


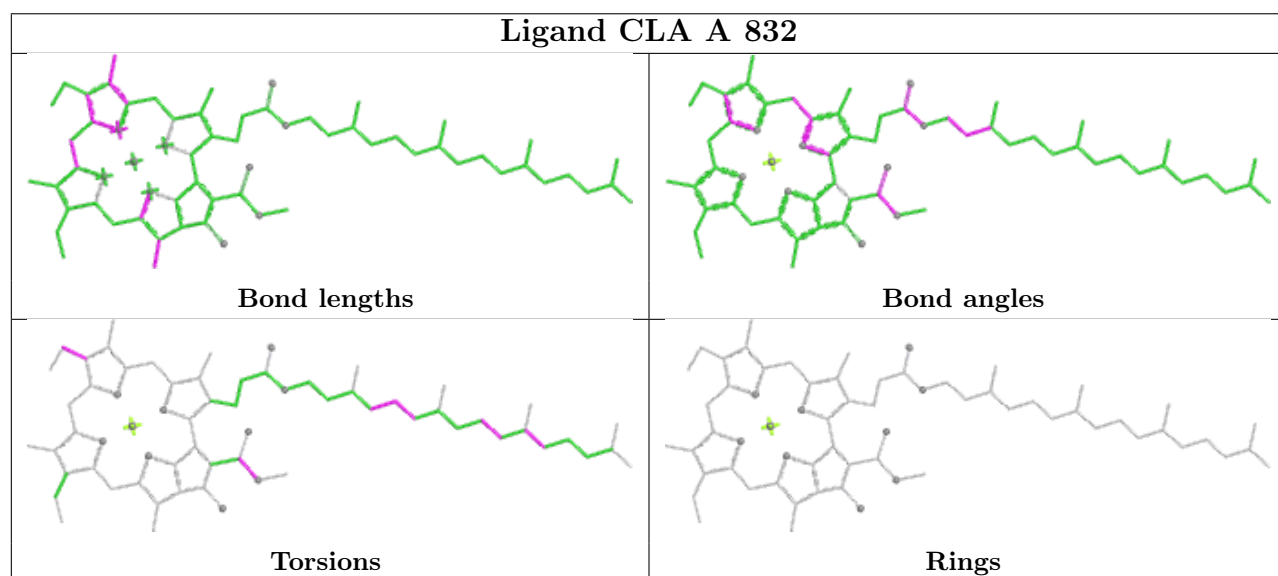
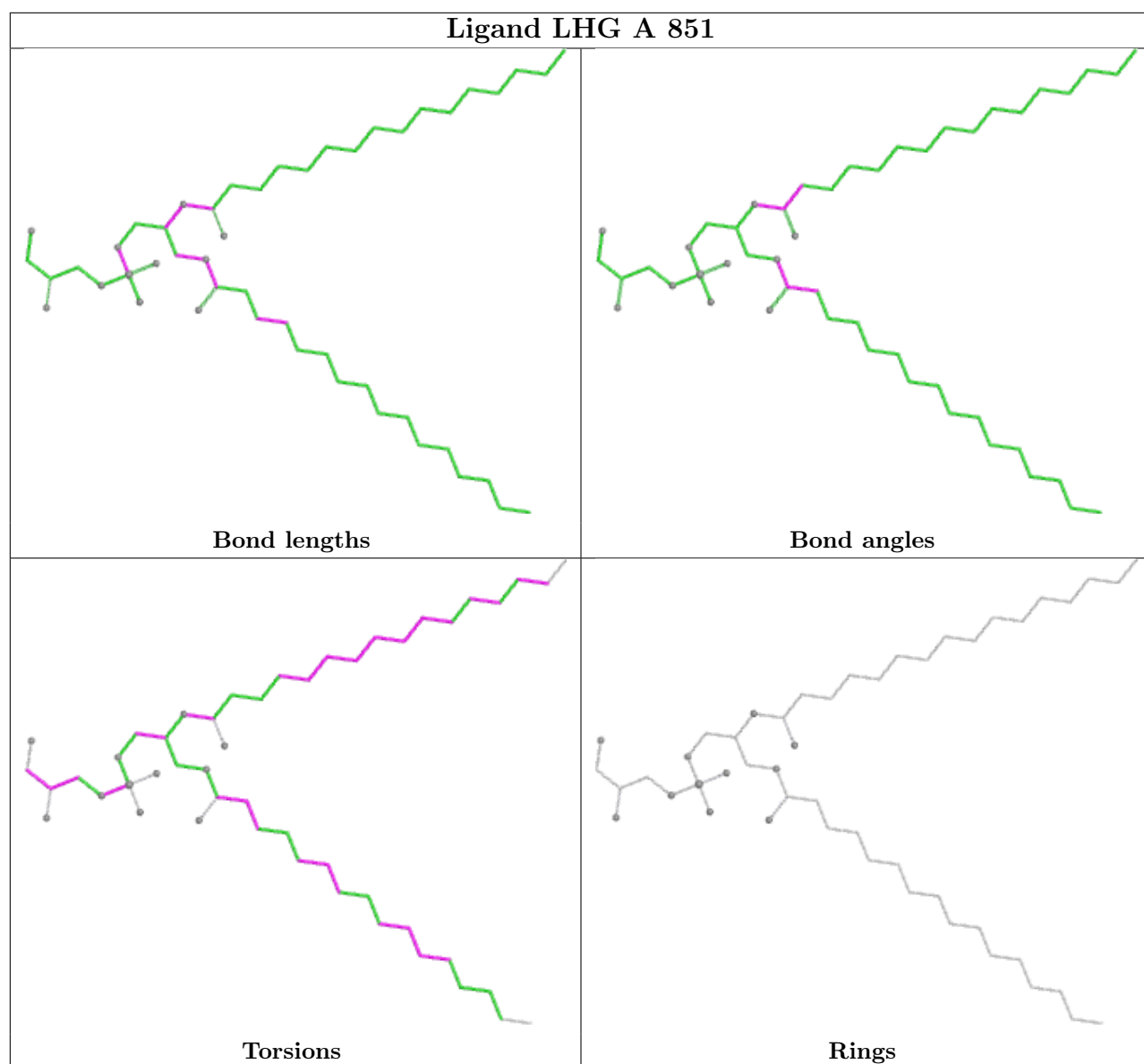
Torsions



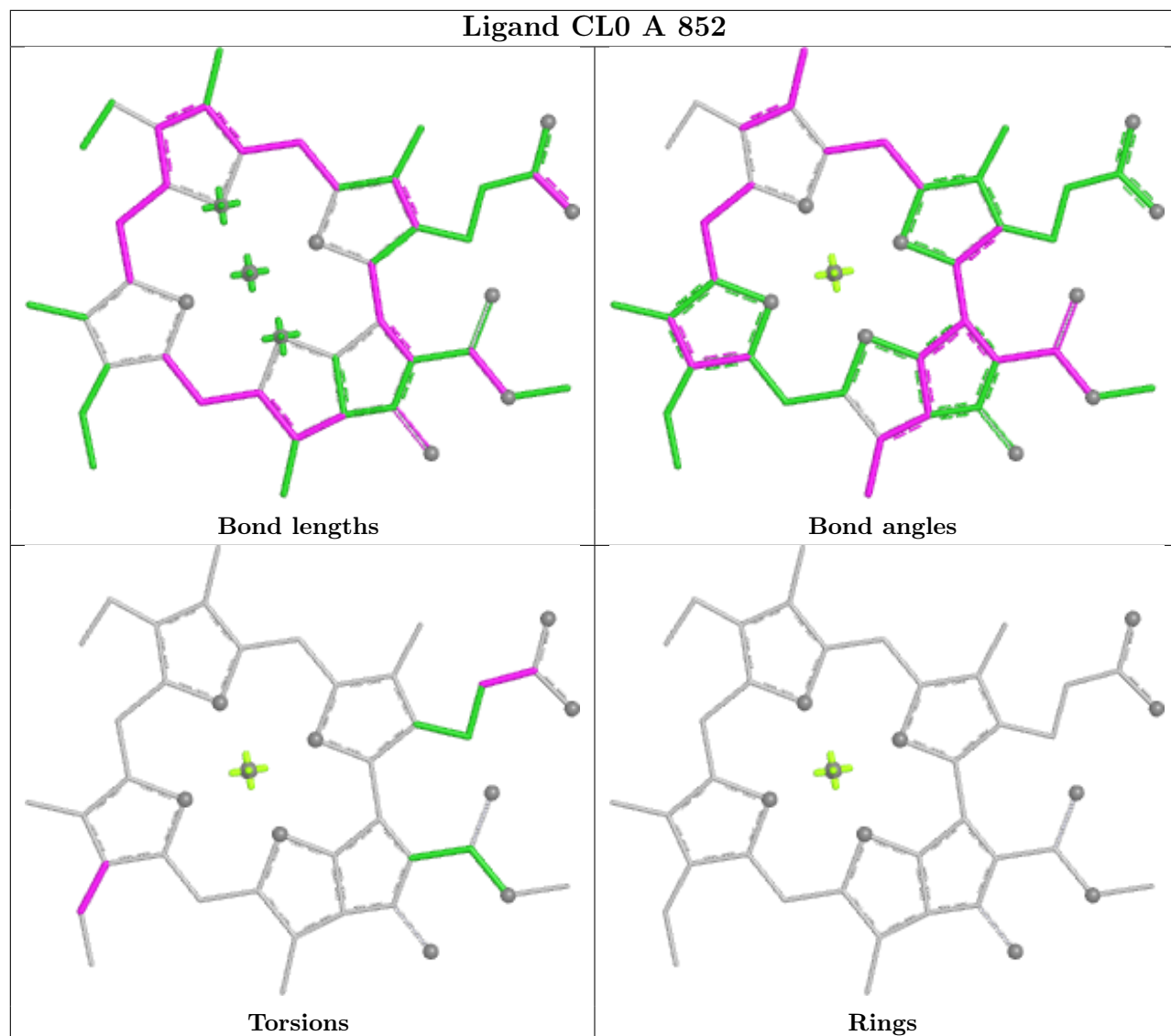
Rings



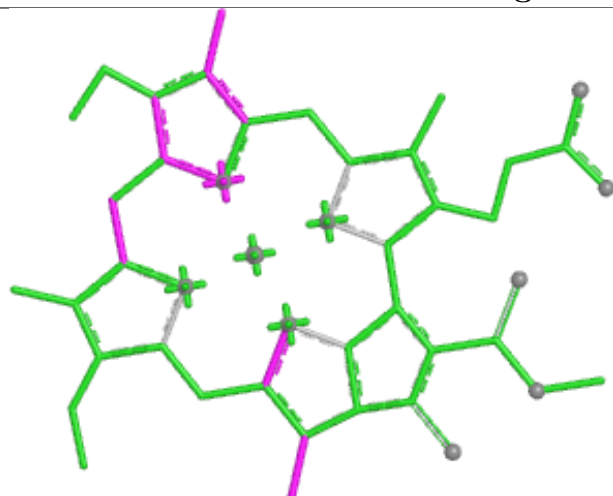




## Ligand CL0 A 852



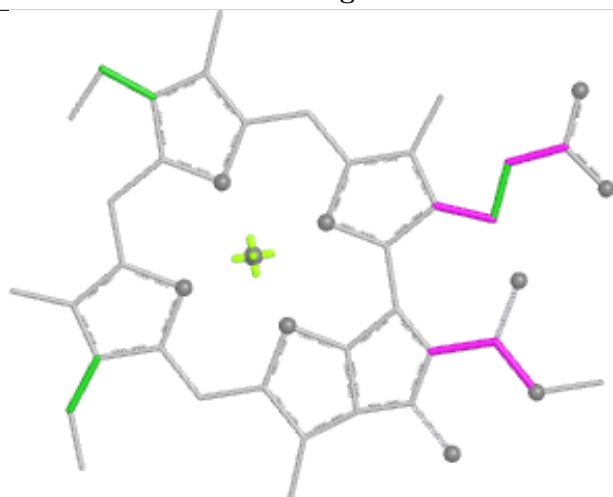
## Ligand CLA w 203



Bond lengths



Bond angles

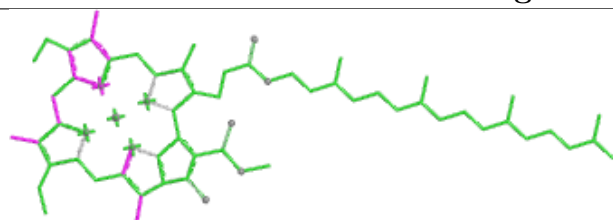


Torsions

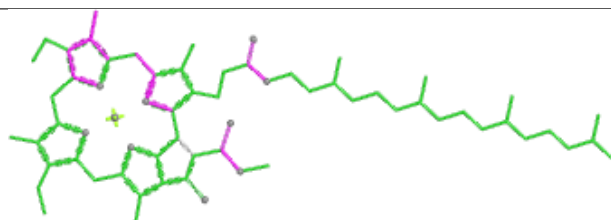


Rings

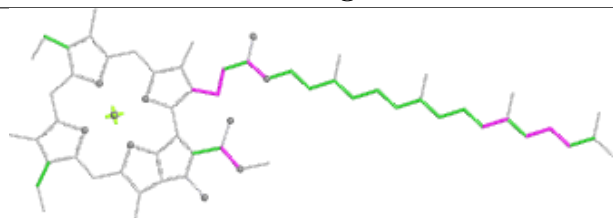
## Ligand CLA B 829



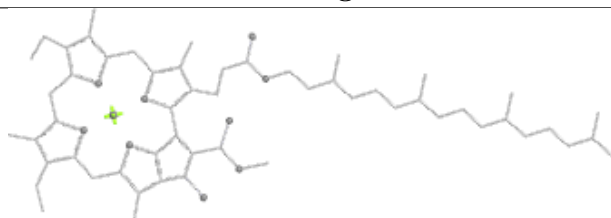
Bond lengths



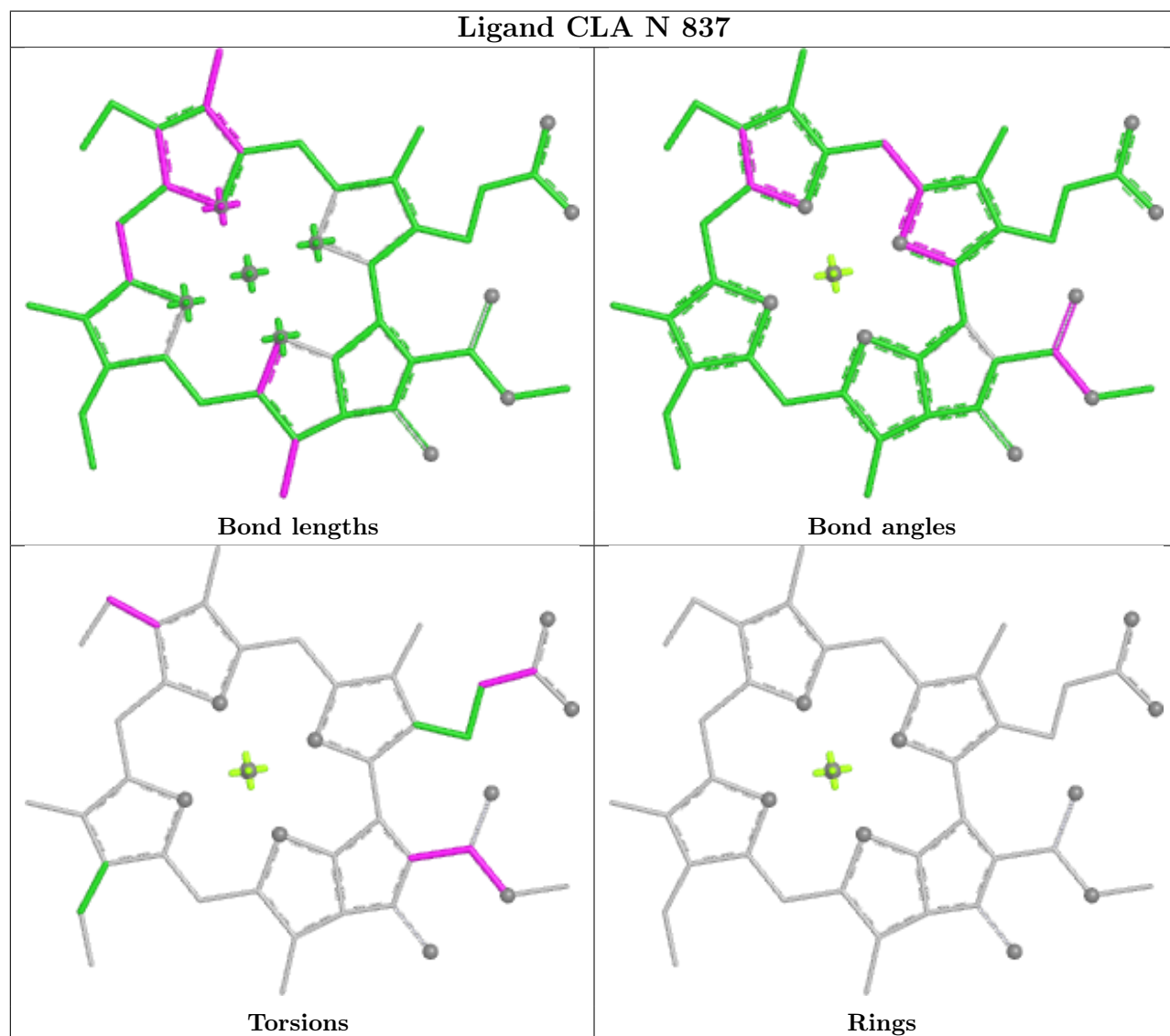
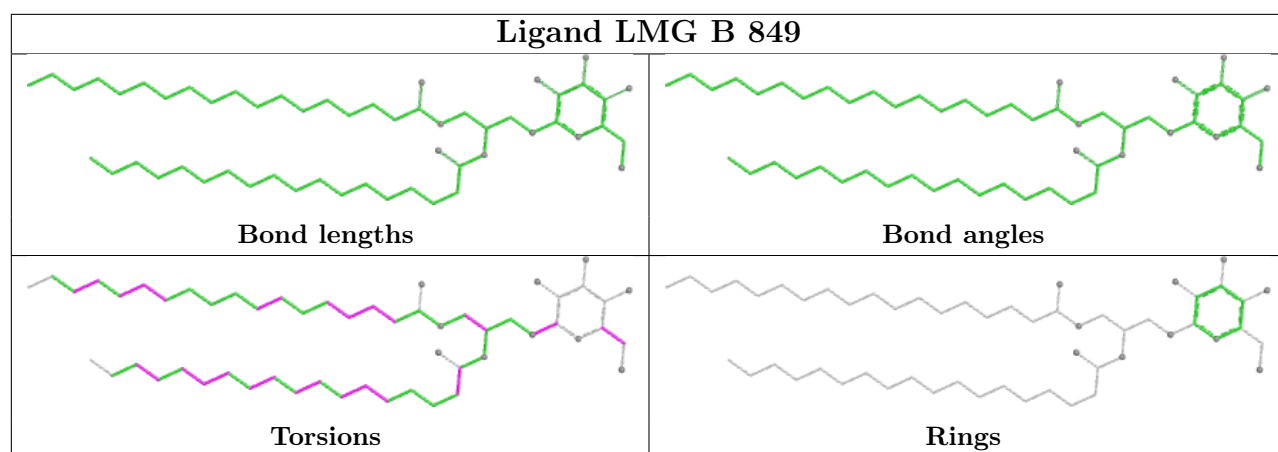
Bond angles



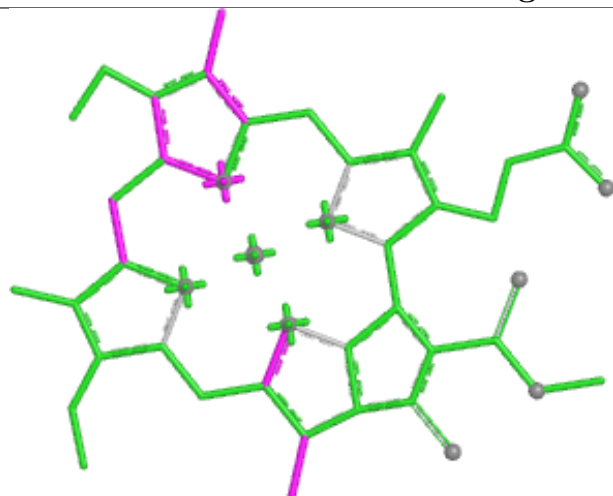
Torsions



Rings



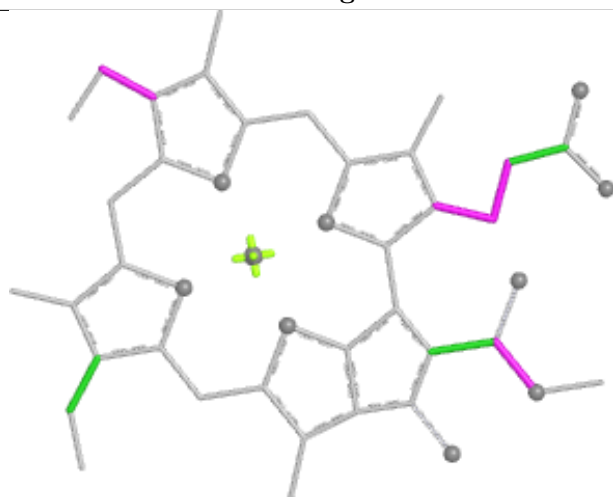
## Ligand CLA a 840



Bond lengths



Bond angles

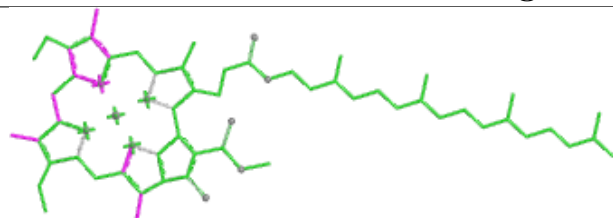


Torsions

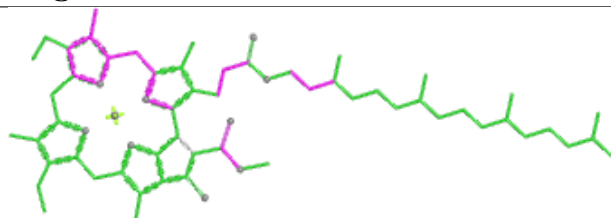


Rings

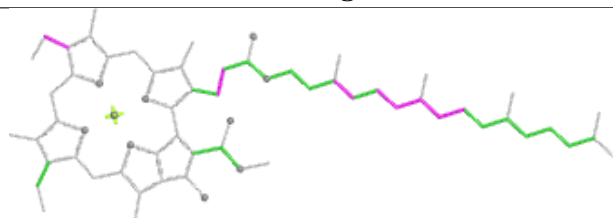
## Ligand CLA g 852



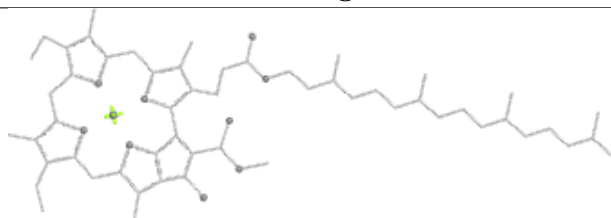
Bond lengths



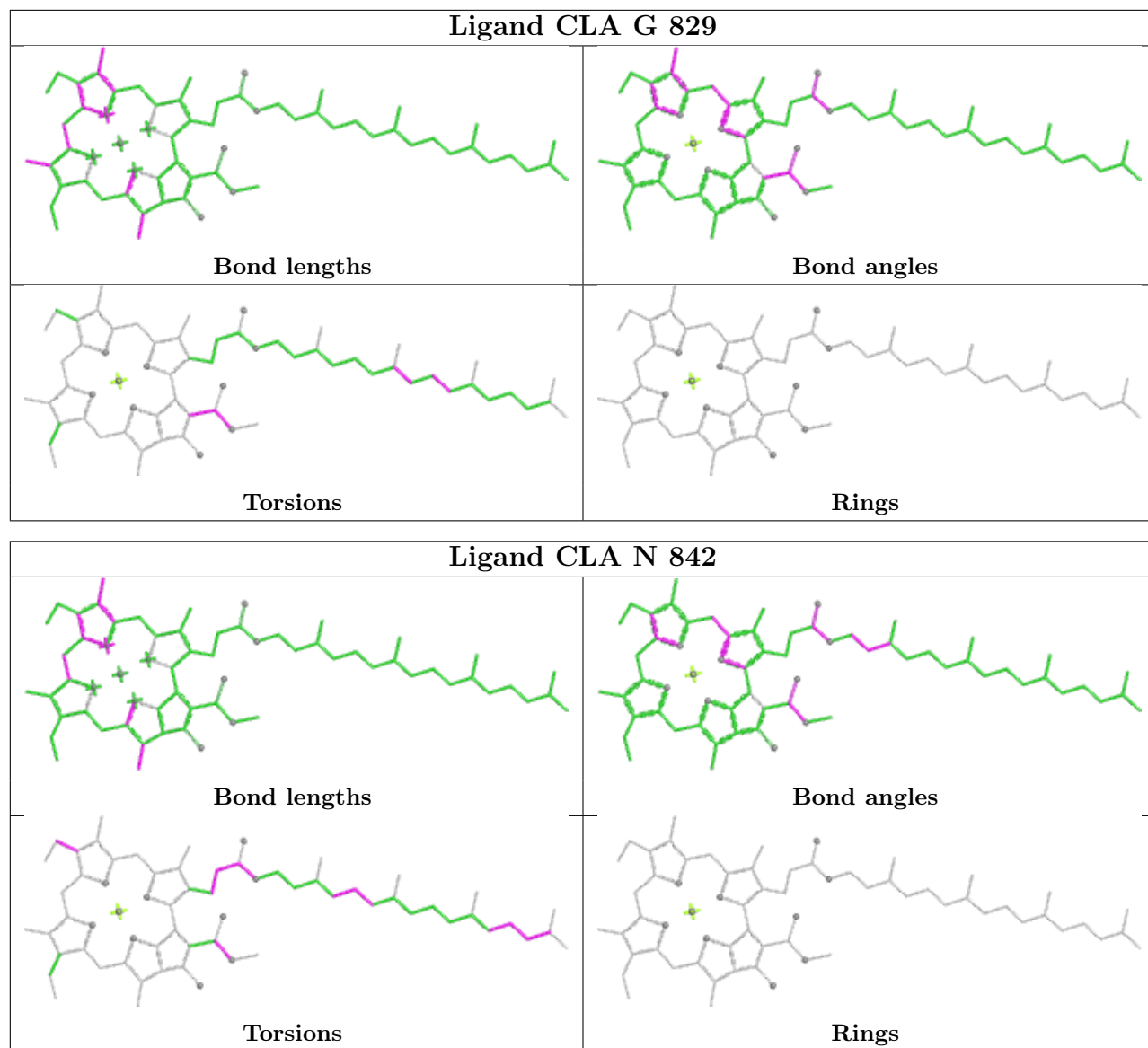
Bond angles

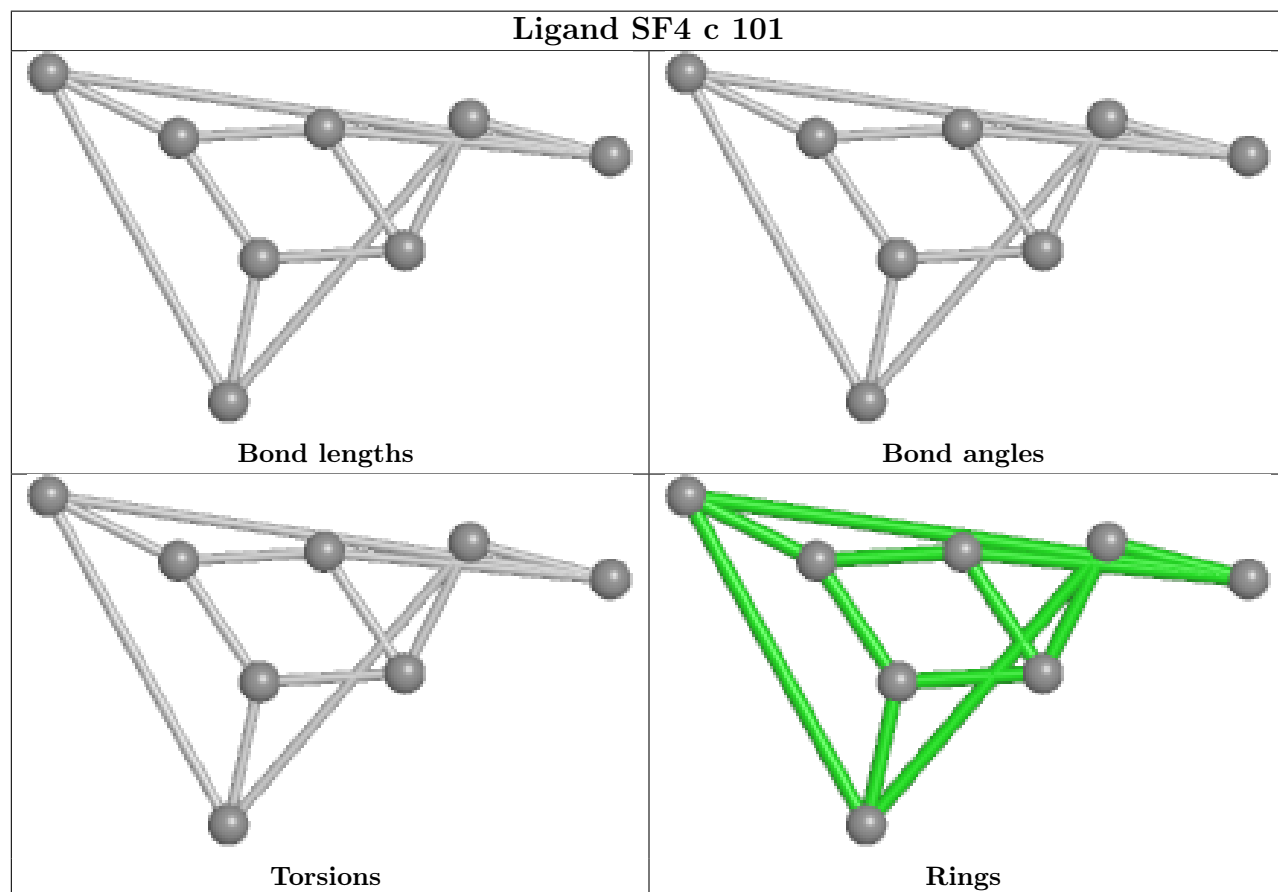
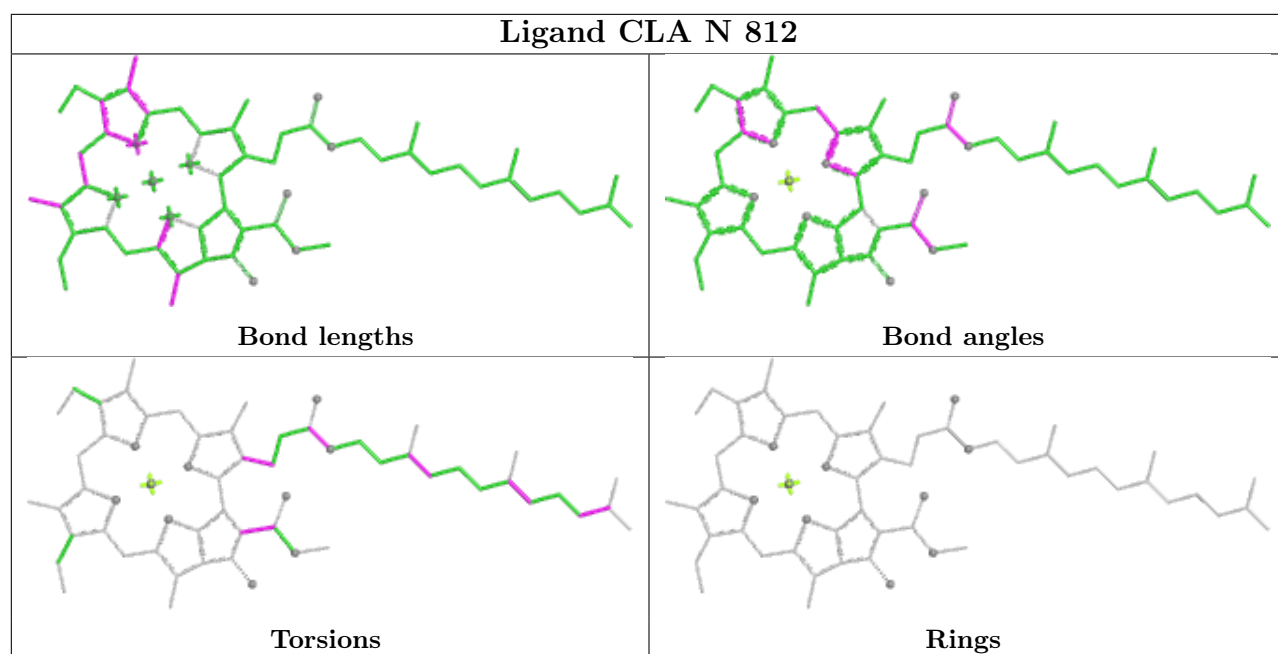


Torsions



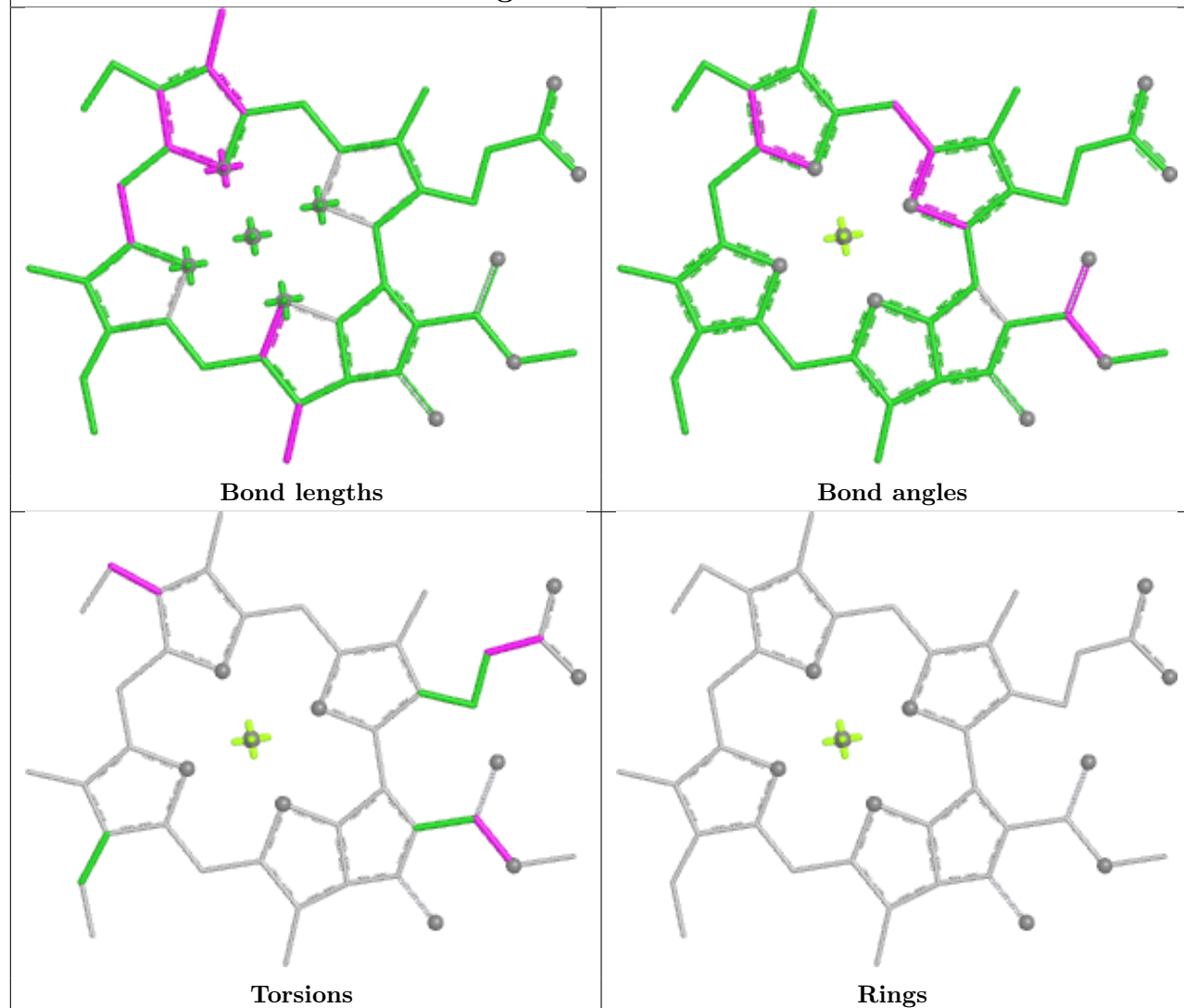
Rings



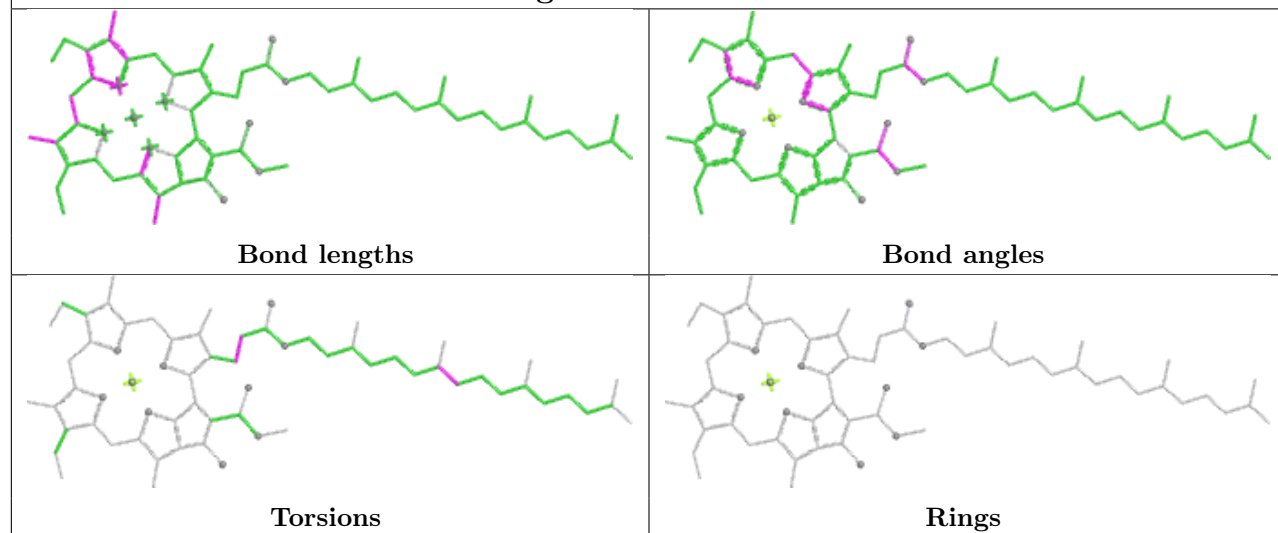


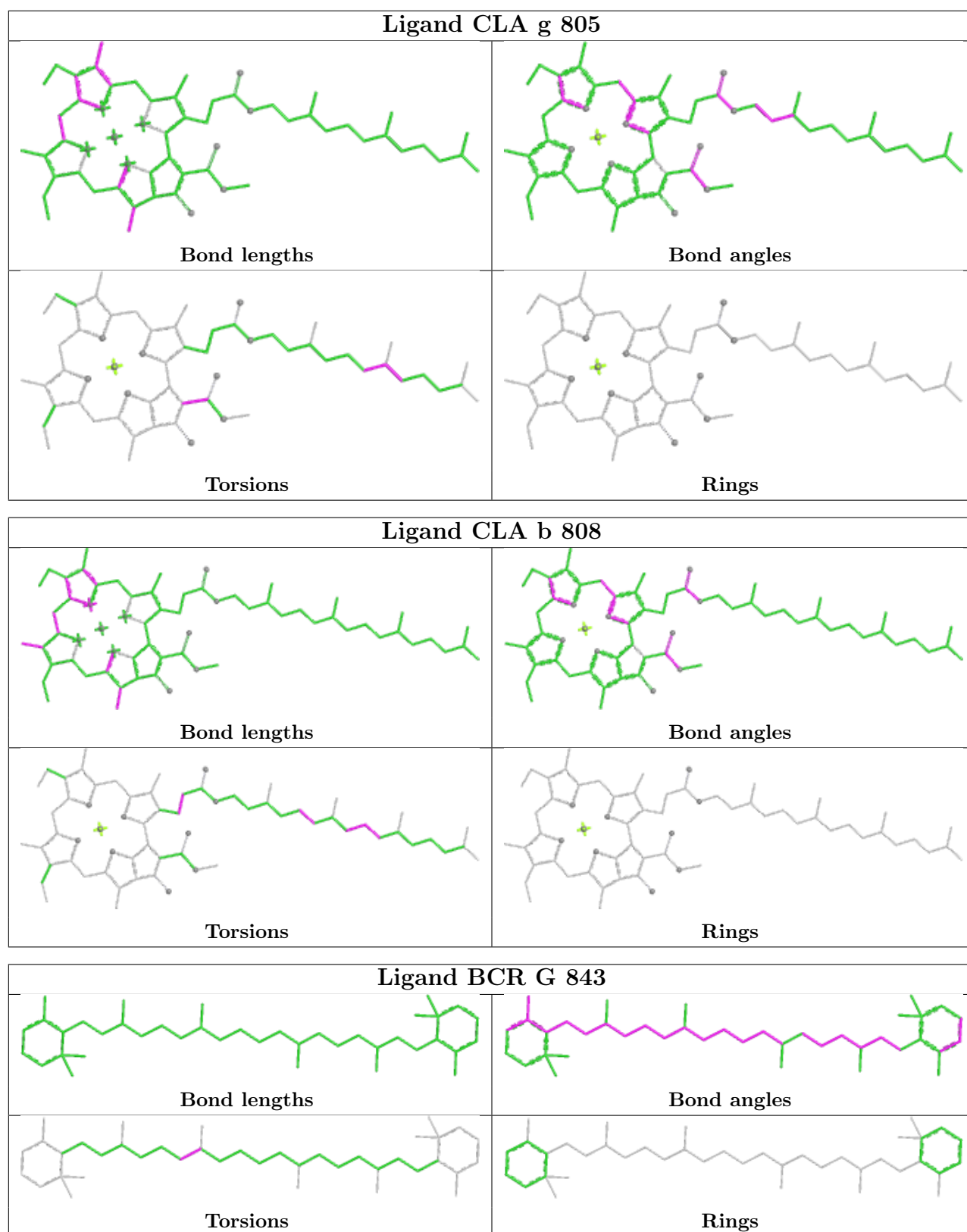


## Ligand CLA a 822

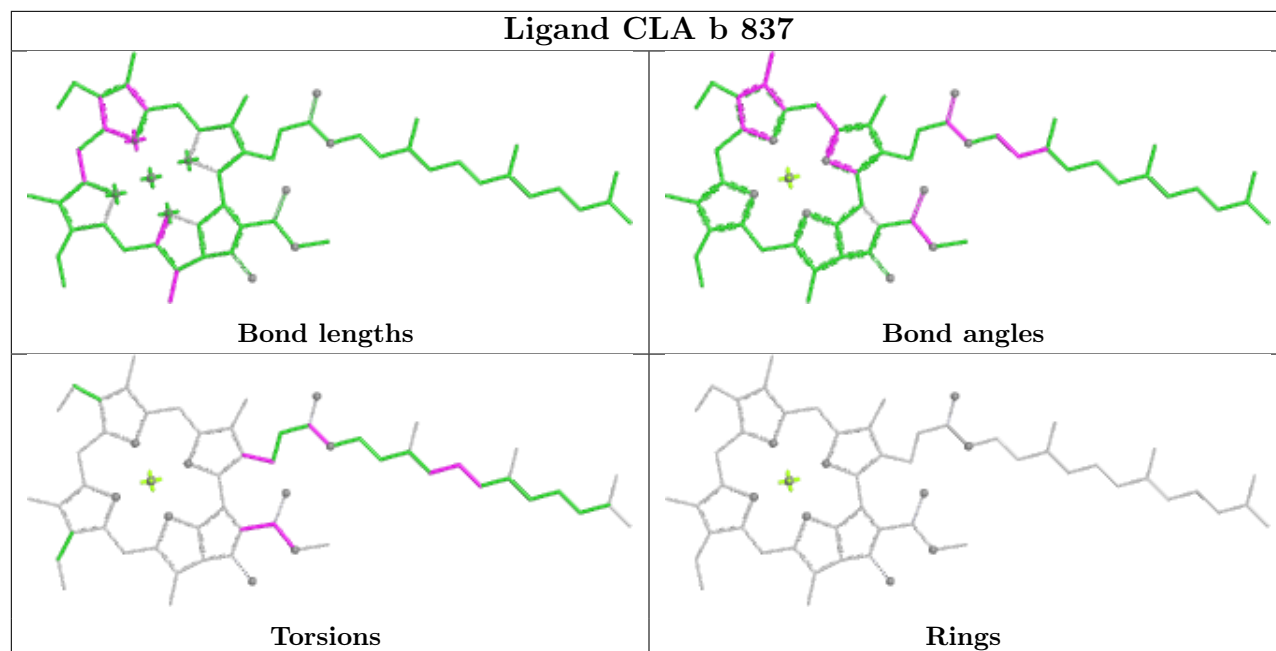


## Ligand CLA a 839

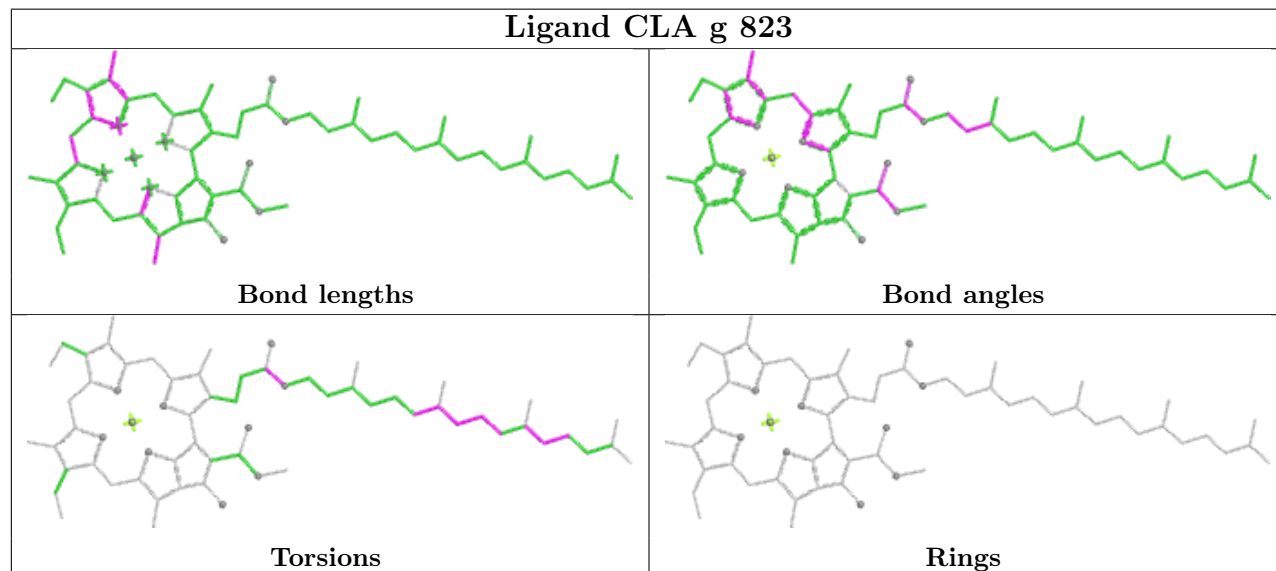


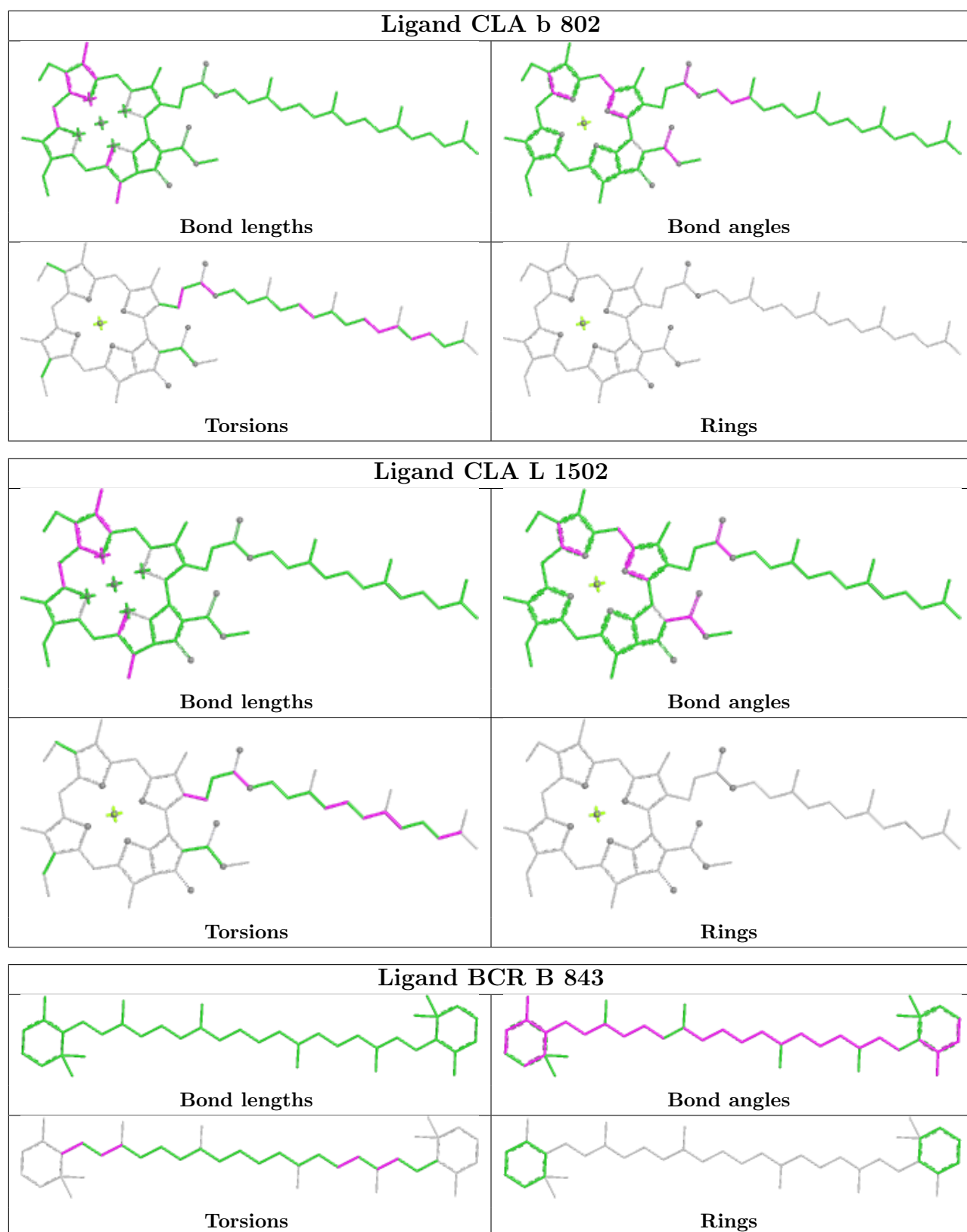


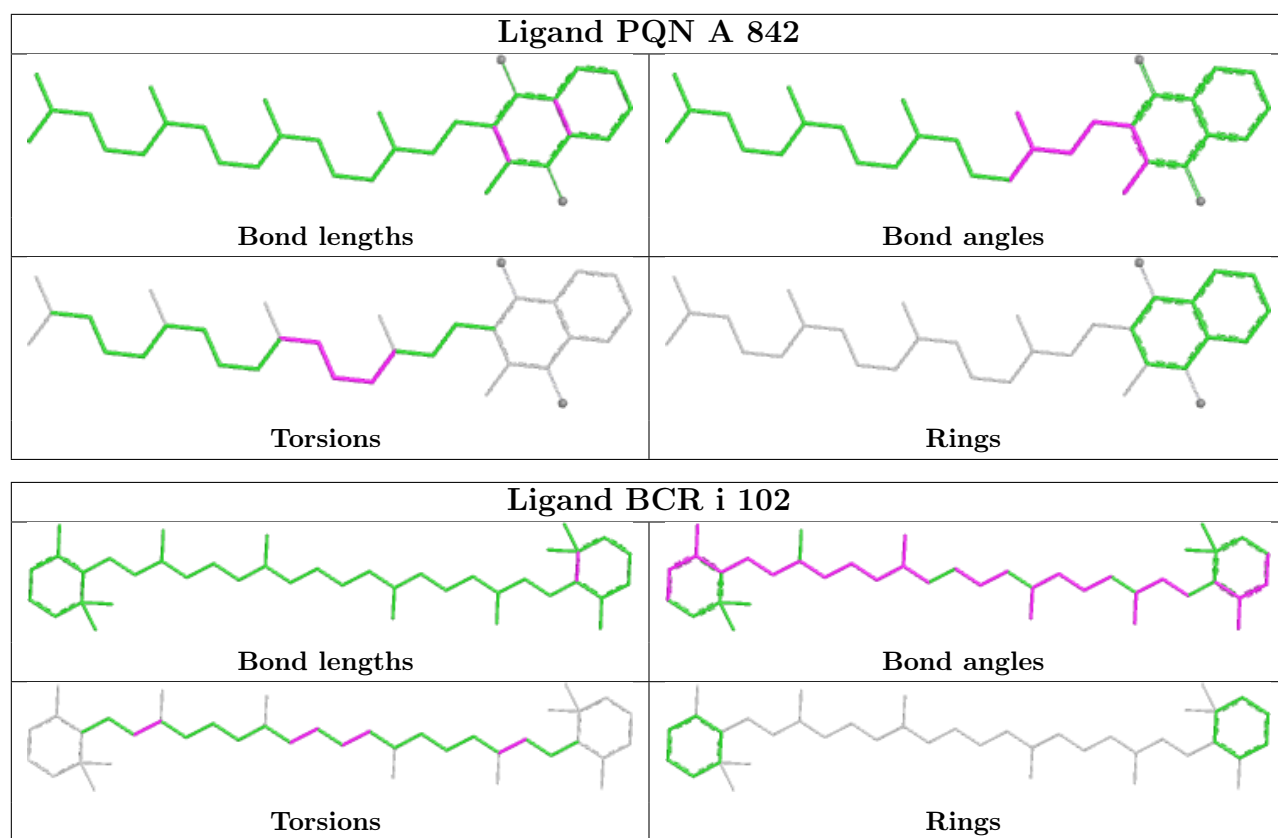
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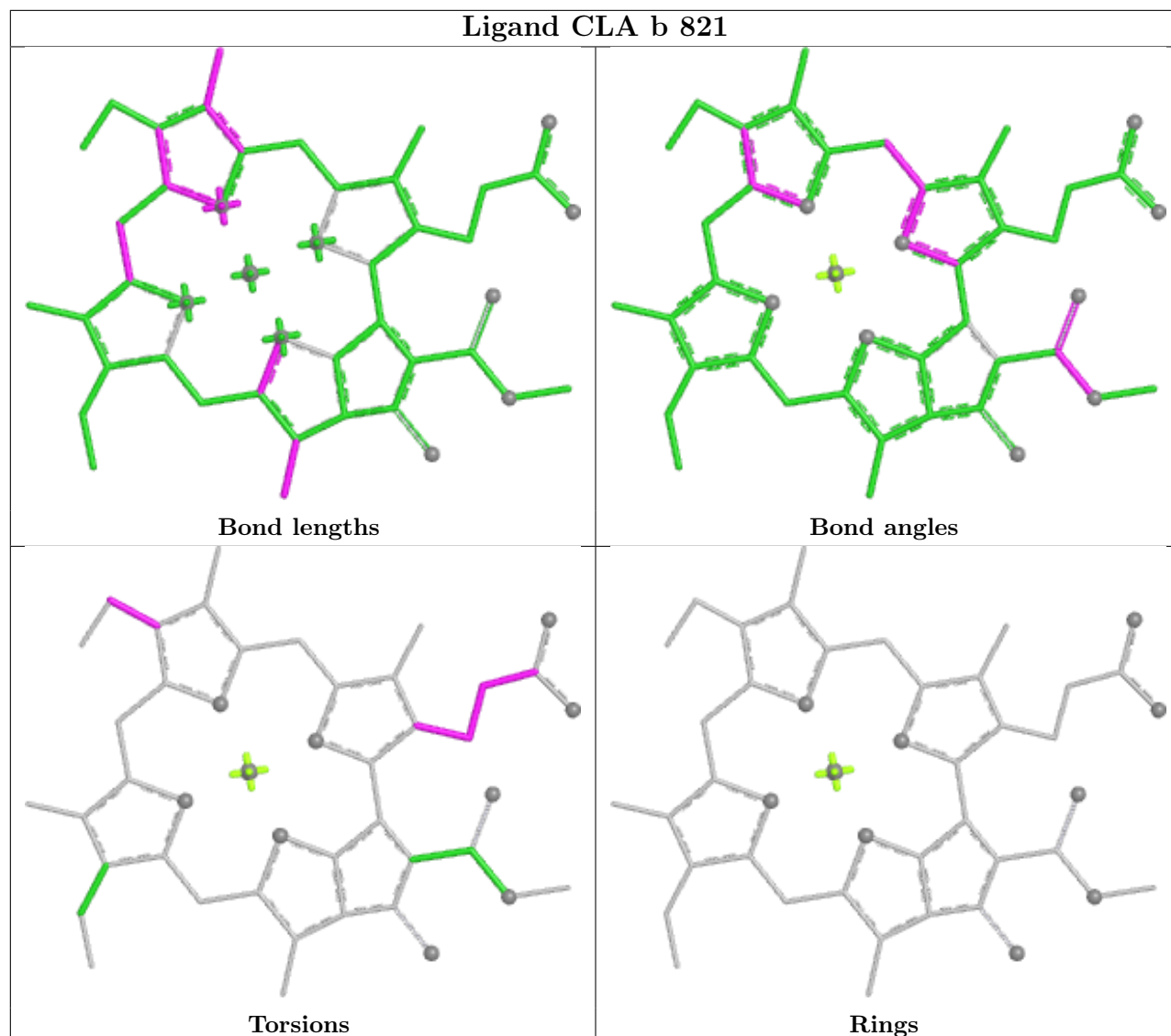
## Ligand CLA g 823



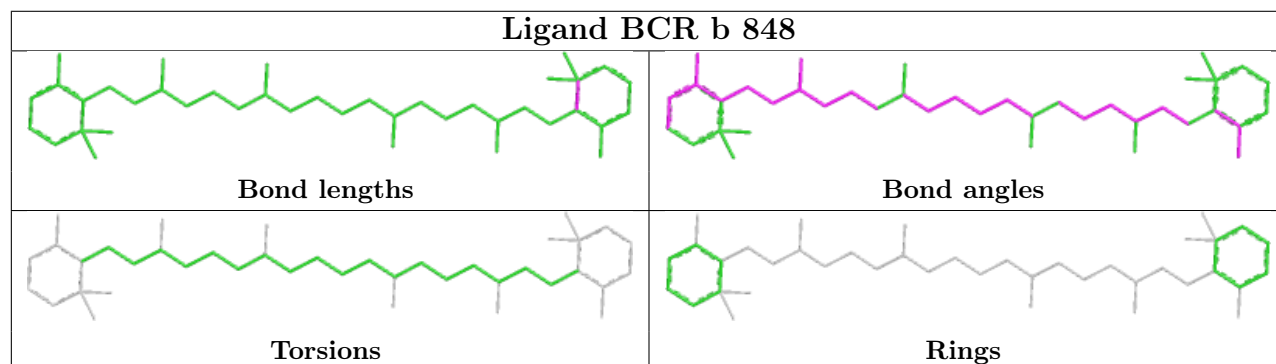




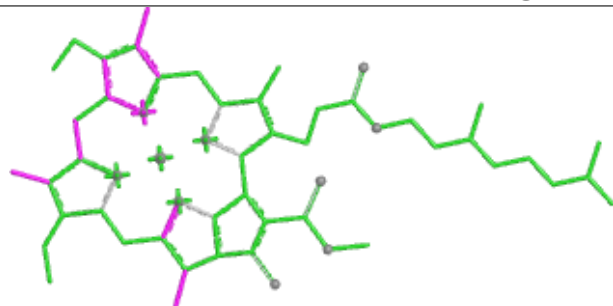
## Ligand CLA b 821



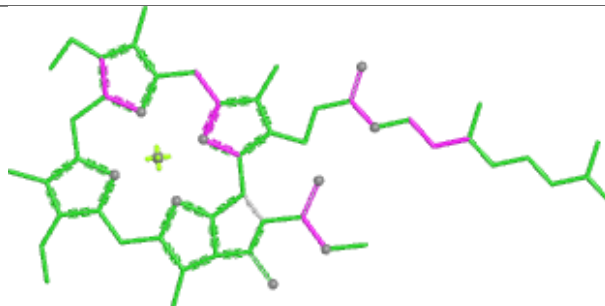
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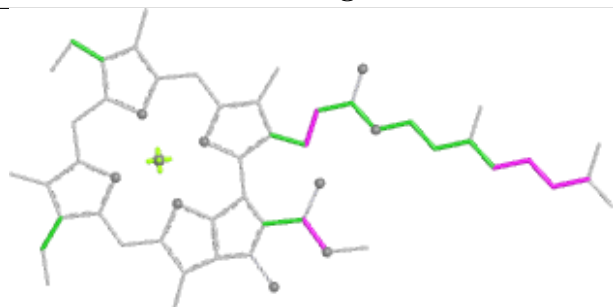
## Ligand CLA n 852



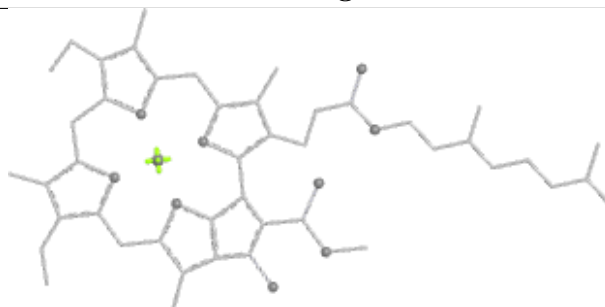
Bond lengths



Bond angles

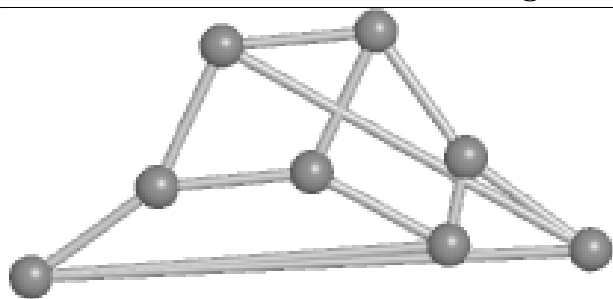


Torsions

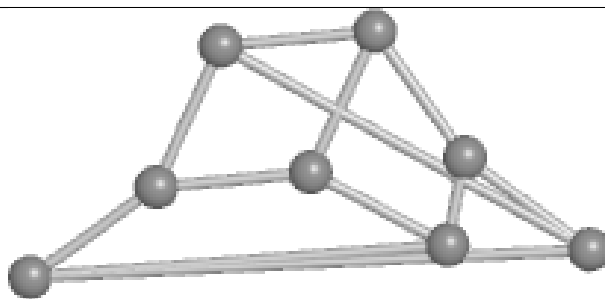


Rings

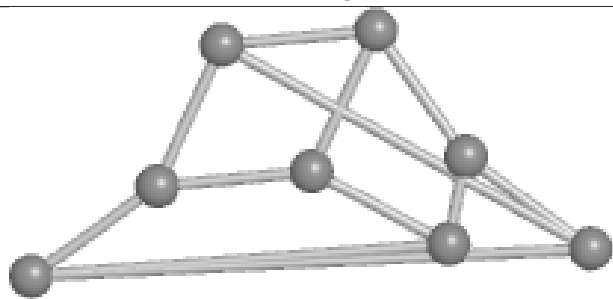
## Ligand SF4 C 102



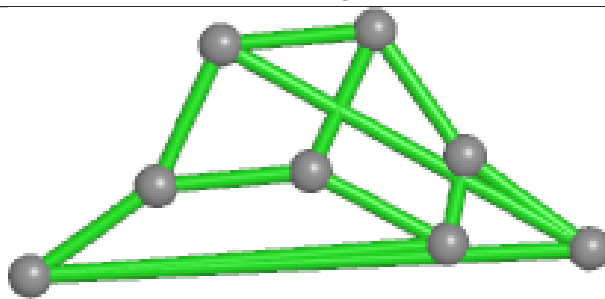
Bond lengths



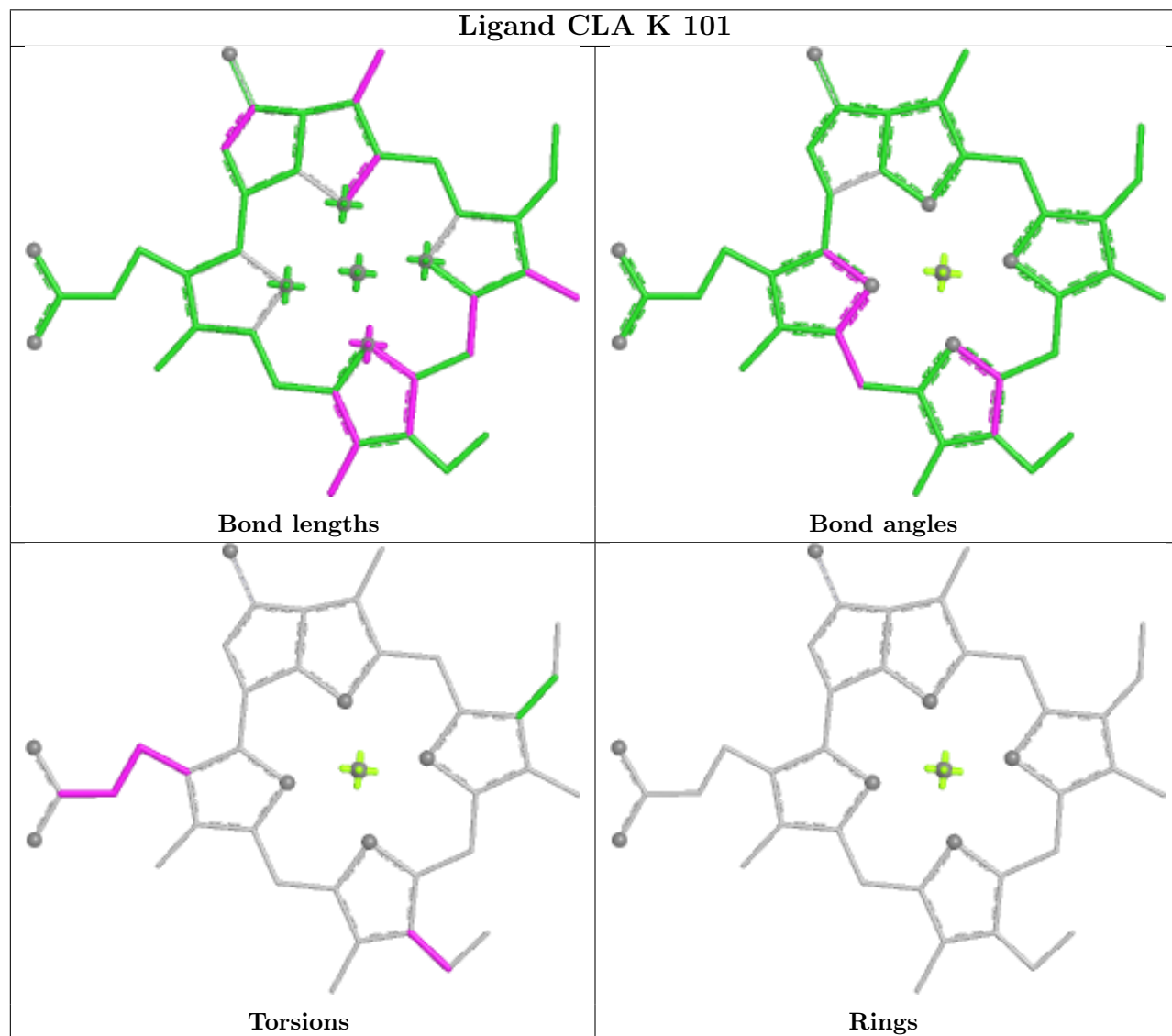
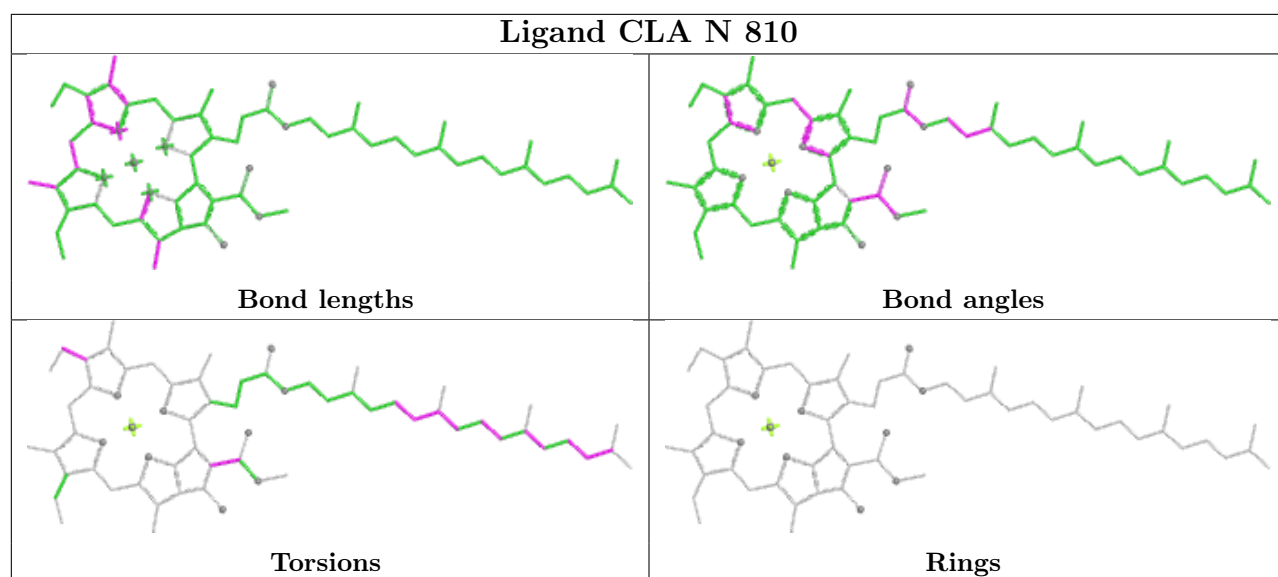
Bond angles



Torsions

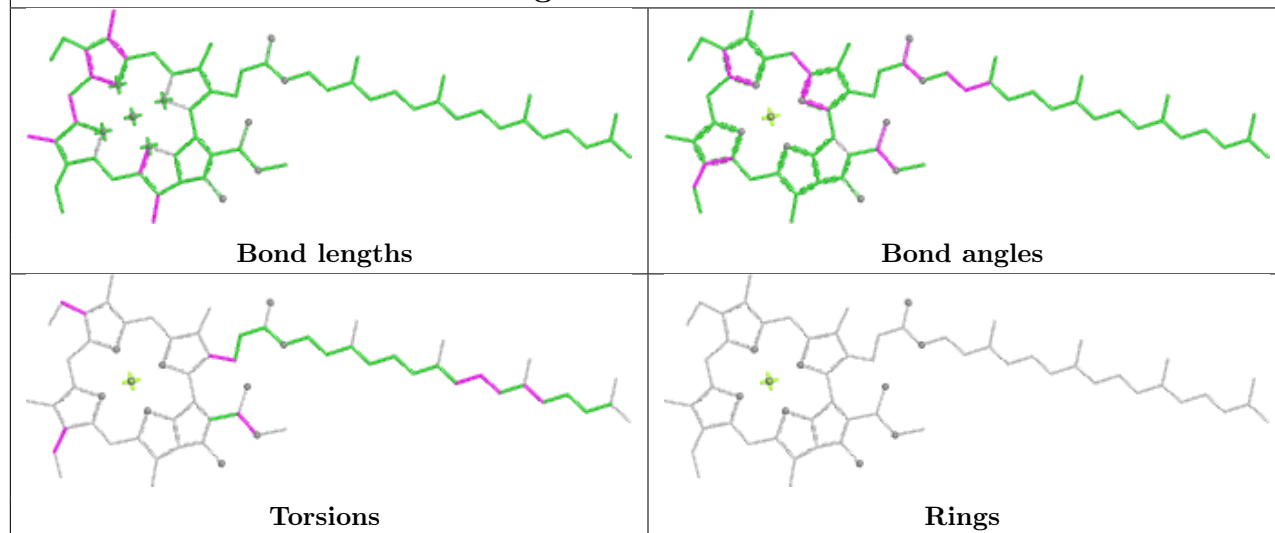


Rings

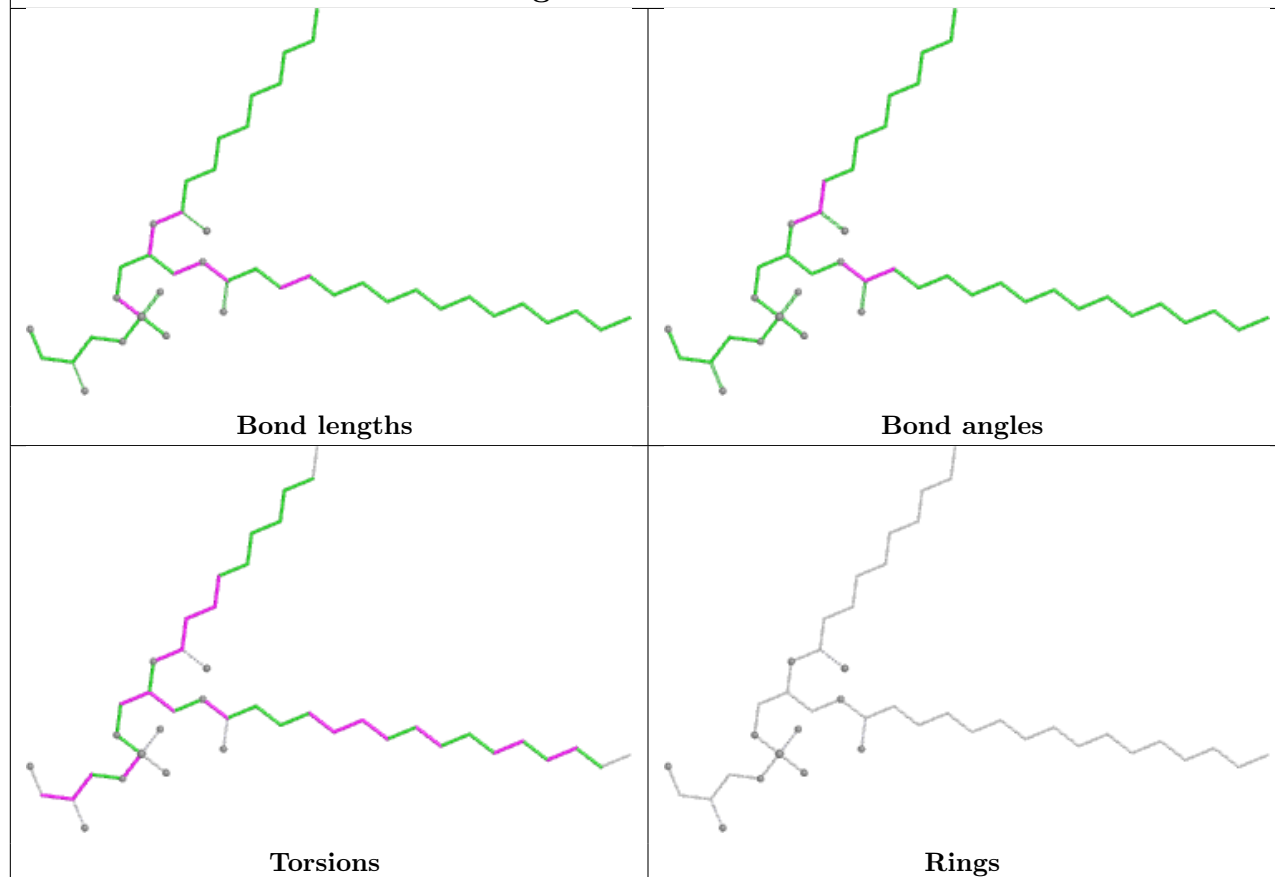


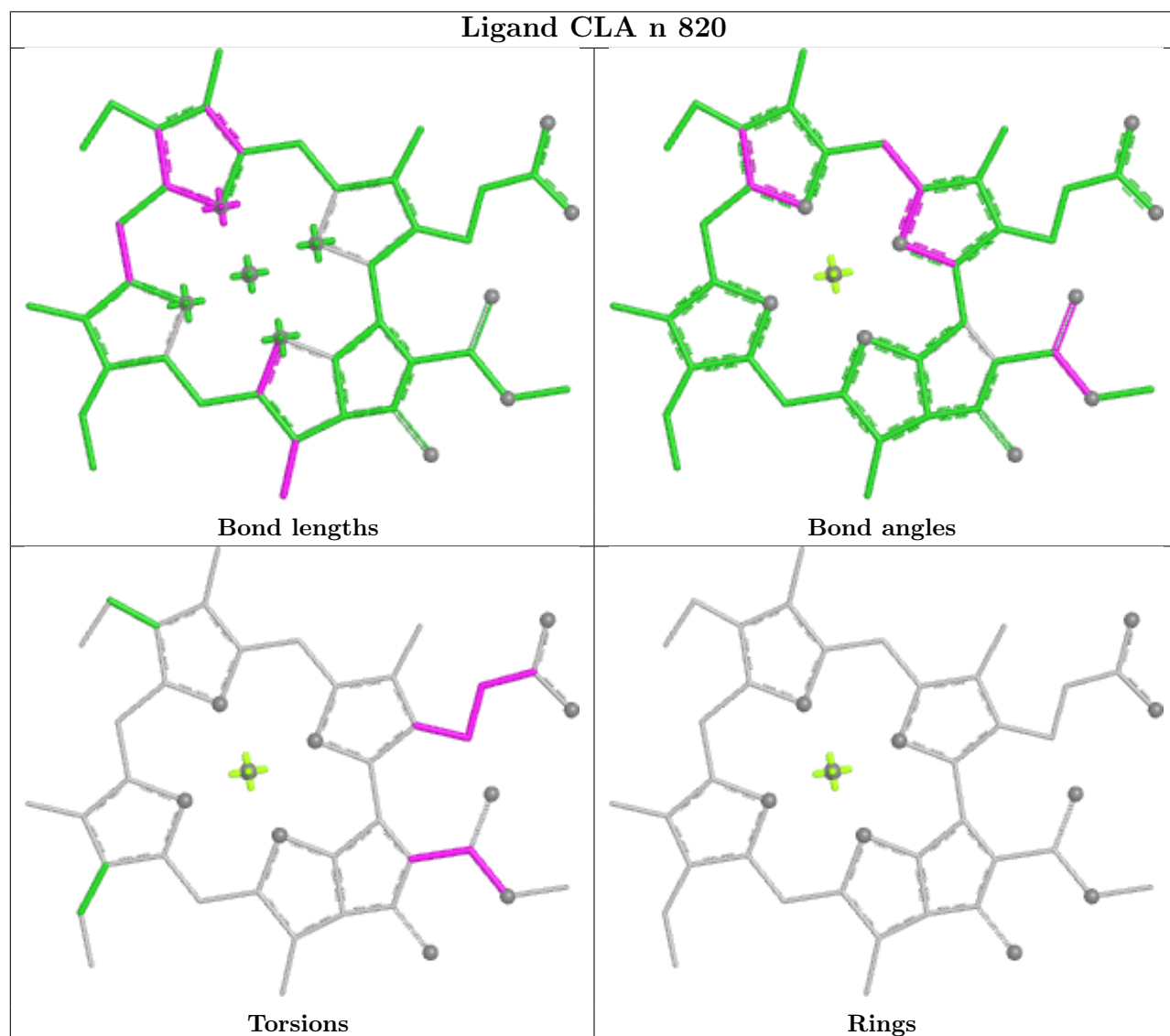
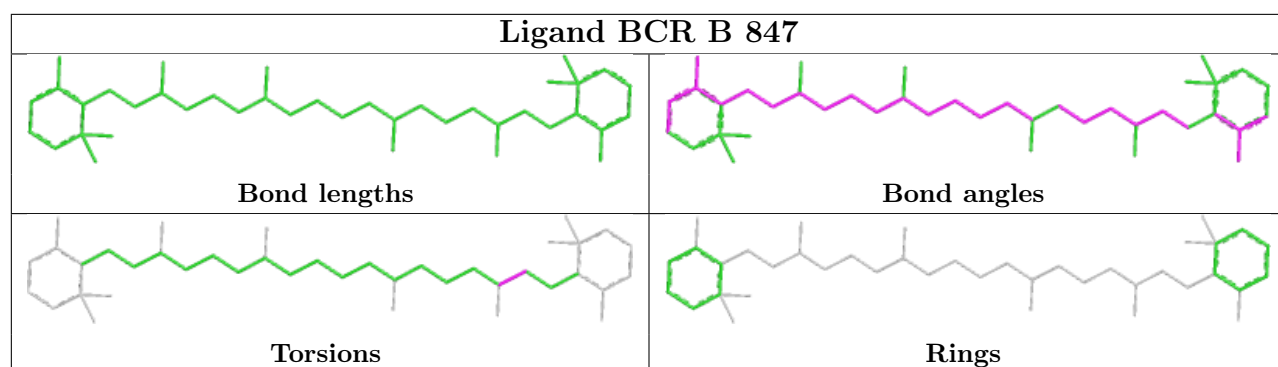


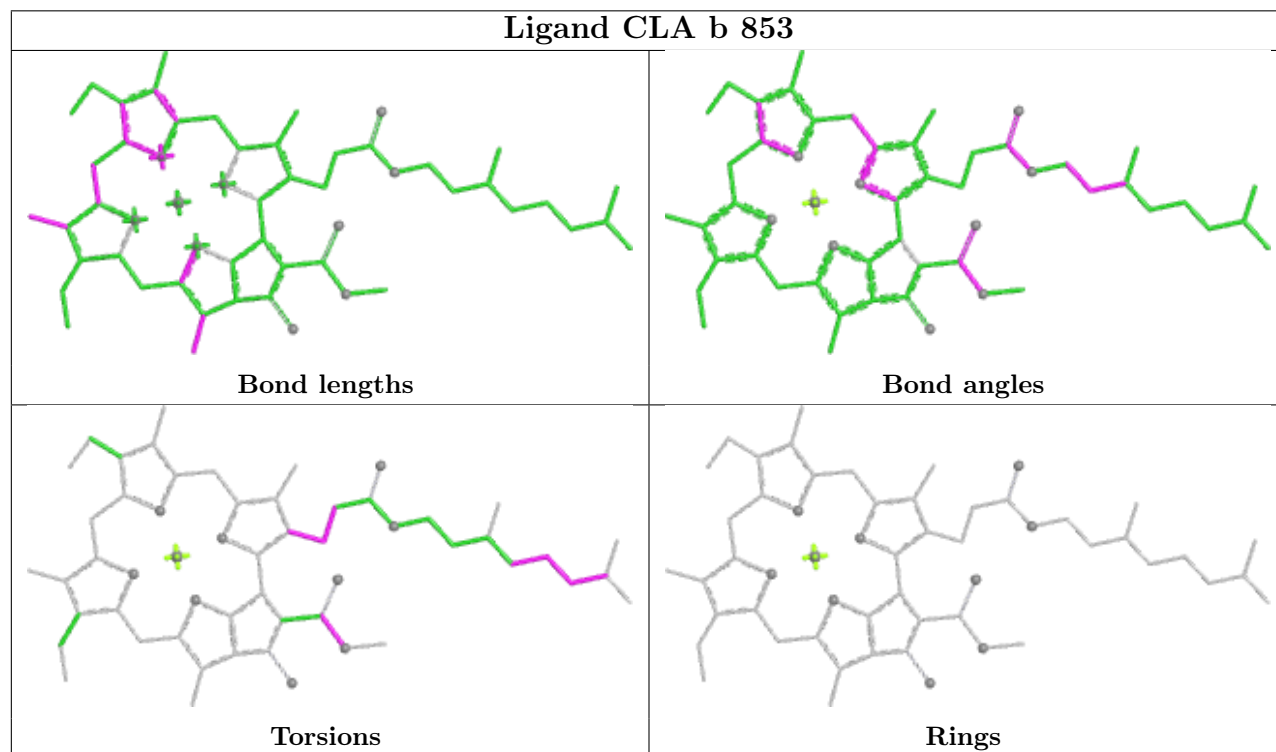
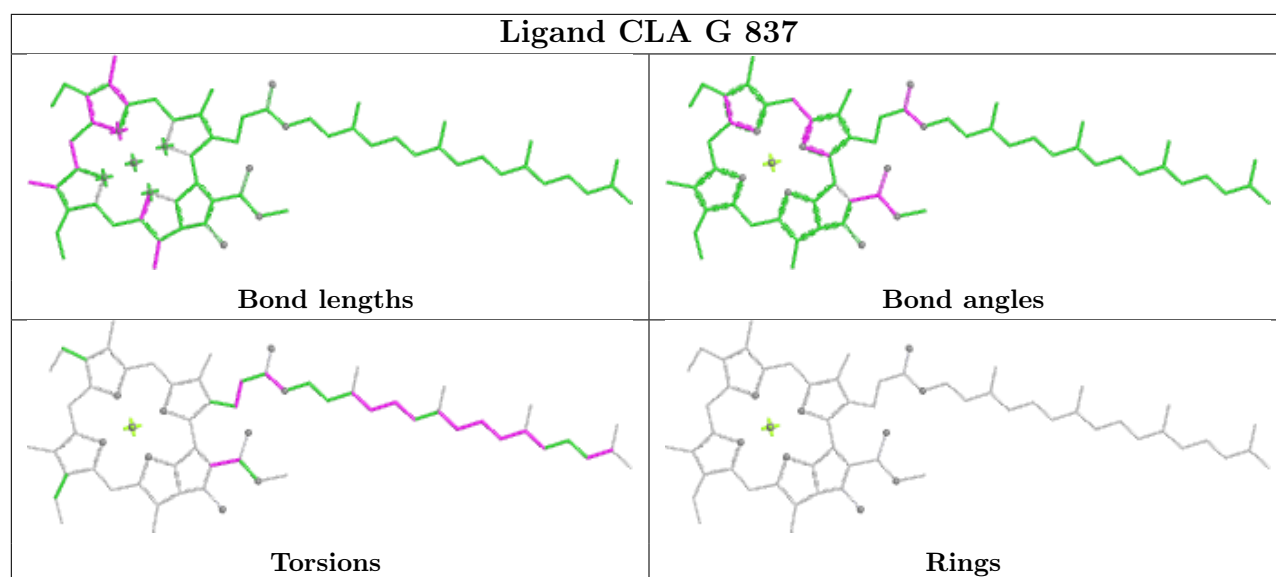
## Ligand CLA b 805

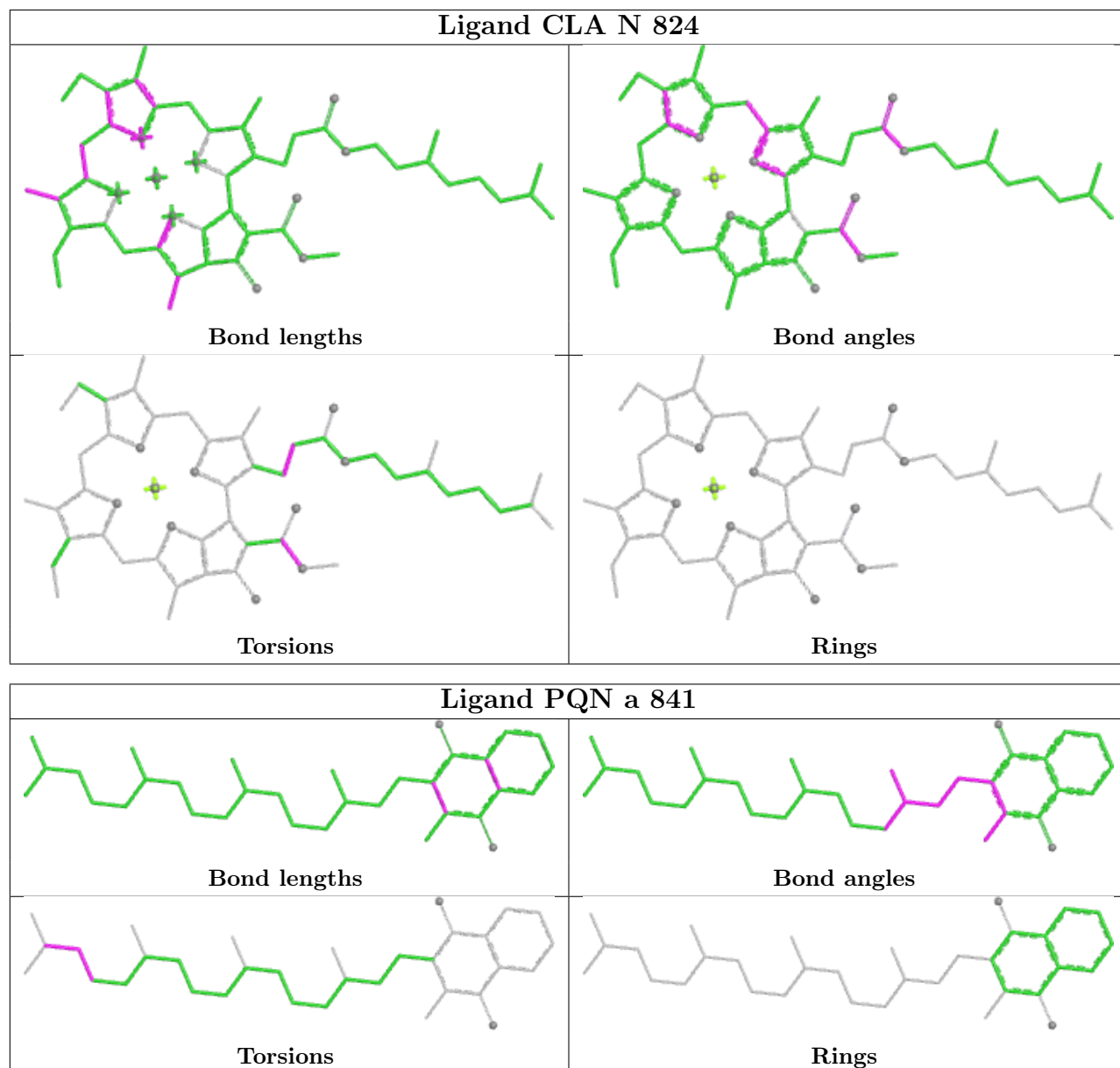


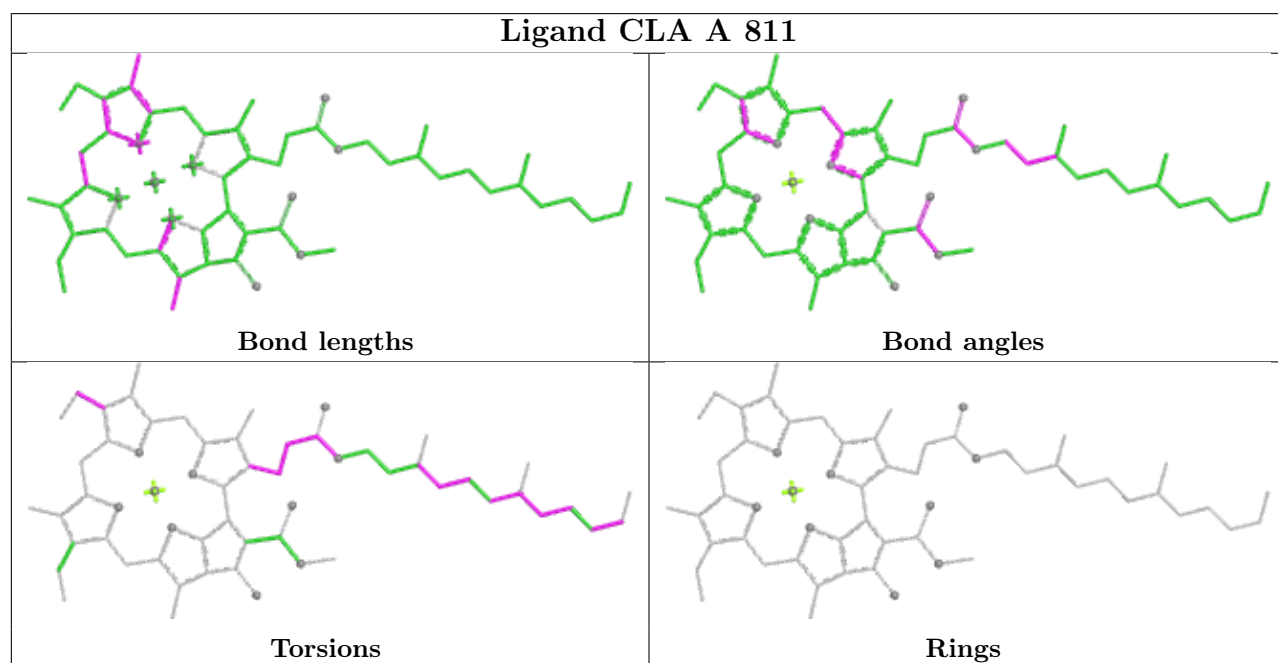
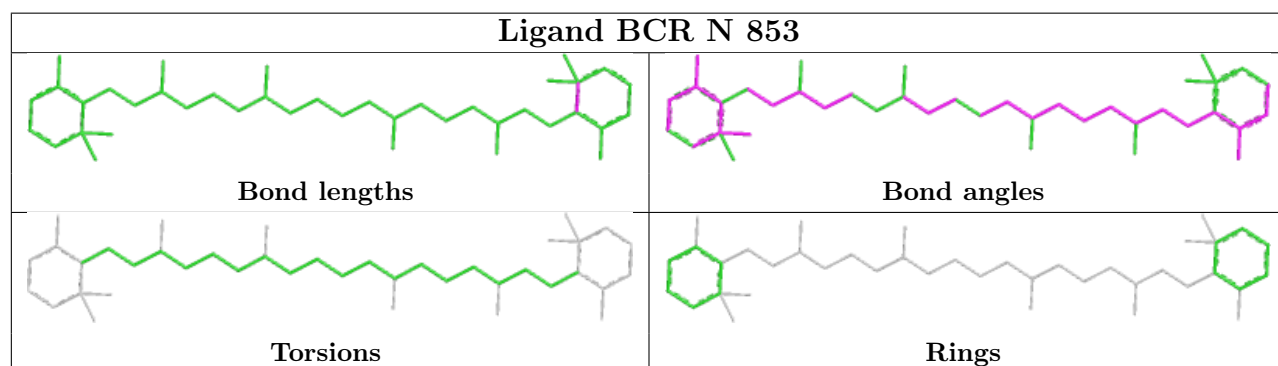
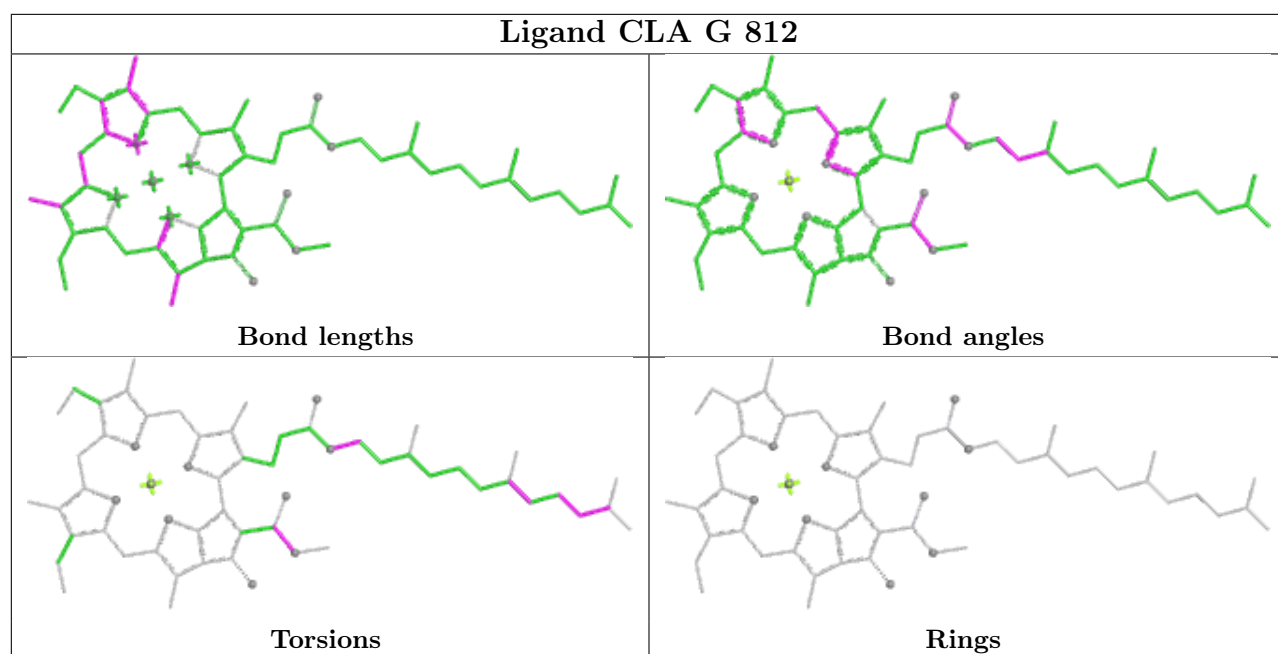
## Ligand LHG S 202

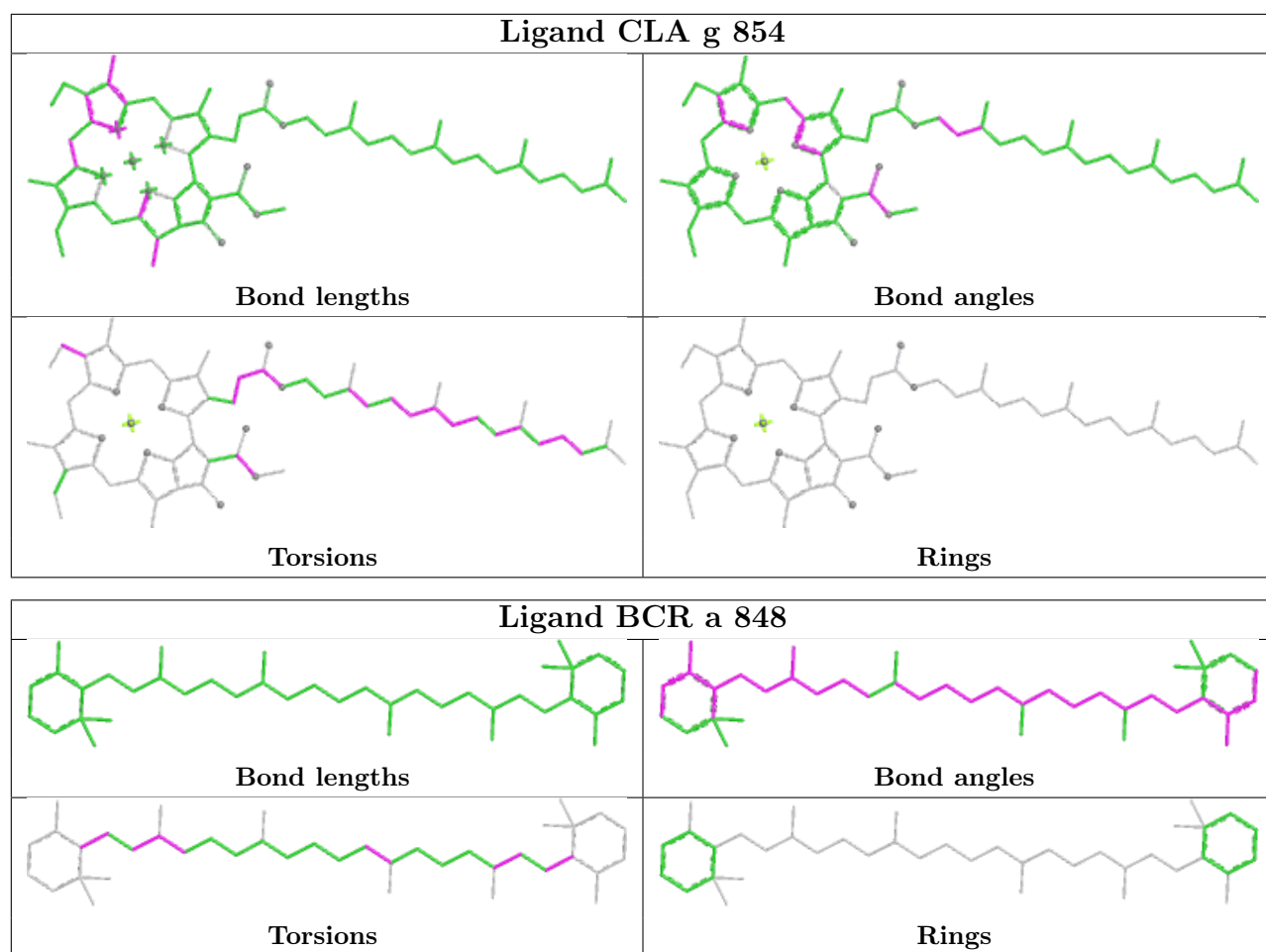




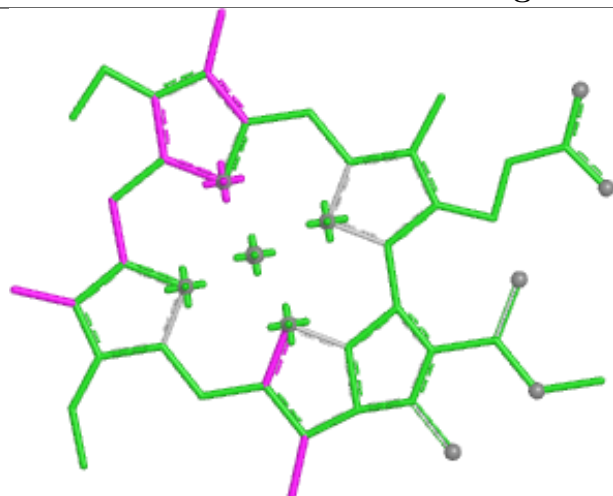




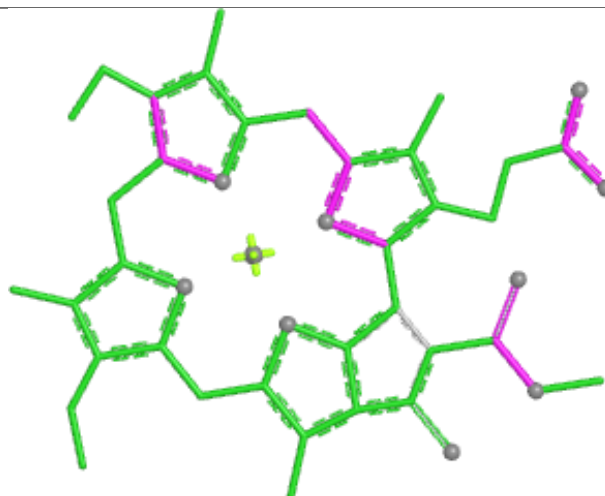




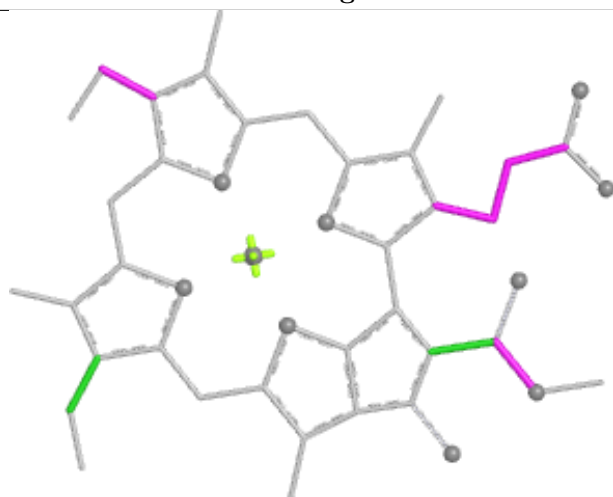
## Ligand CLA A 855



Bond lengths



Bond angles

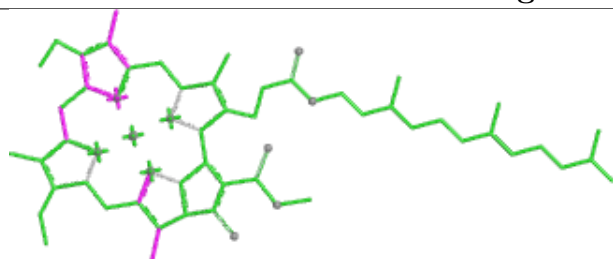


Torsions

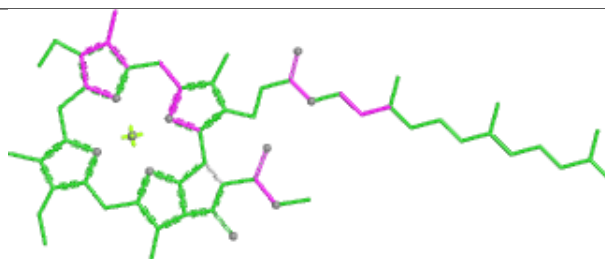


Rings

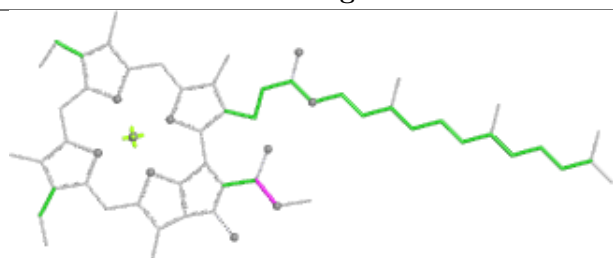
## Ligand CLA n 836



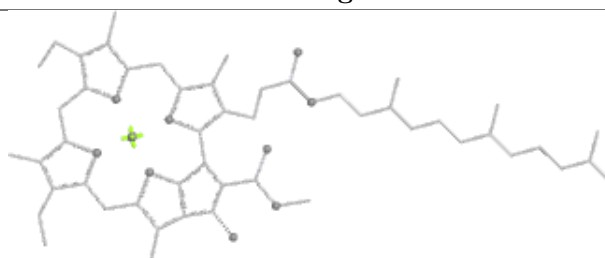
Bond lengths



Bond angles

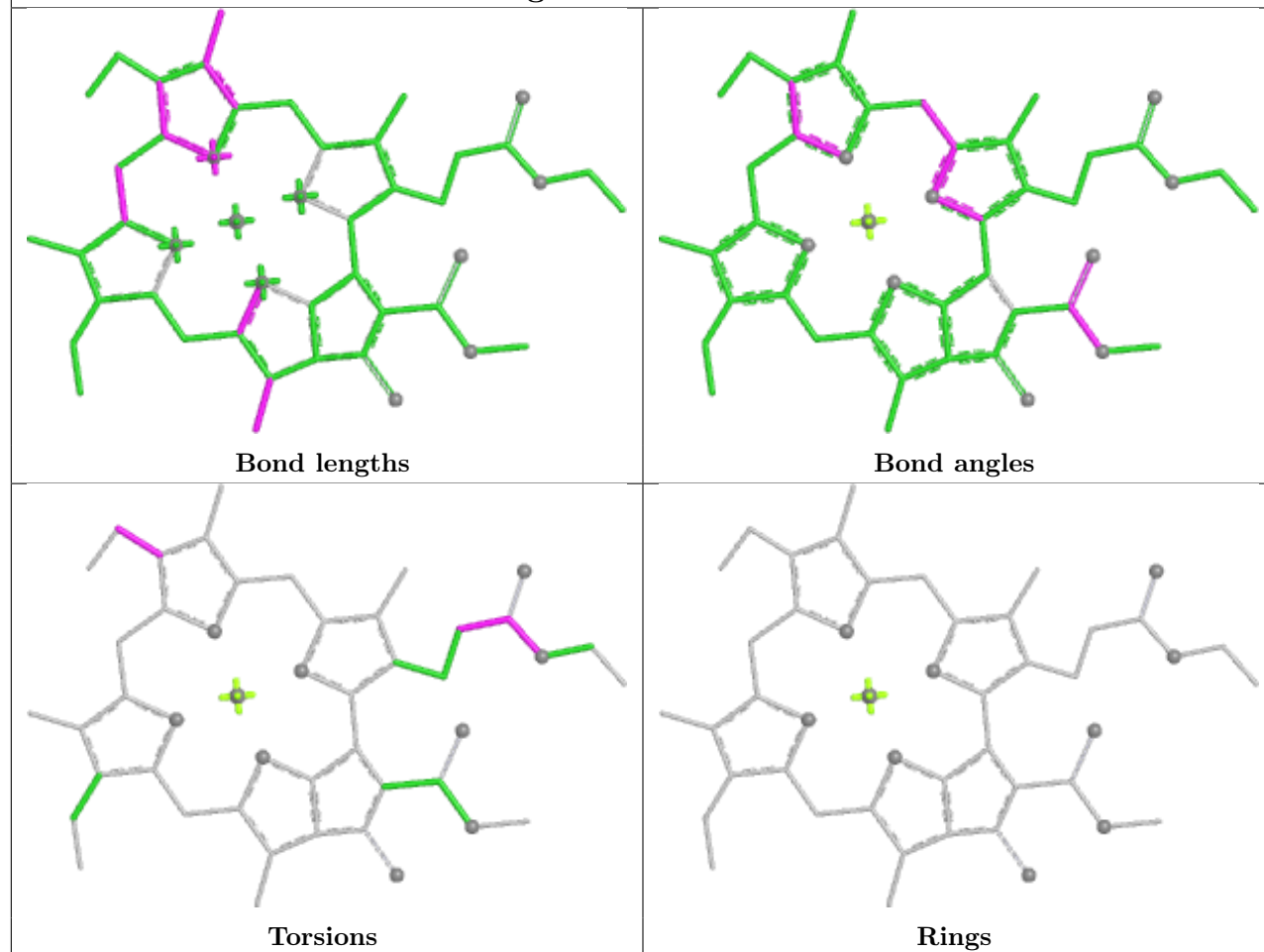


Torsions

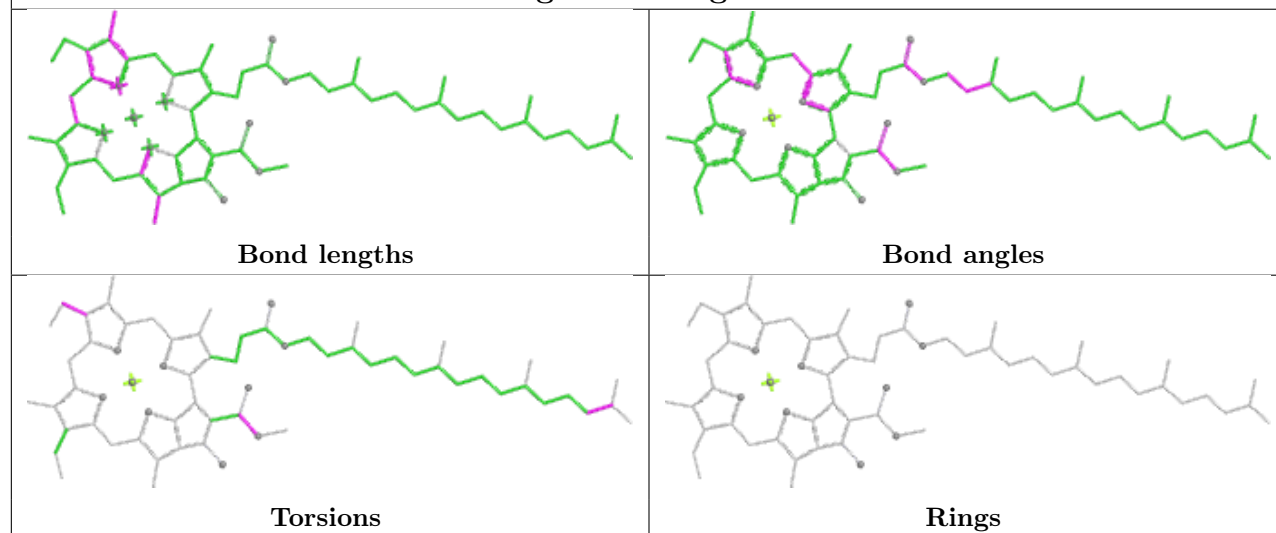


Rings

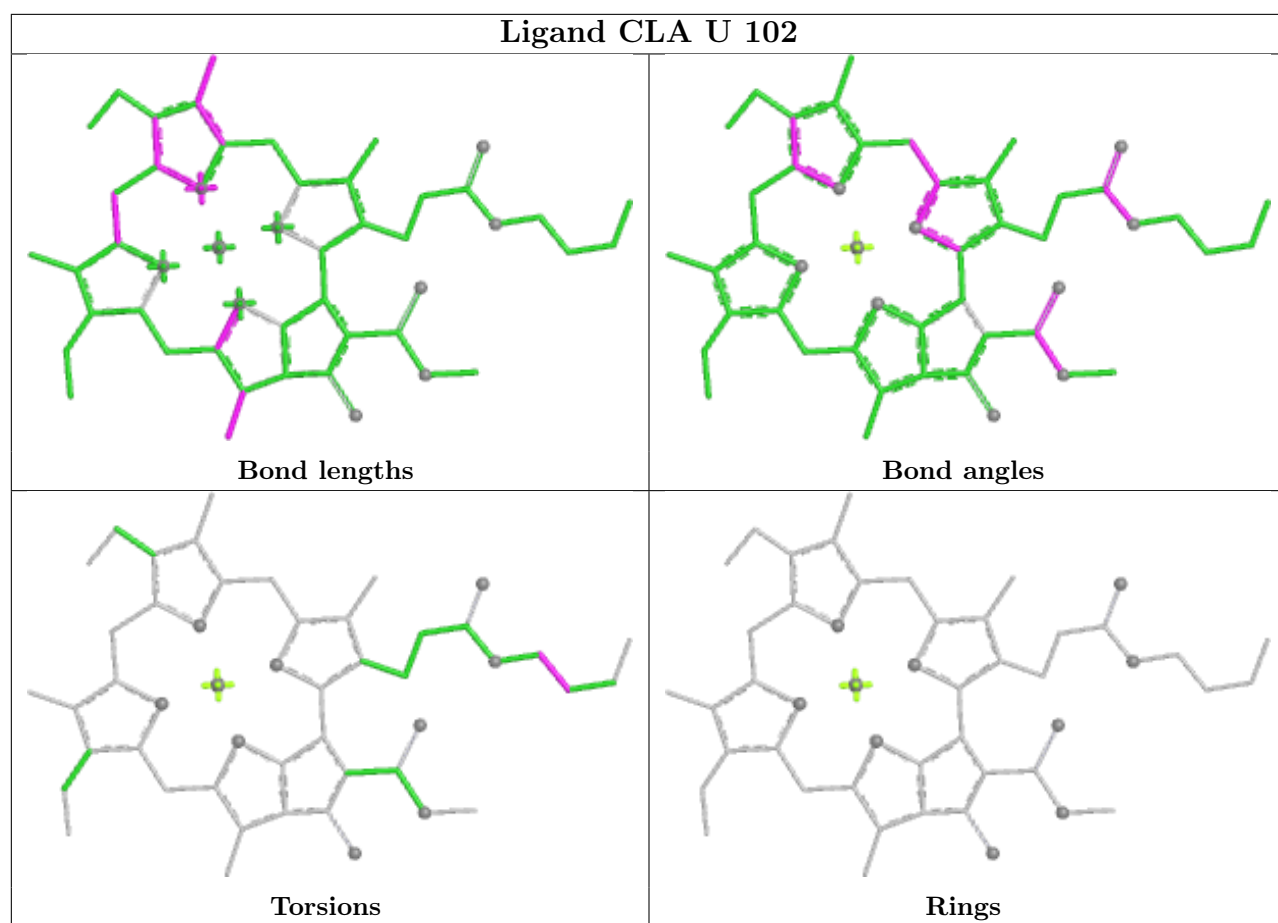
## Ligand CLA B 839

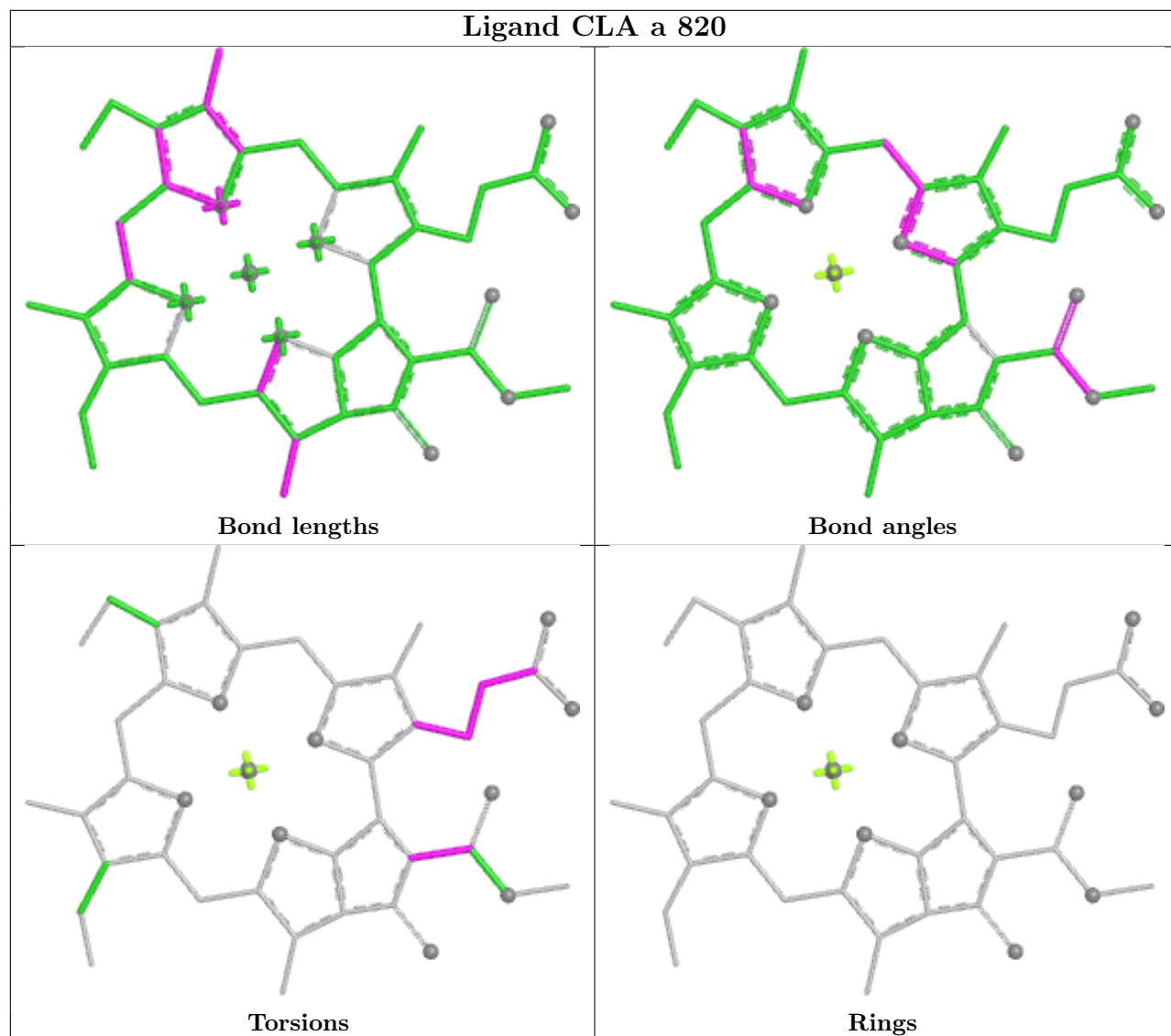


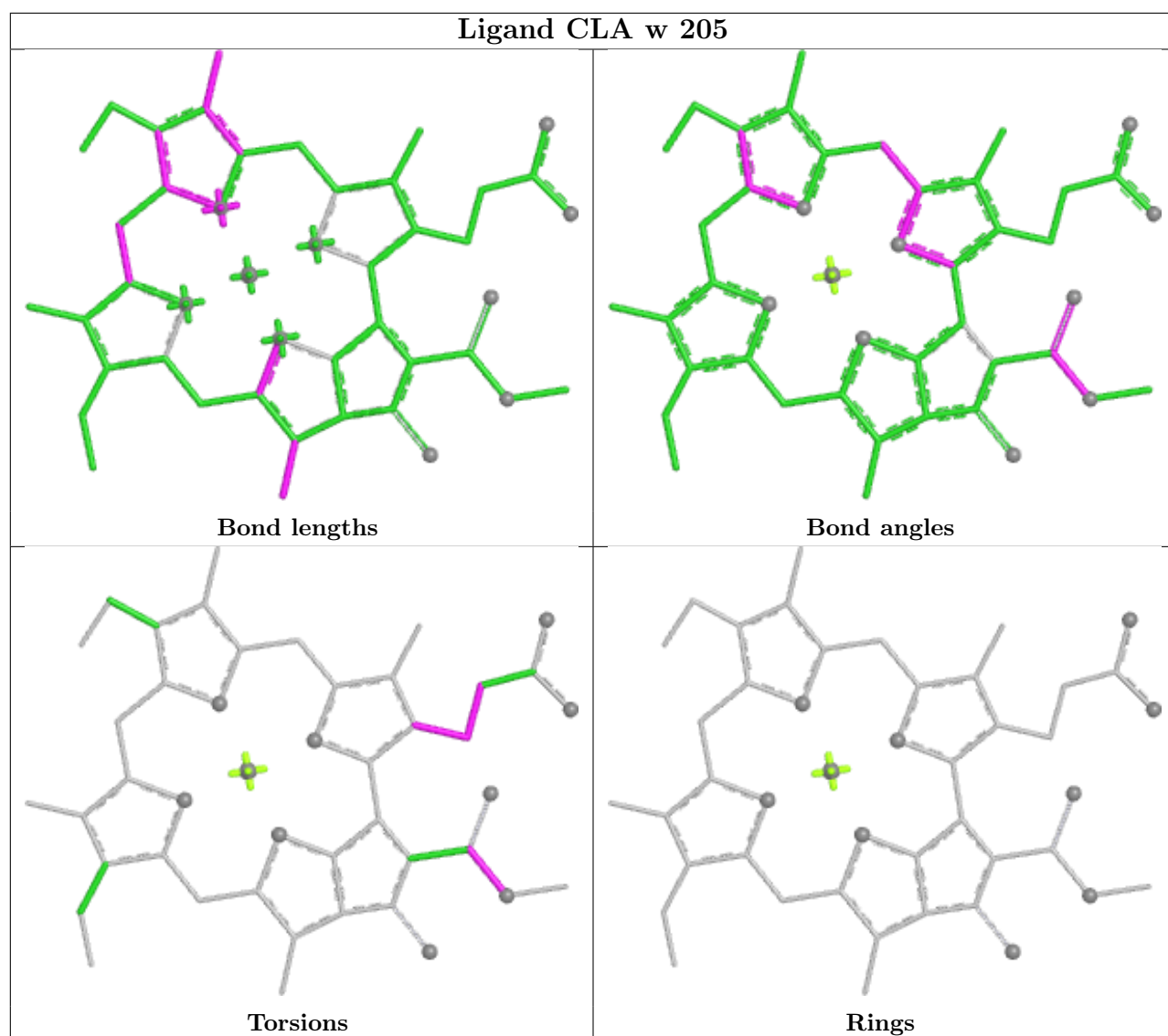
## Ligand CLA g 831

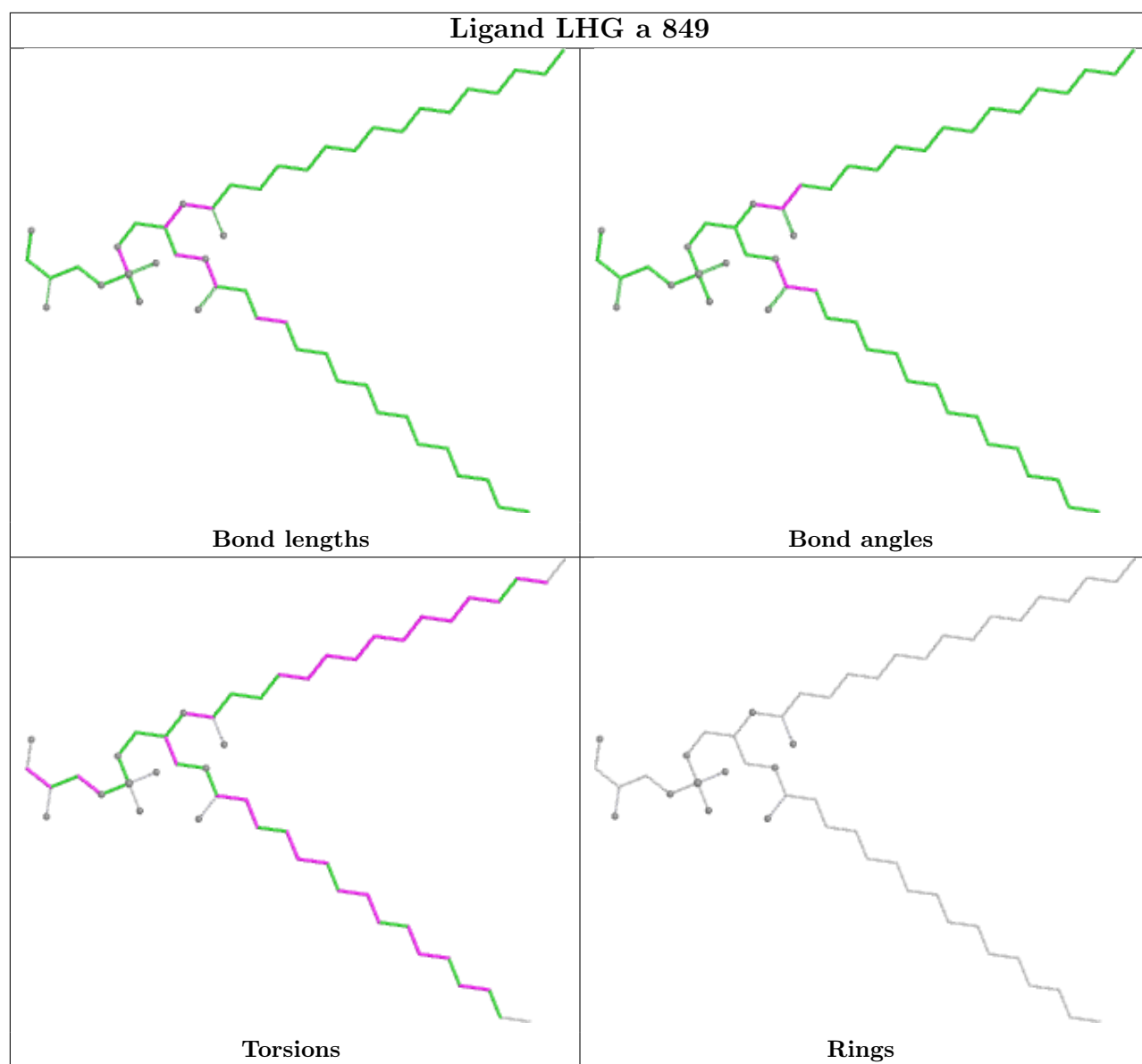


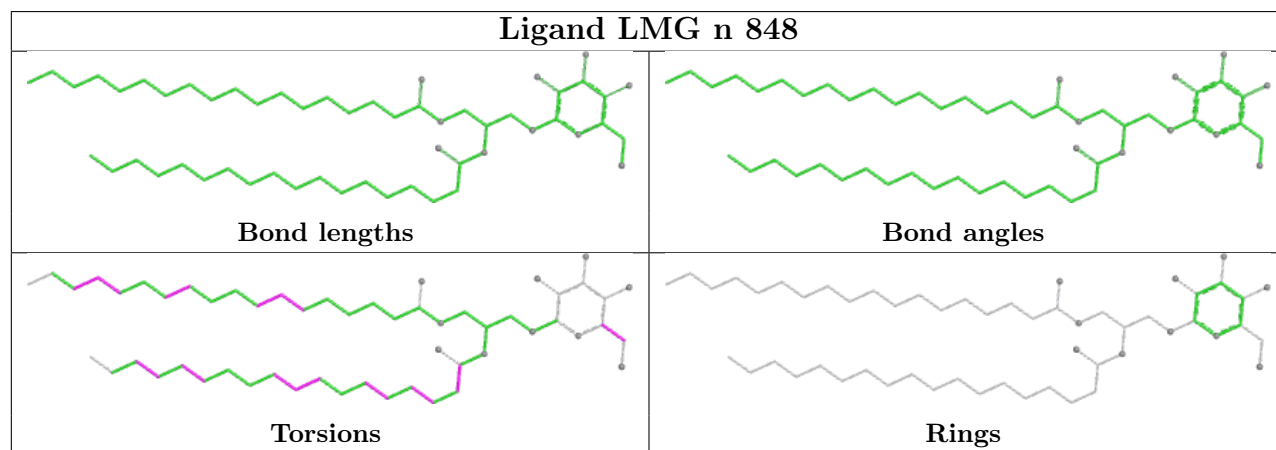
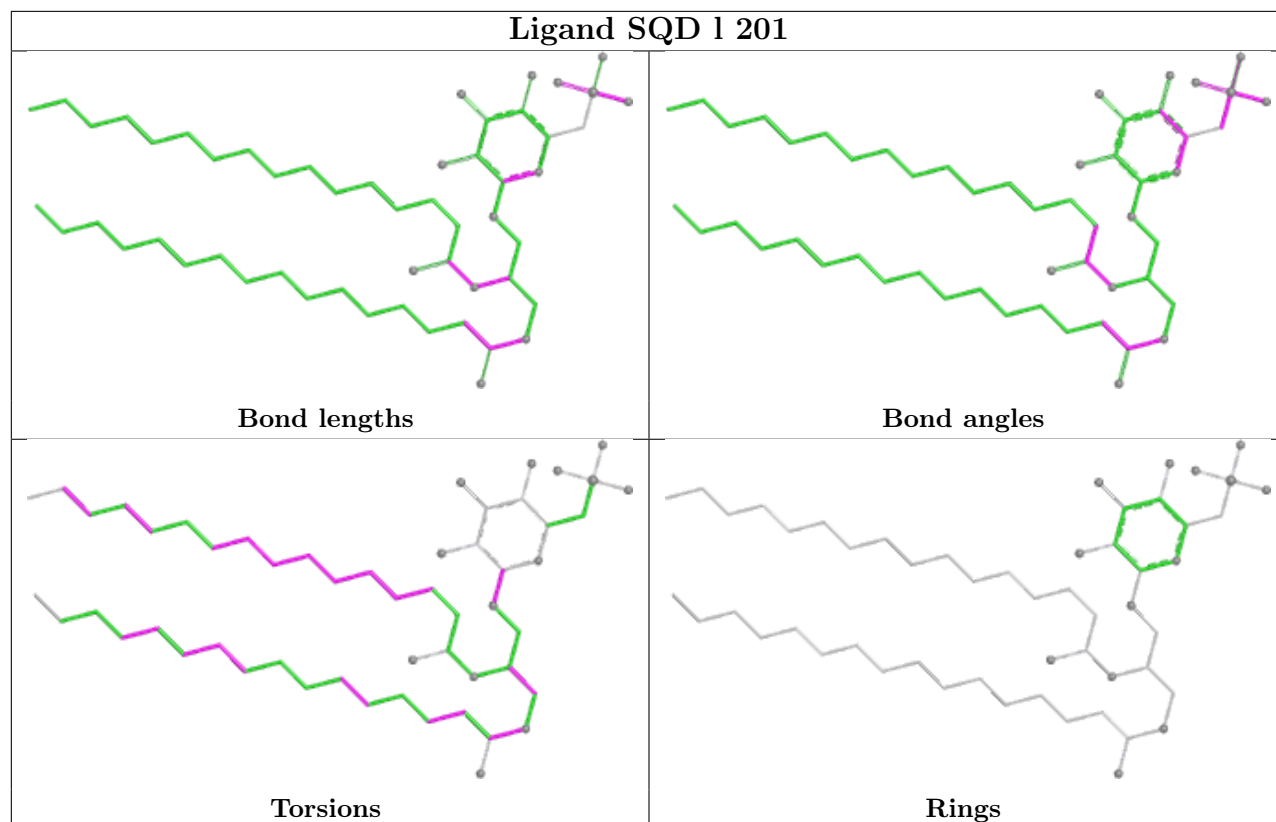




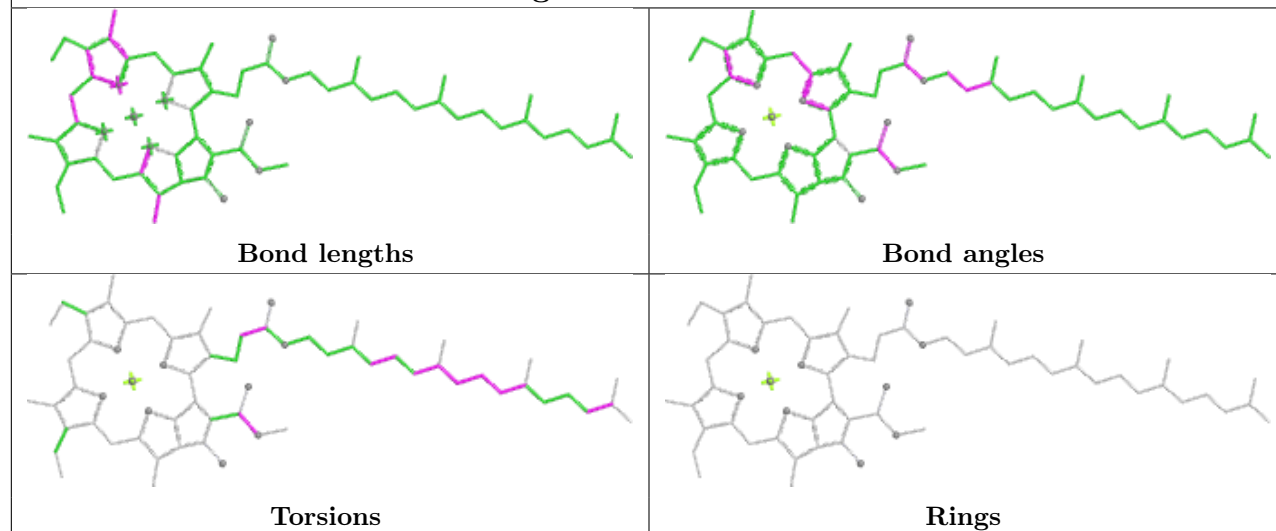




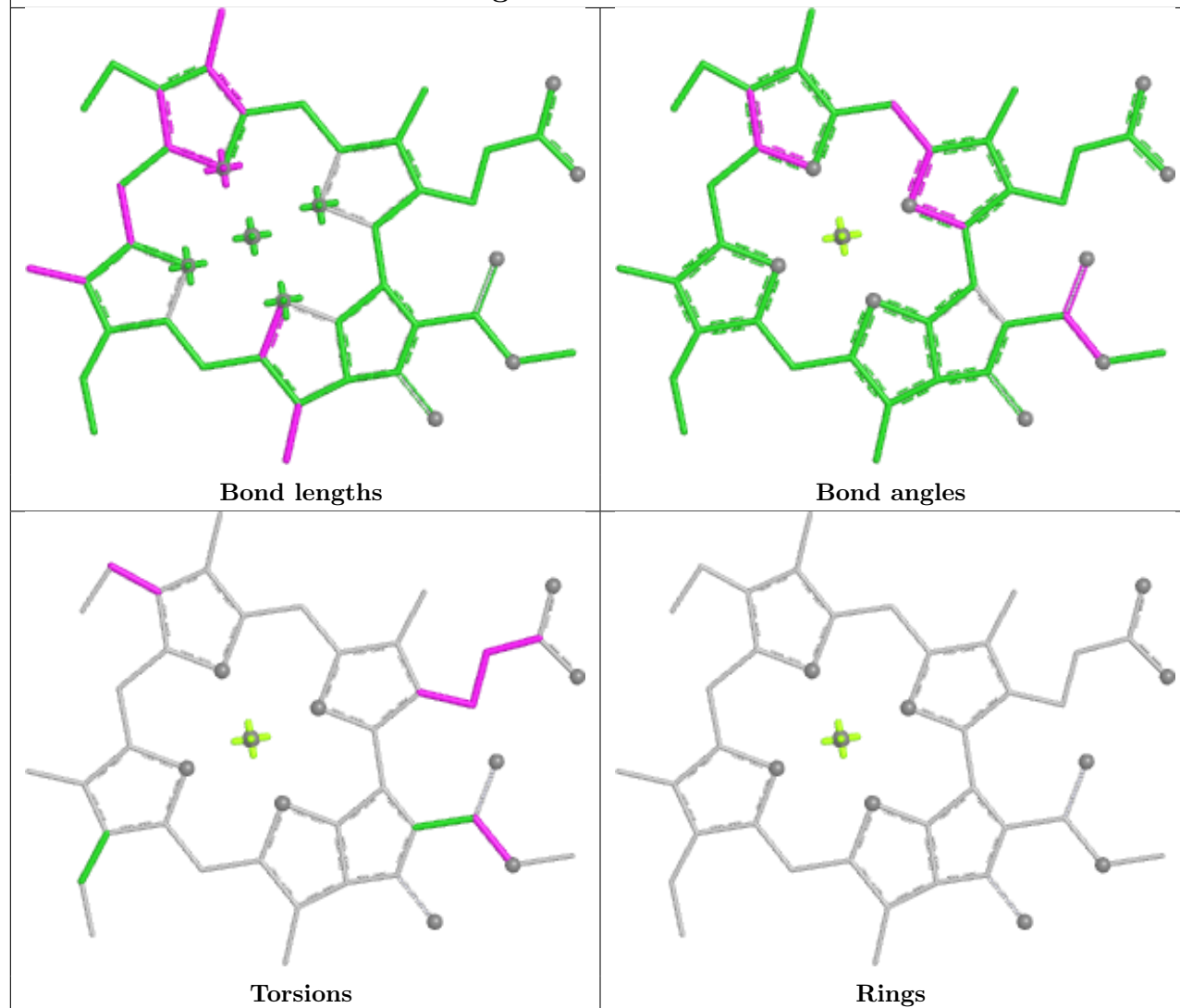


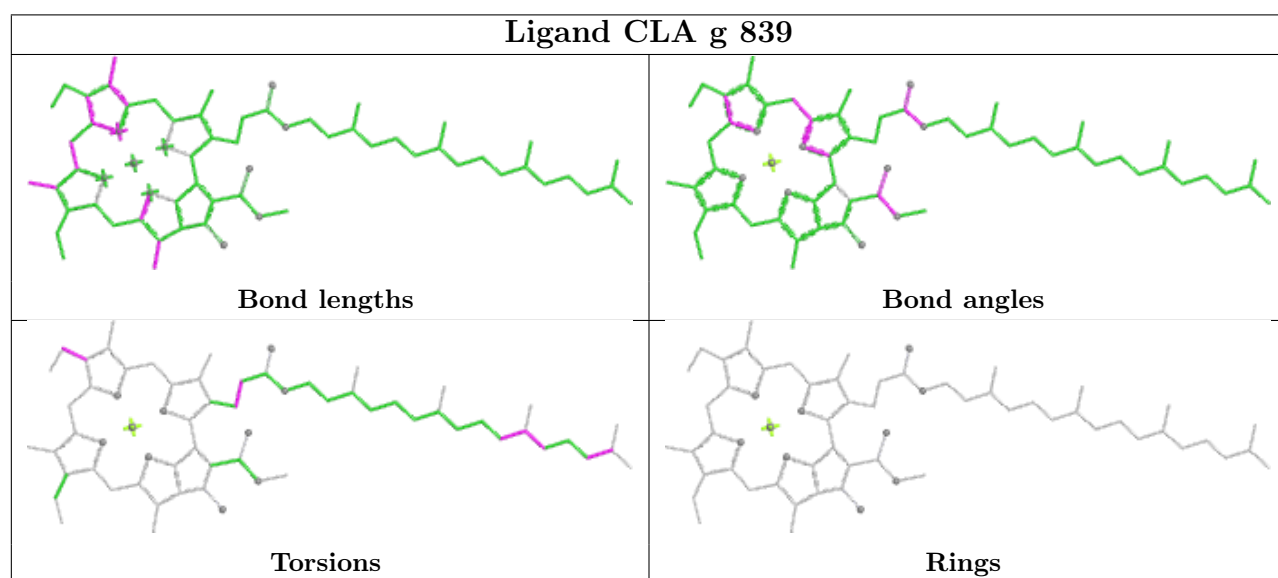
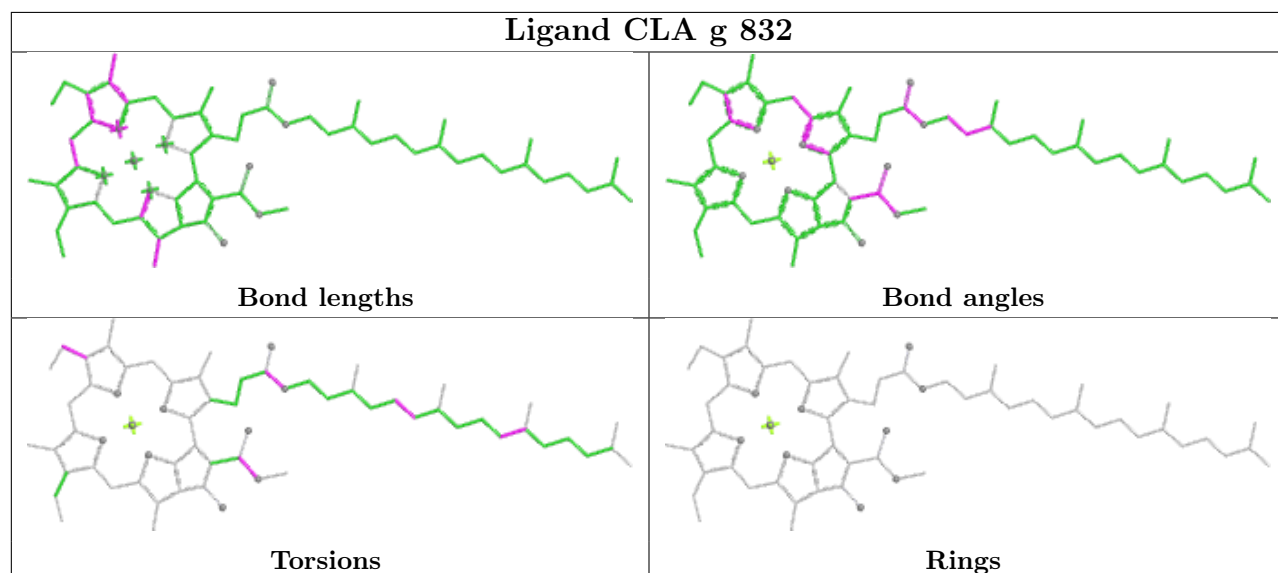
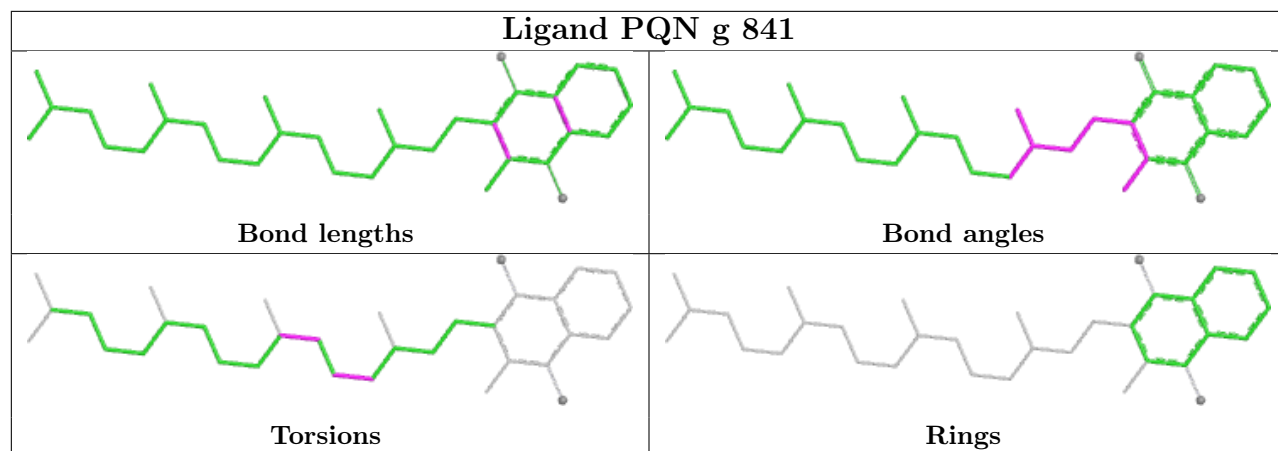


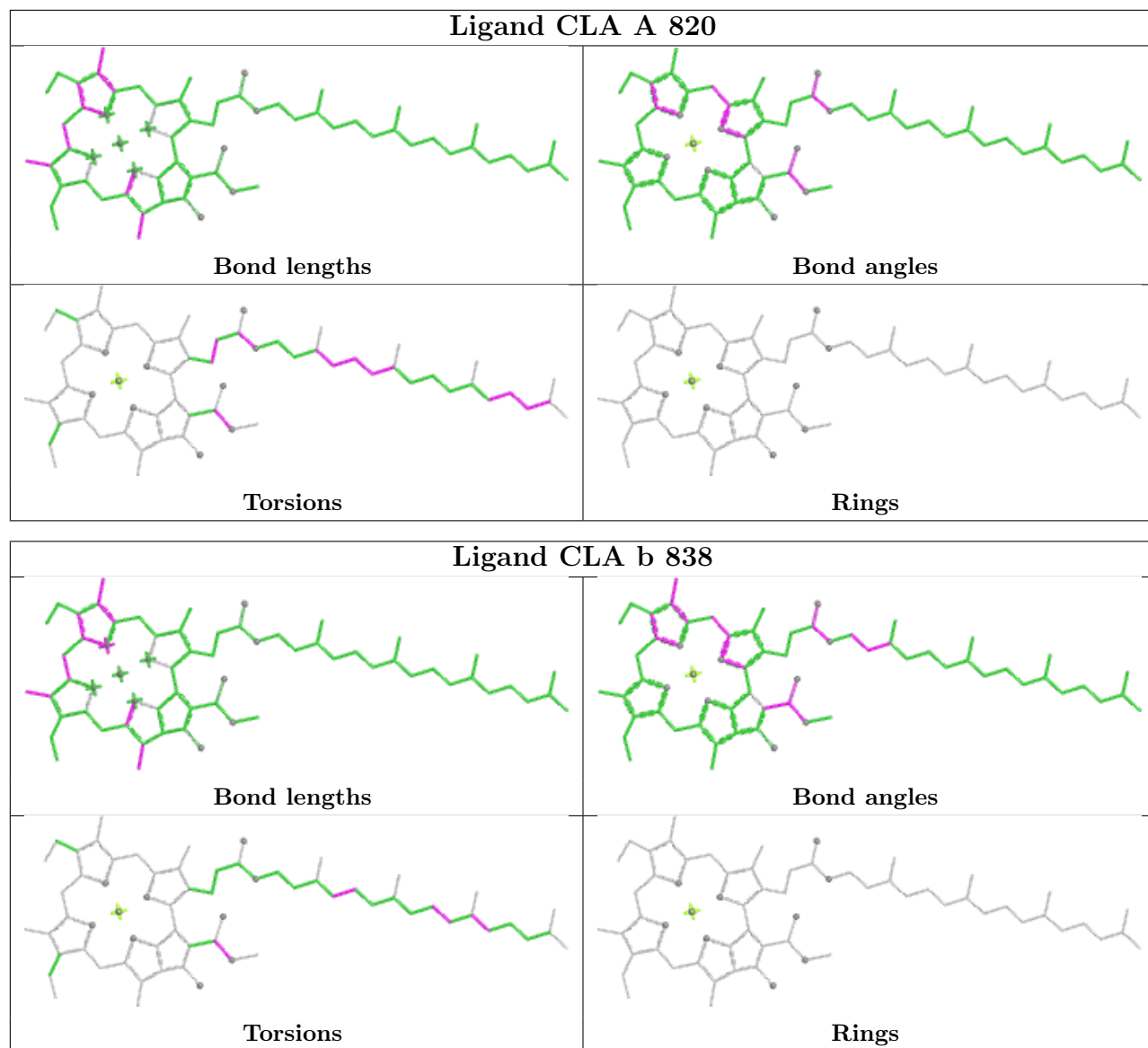
## Ligand CLA B 850



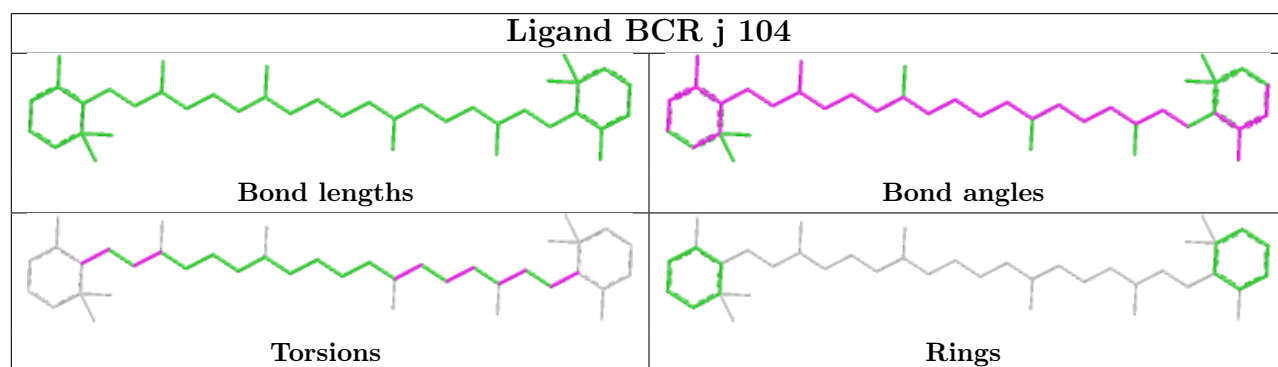
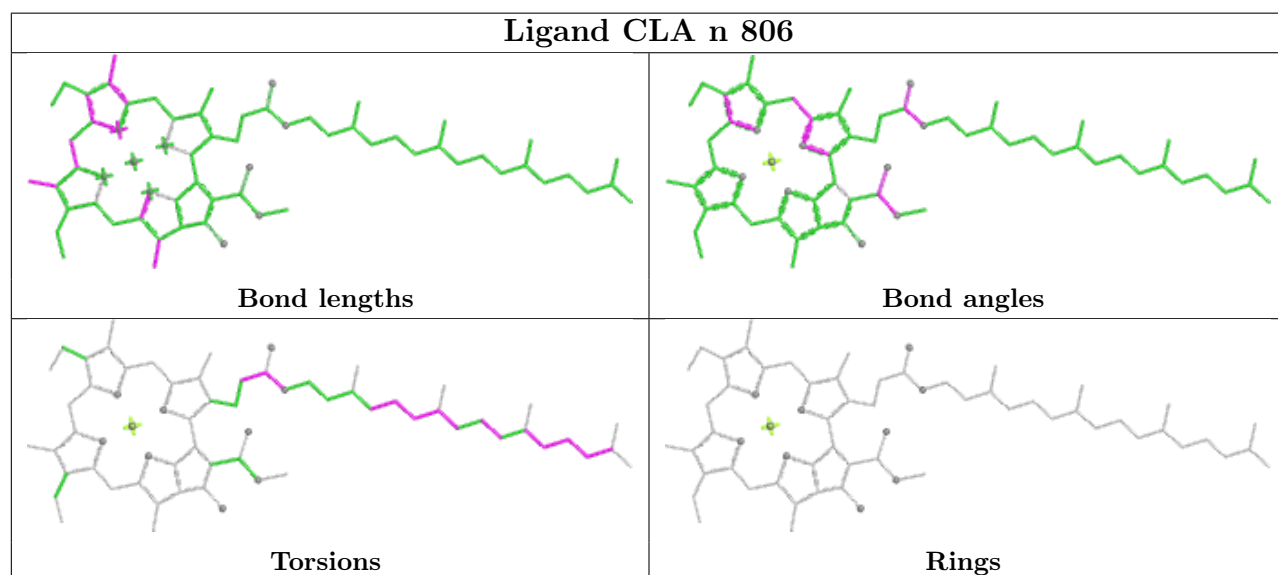
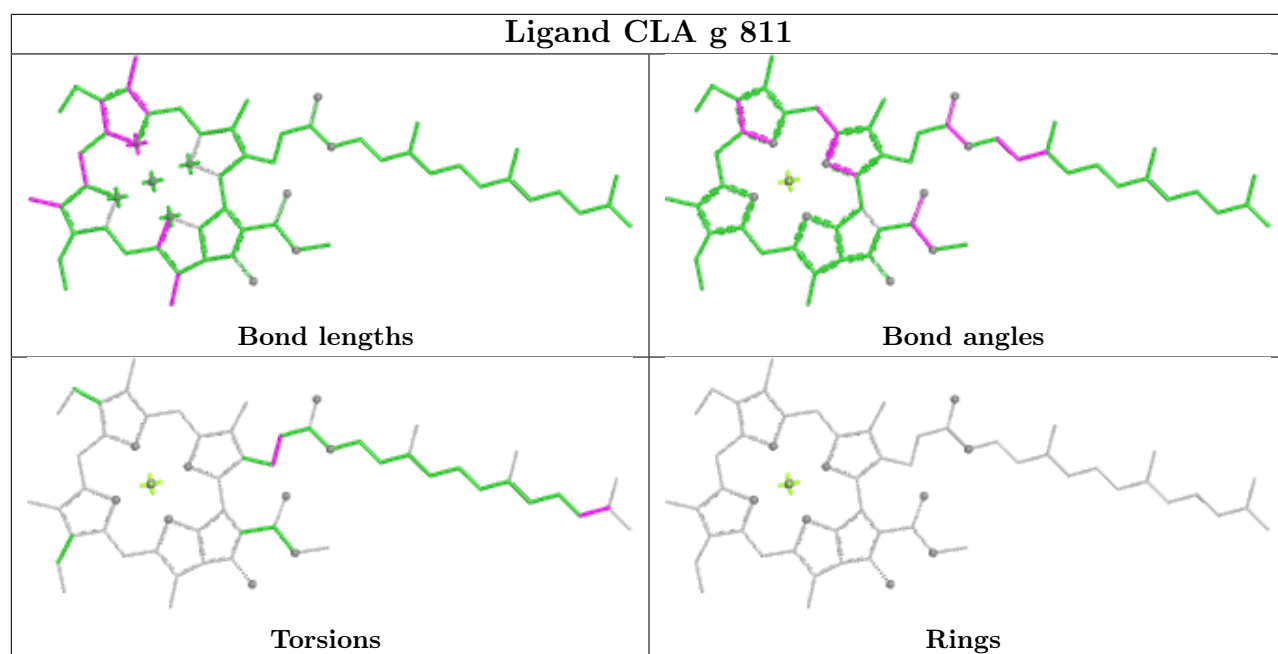
## Ligand CLA B 817



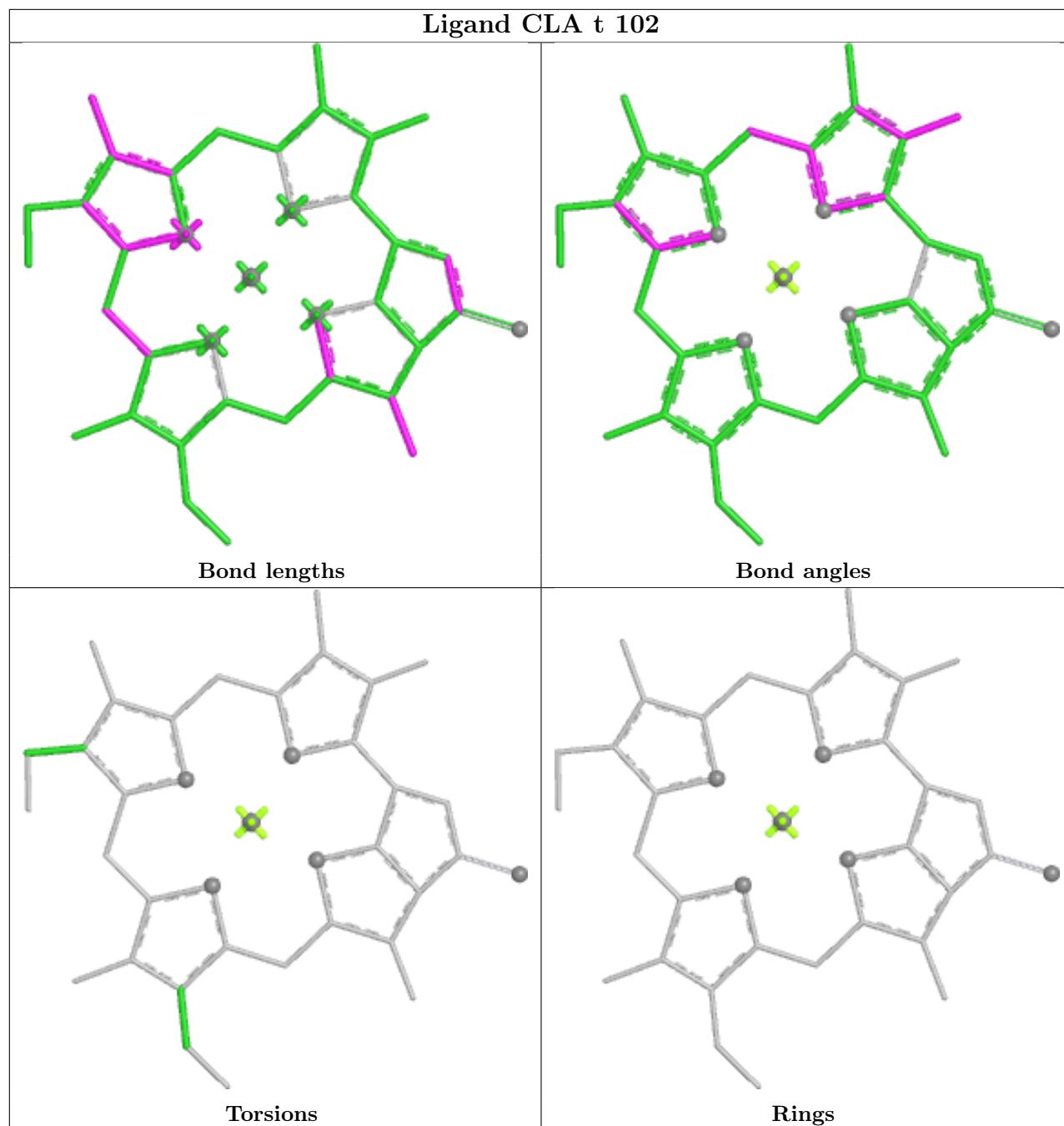




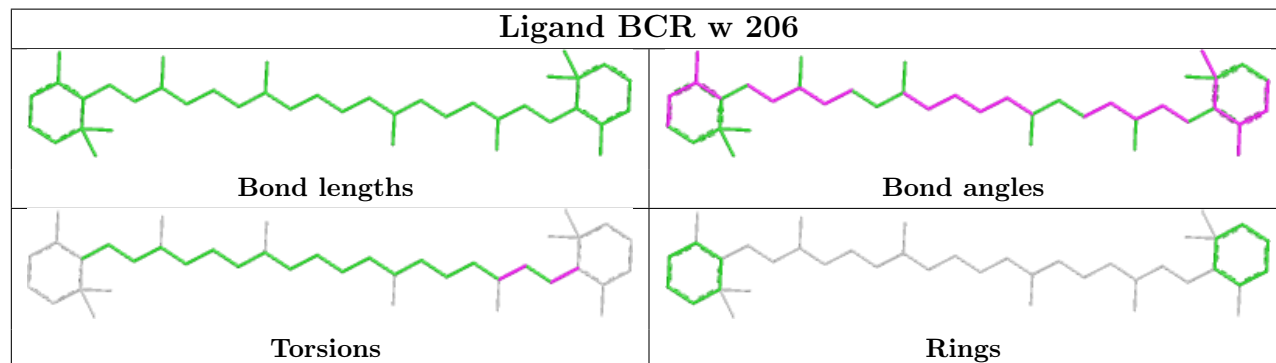


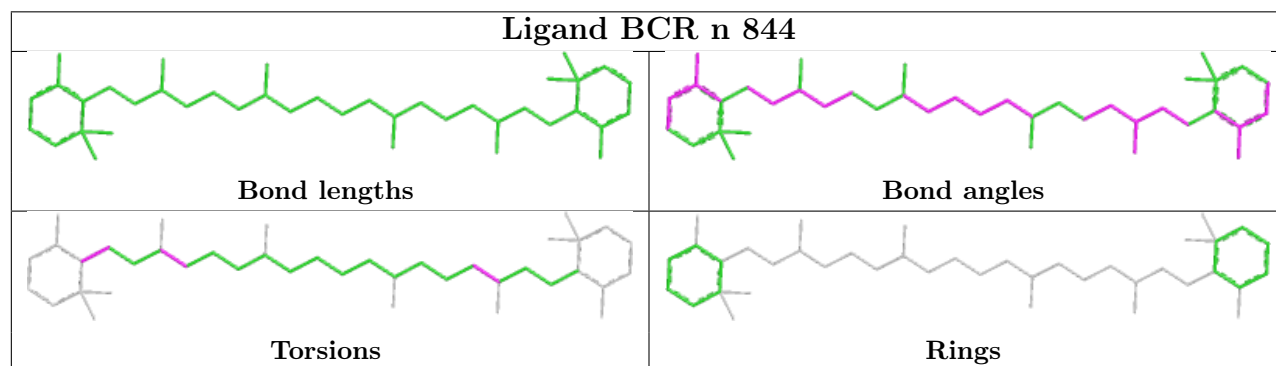
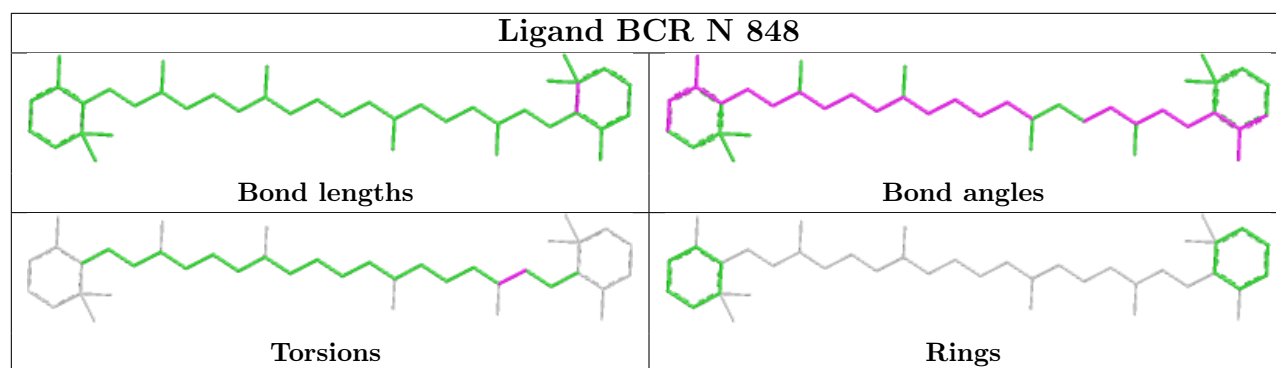
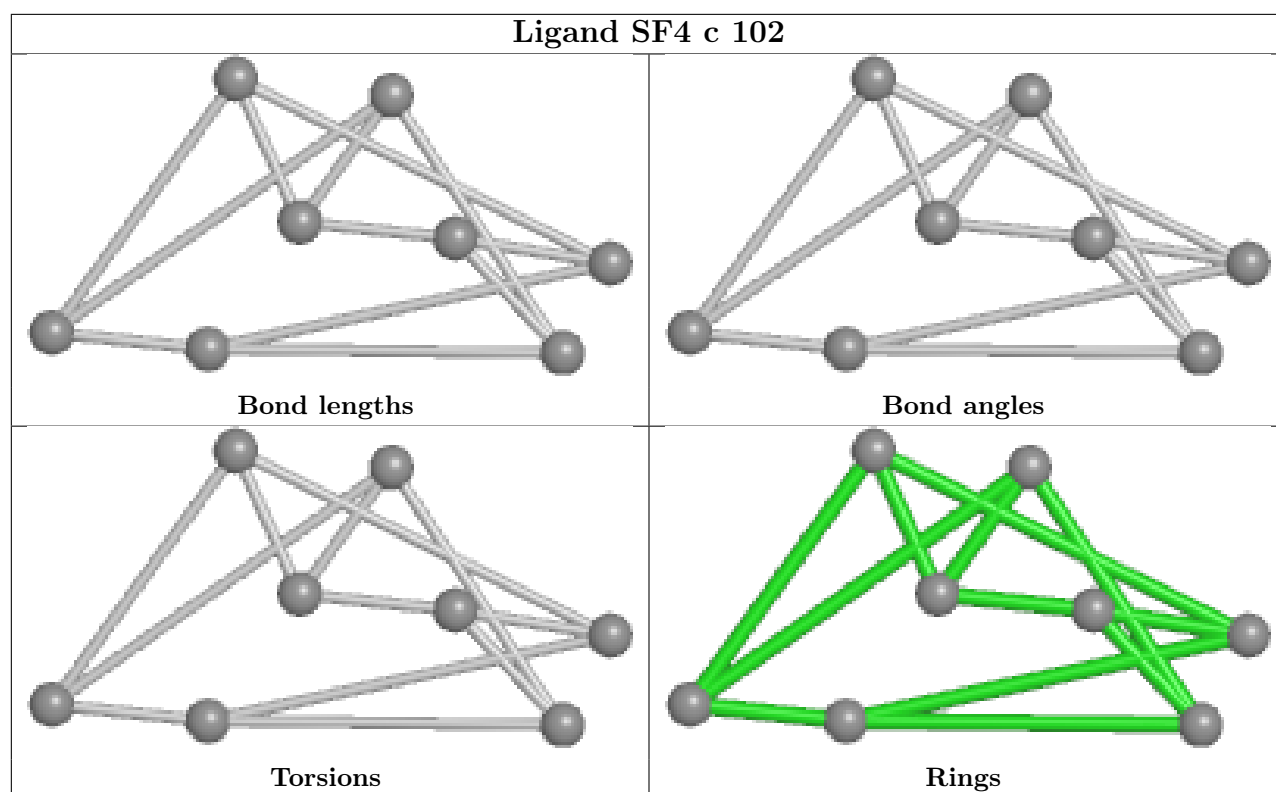


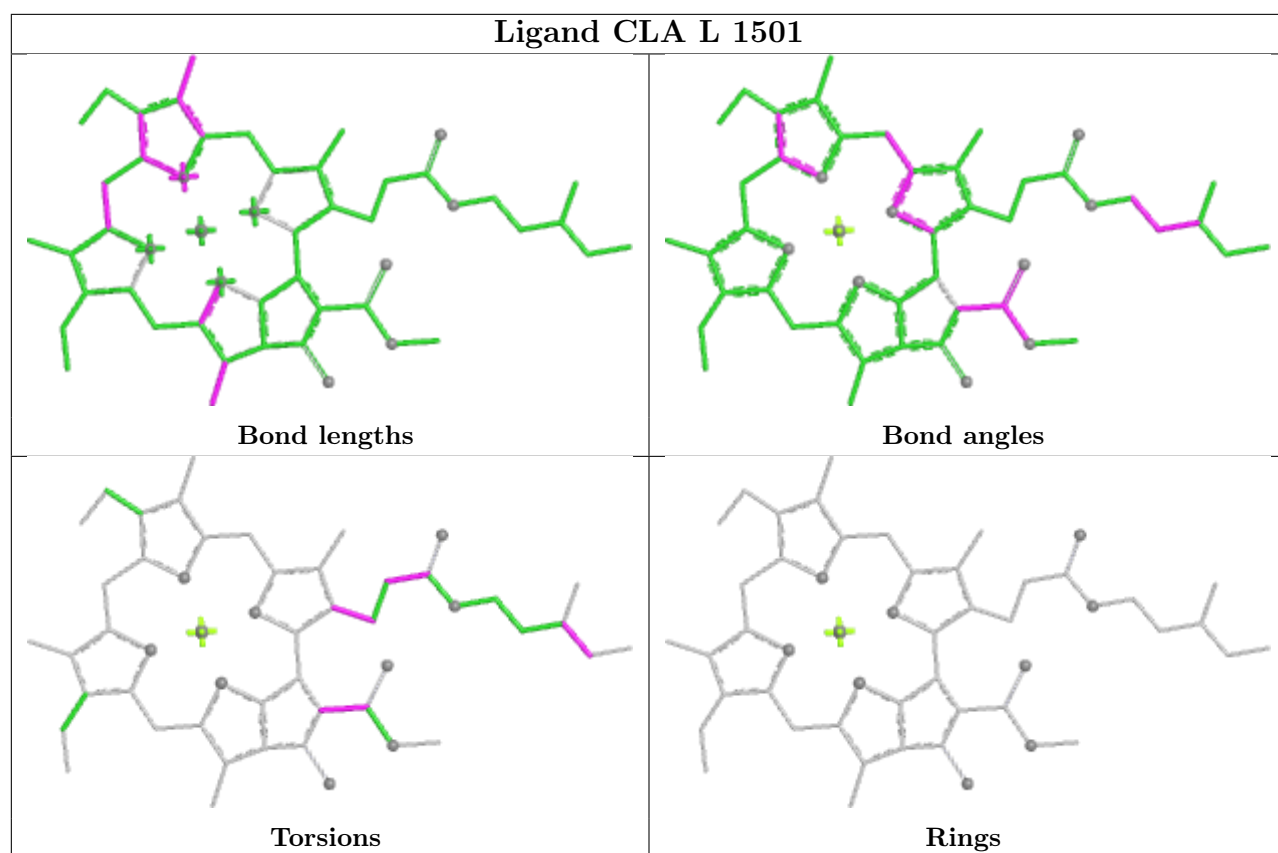
## Ligand CLA t 102



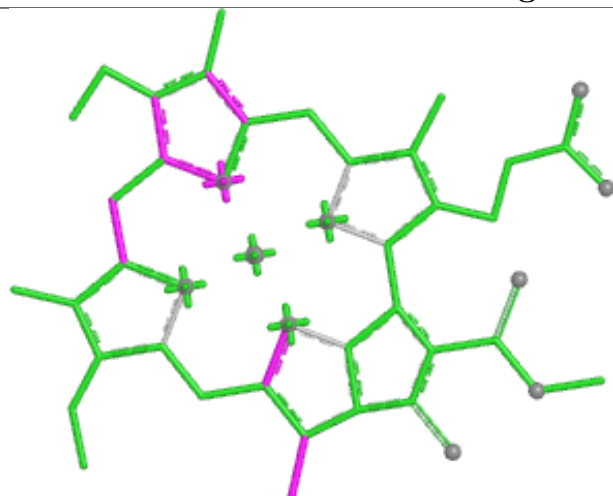
## Ligand BCR w 206



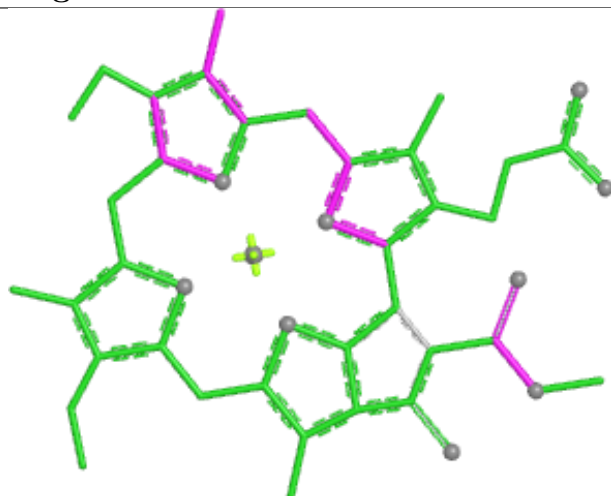




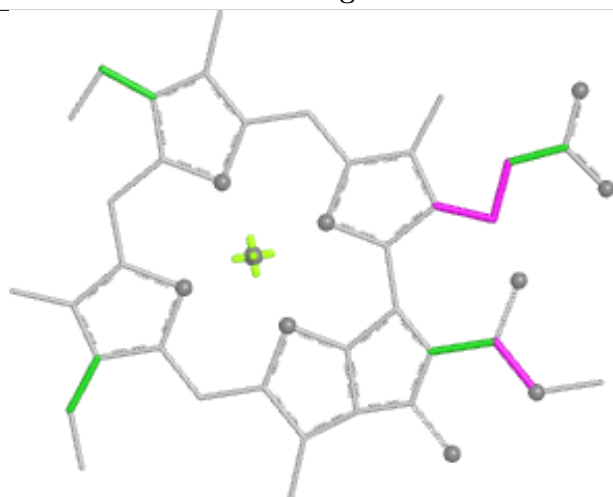
## Ligand CLA g 834



Bond lengths



Bond angles

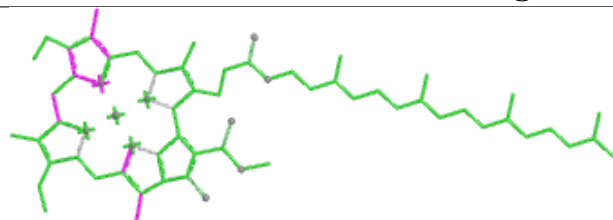


Torsions

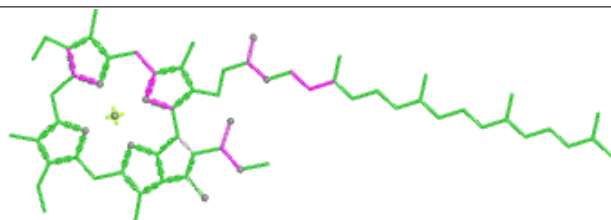


Rings

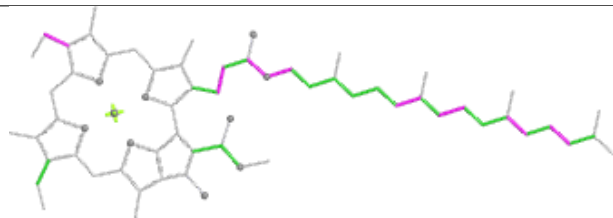
## Ligand CLA N 801



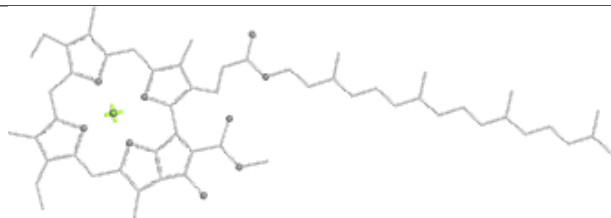
Bond lengths



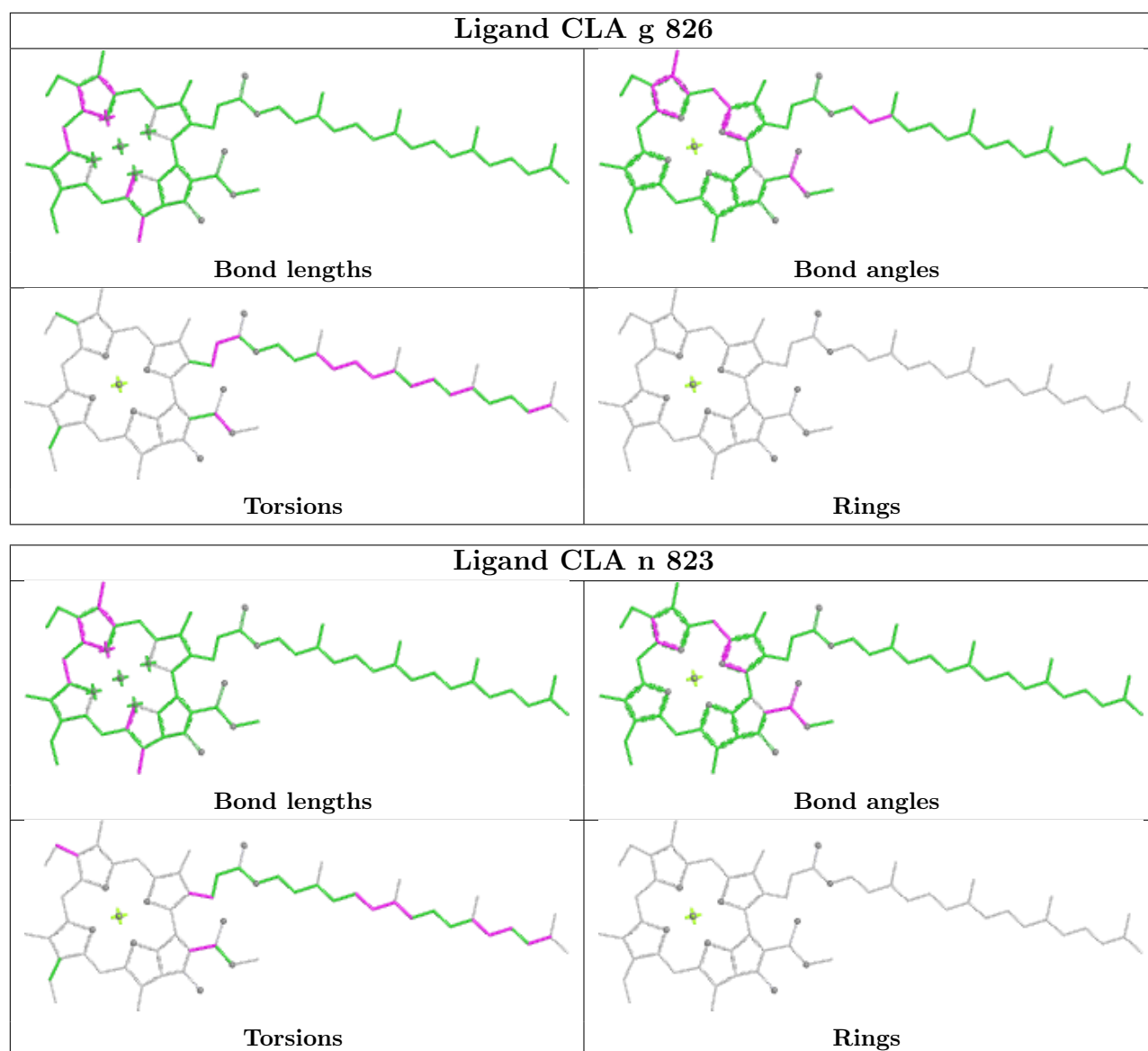
Bond angles



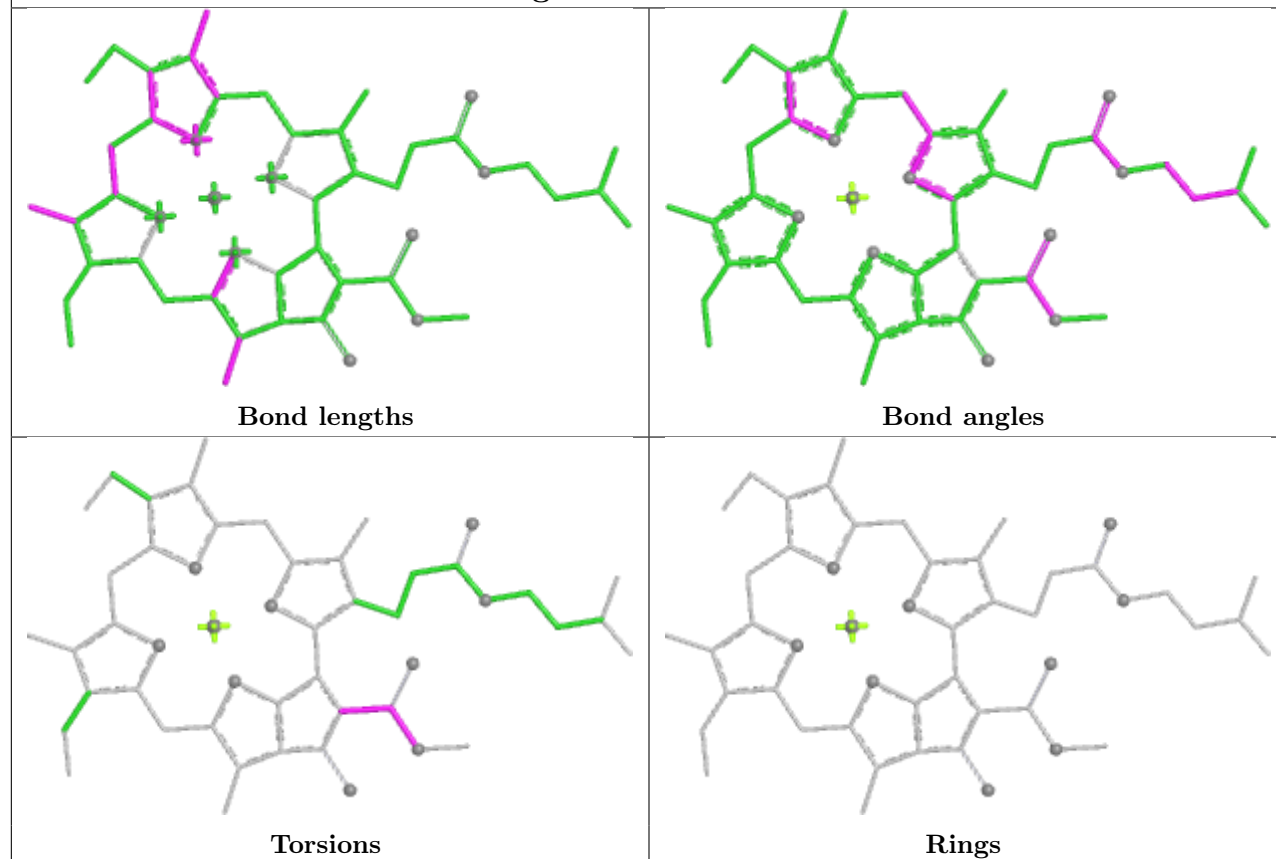
Torsions



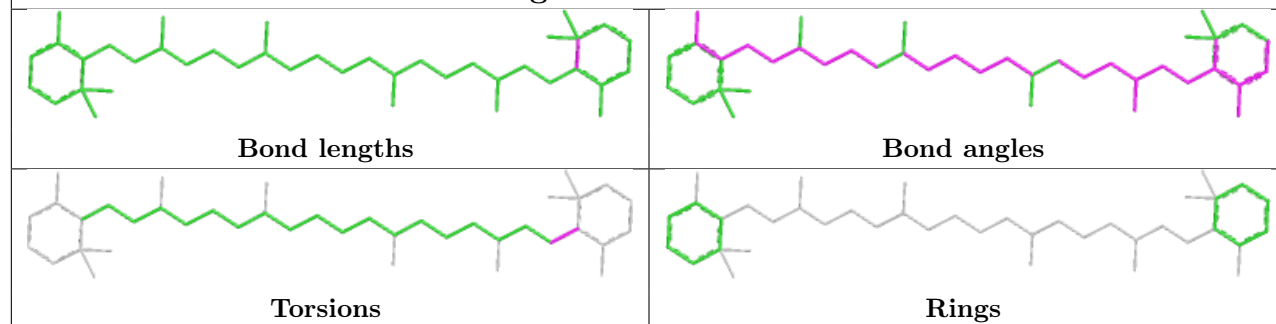
Rings

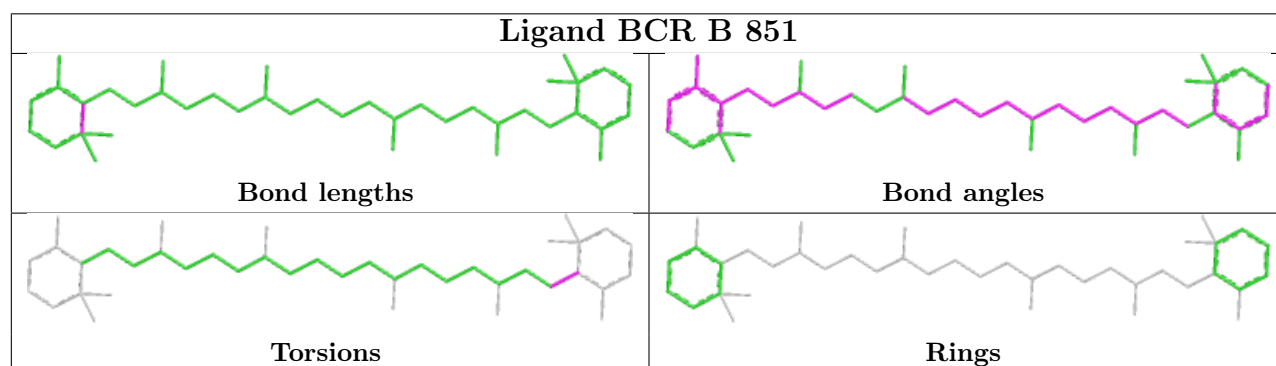
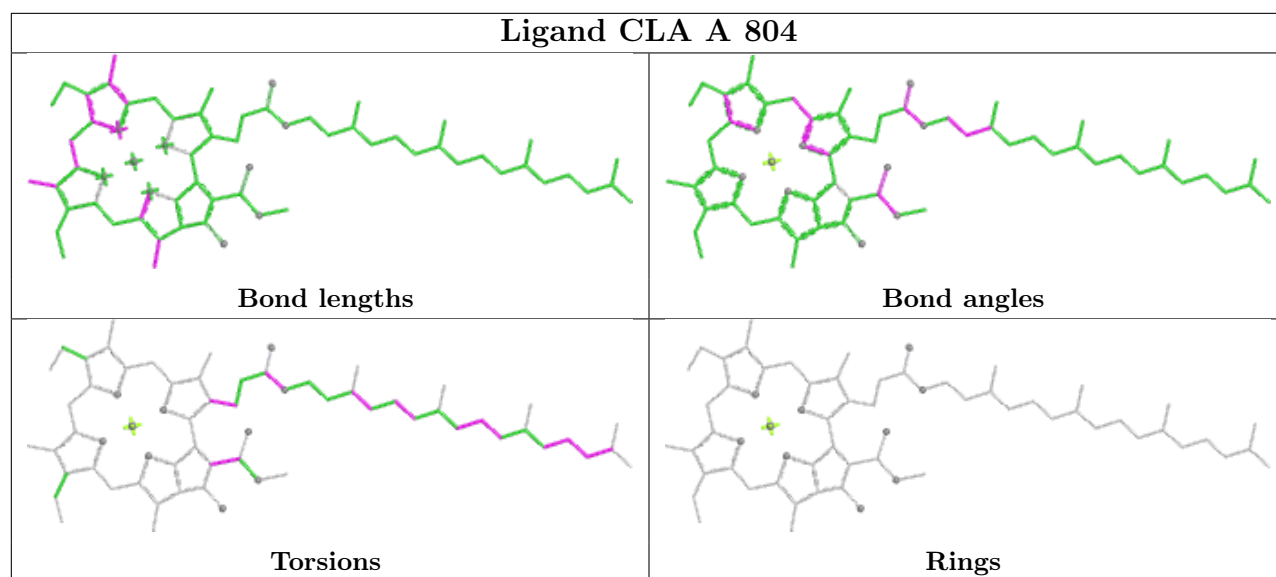
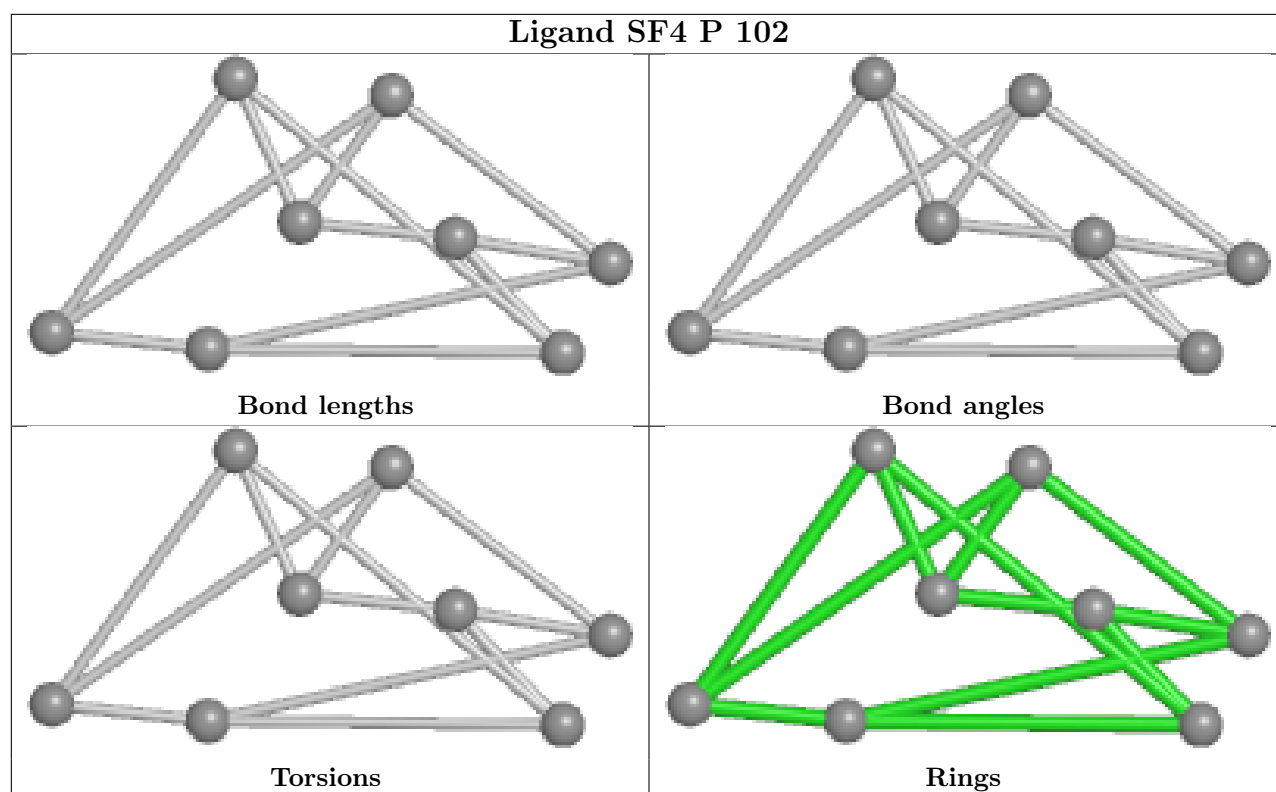


## Ligand CLA B 815

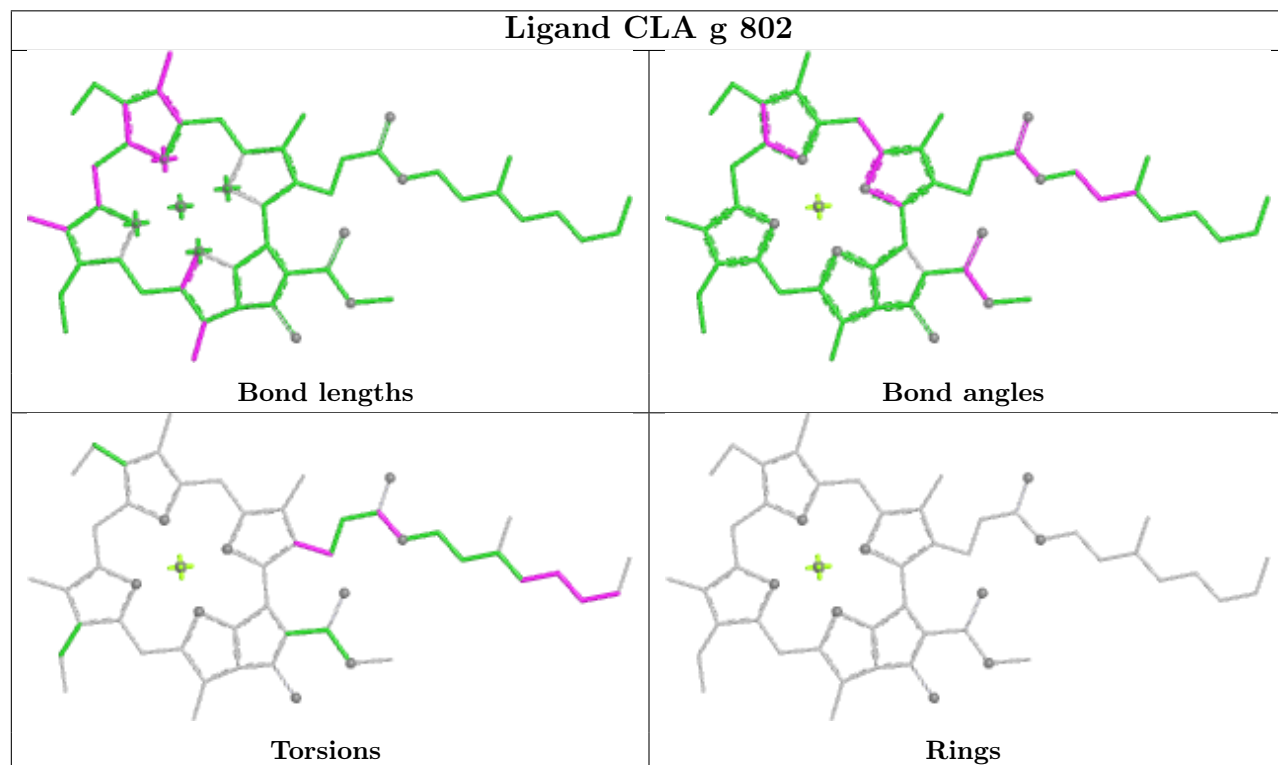
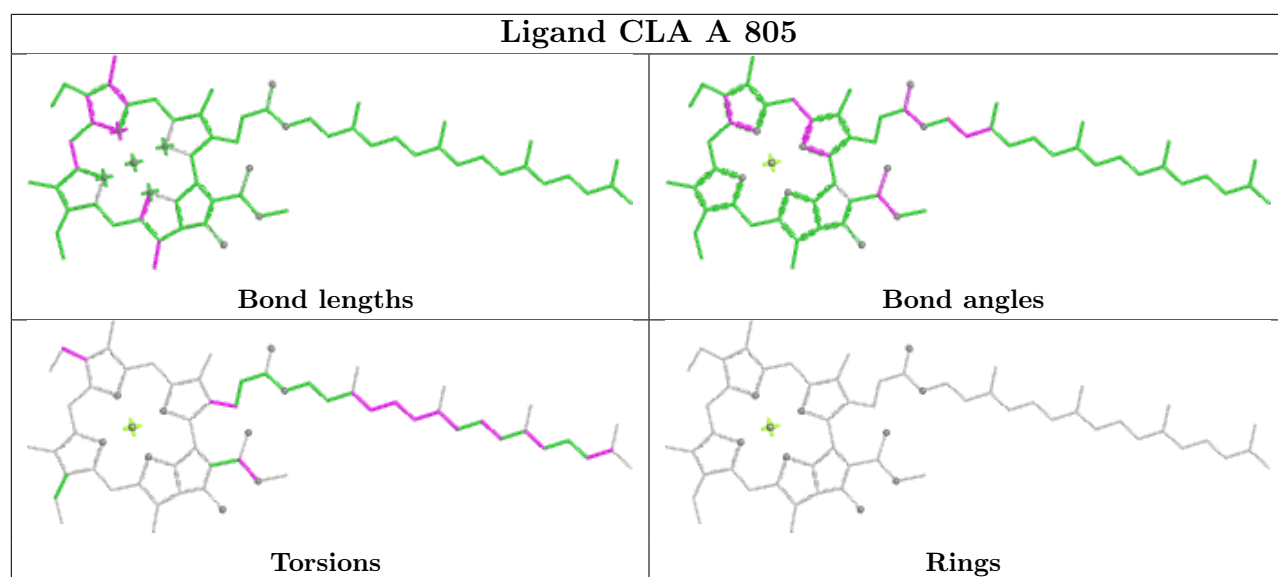


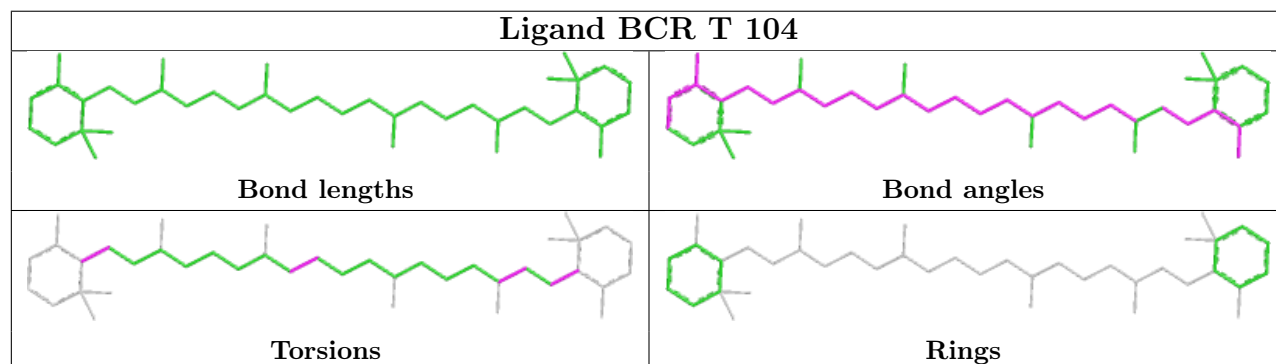
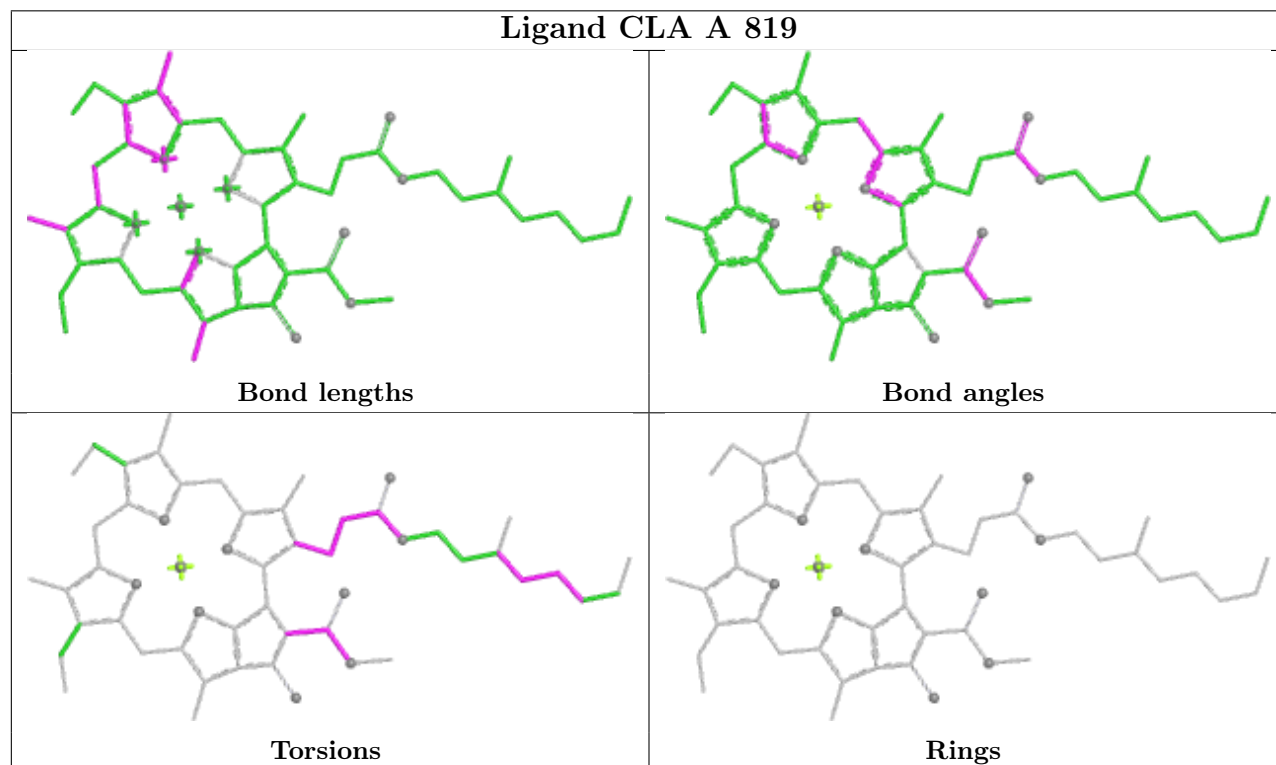
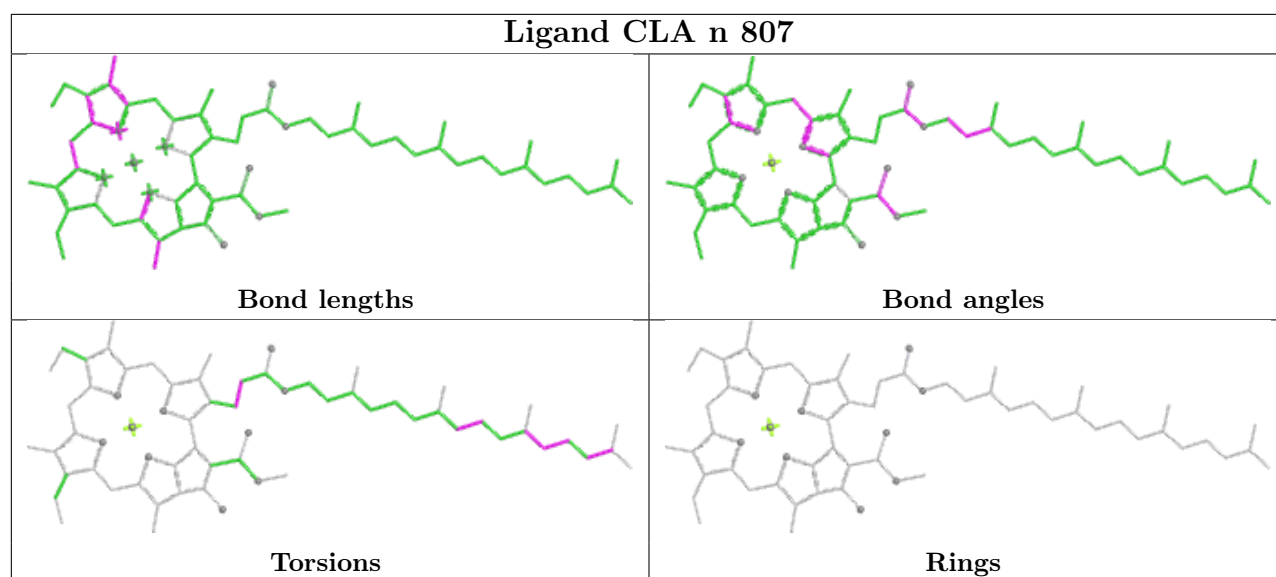
## Ligand BCR A 848

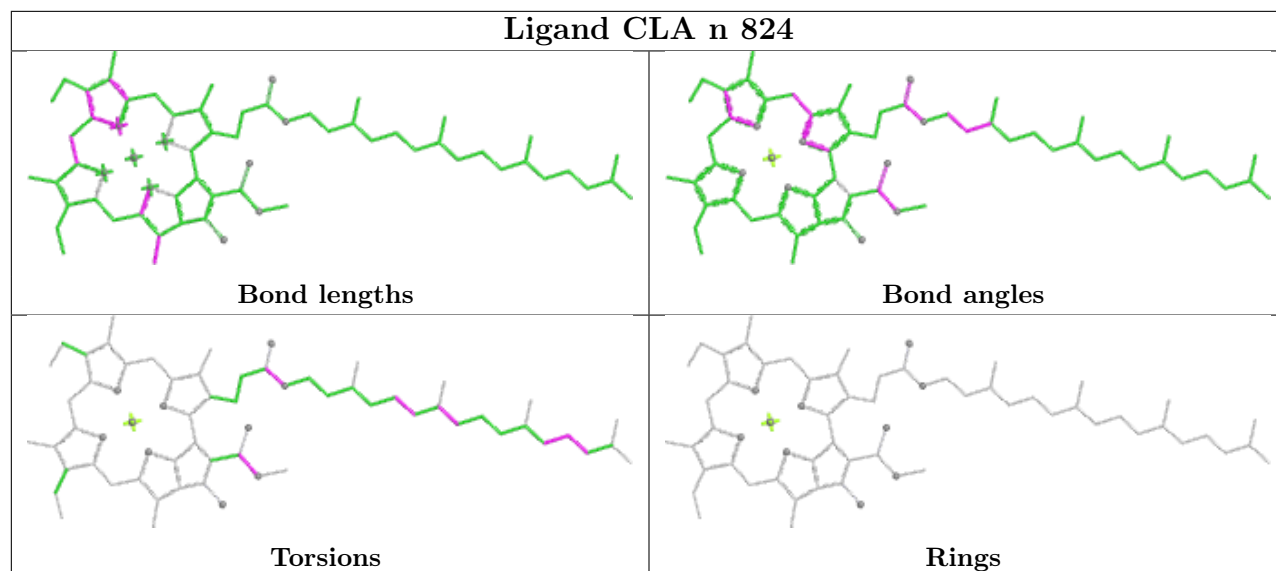
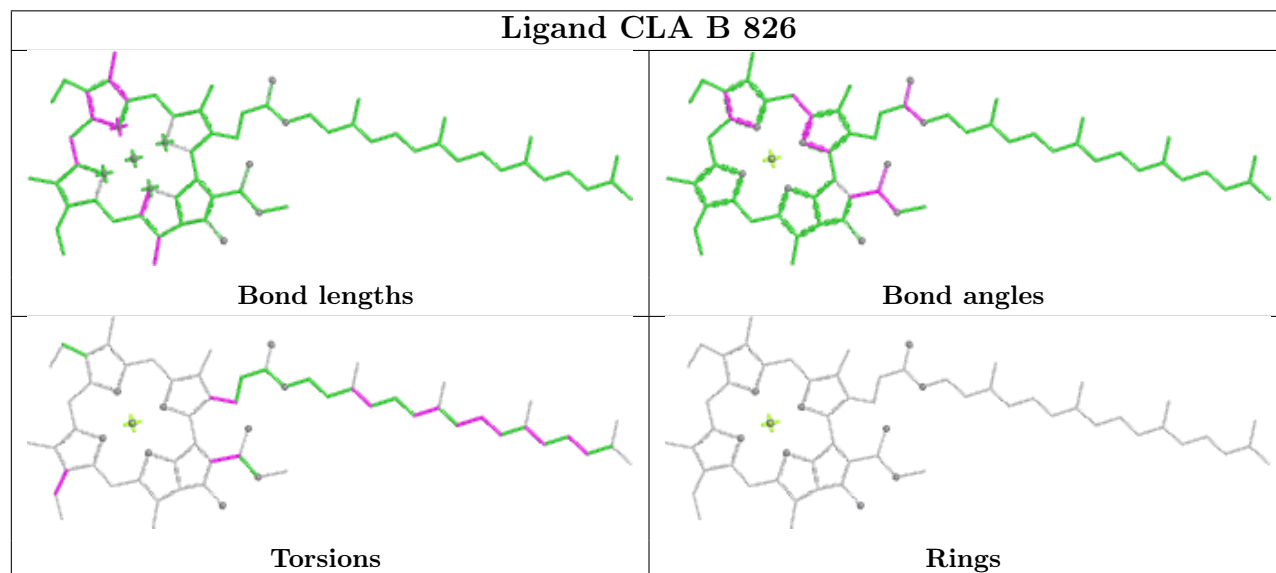
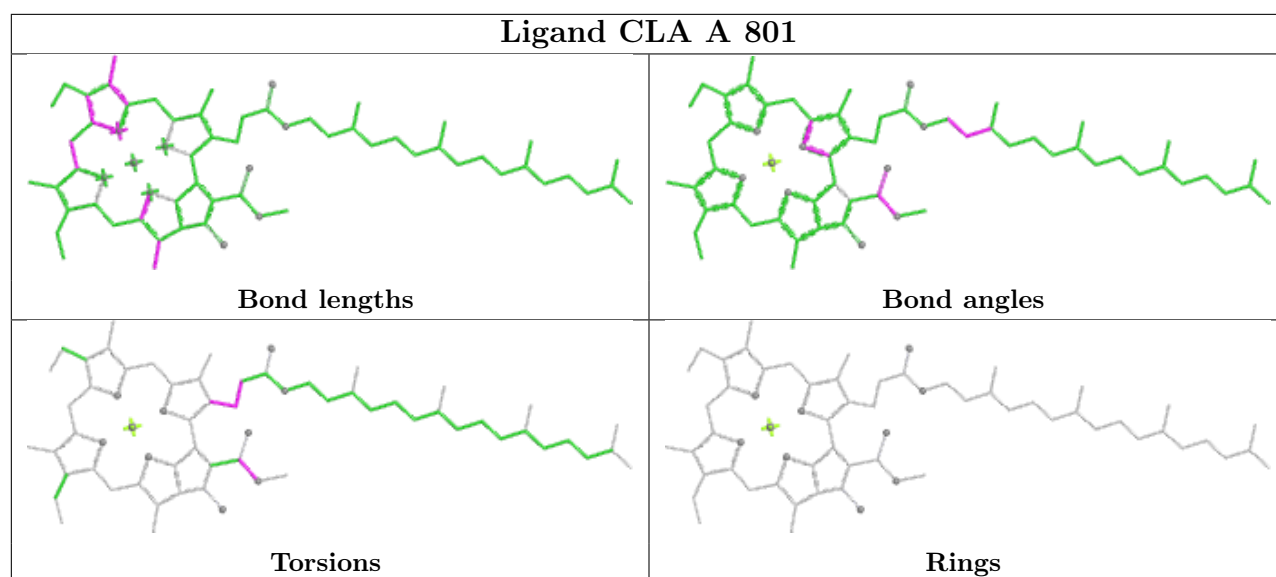


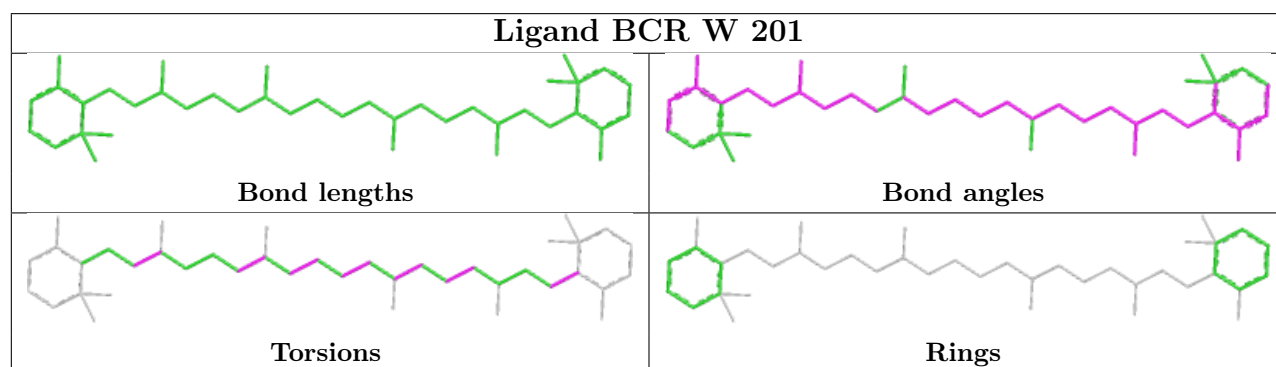
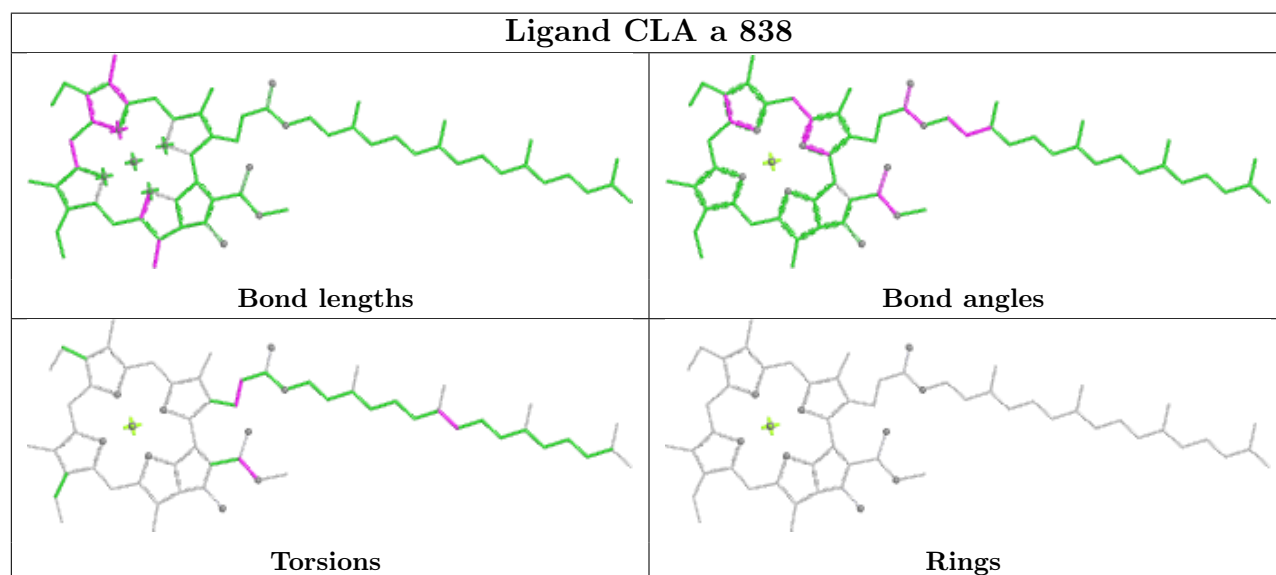
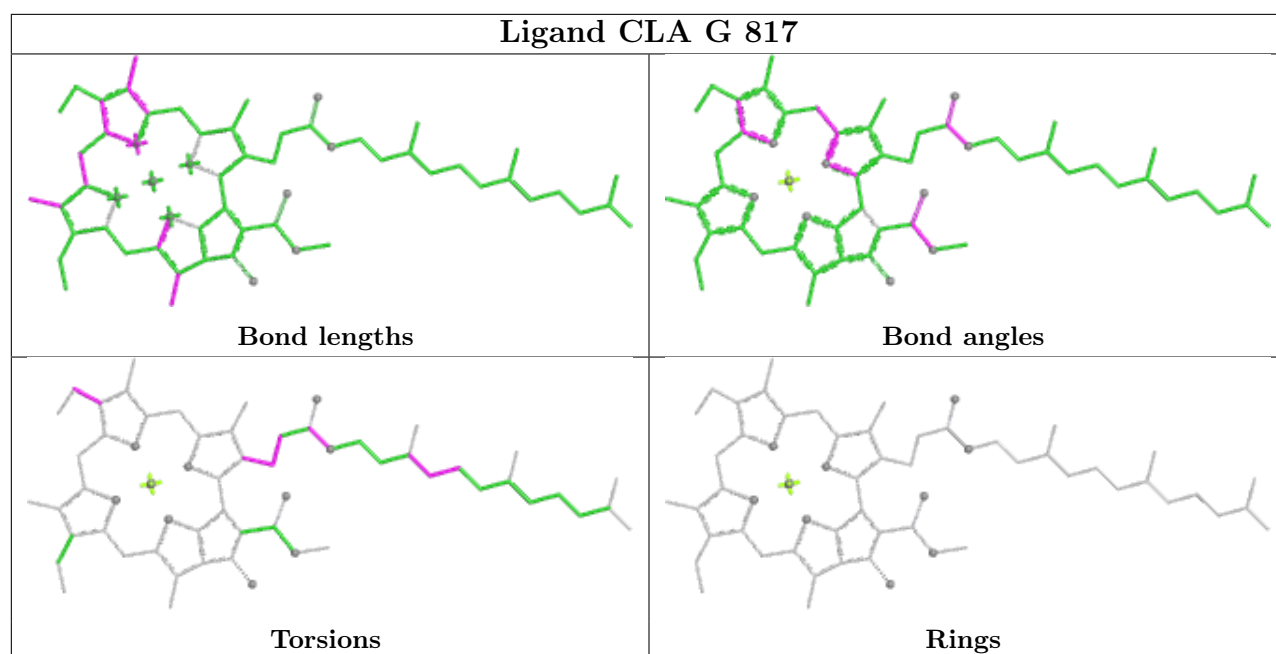


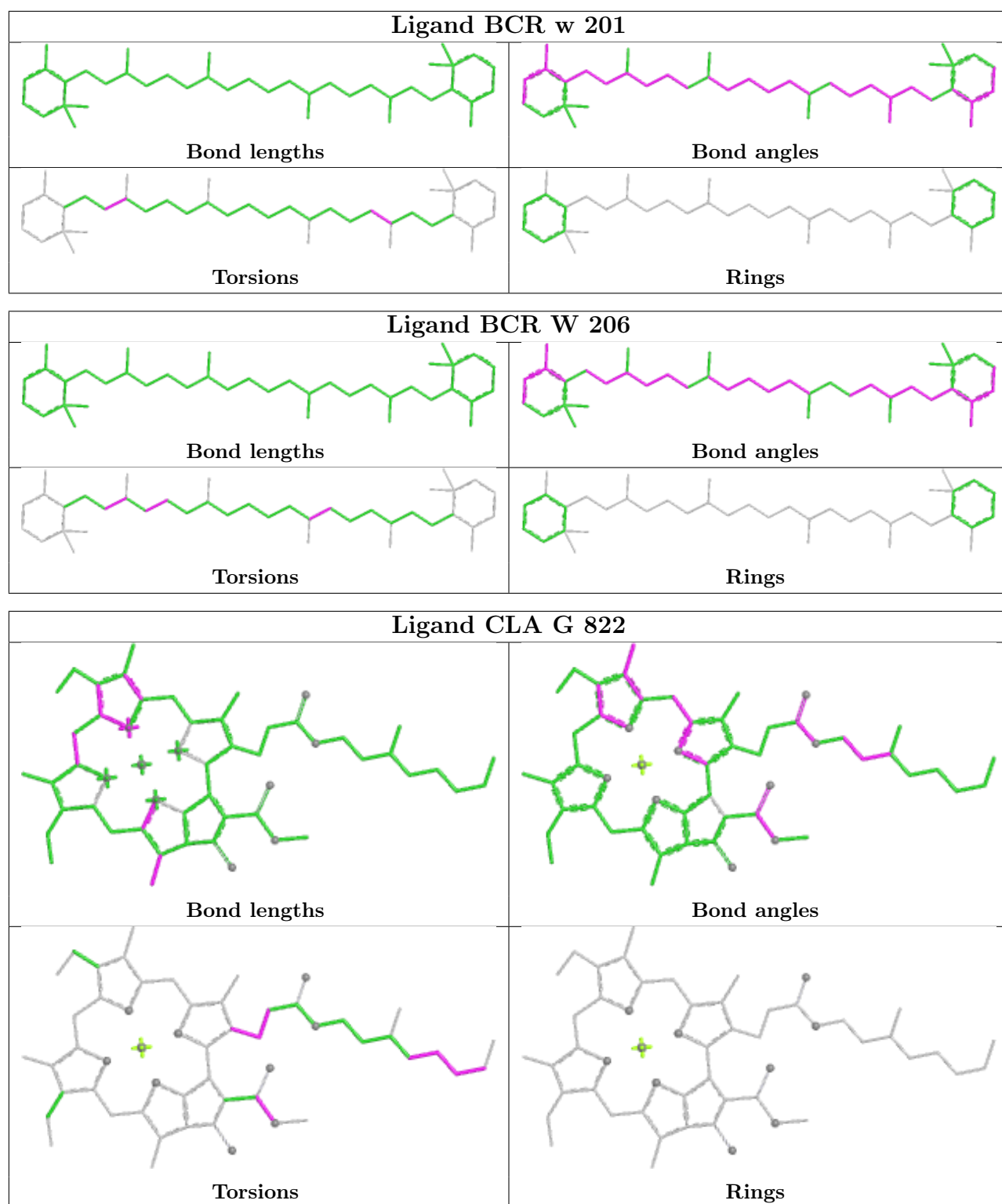


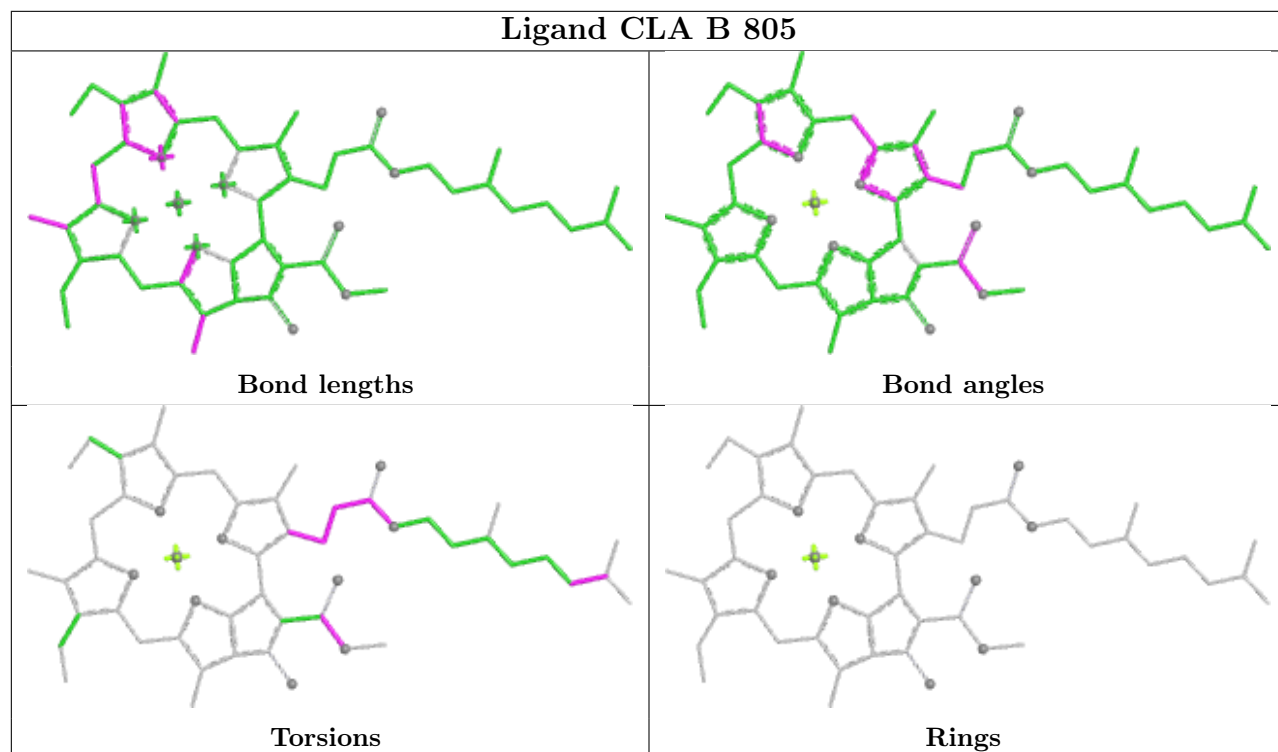
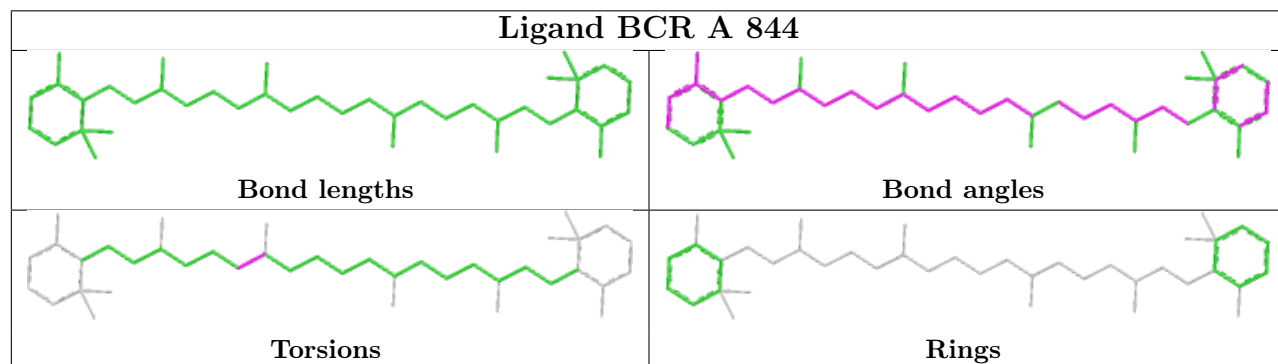
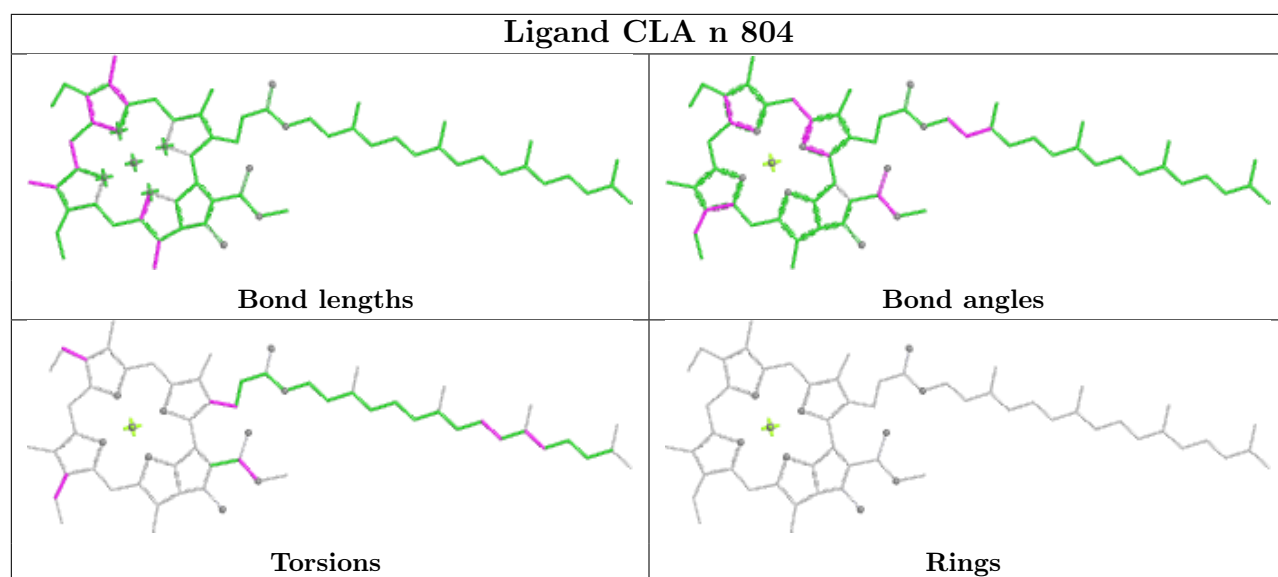




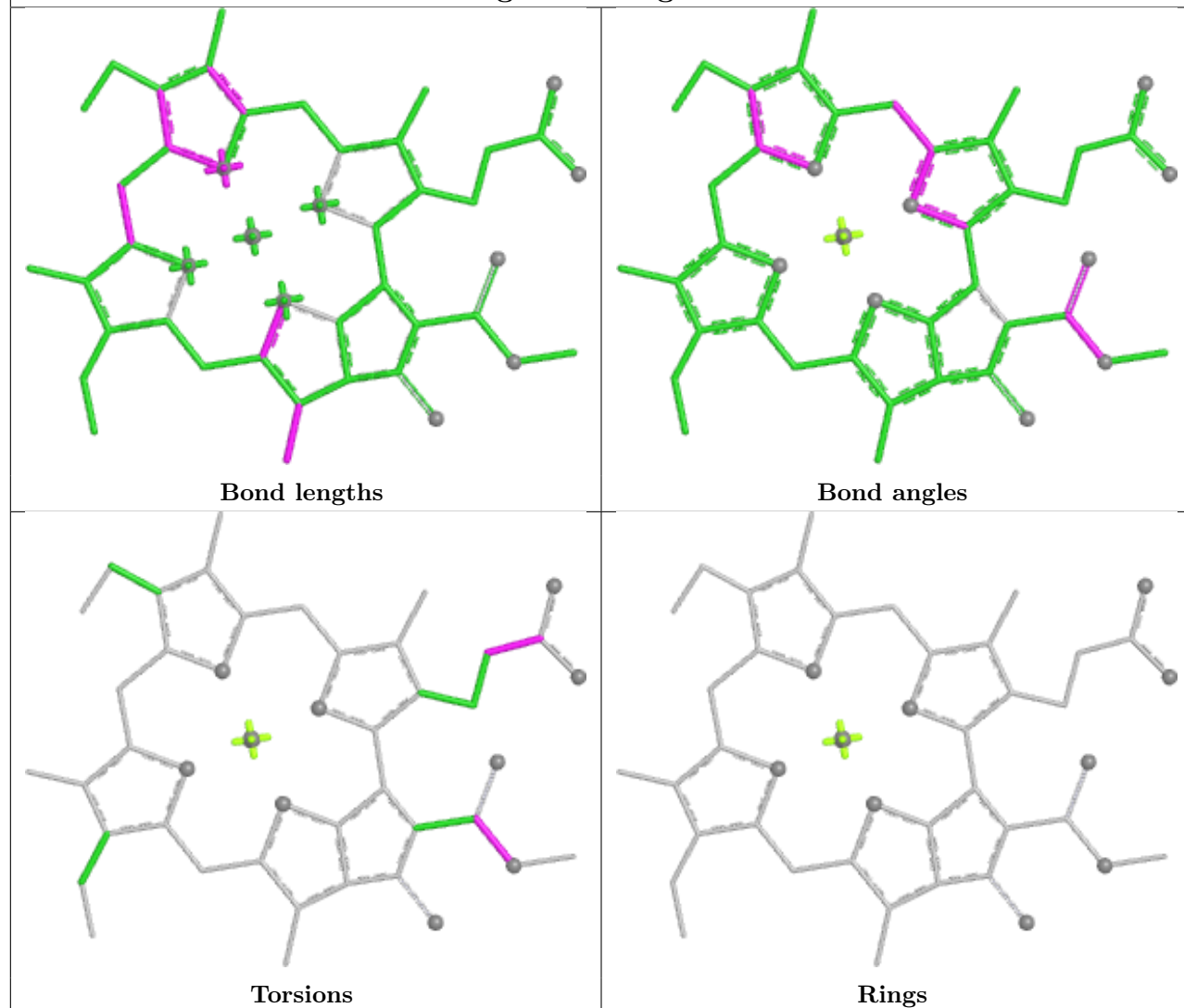




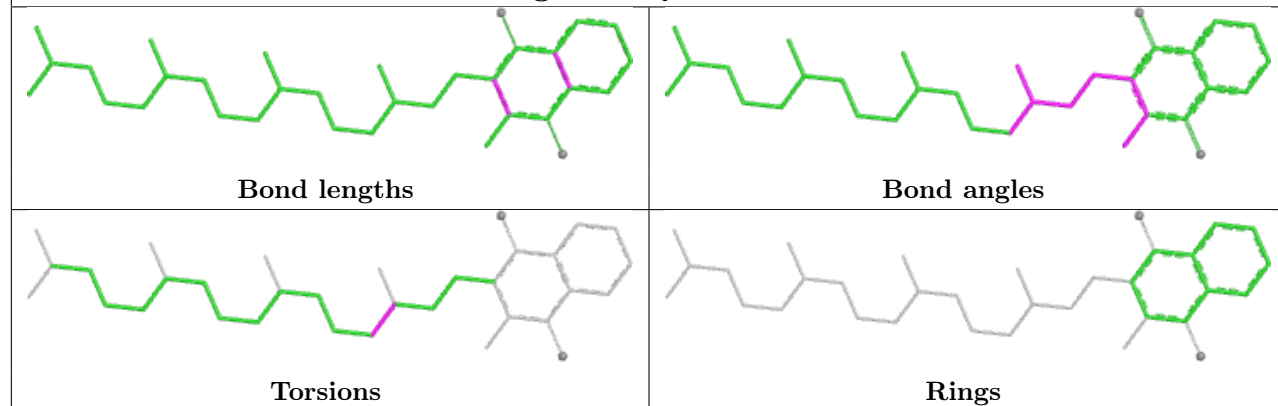


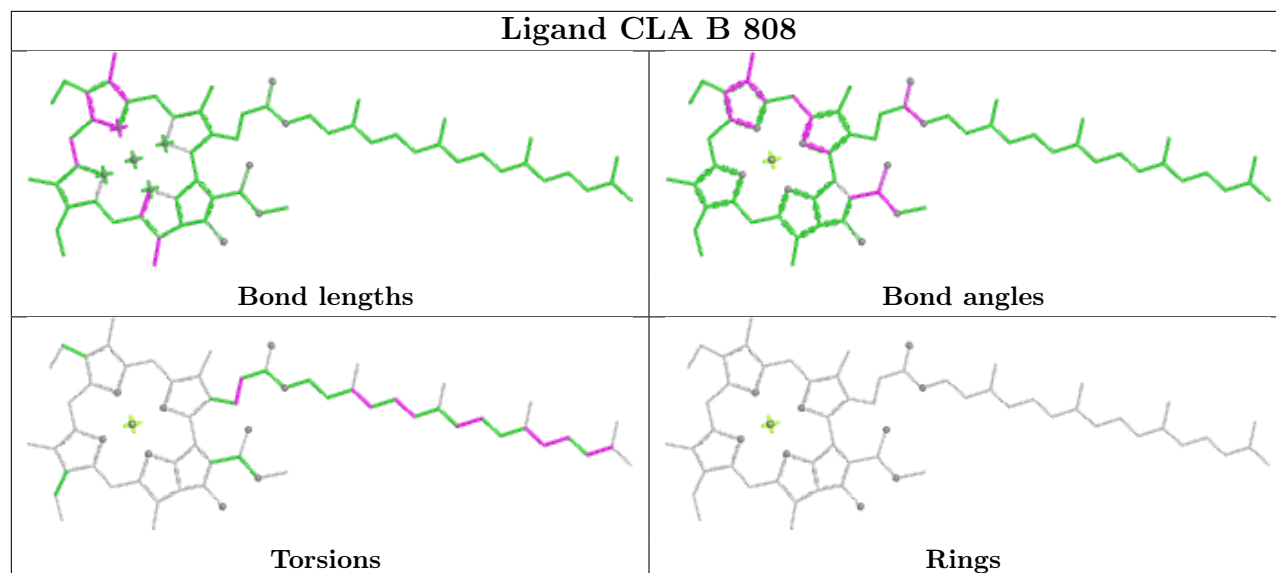
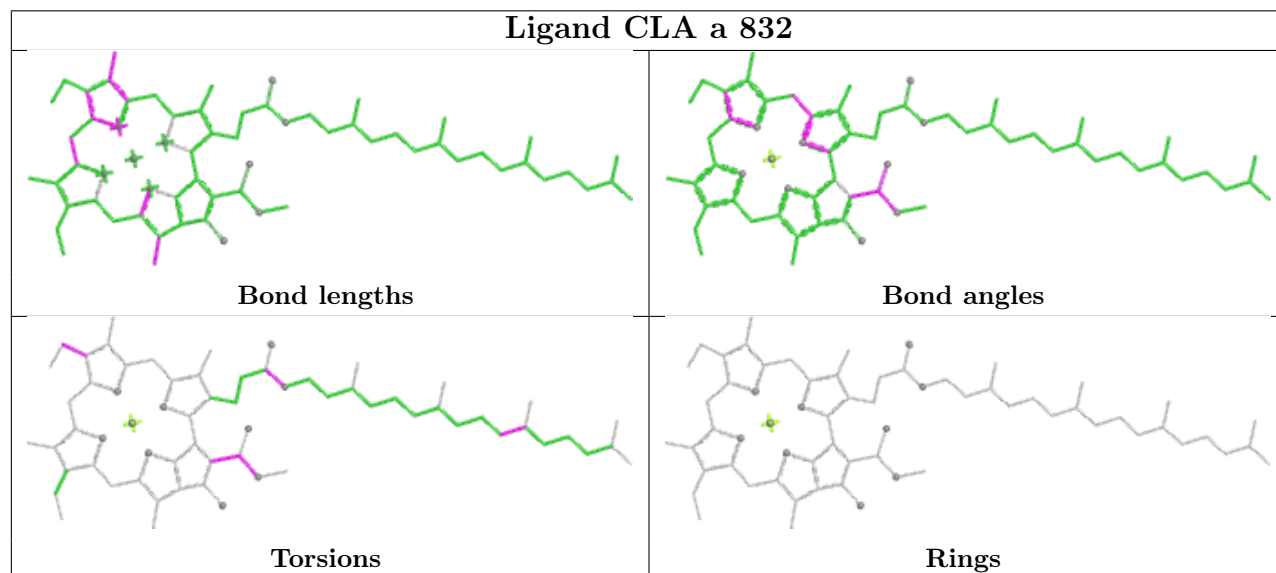
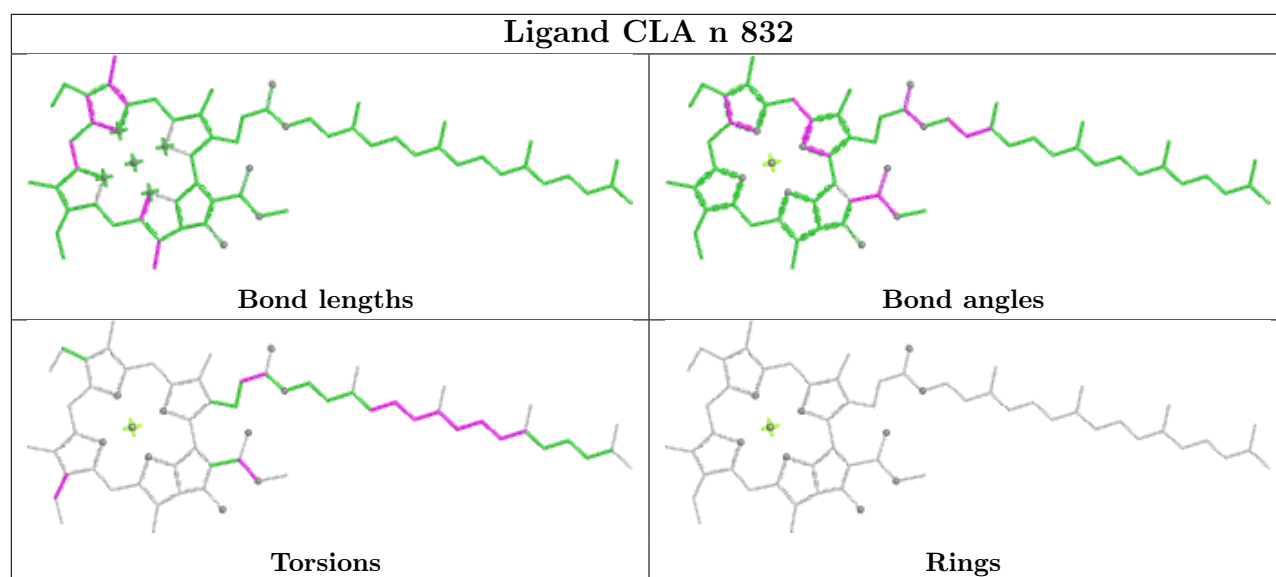


## Ligand CLA g 814

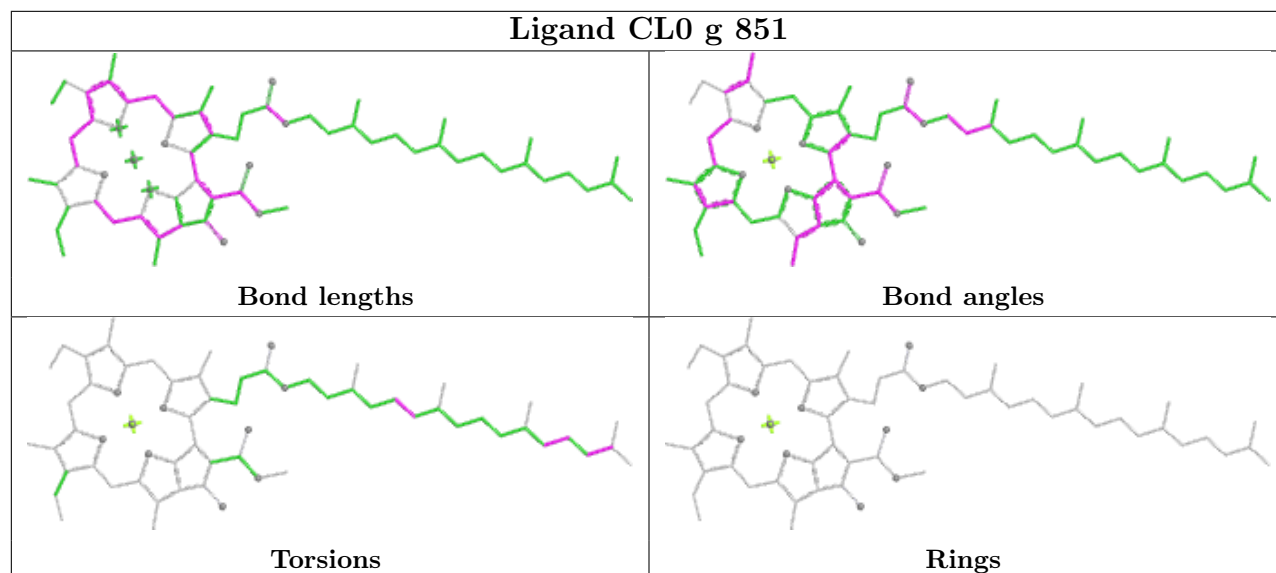
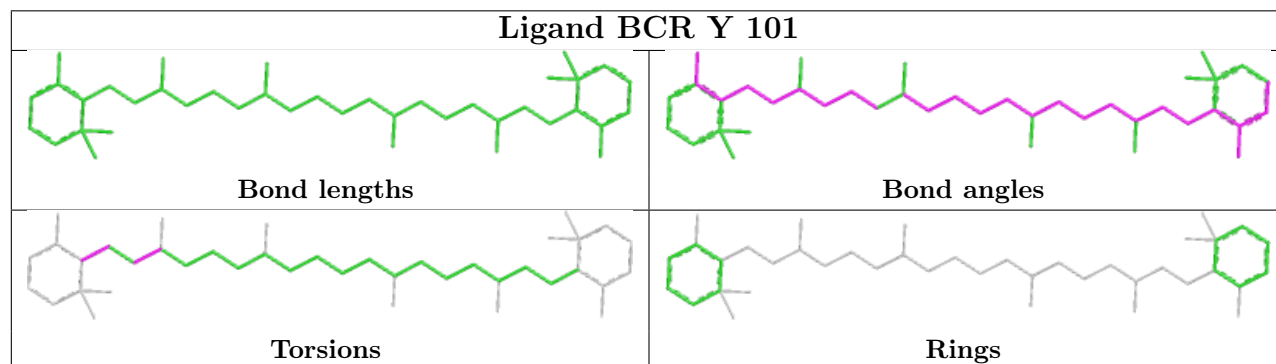
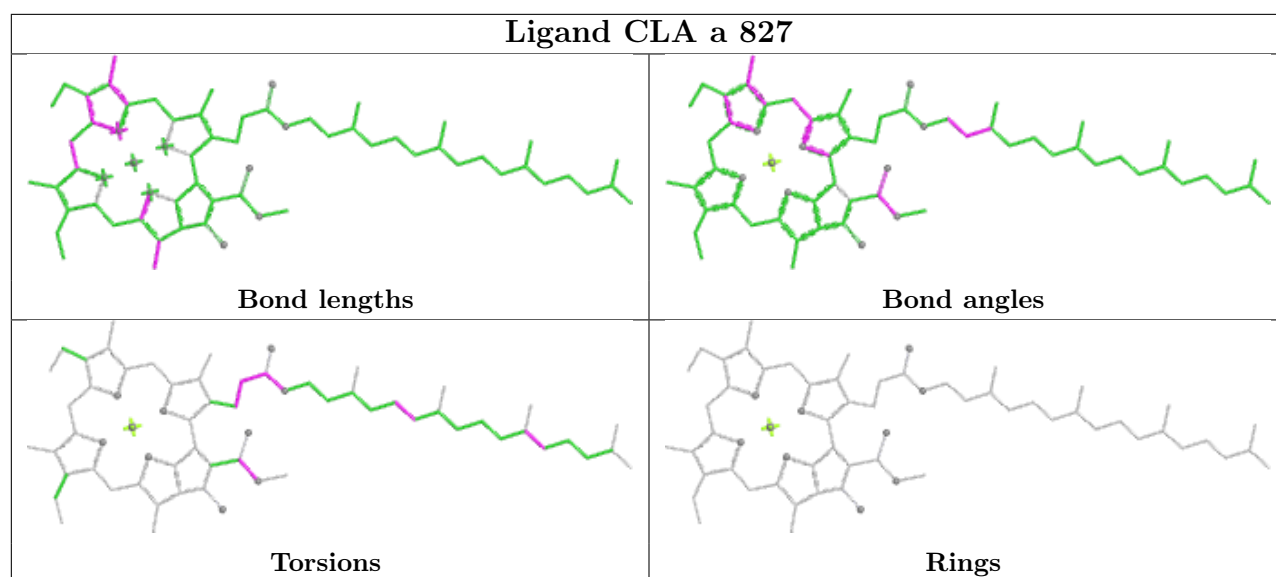


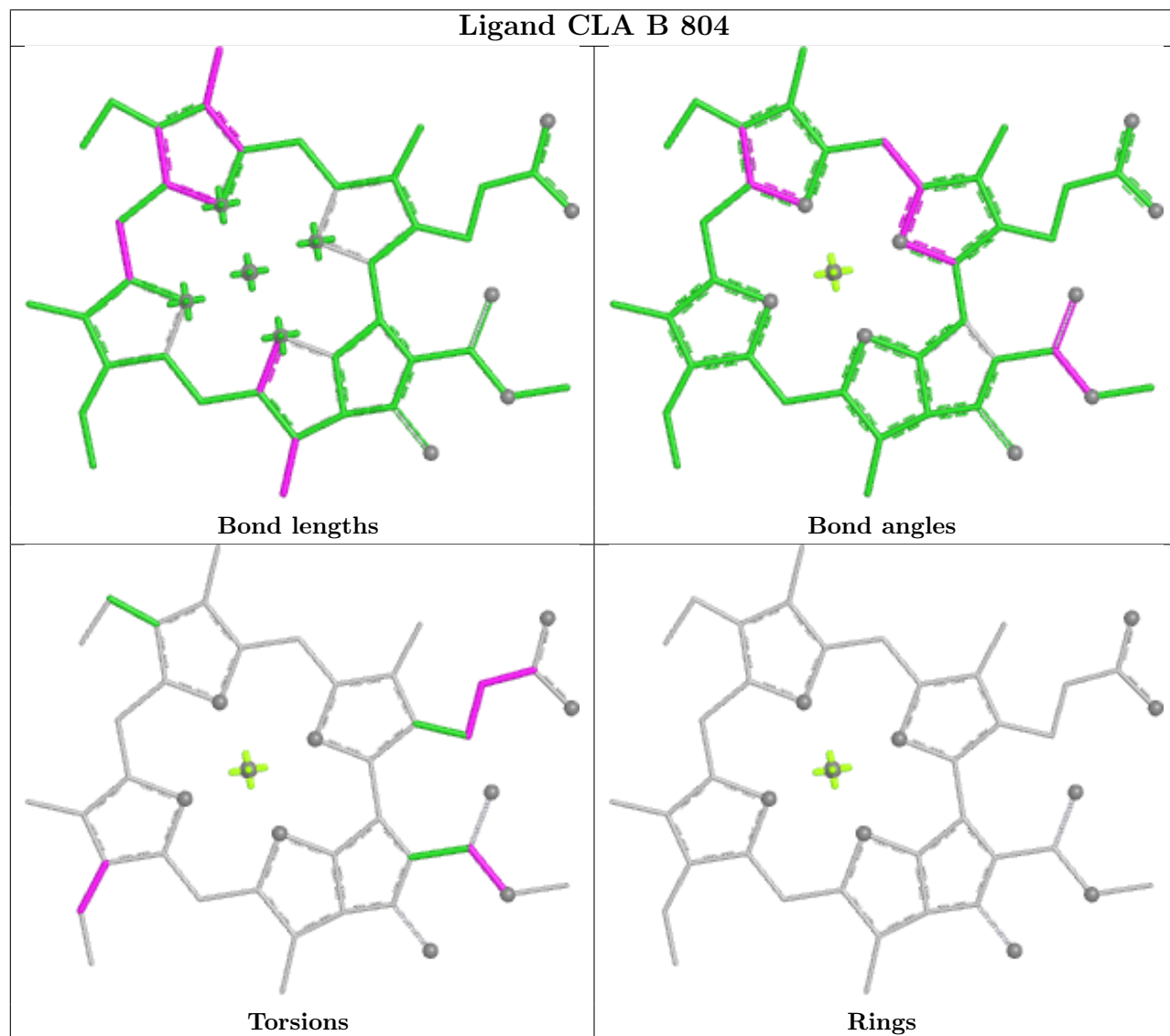
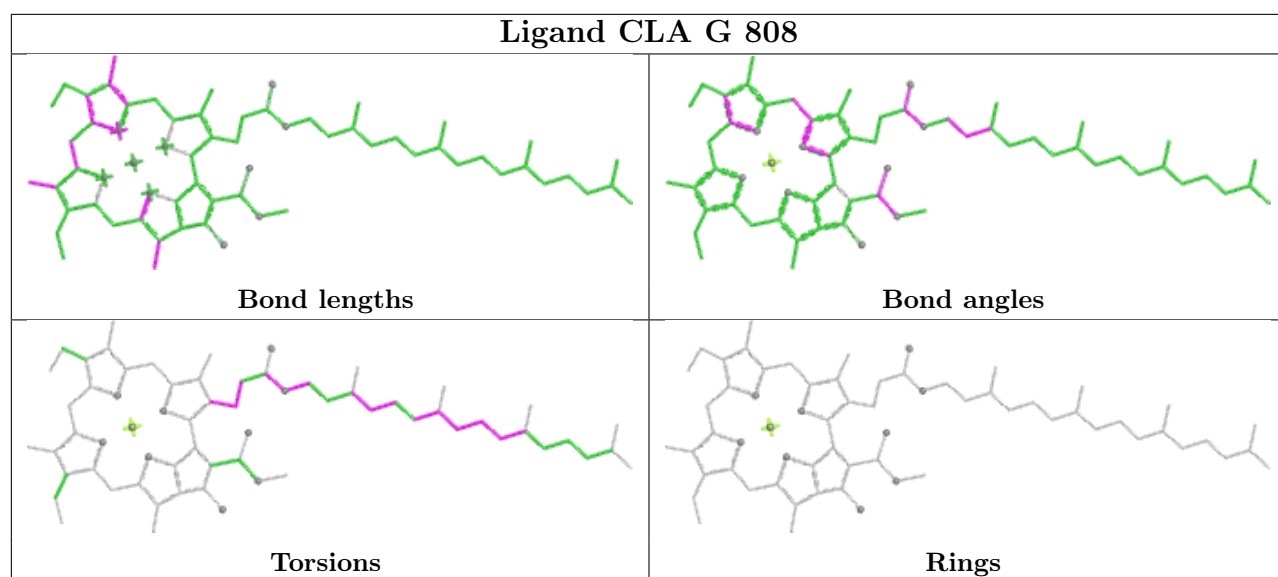
## Ligand PQN b 842



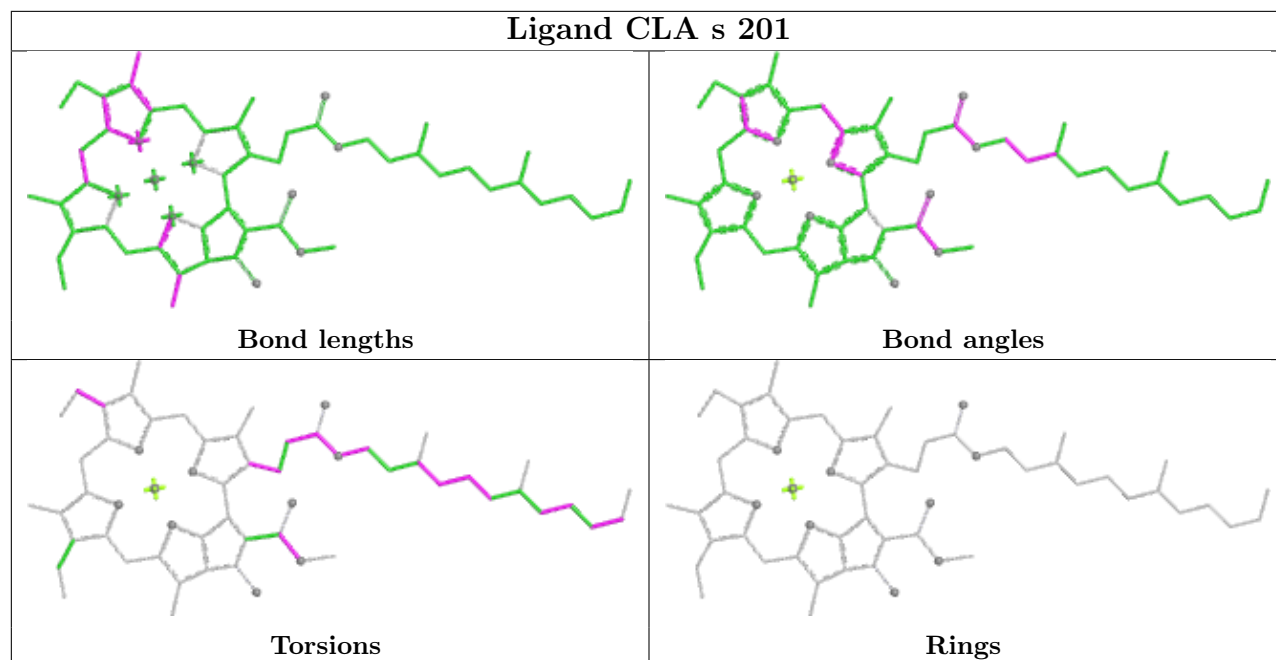




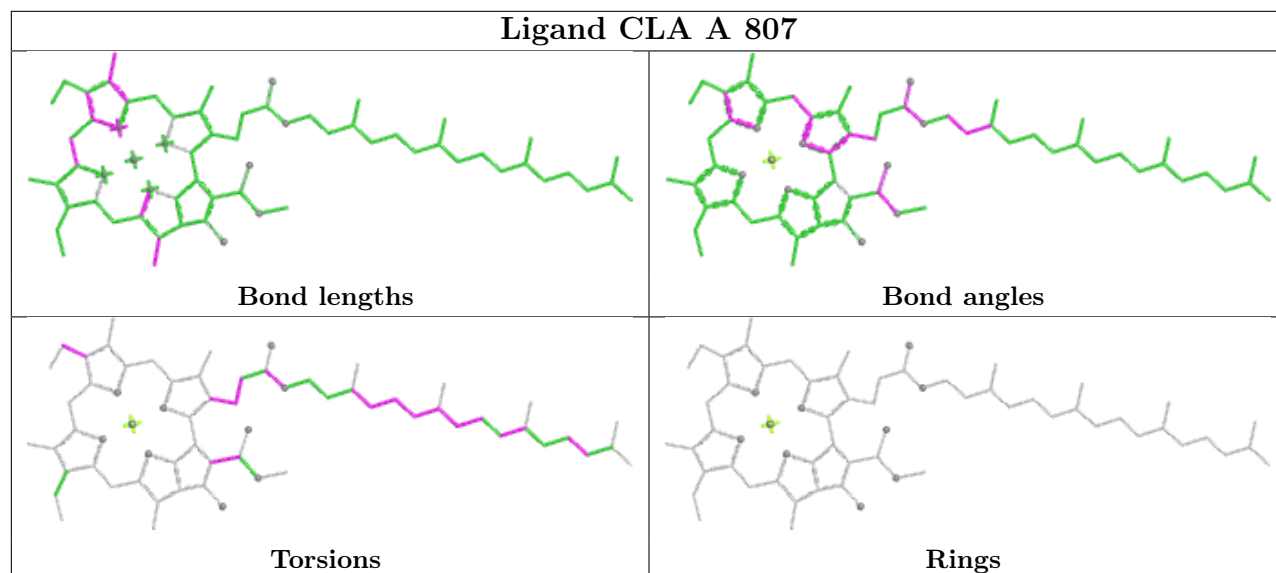




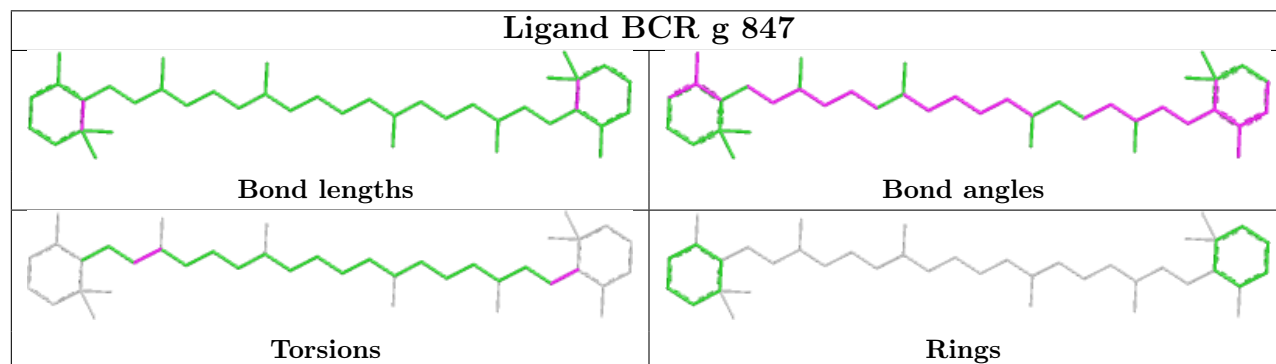
## Ligand CLA s 201

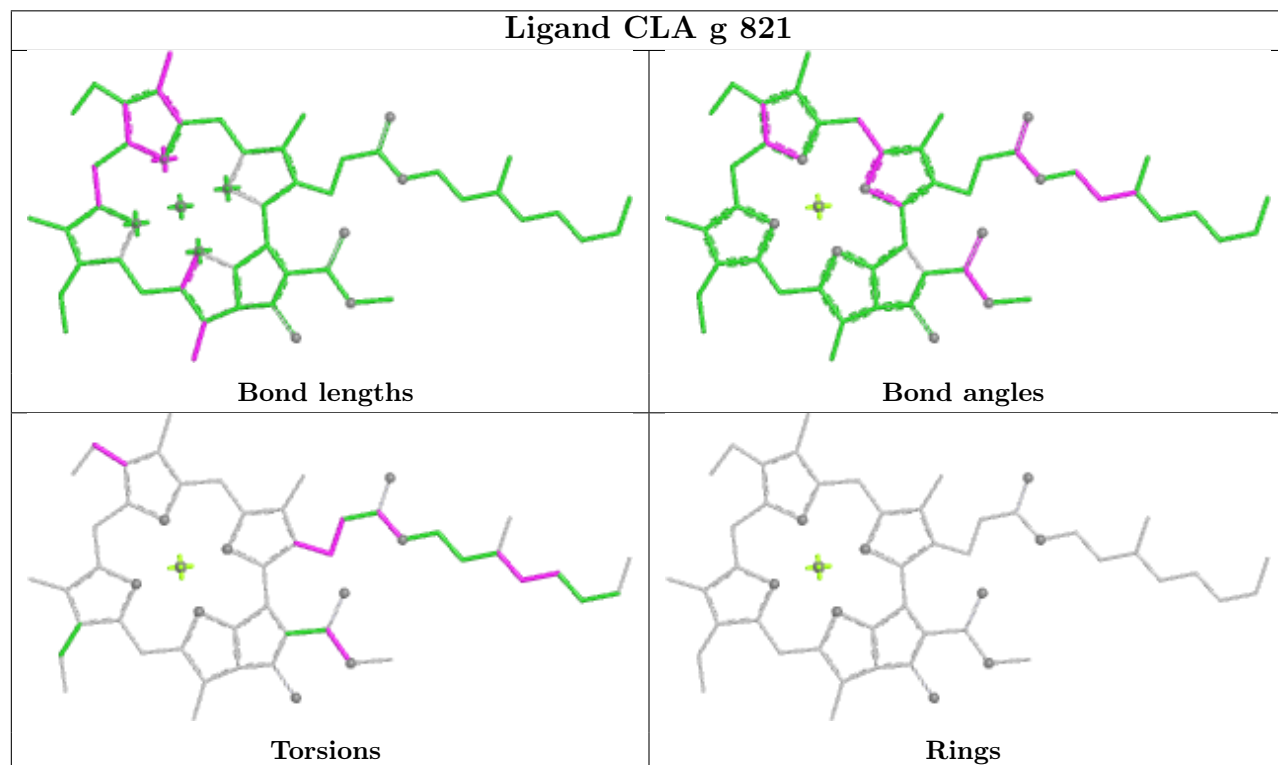
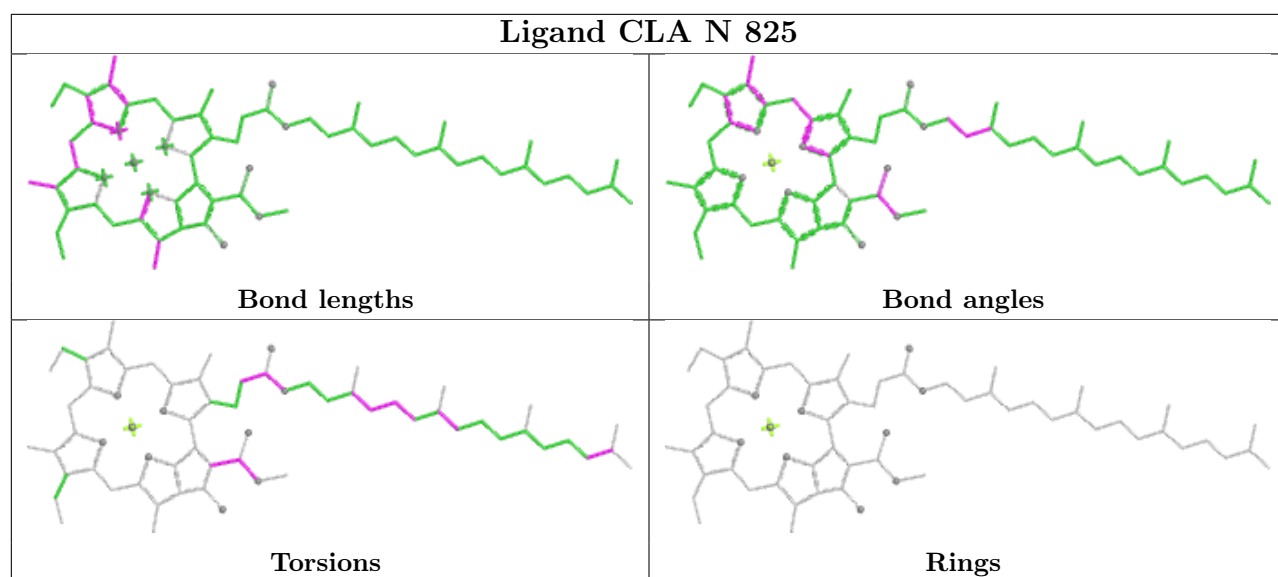


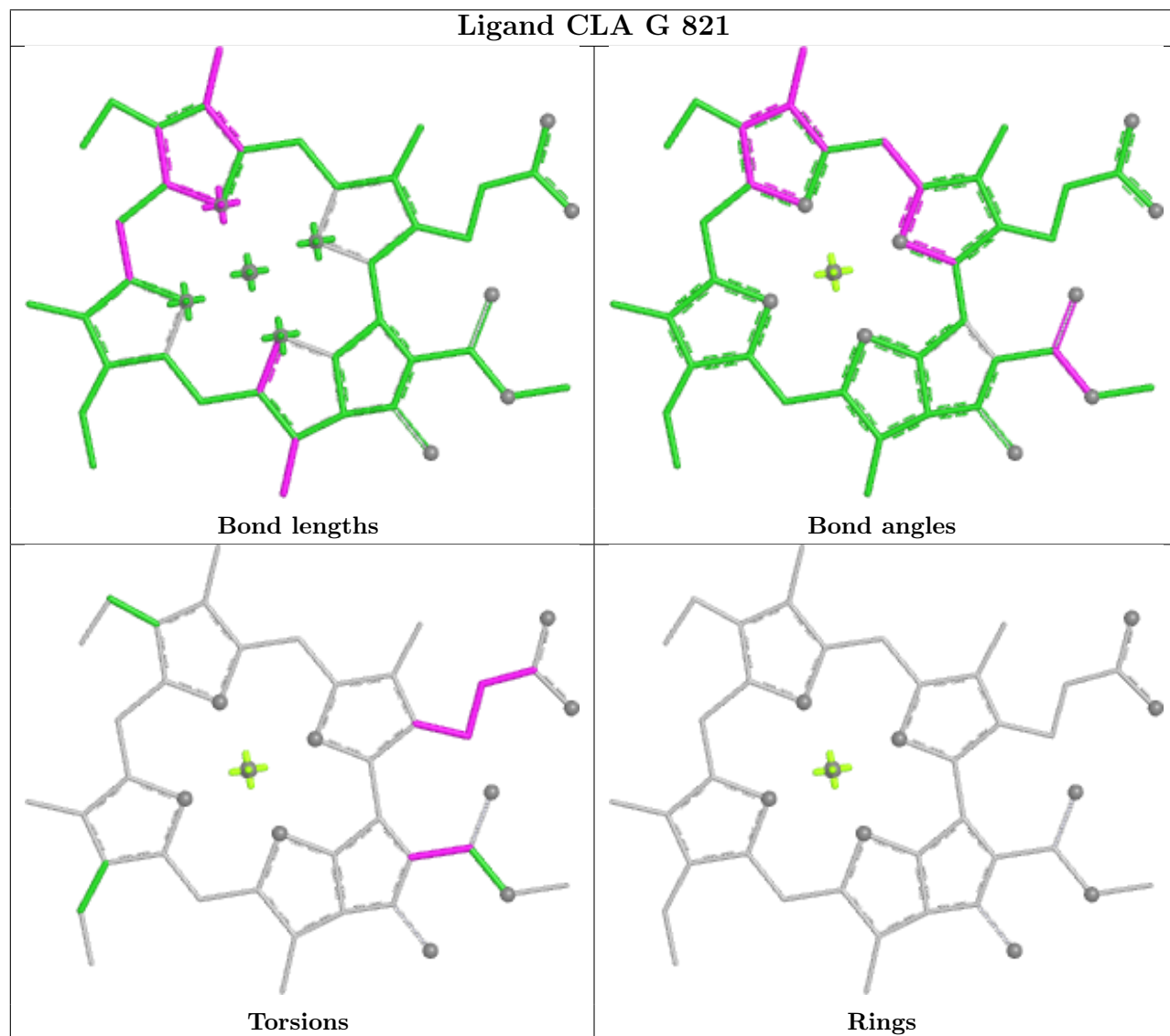
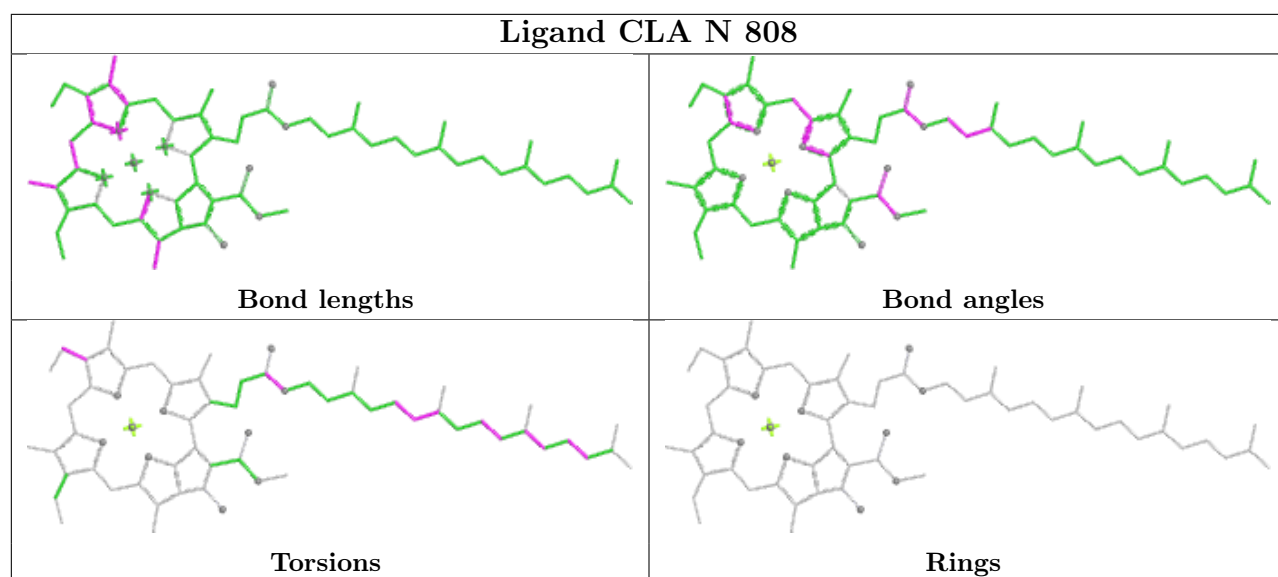
## Ligand CLA A 807

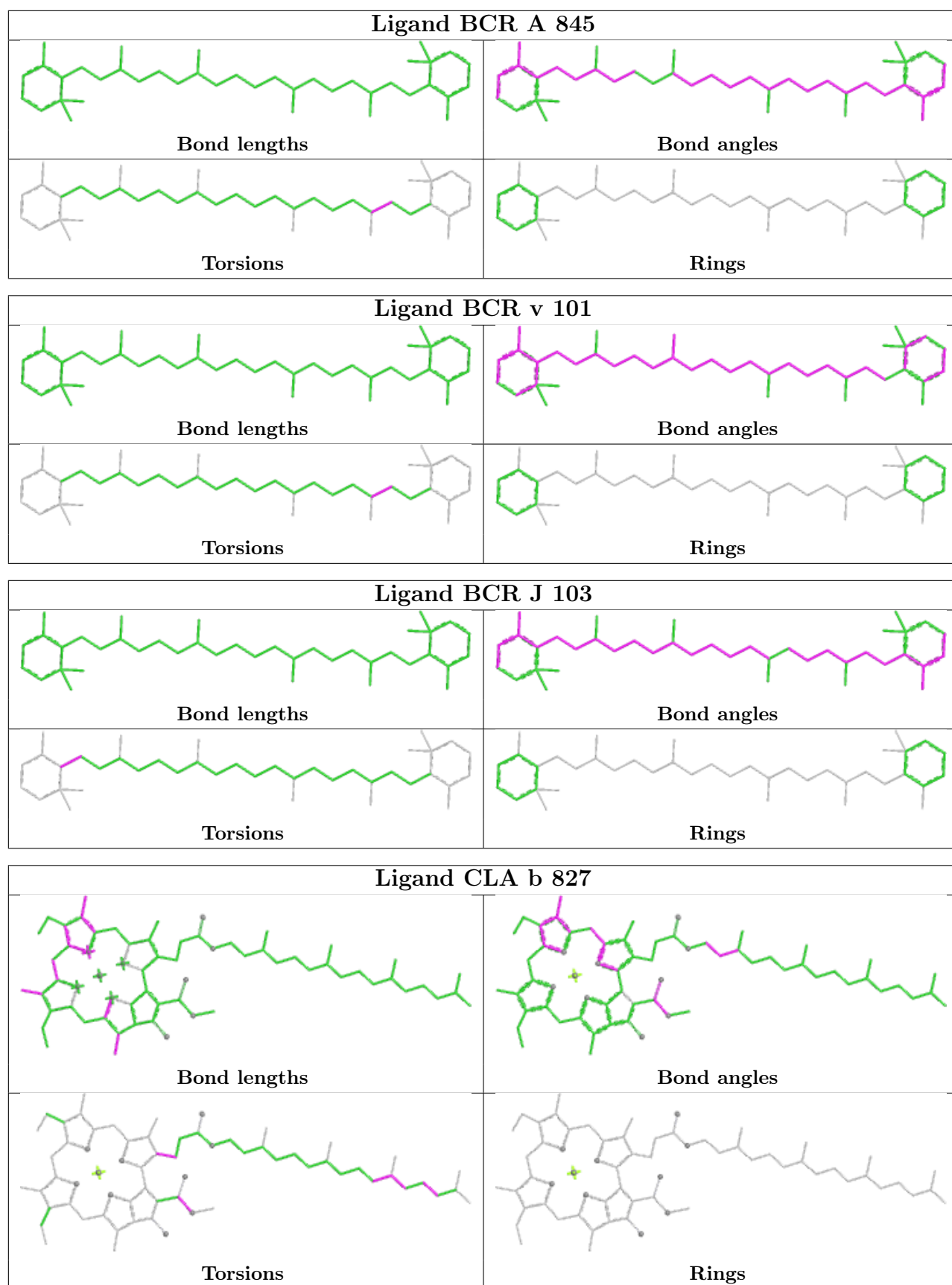


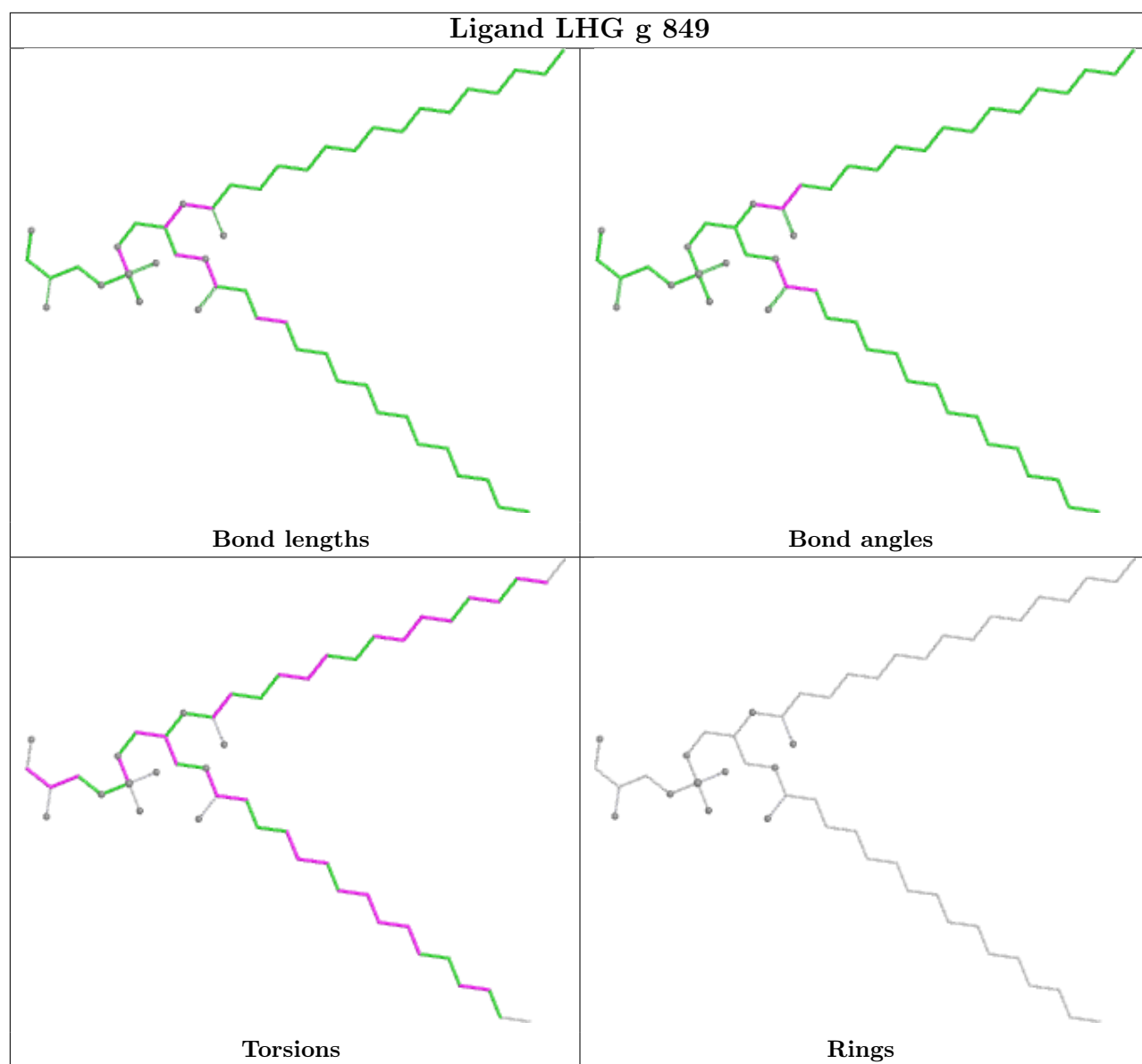
## Ligand BCR g 847



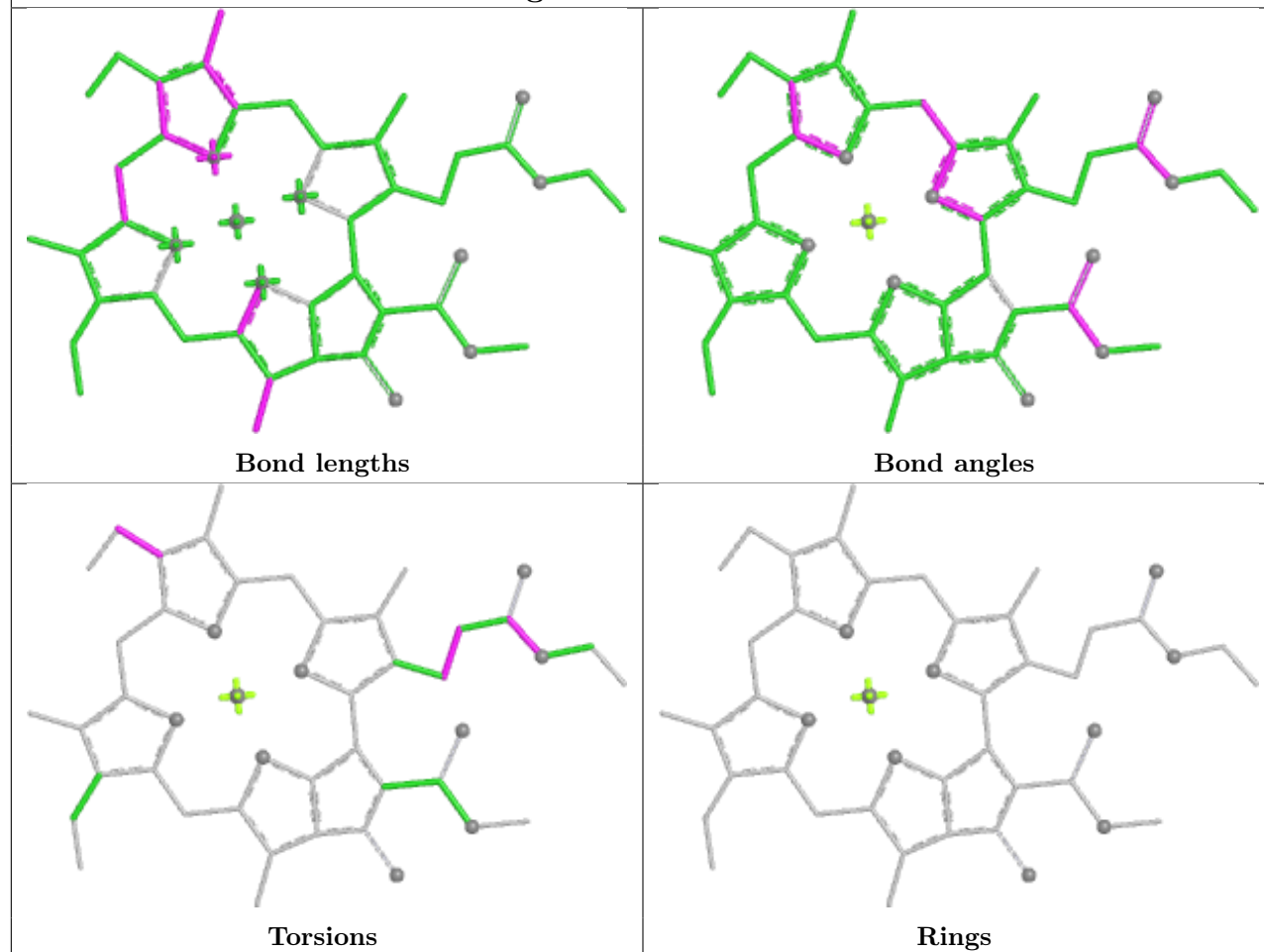




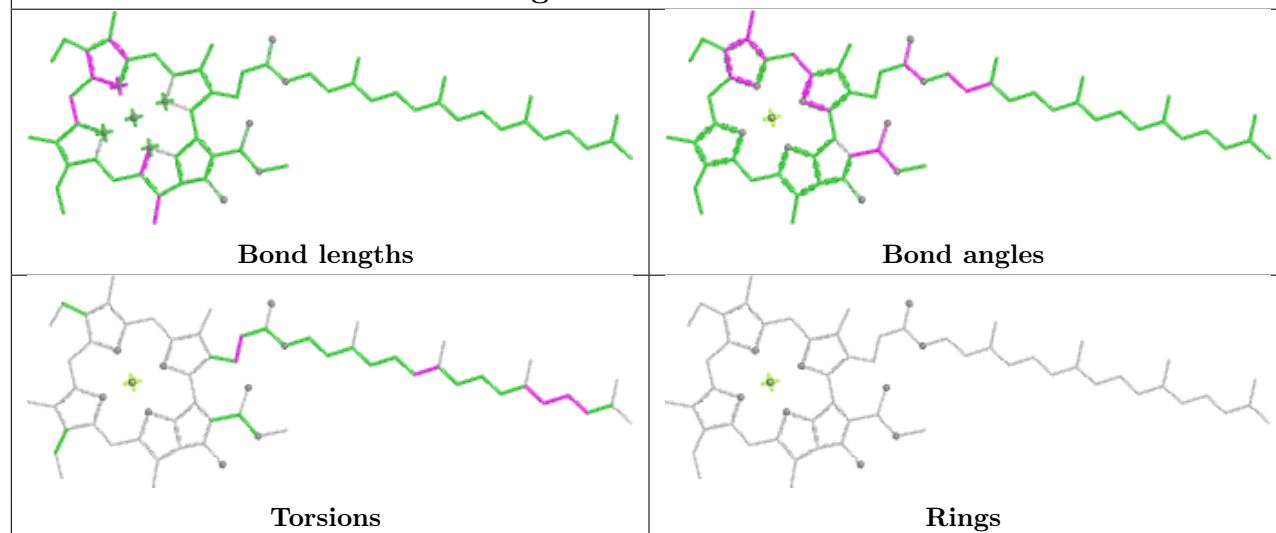




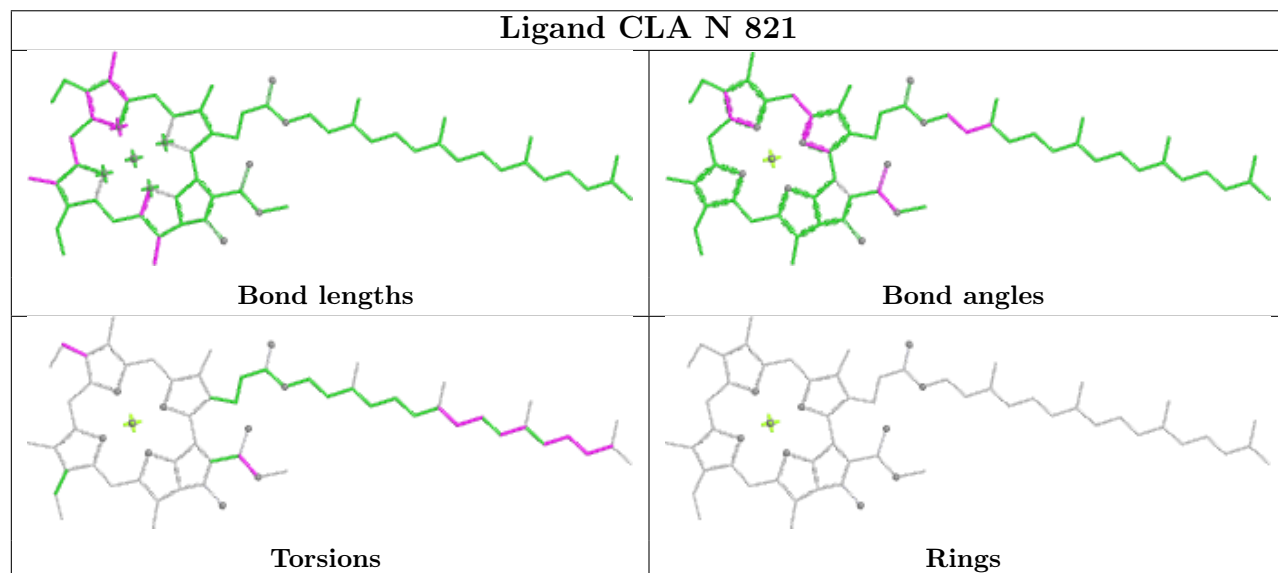
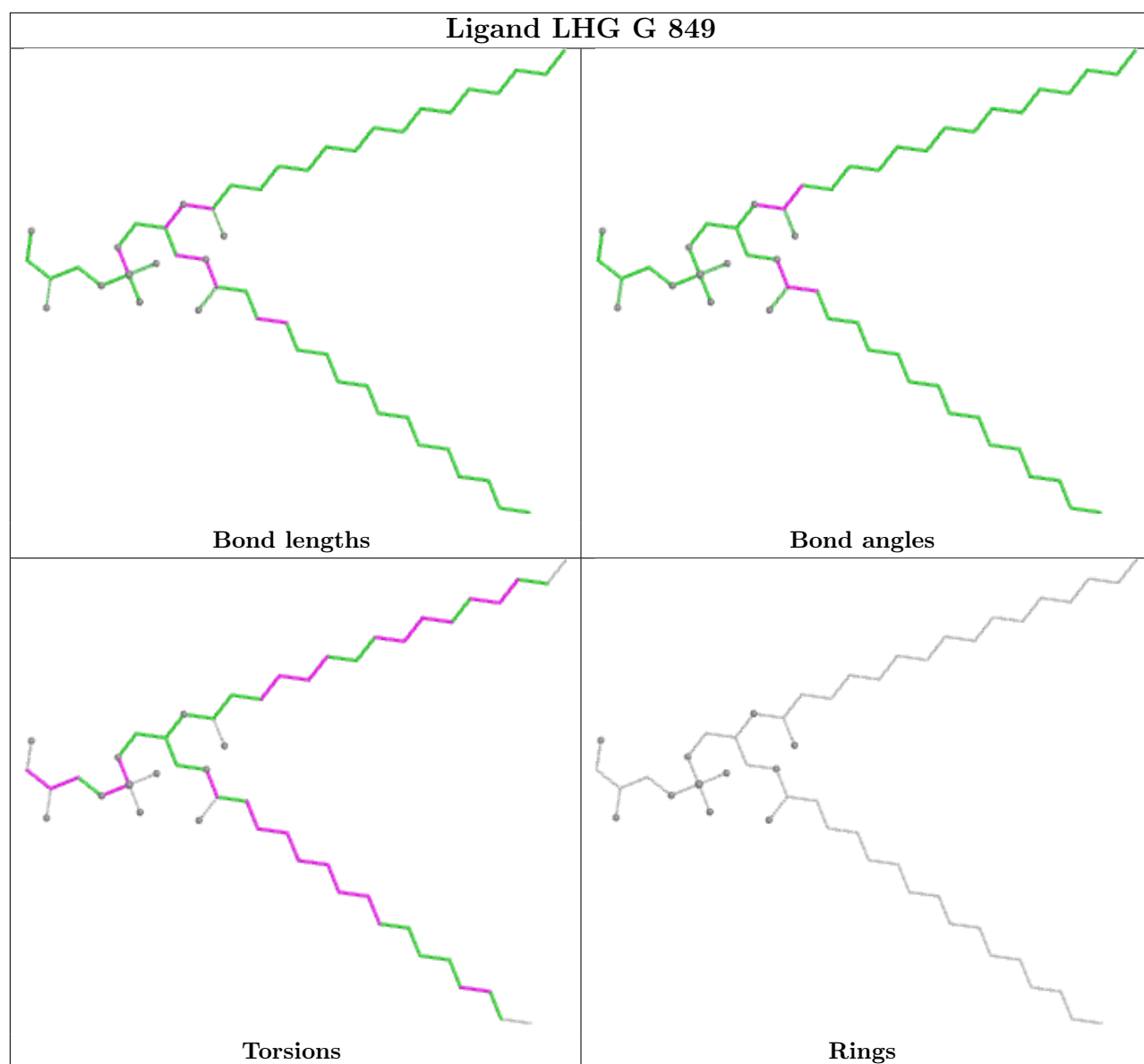
## Ligand CLA N 840



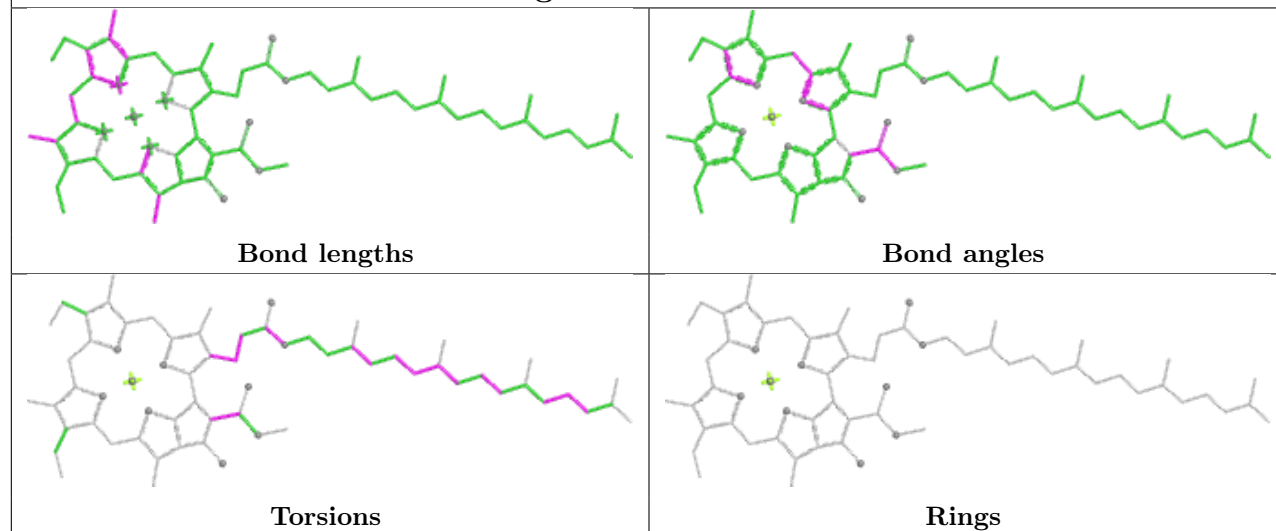
## Ligand CLA N 809



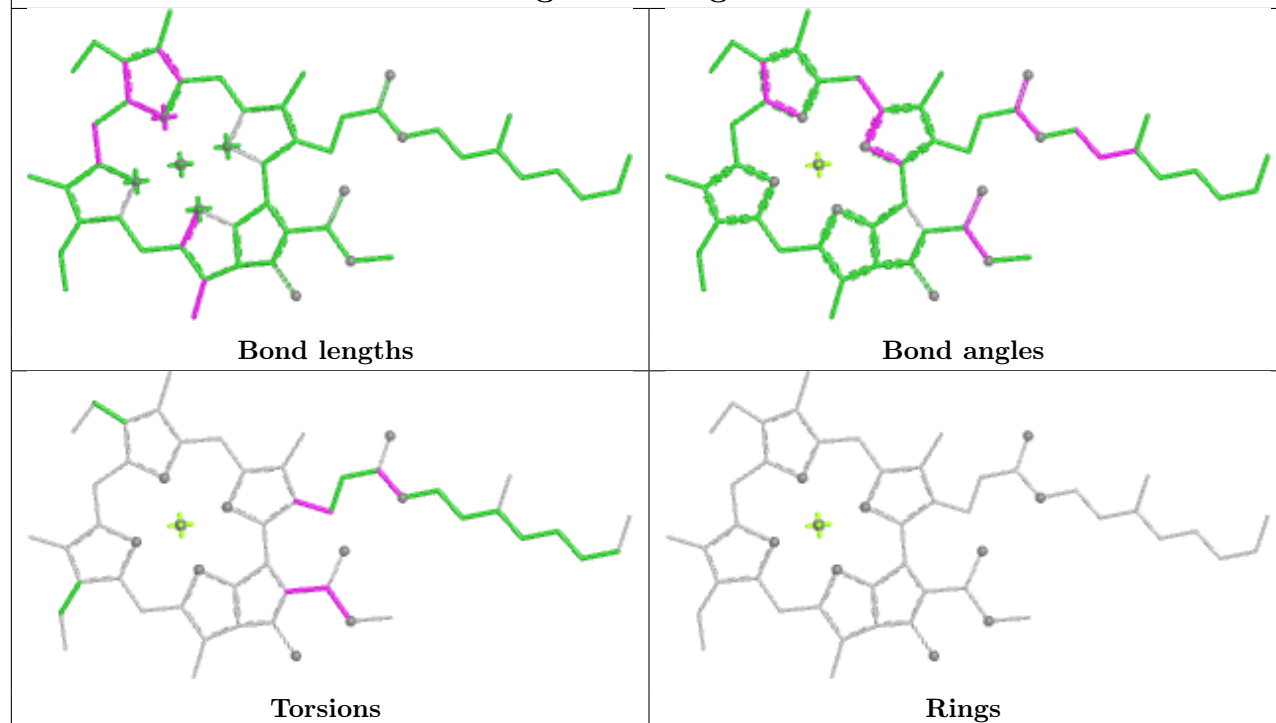




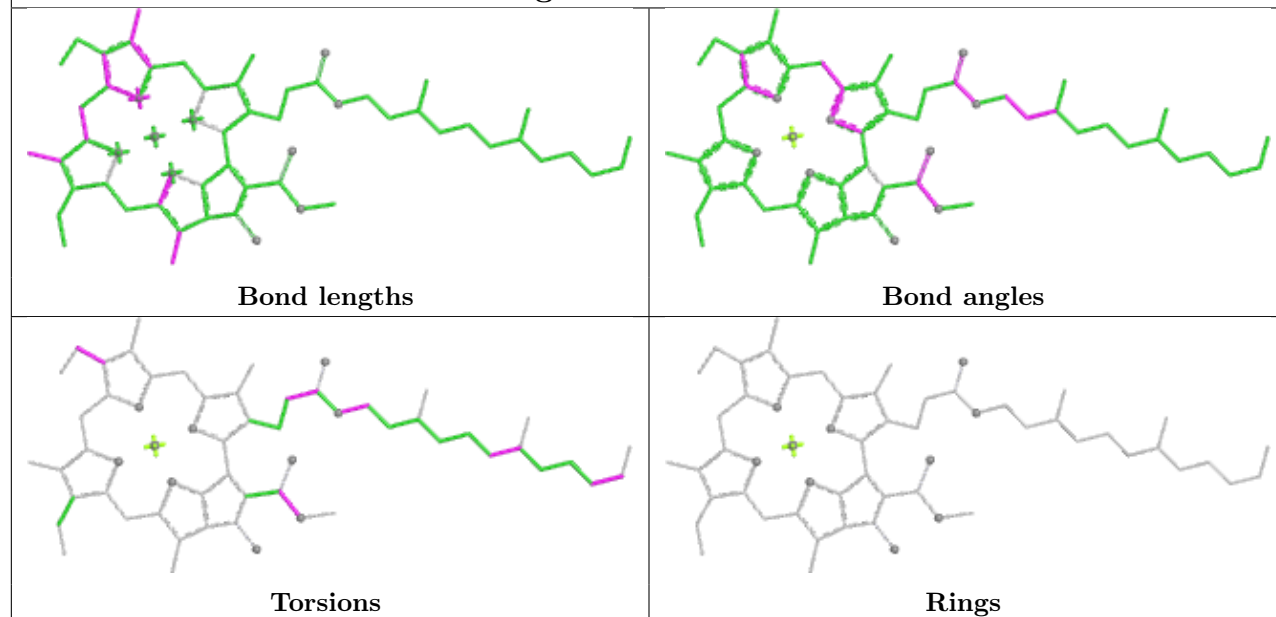
## Ligand CLA b 803



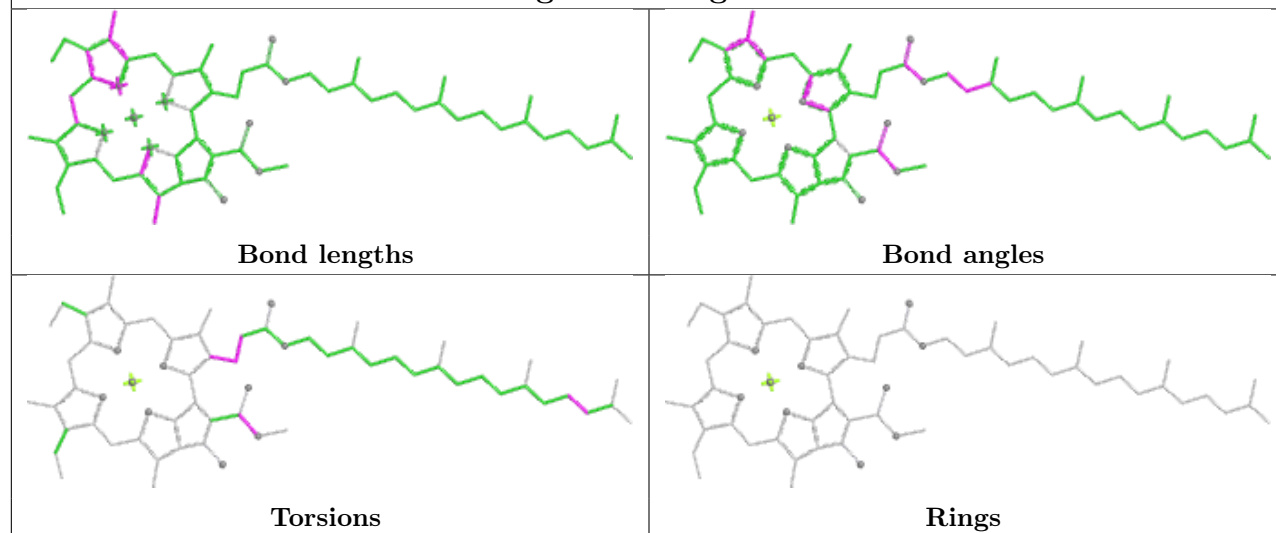
## Ligand CLA g 812



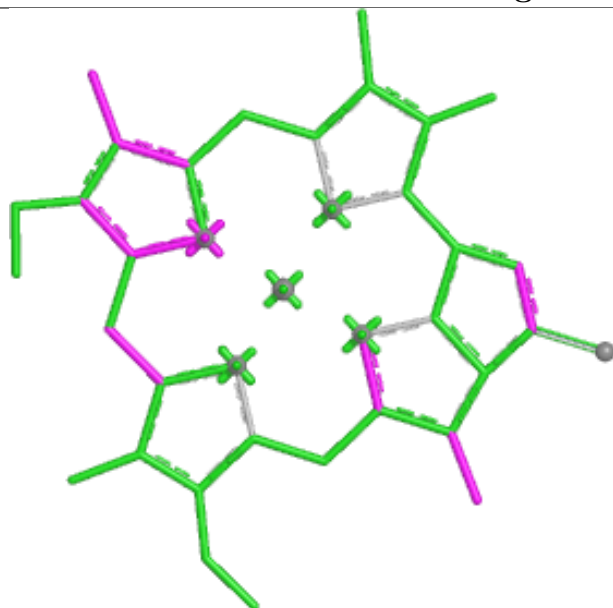
## Ligand CLA S 201



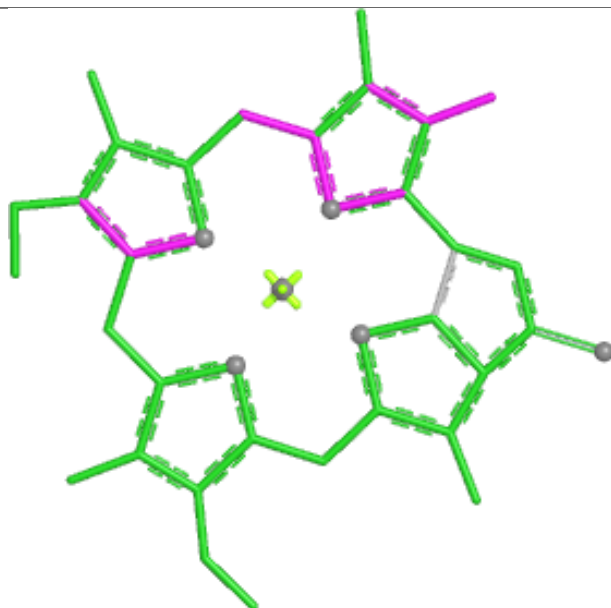
## Ligand CLA g 853



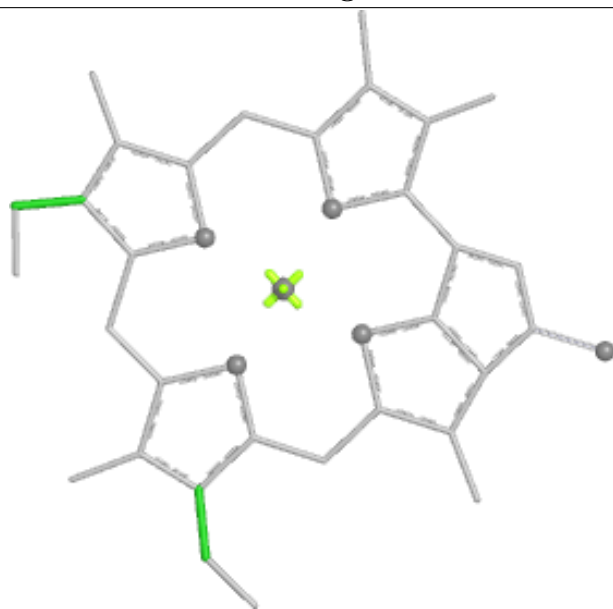
## Ligand CLA T 102



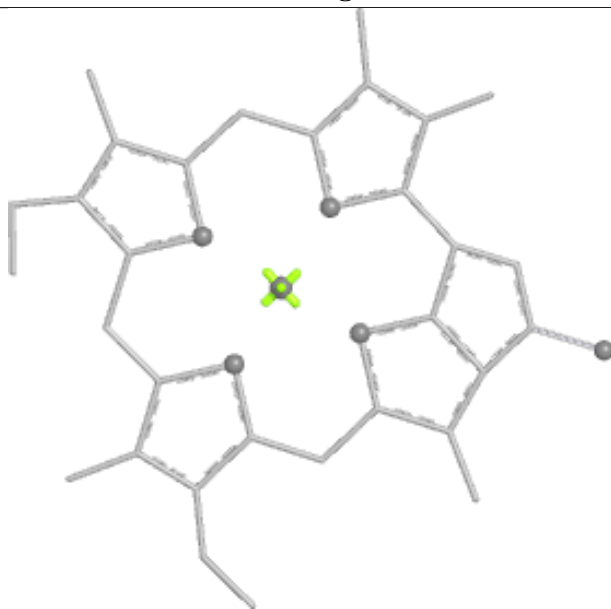
Bond lengths



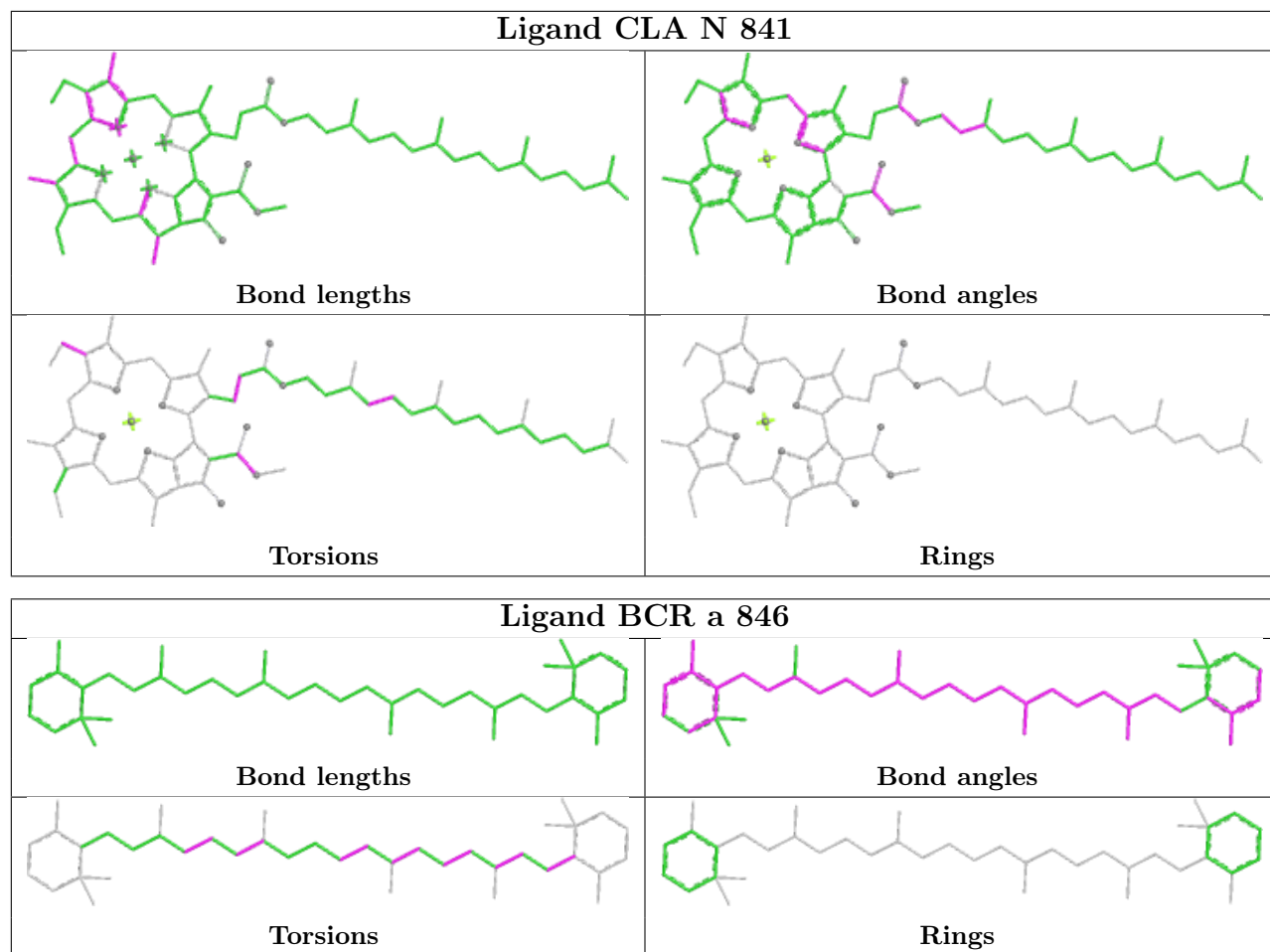
Bond angles



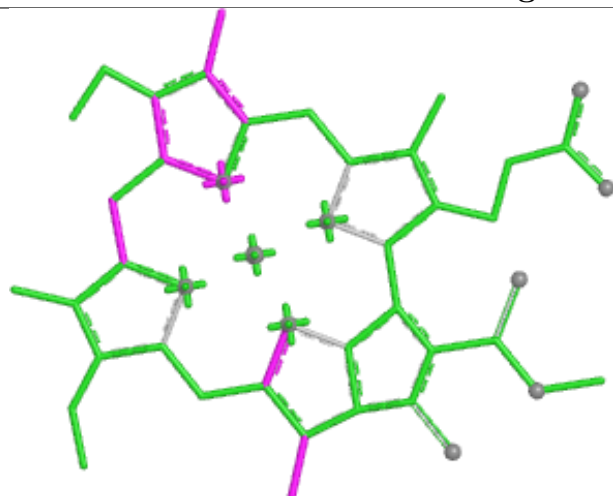
Torsions



Rings



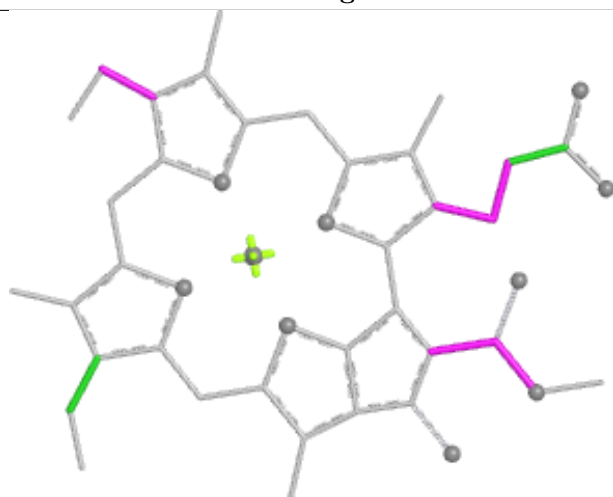
## Ligand CLA J 101



Bond lengths



Bond angles

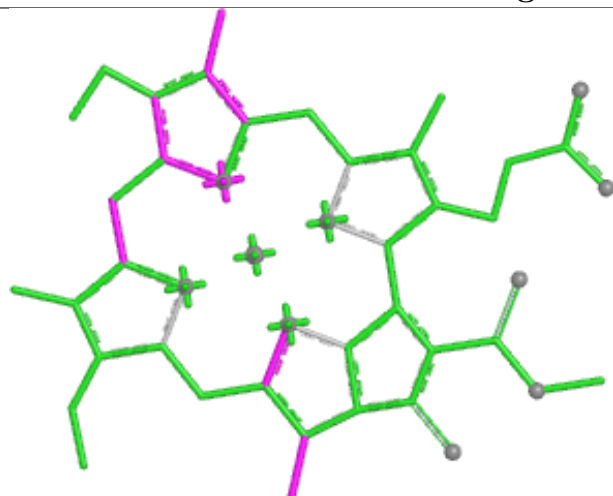


Torsions

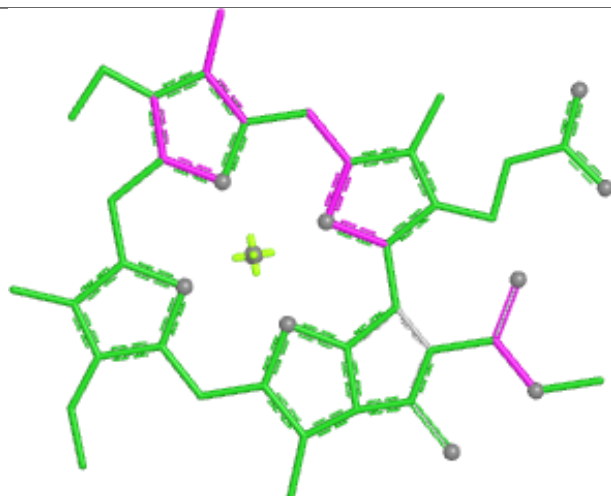


Rings

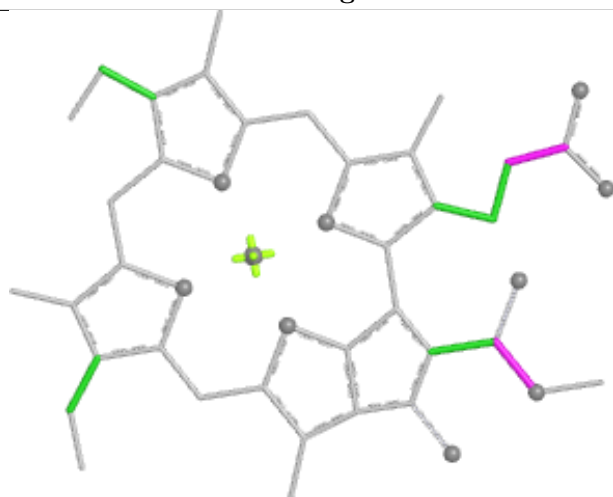
## Ligand CLA S 203



Bond lengths



Bond angles

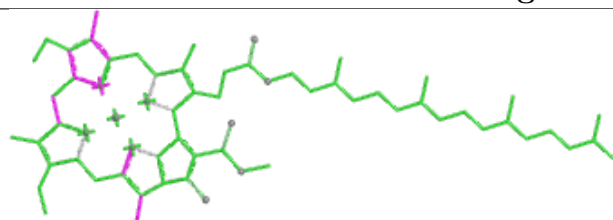


Torsions

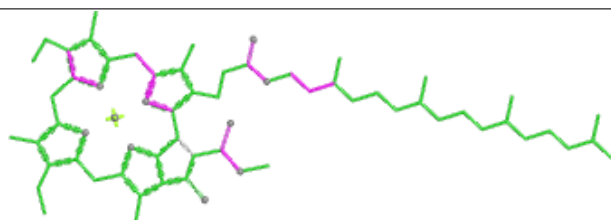


Rings

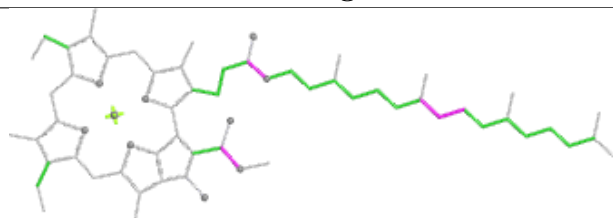
## Ligand CLA n 819



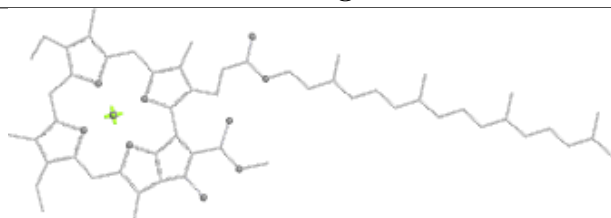
Bond lengths



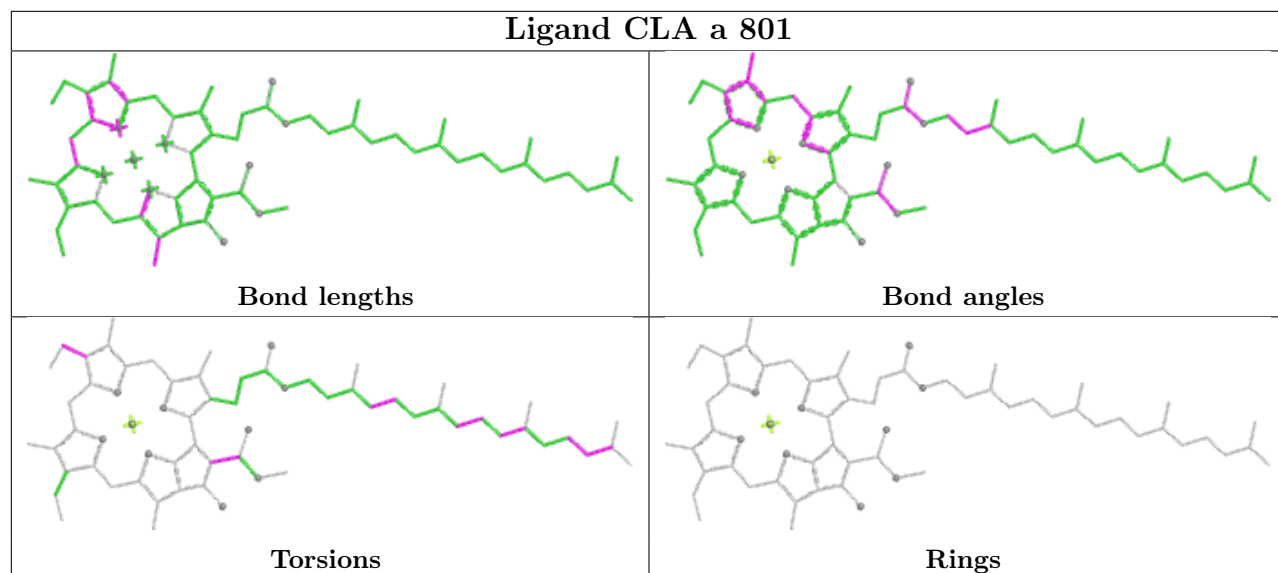
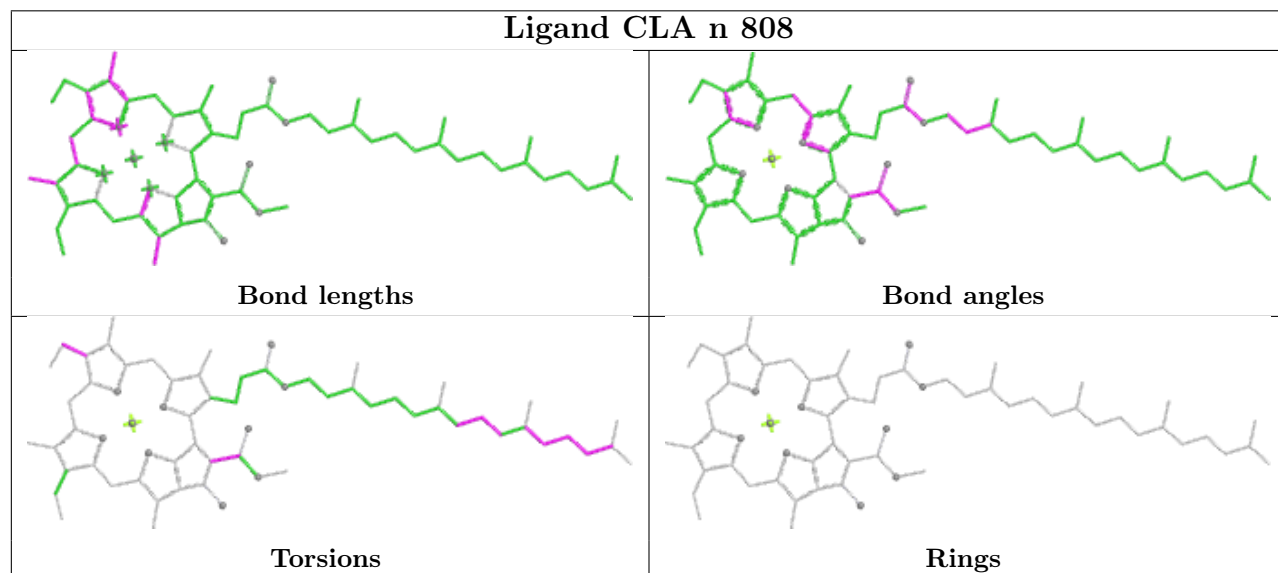
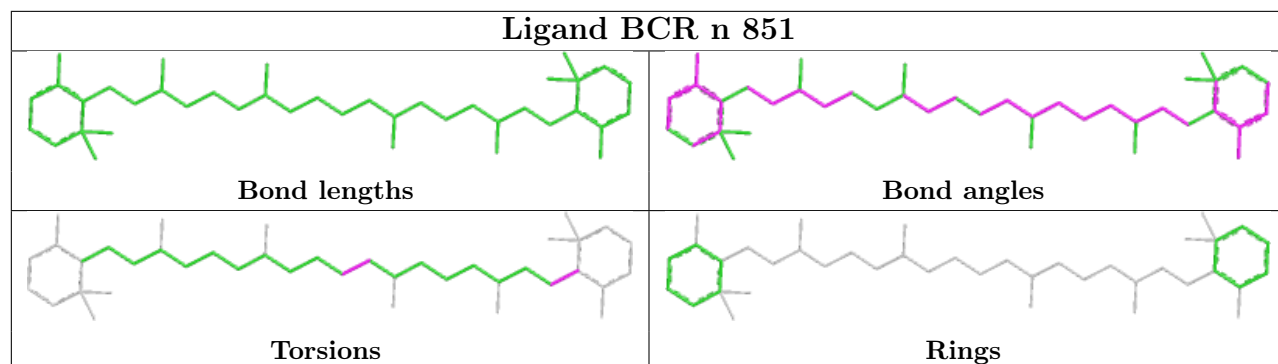
Bond angles



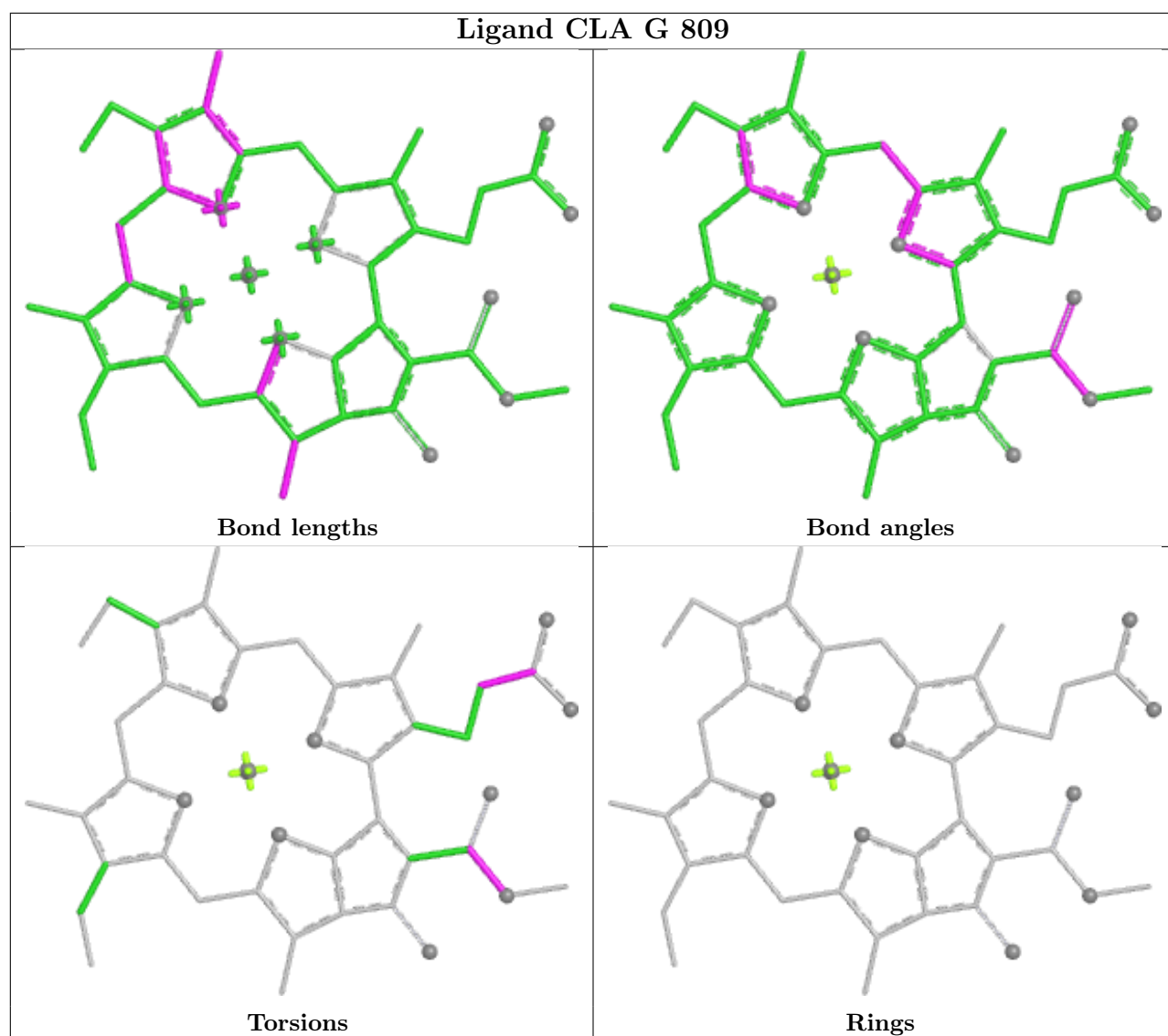
Torsions

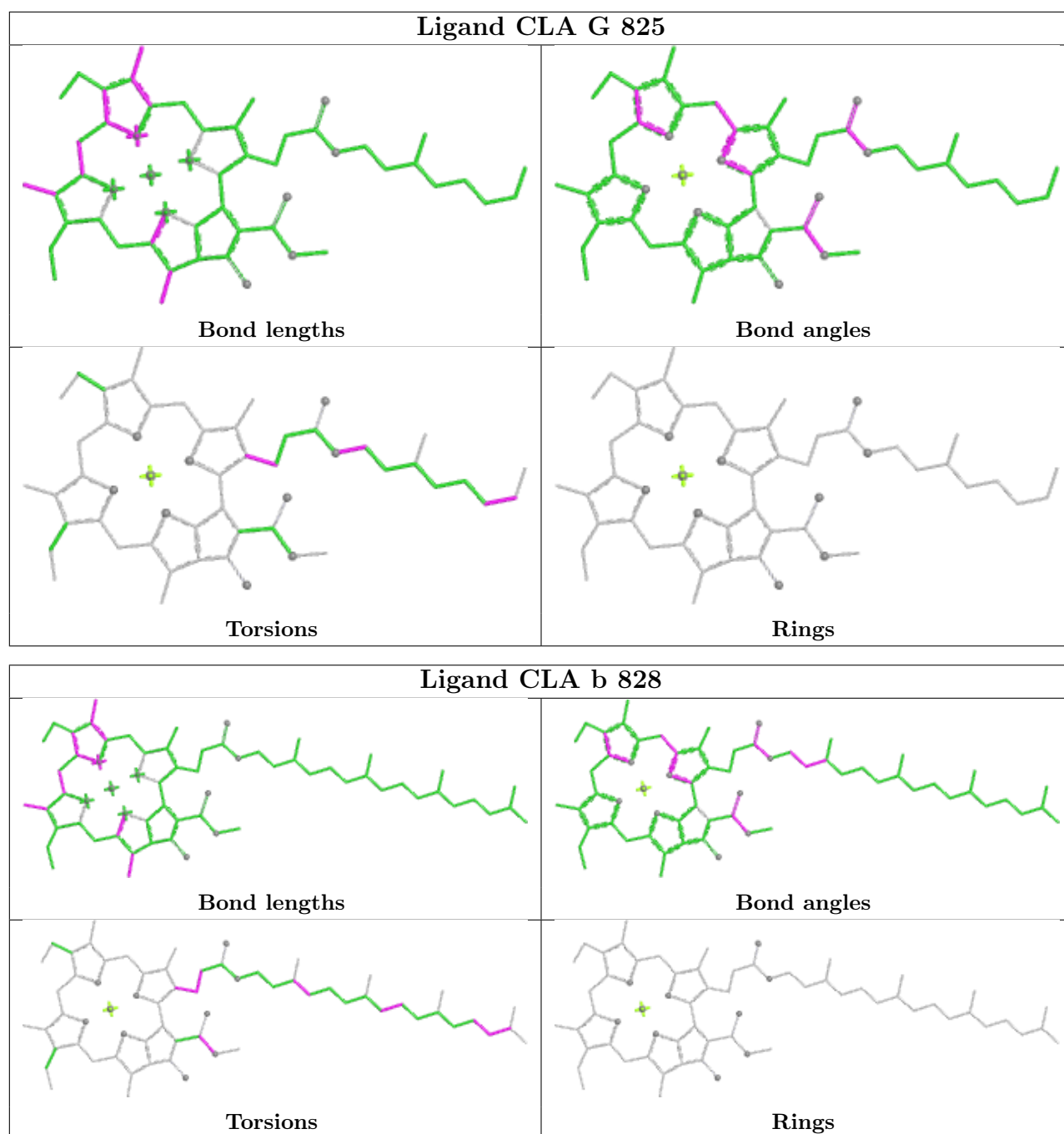


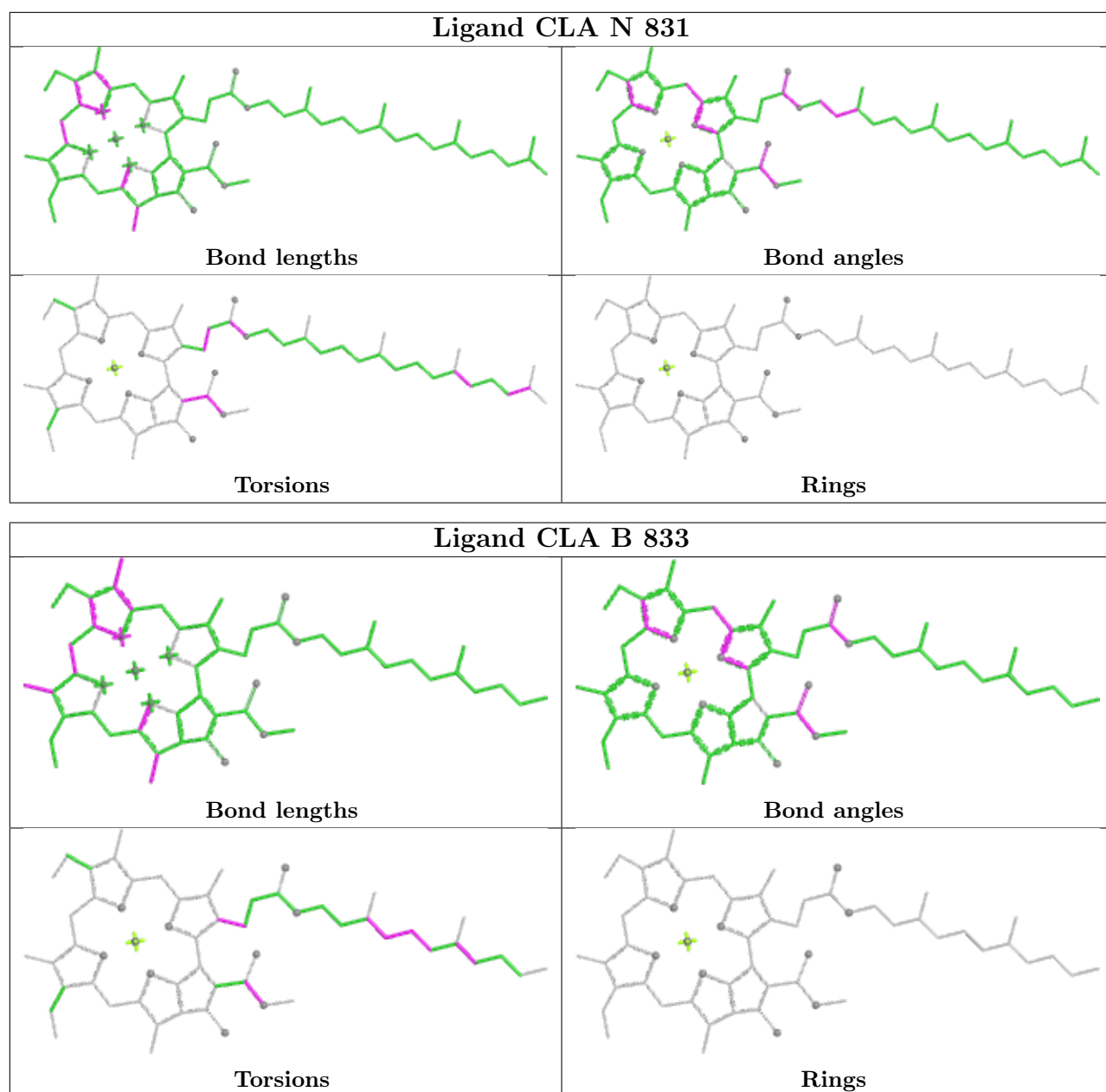
Rings

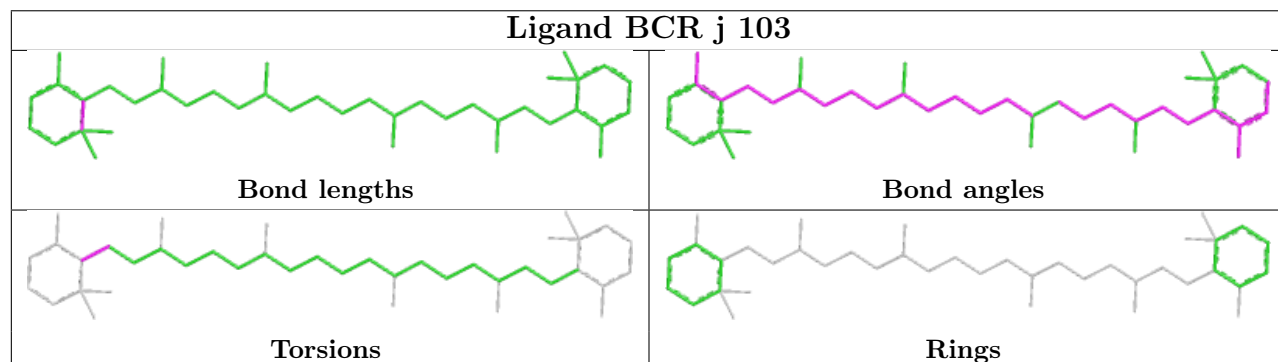
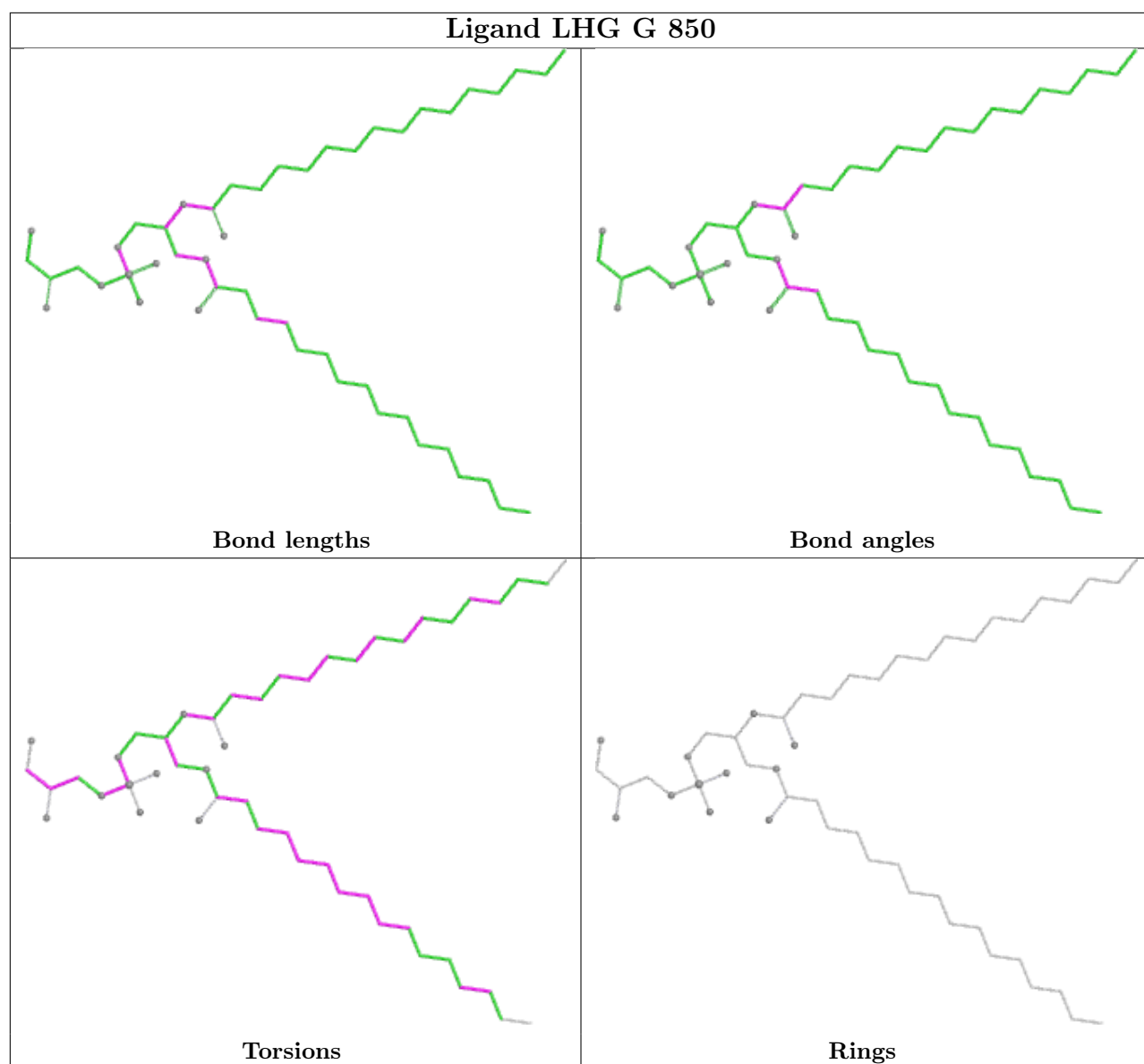


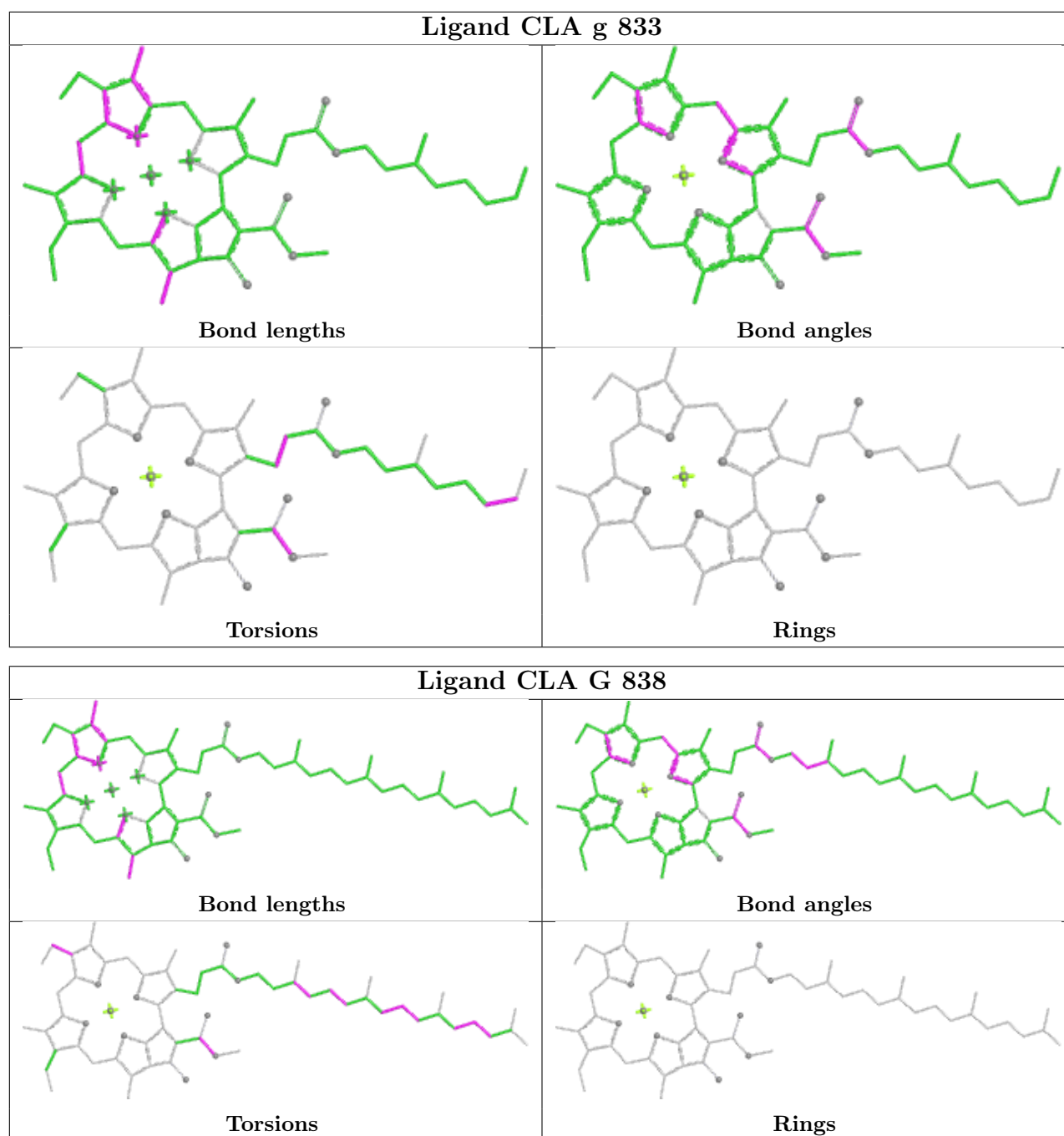




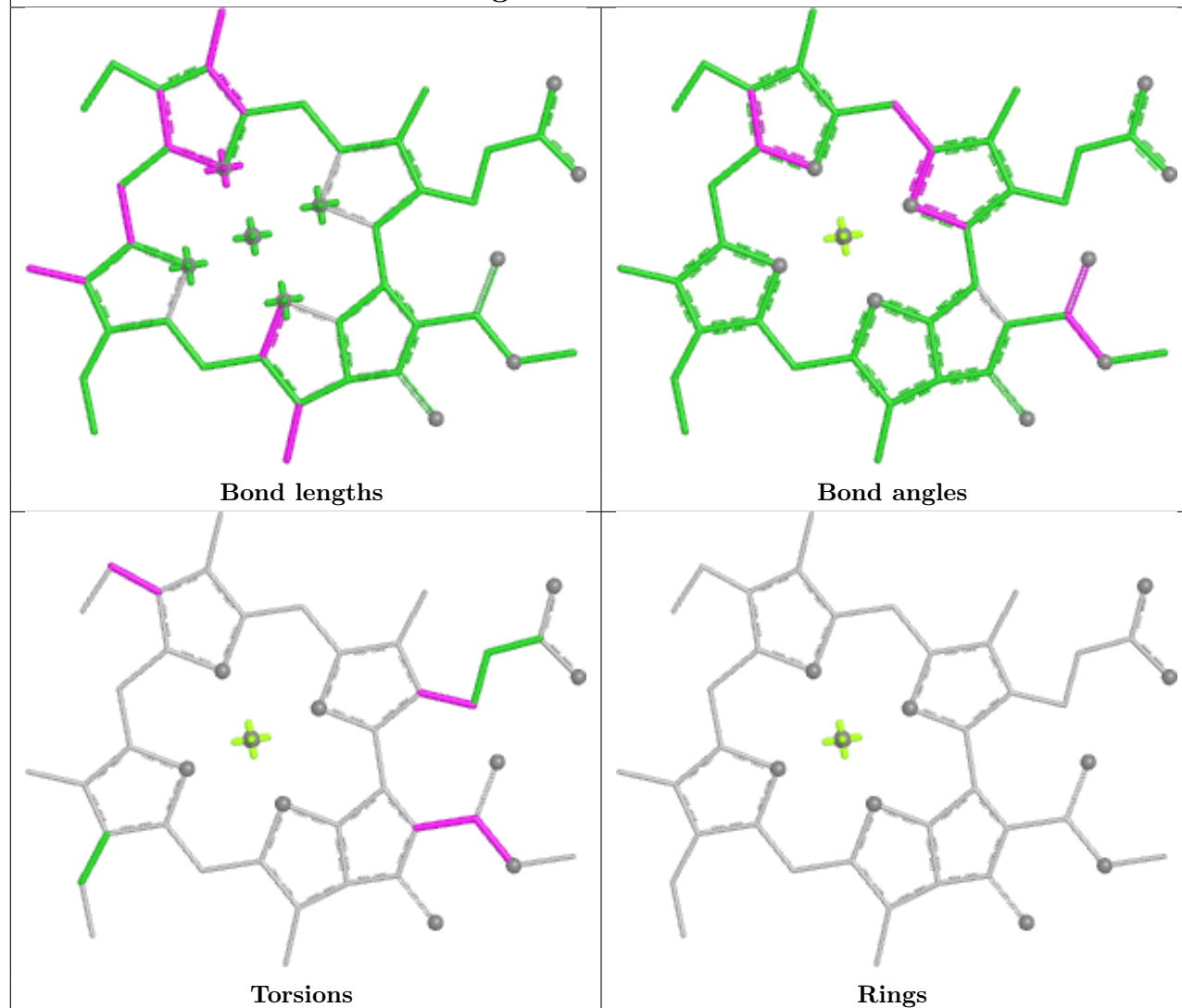




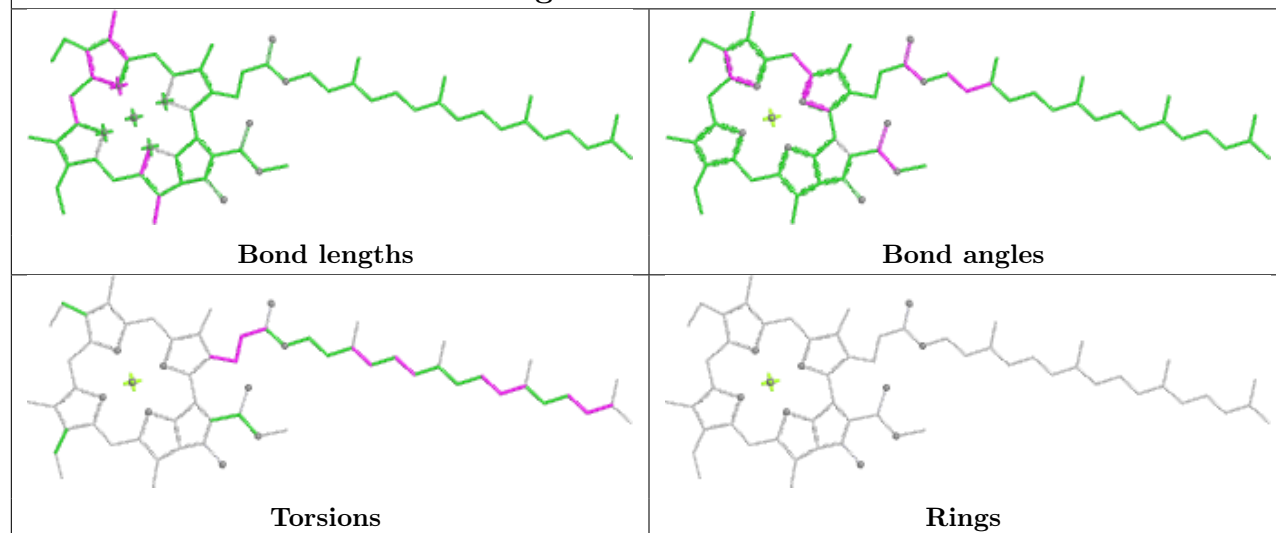




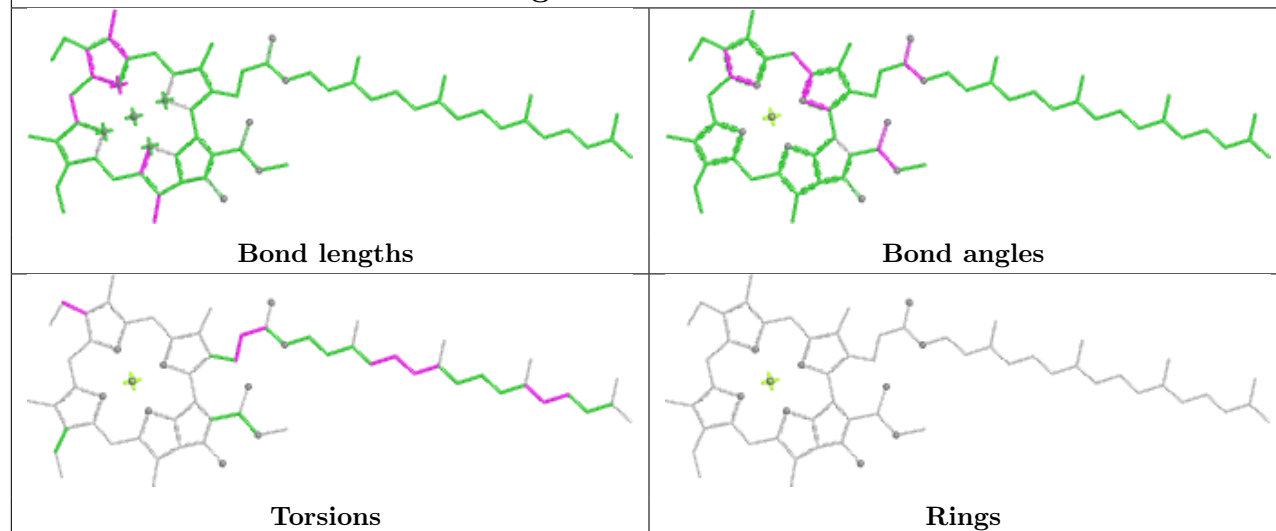
## Ligand CLA G 840



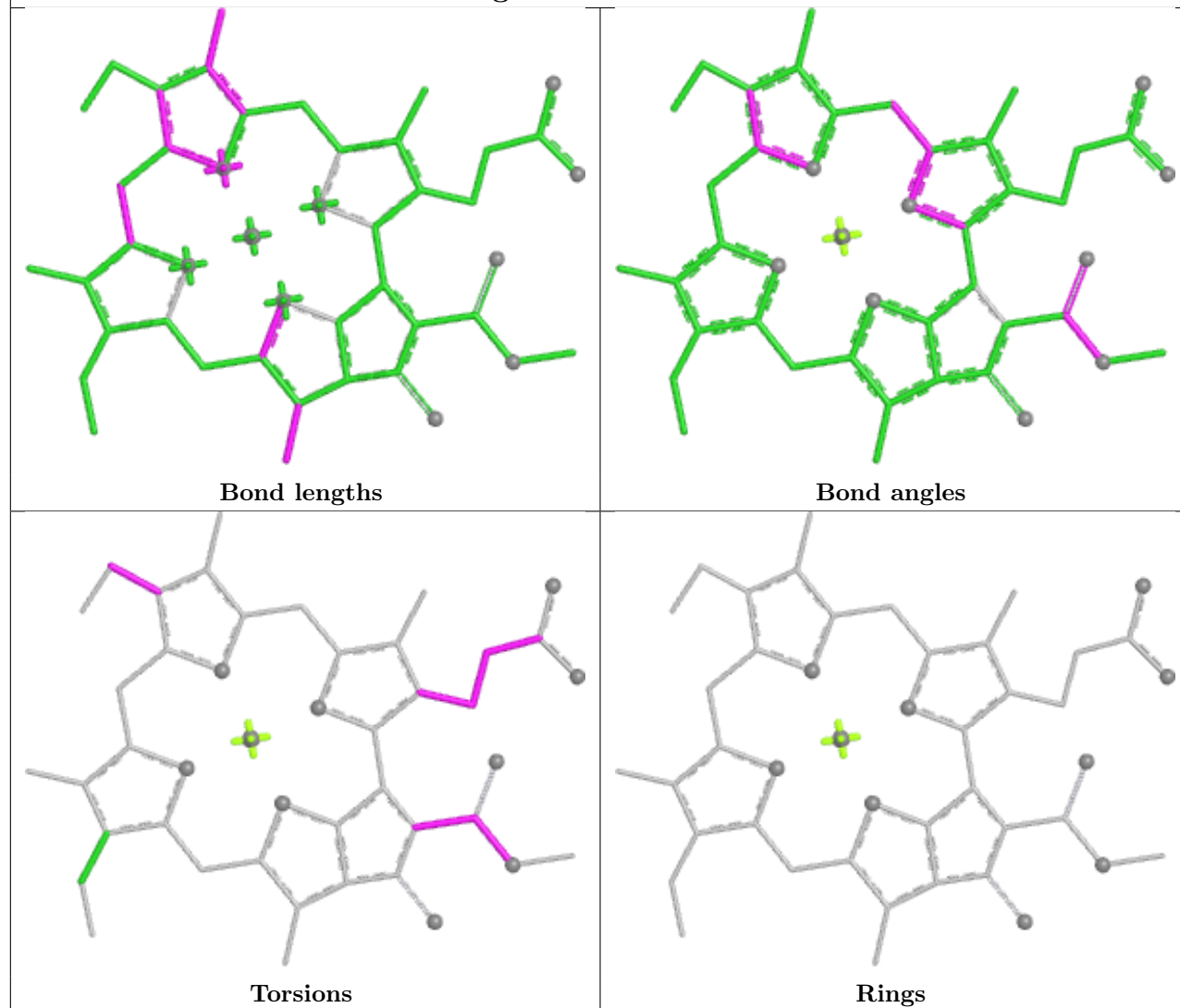
## Ligand CLA b 810

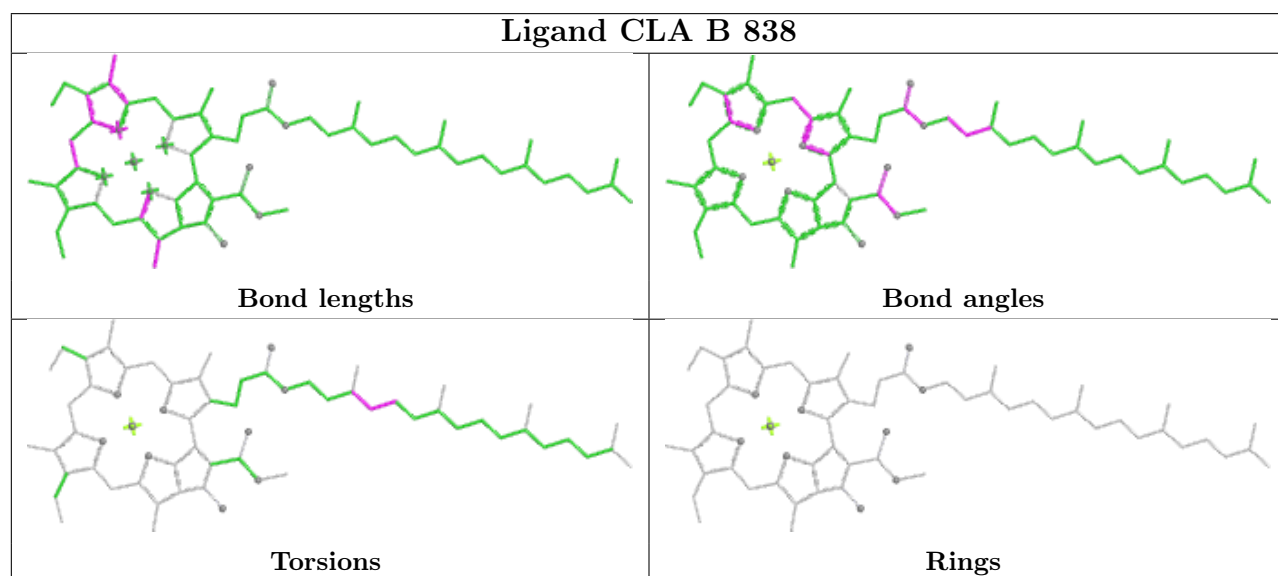
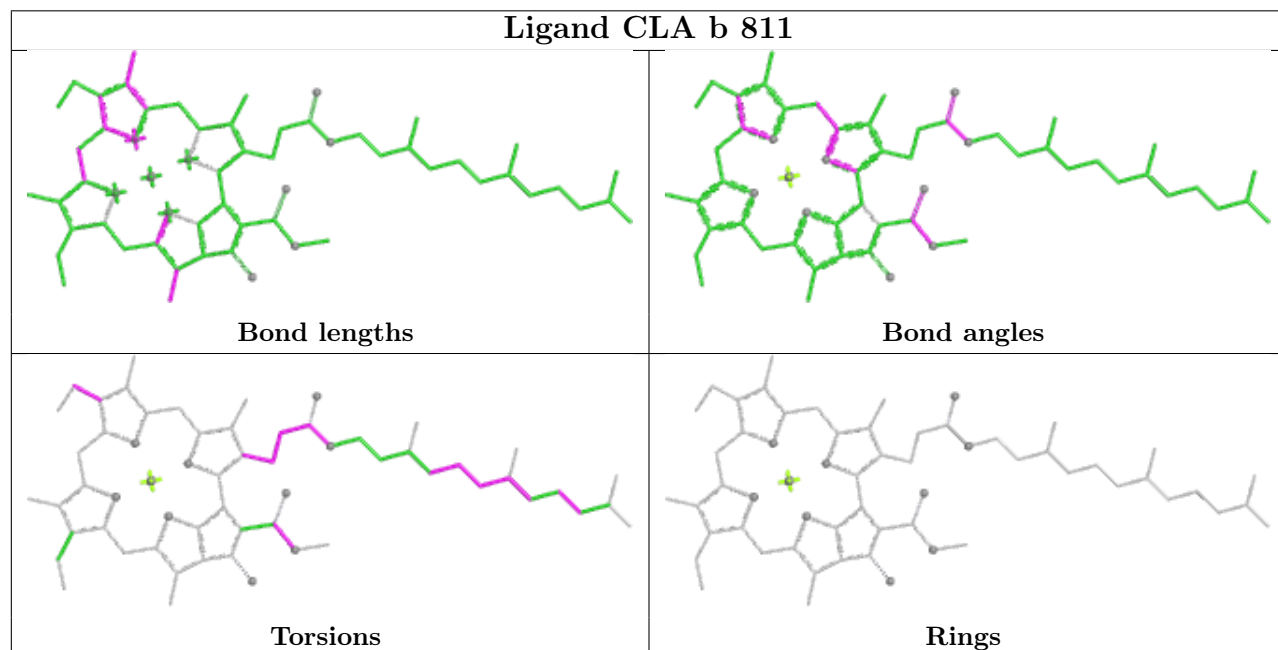
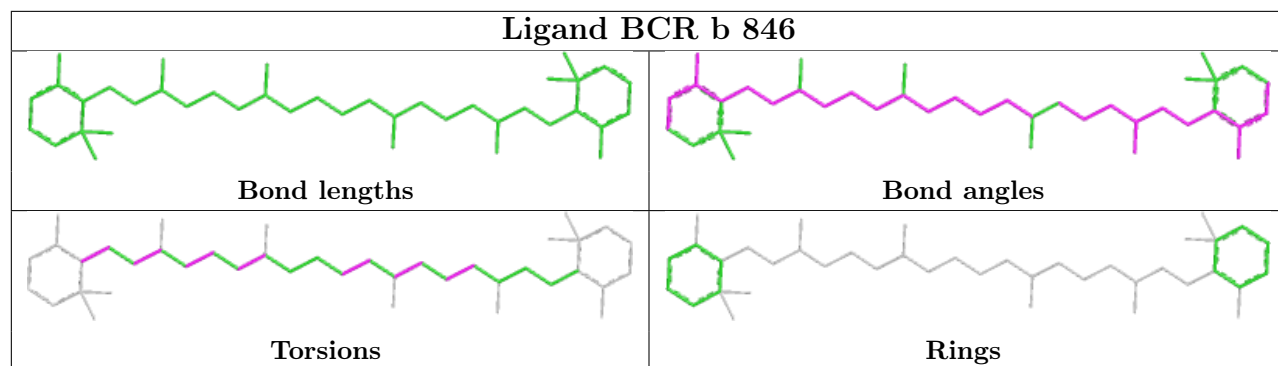


## Ligand CLA A 837



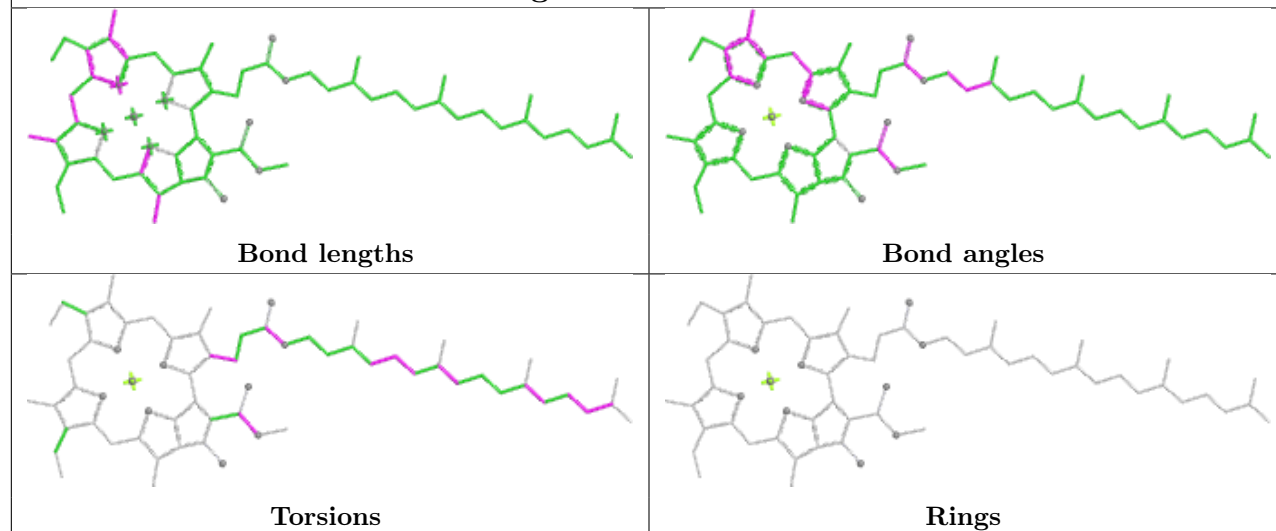
## Ligand CLA T 101



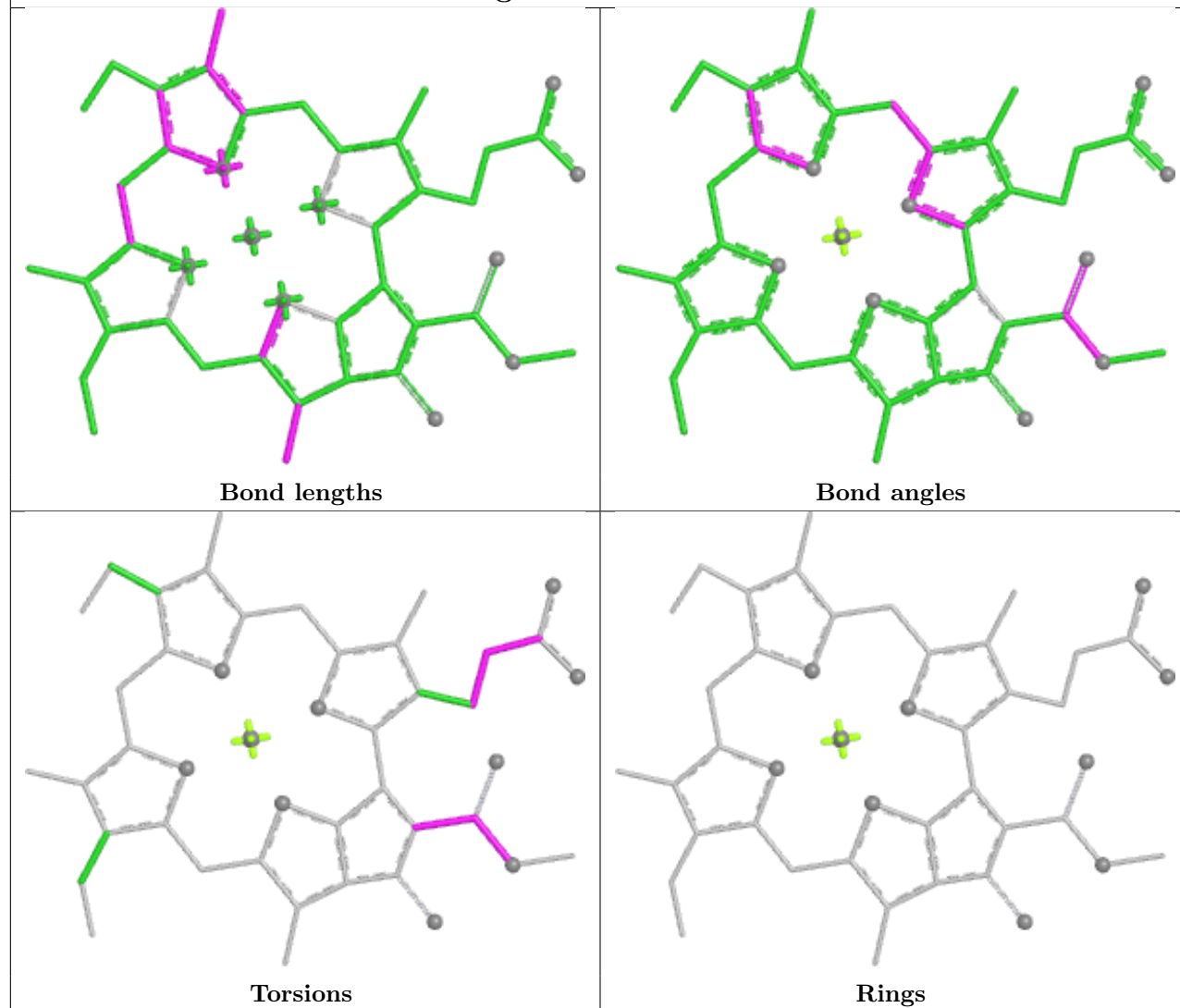


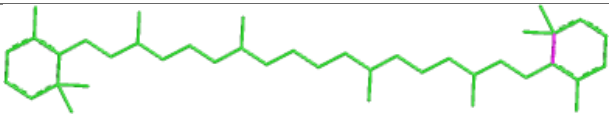
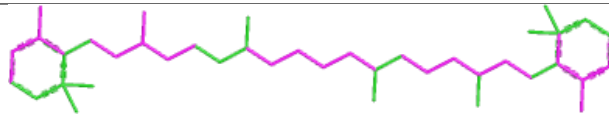
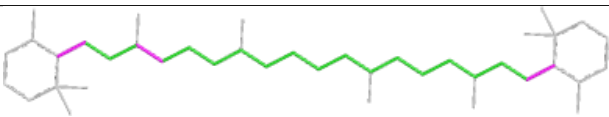
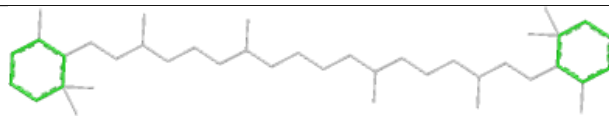



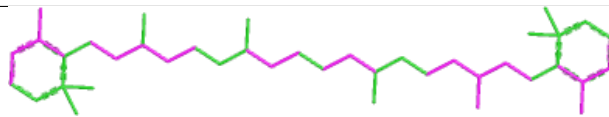
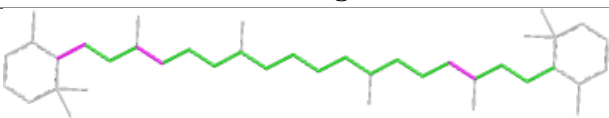
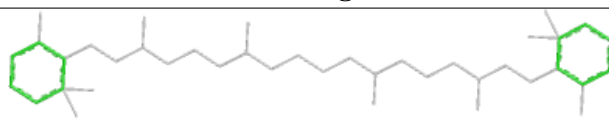
## Ligand CLA G 805

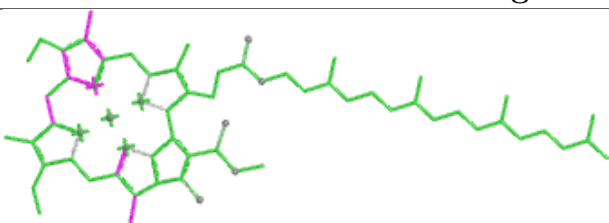
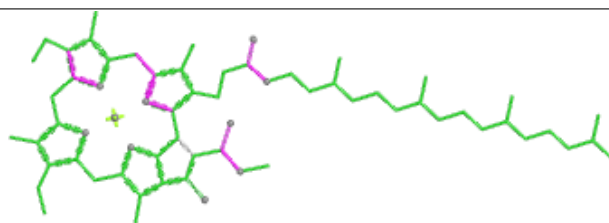
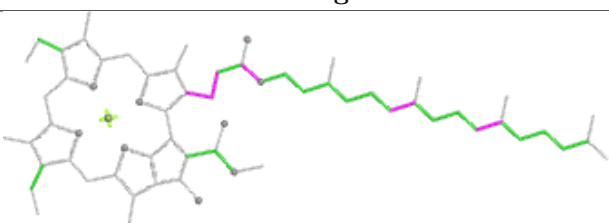
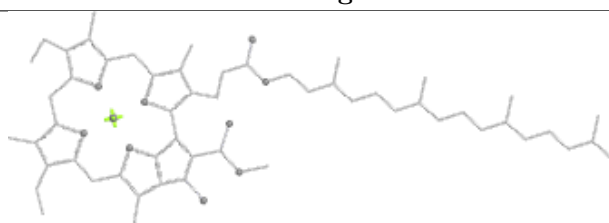


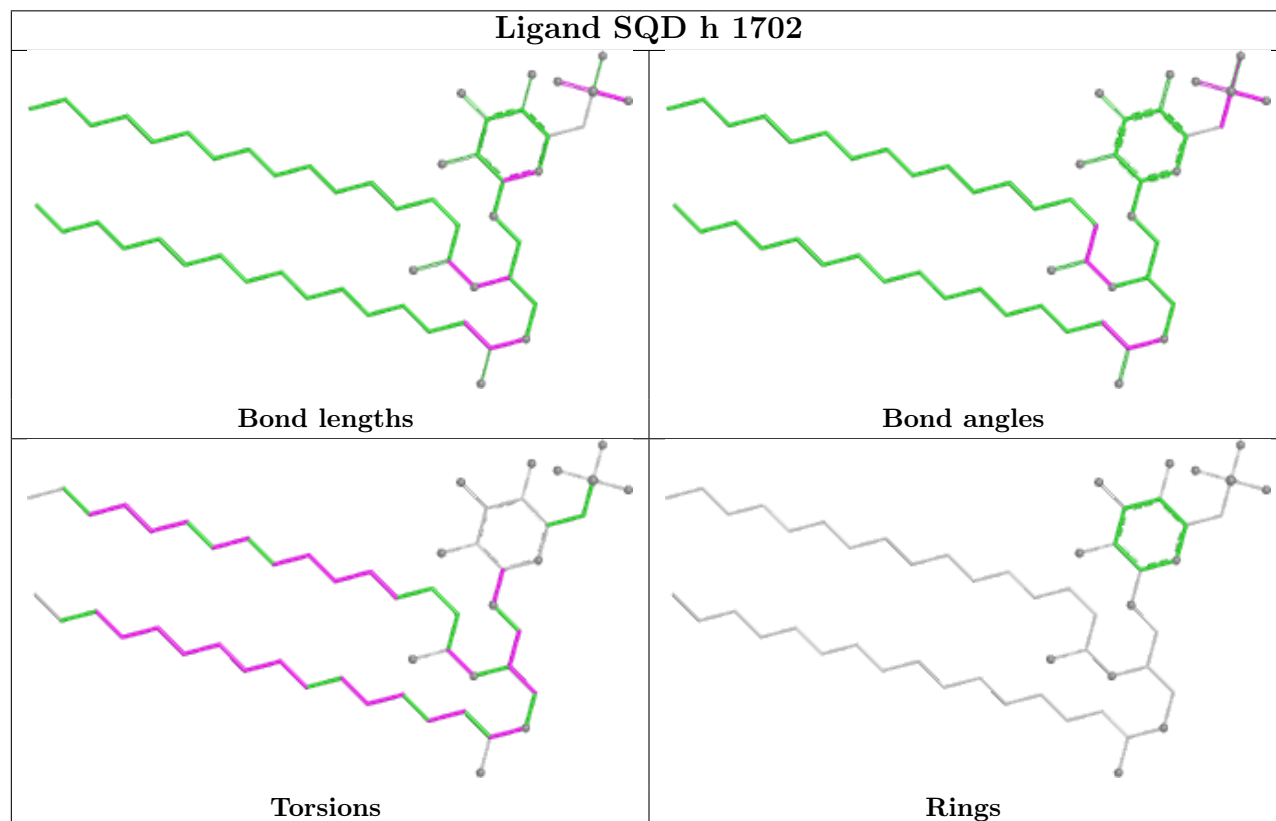
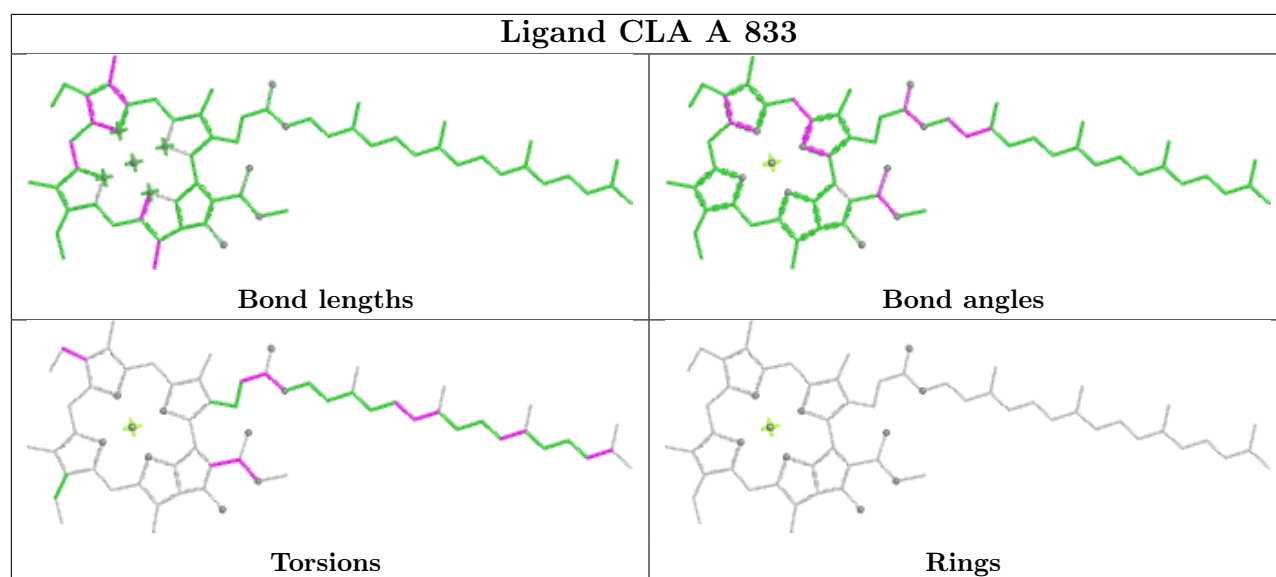
## Ligand CLA a 813



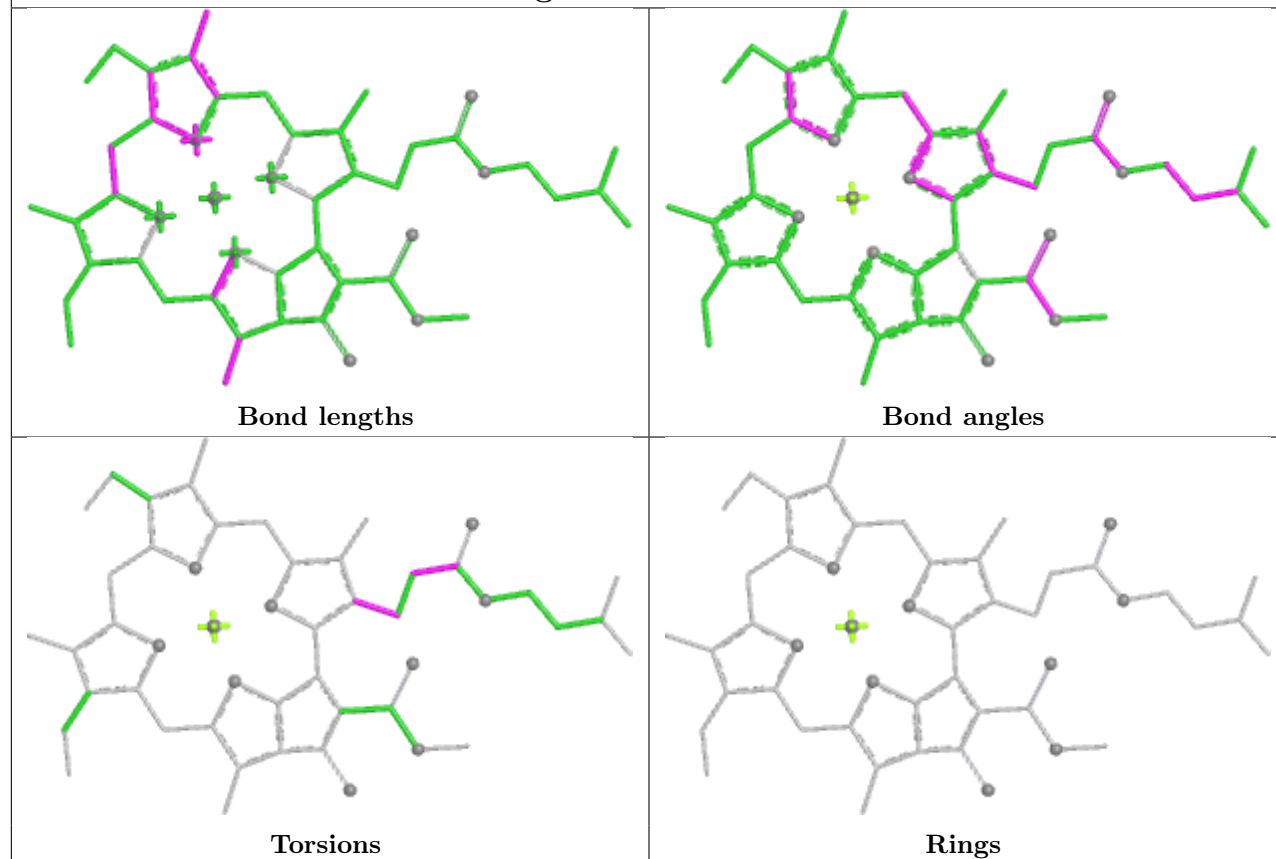
| Ligand BCR n 843  |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

| Ligand BCR b 845  |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

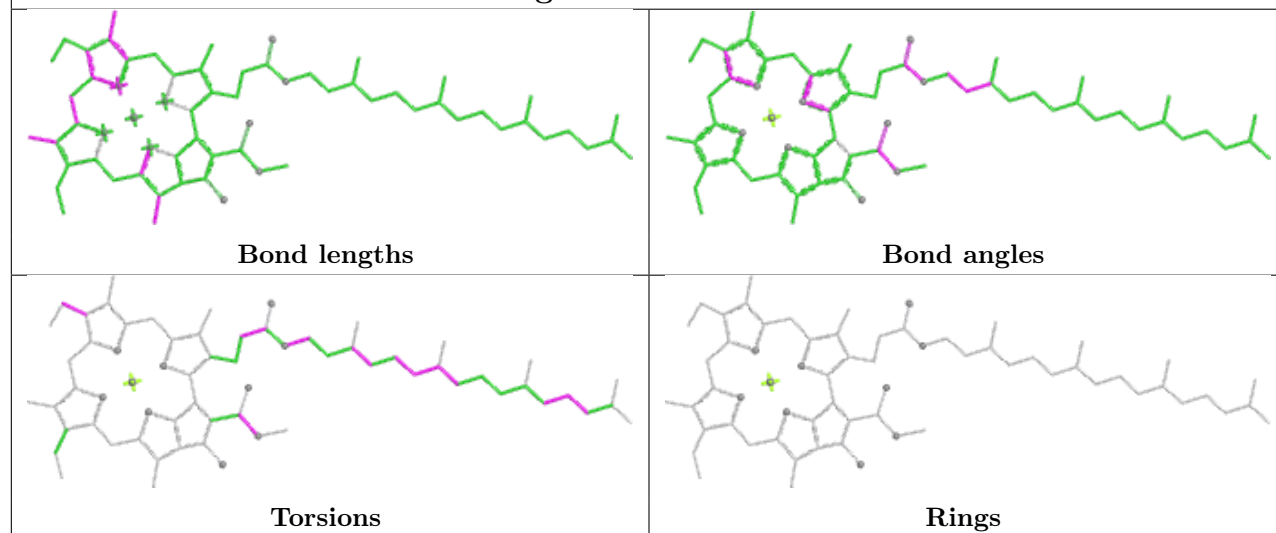
| Ligand CLA n 818  |  |
|---|--|
|   |   |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |



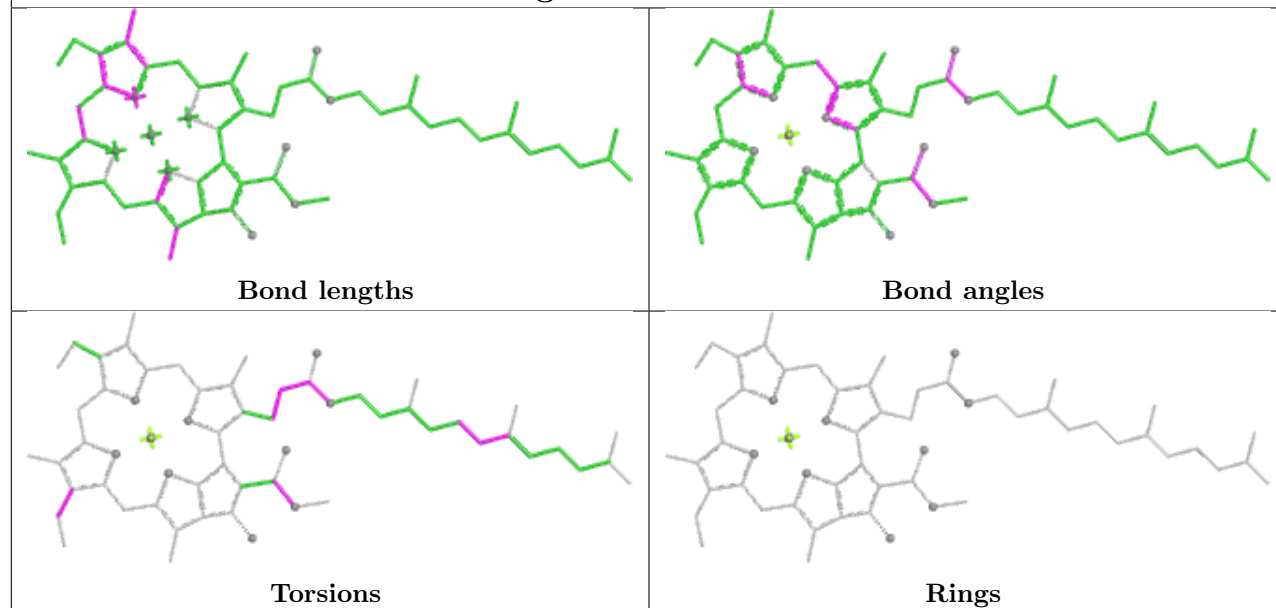
## Ligand CLA n 814



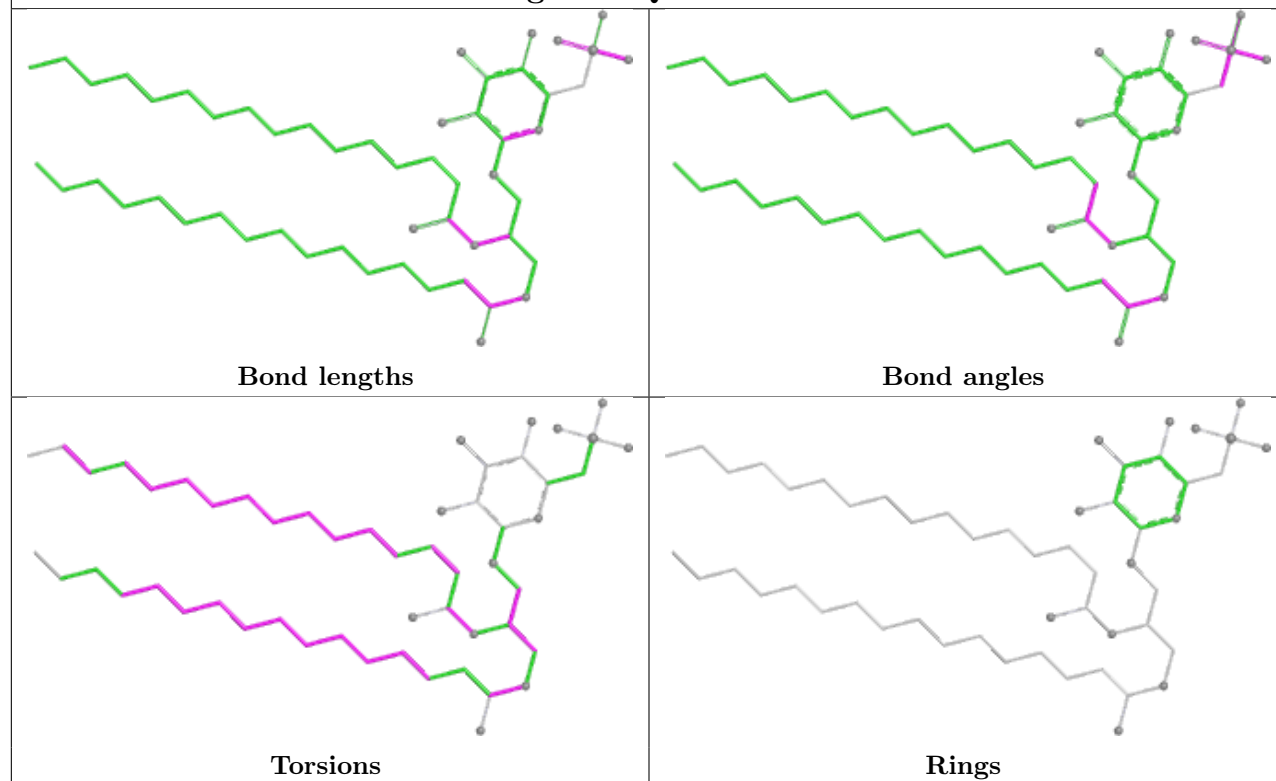
## Ligand CLA b 804

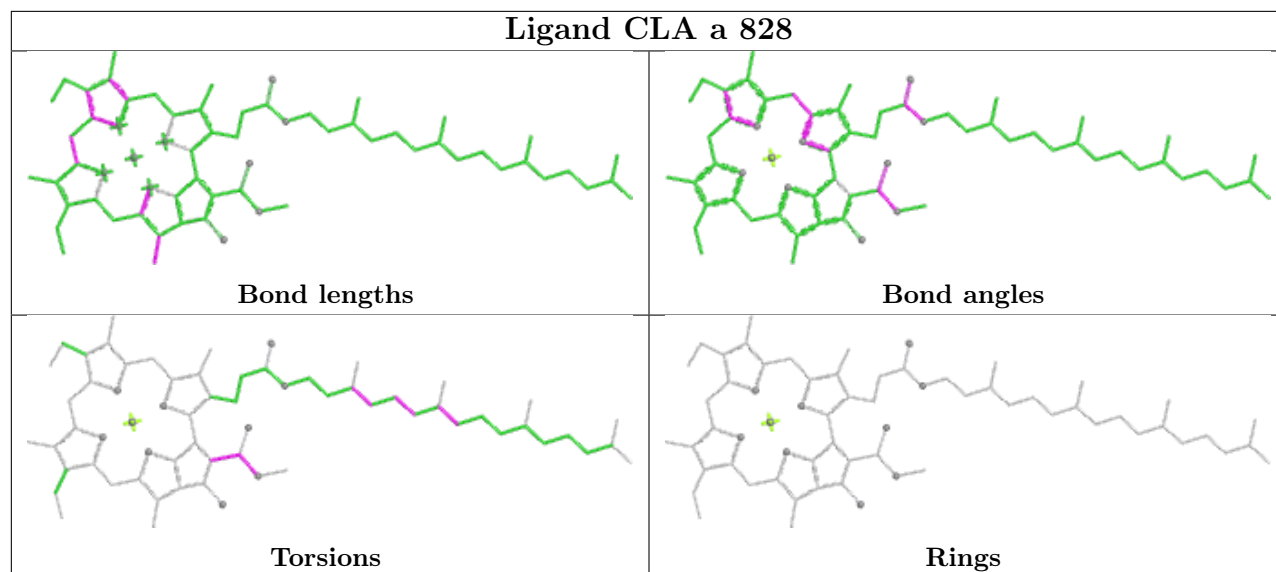
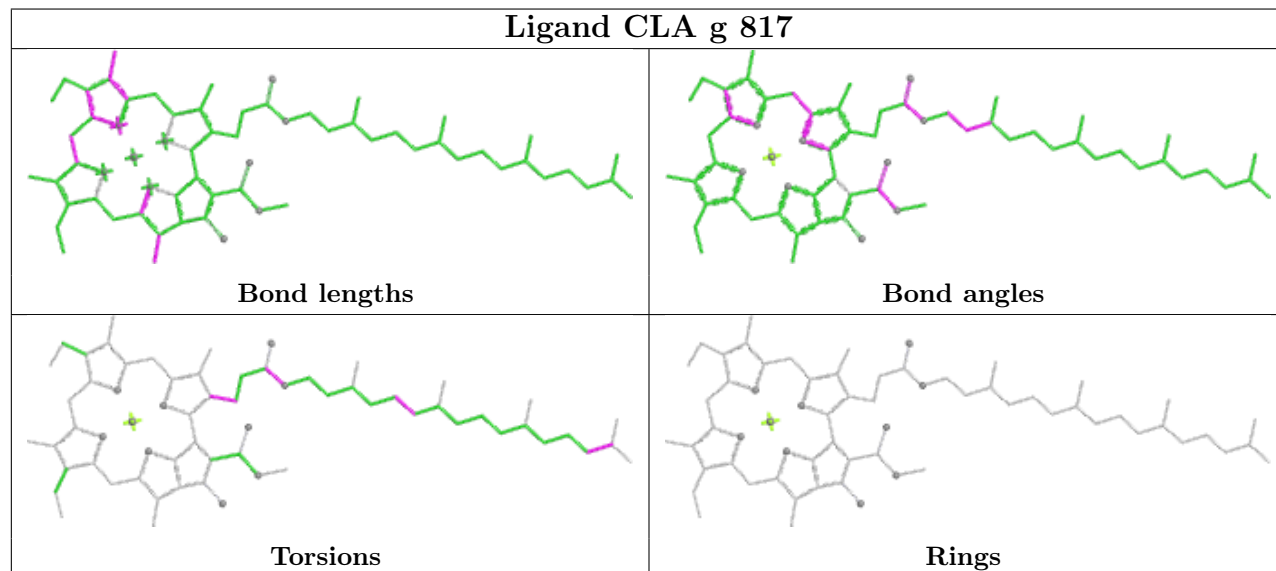


## Ligand CLA a 811

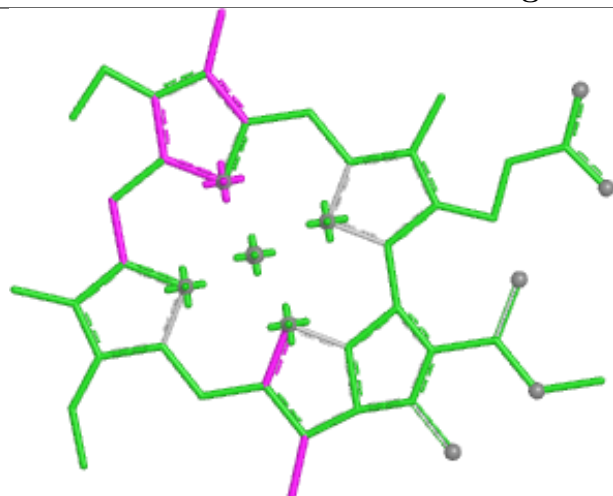


## Ligand SQD x 1702

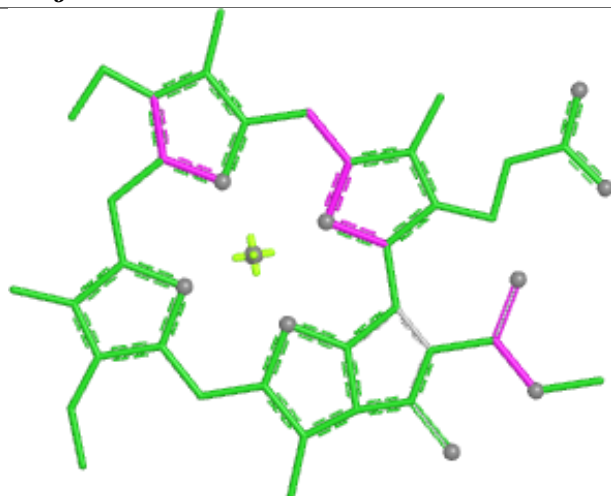


**Ligand CLA a 828****Ligand CLA g 817**

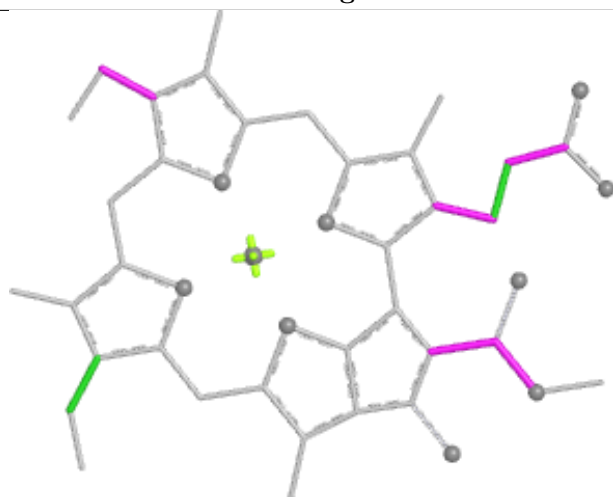
## Ligand CLA j 101



Bond lengths



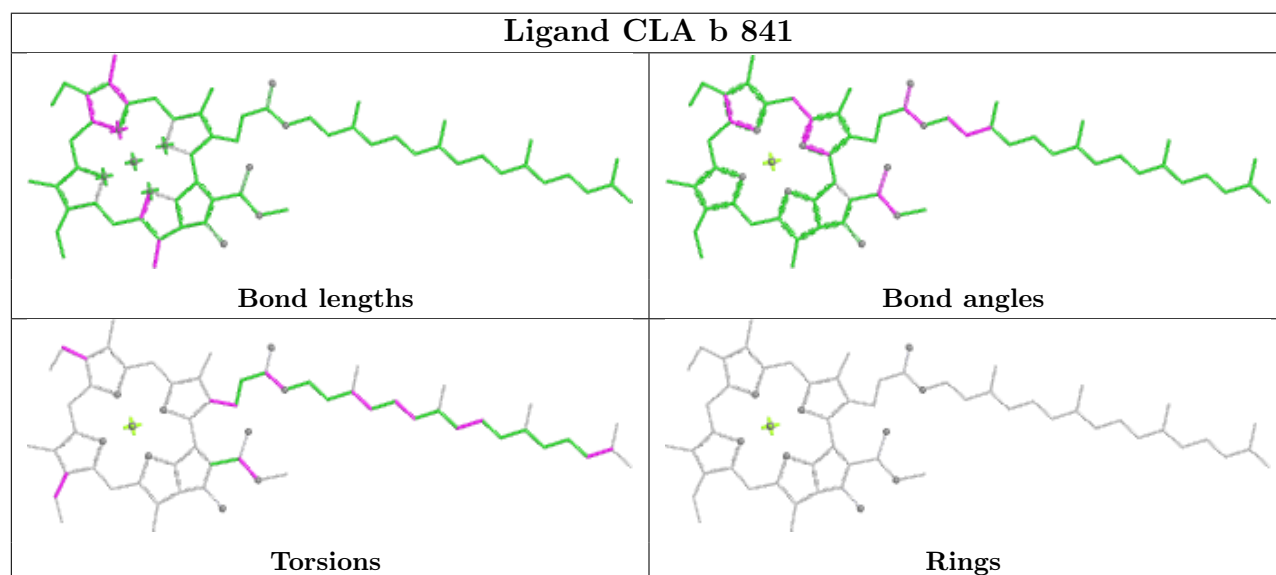
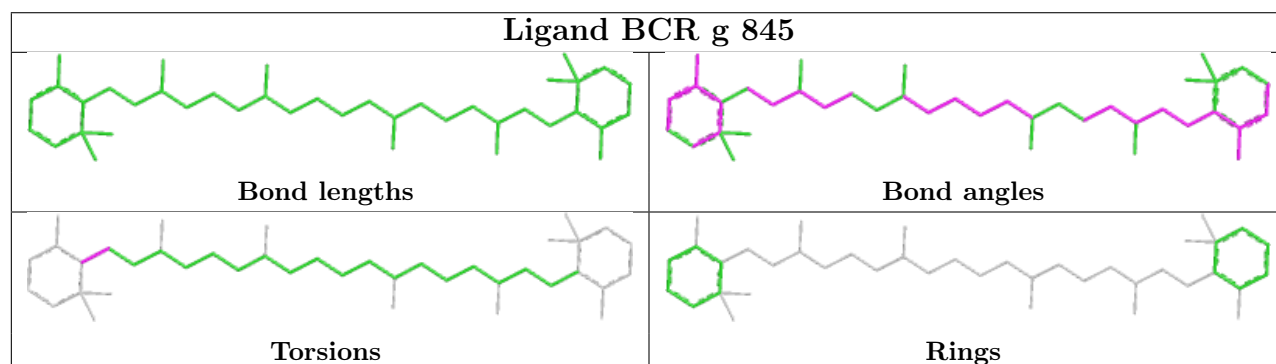
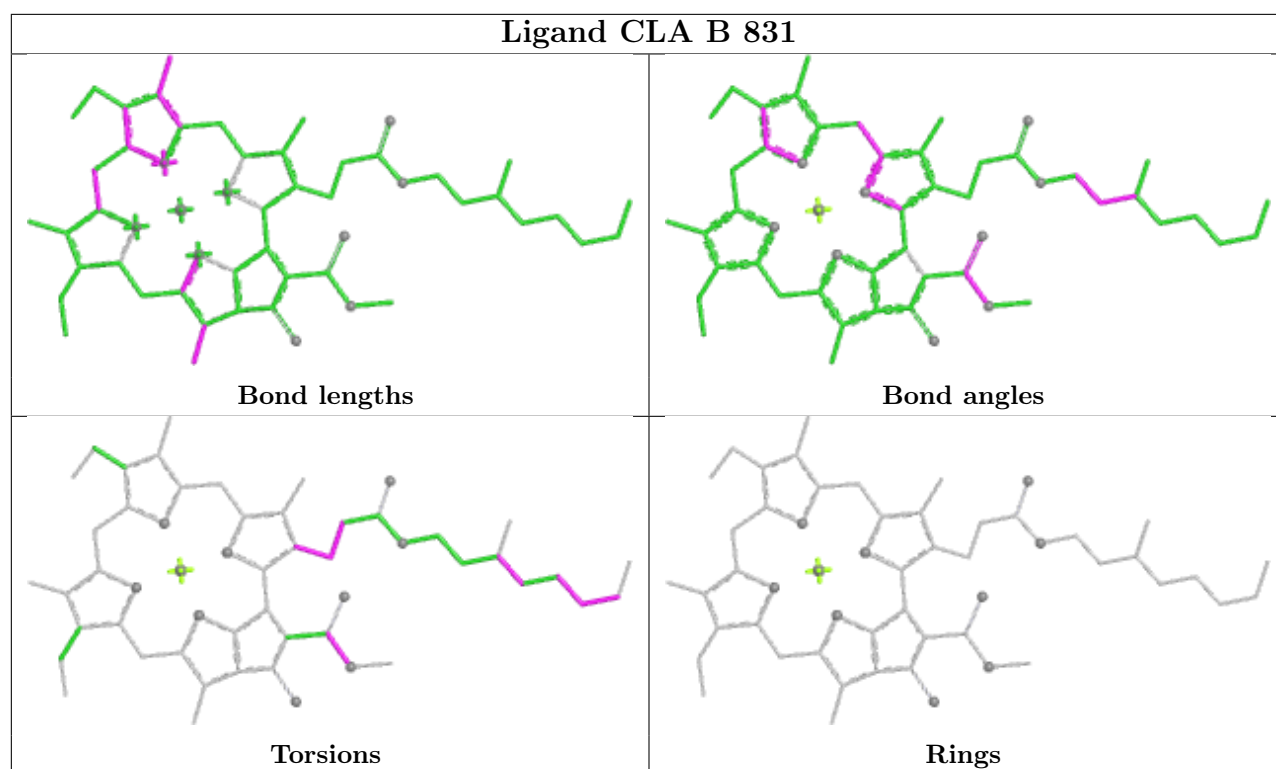
Bond angles



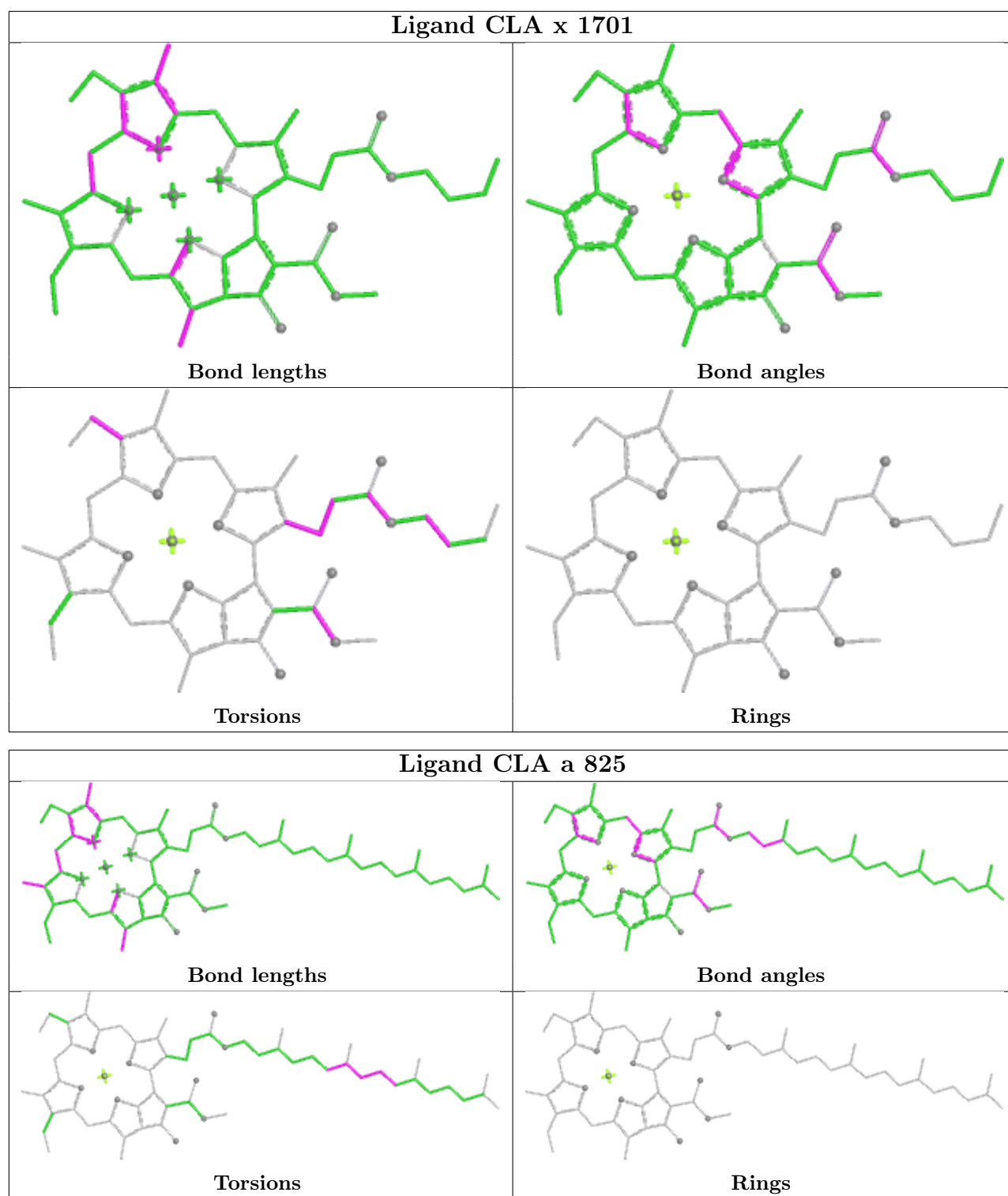
Torsions



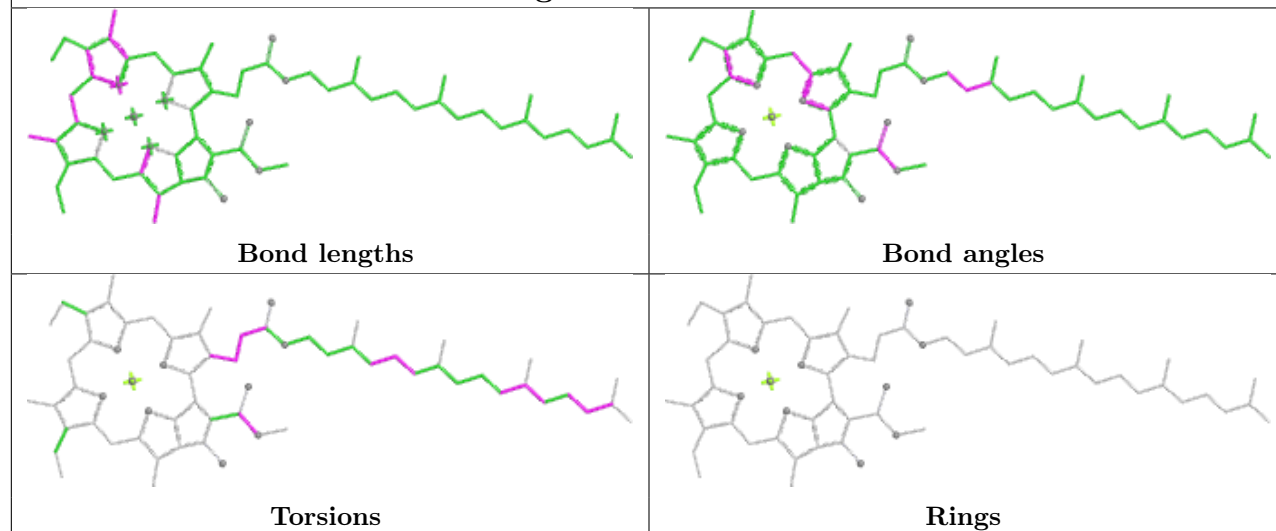
Rings



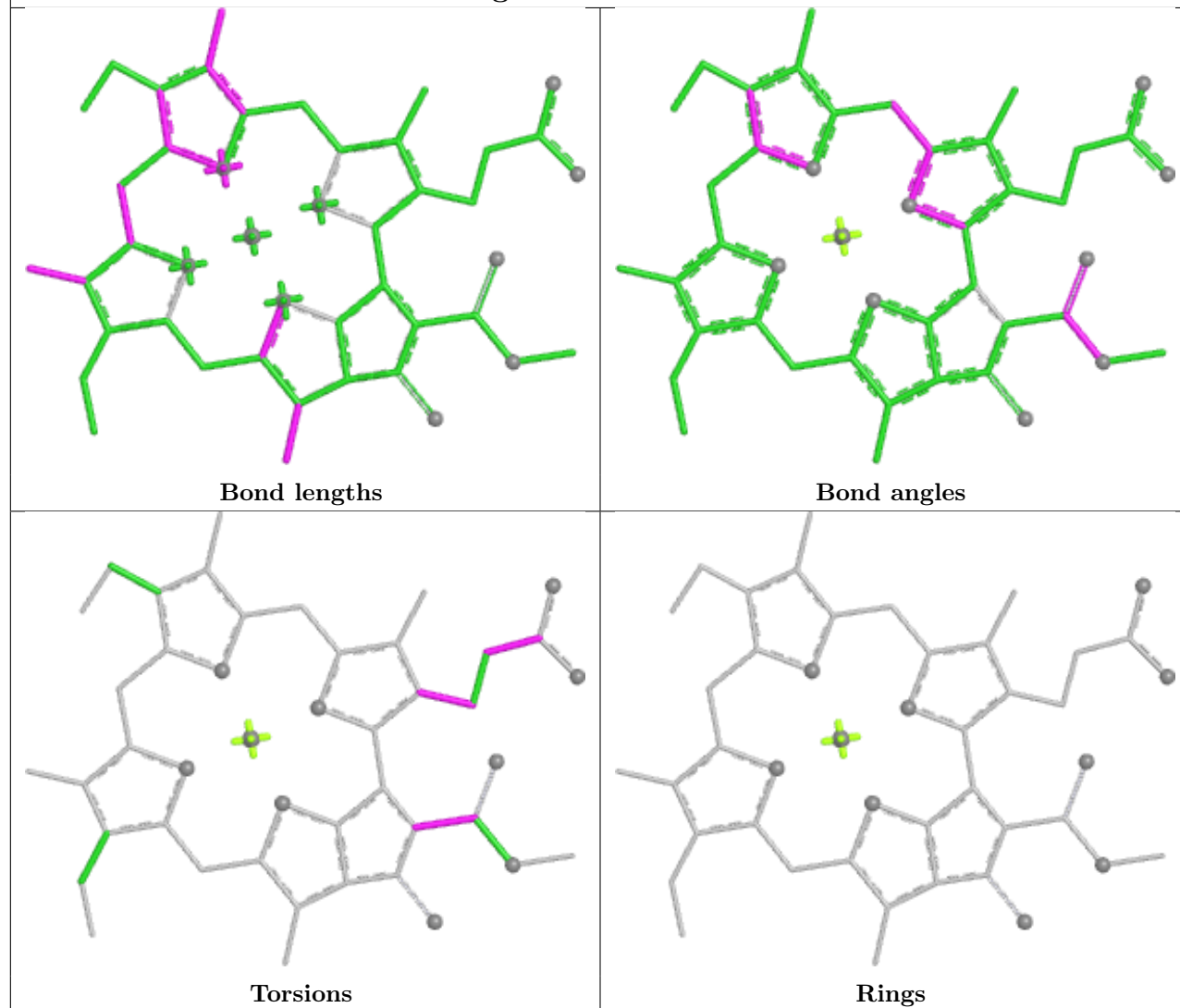


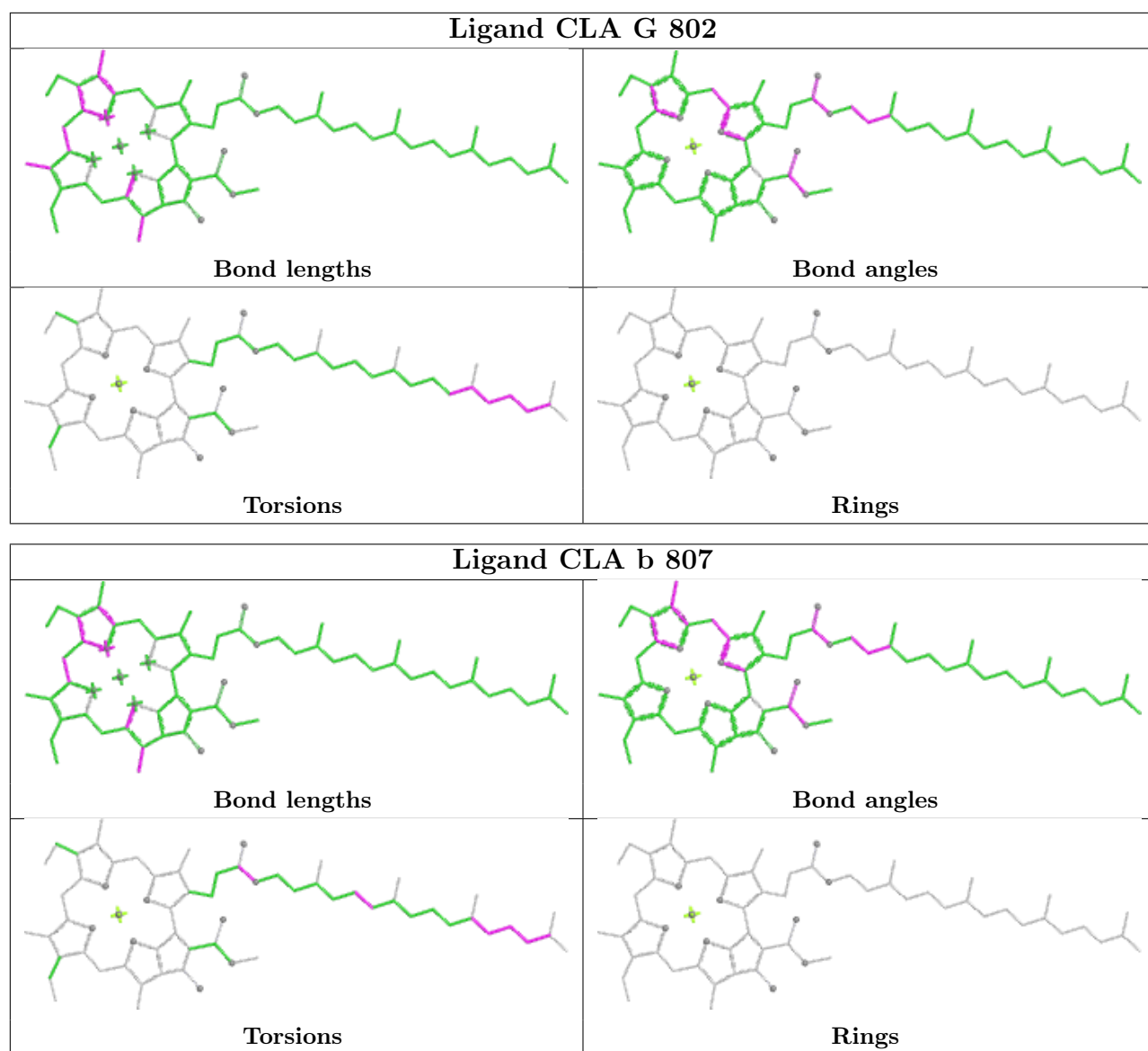


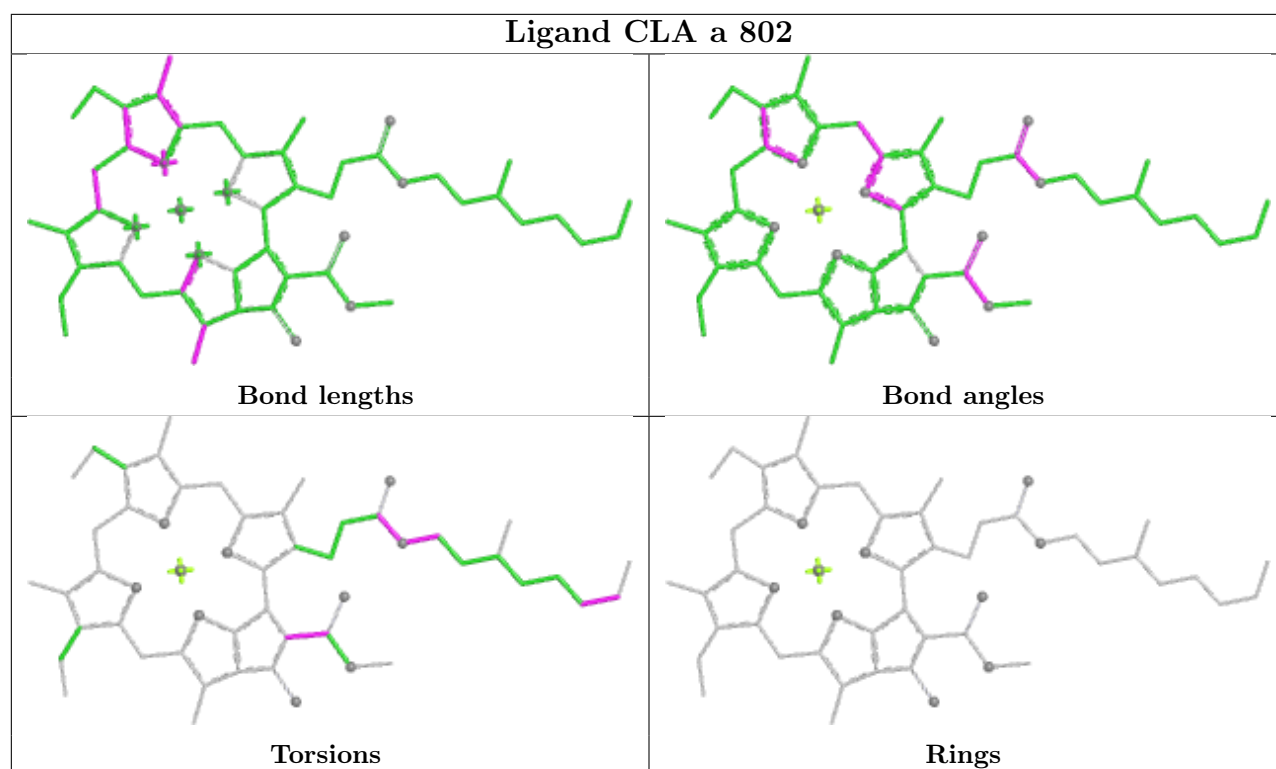
## Ligand CLA n 809



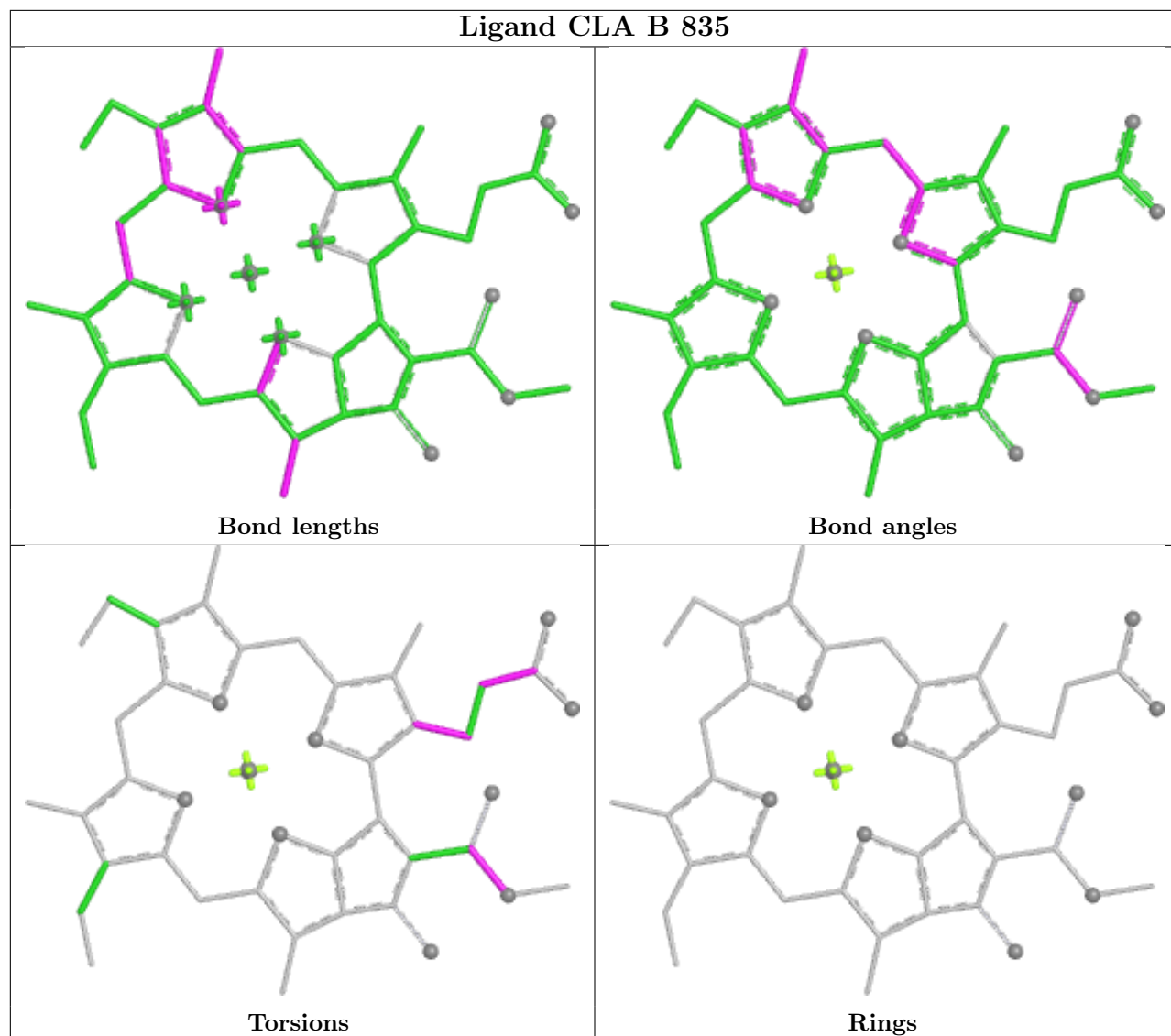
## Ligand CLA B 822



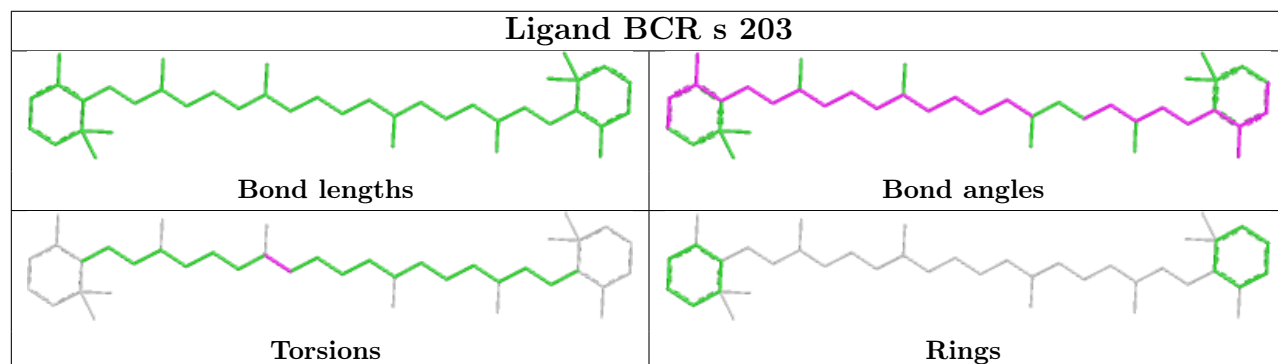




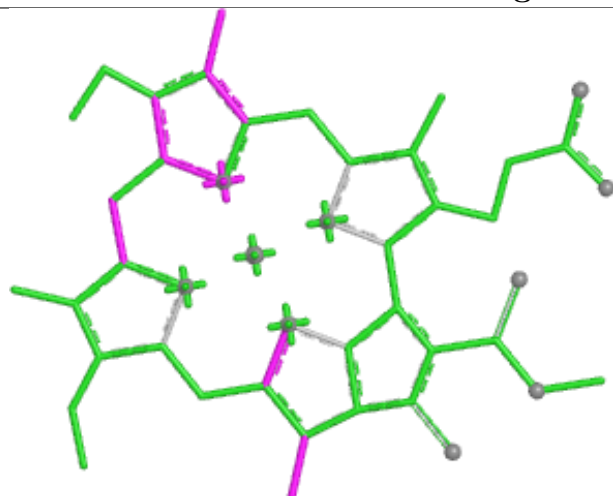
## Ligand CLA B 835



## Ligand BCR s 203



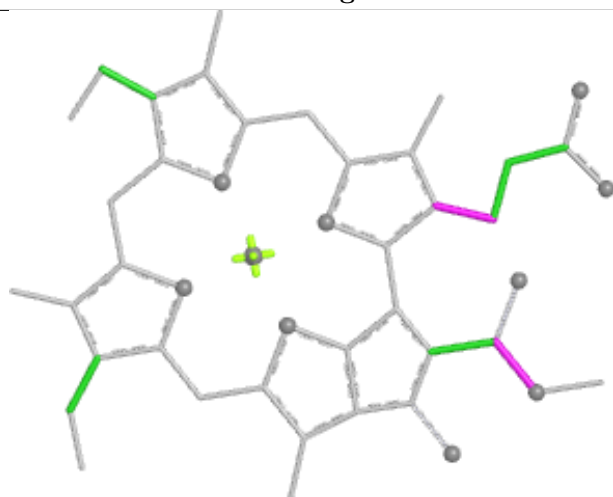
## Ligand CLA A 823



Bond lengths



Bond angles

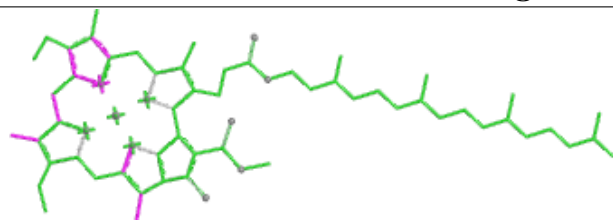


Torsions

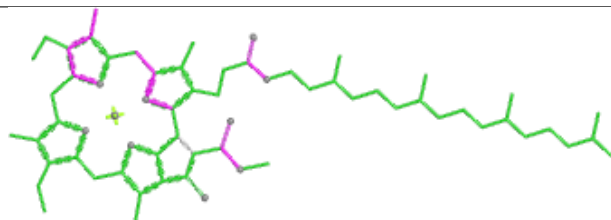


Rings

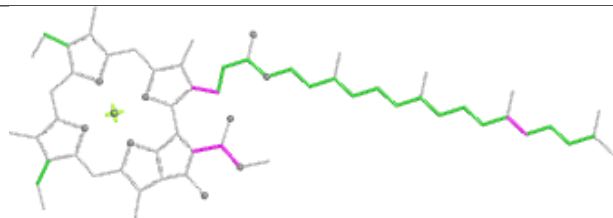
## Ligand CLA B 830



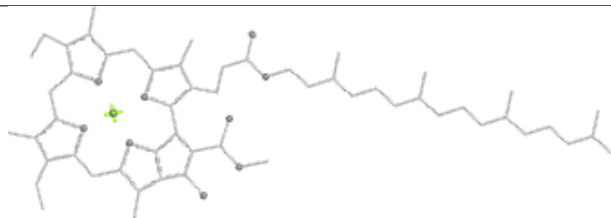
Bond lengths



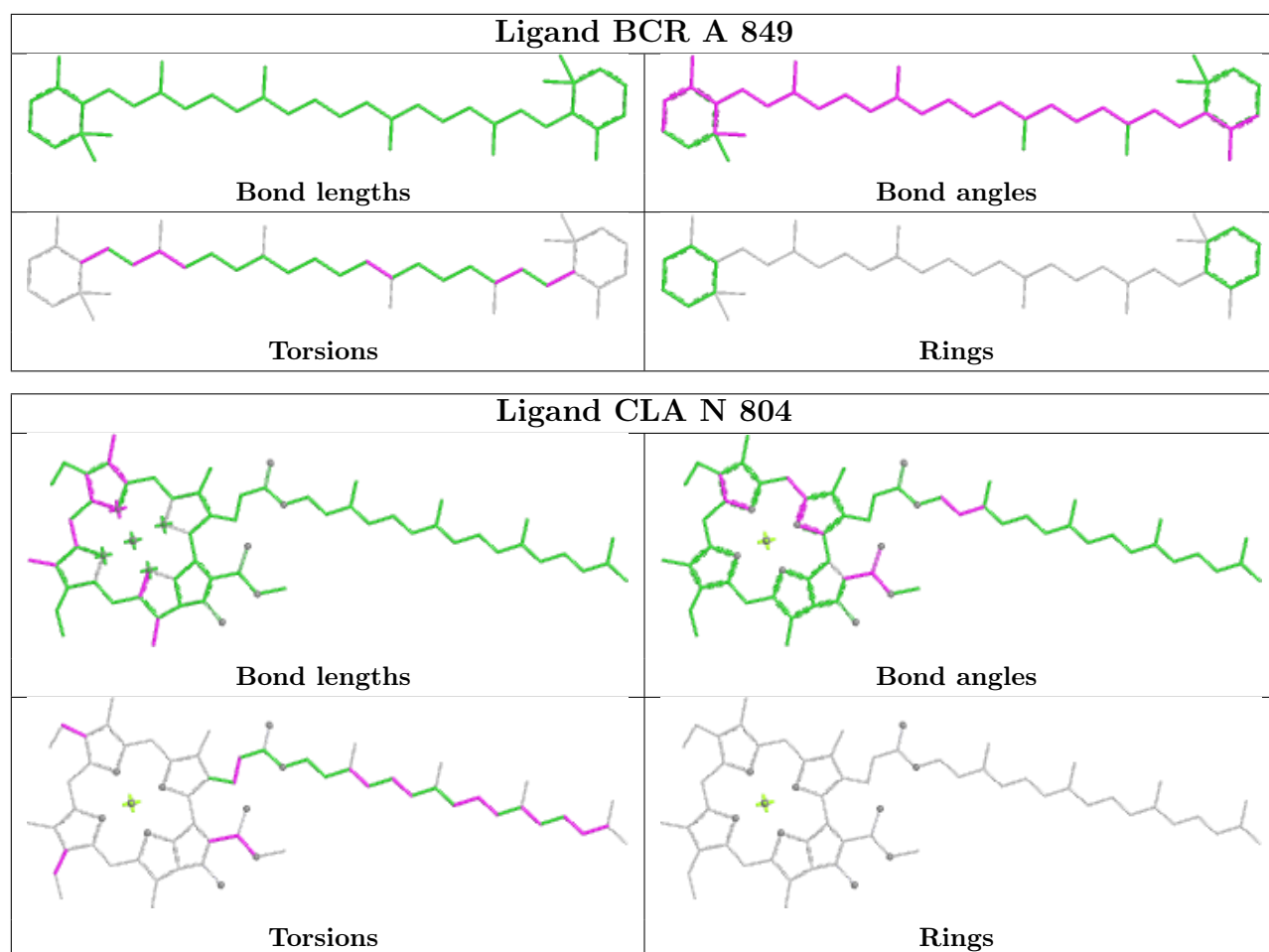
Bond angles



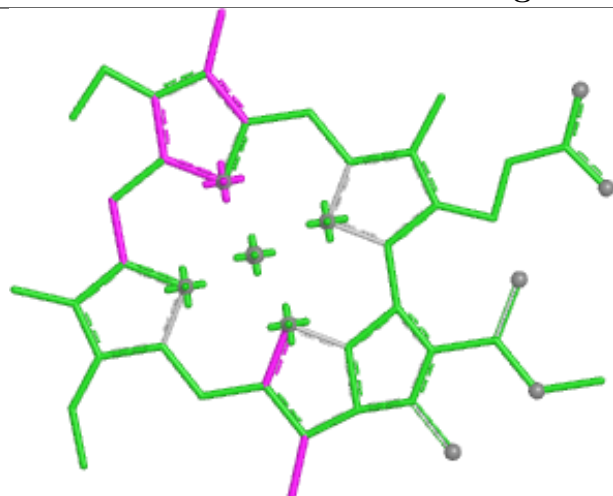
Torsions



Rings



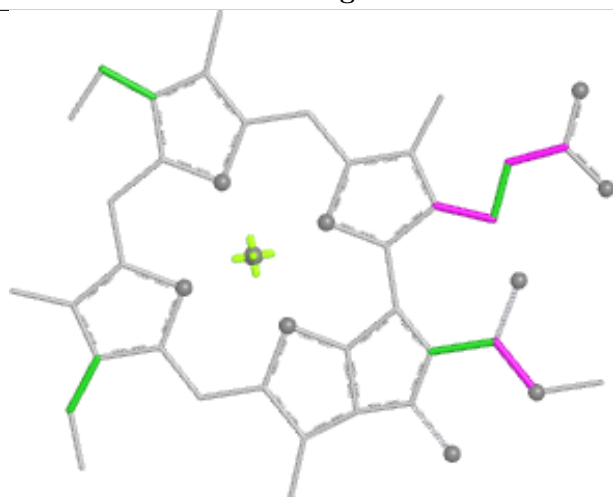
## Ligand CLA A 814



Bond lengths



Bond angles

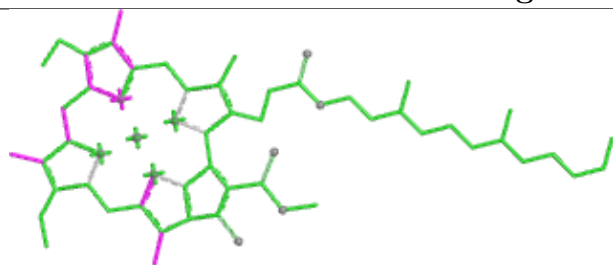


Torsions

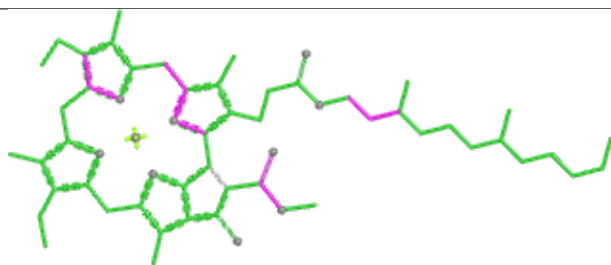


Rings

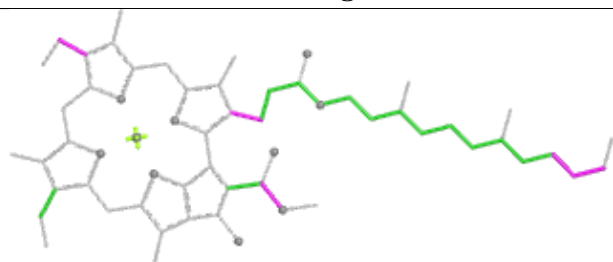
## Ligand CLA F 201



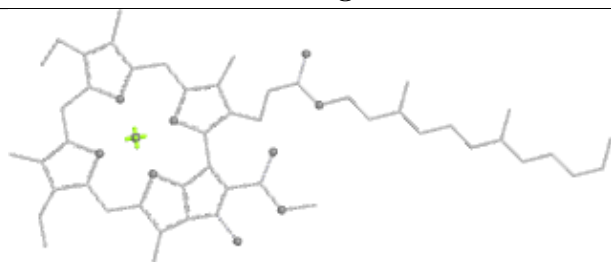
Bond lengths



Bond angles

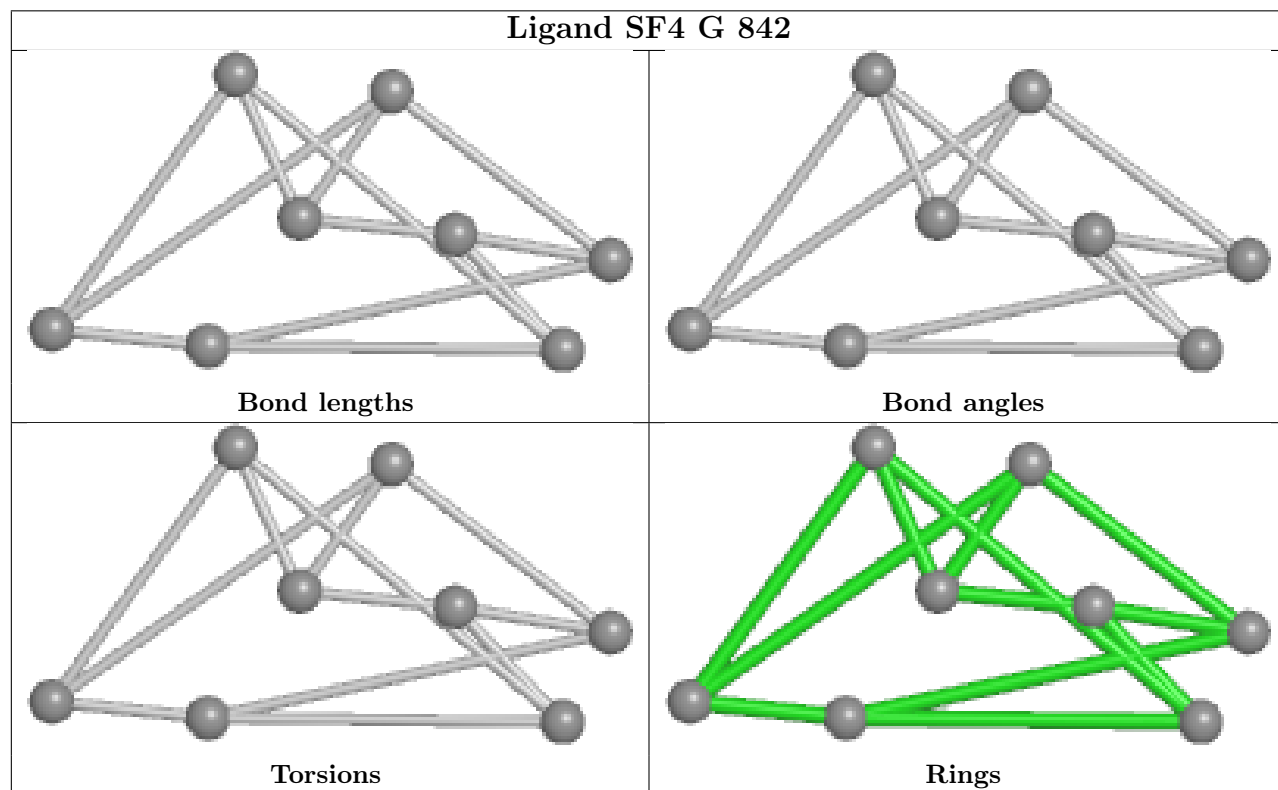
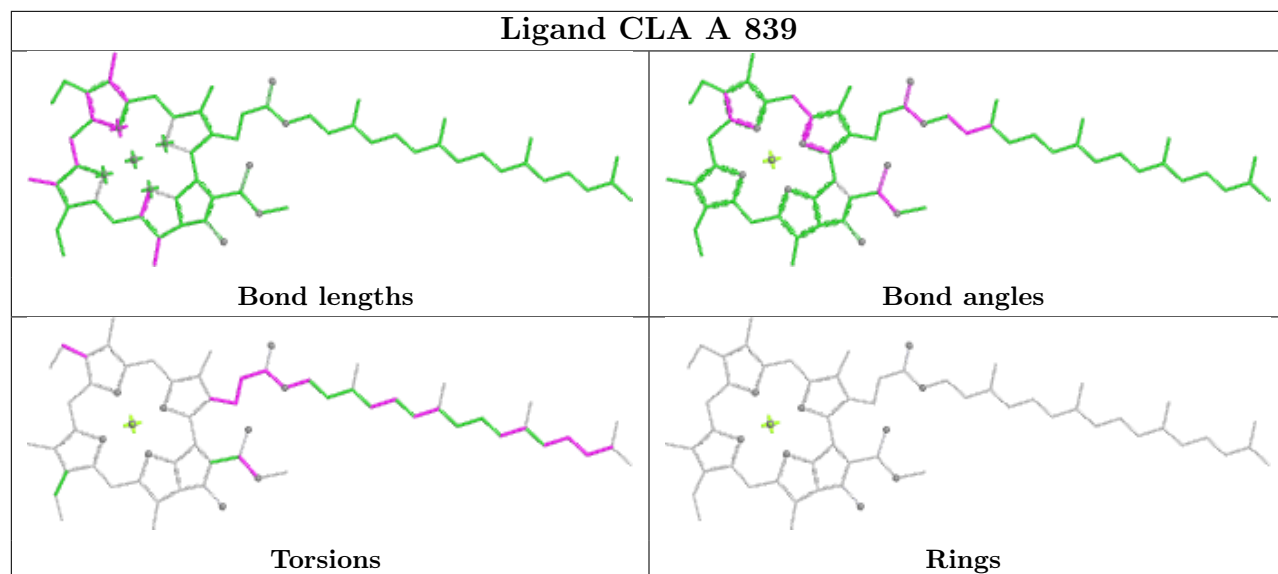


Torsions

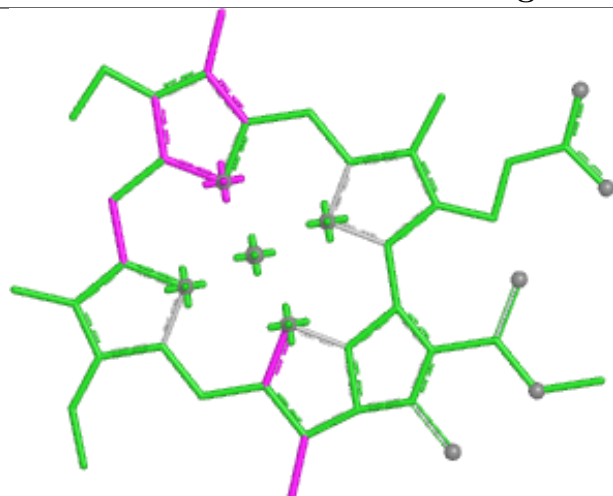


Rings





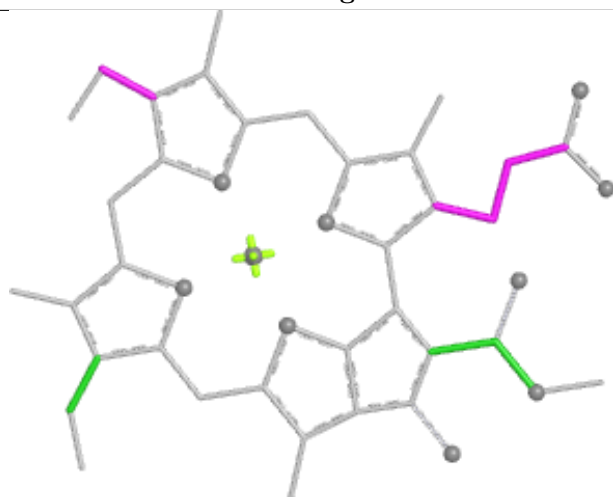
## Ligand CLA n 816



Bond lengths



Bond angles

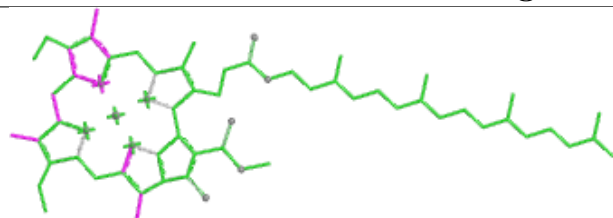


Torsions

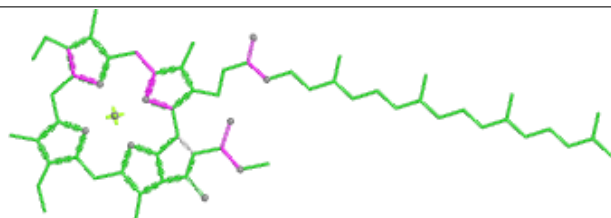


Rings

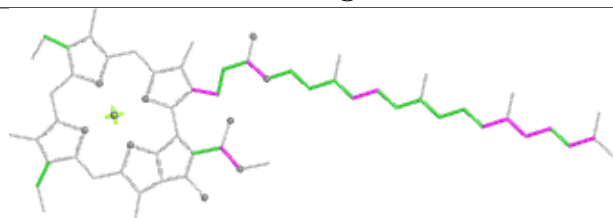
## Ligand CLA n 817



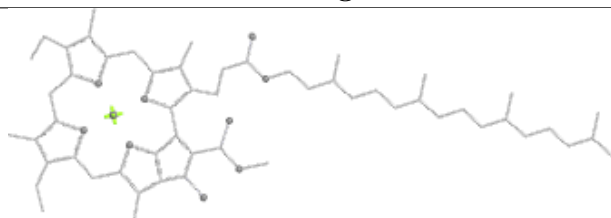
Bond lengths



Bond angles

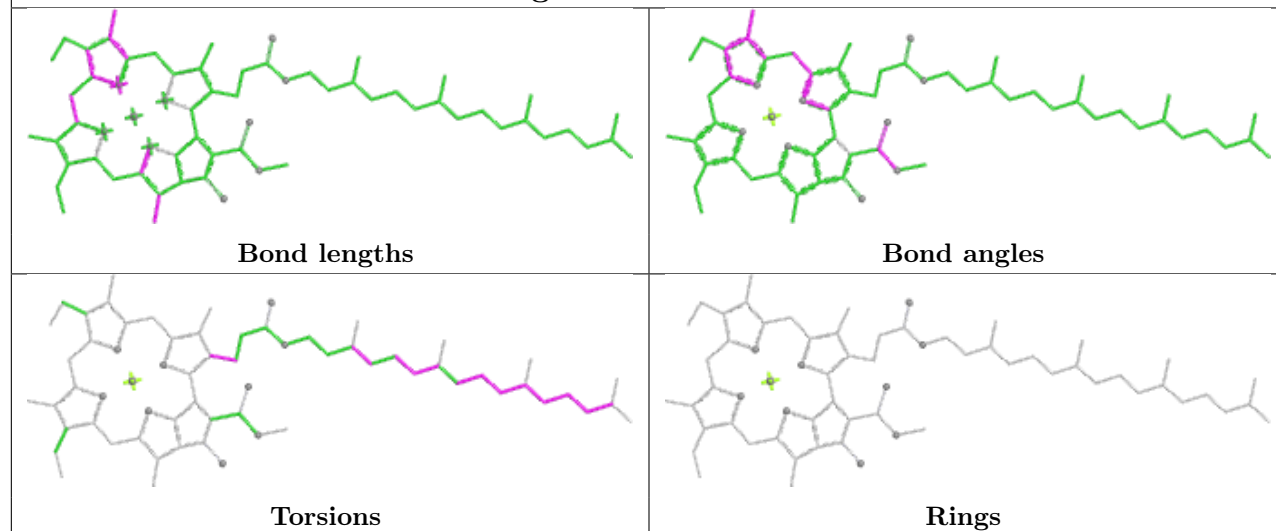


Torsions

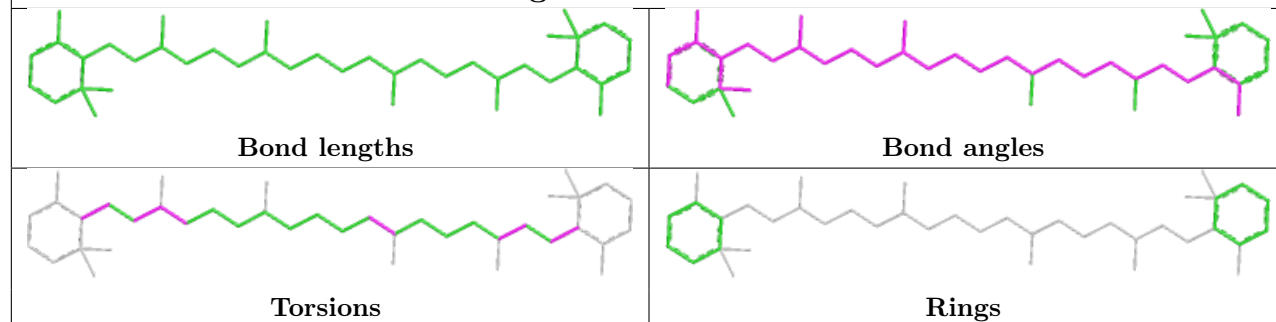


Rings

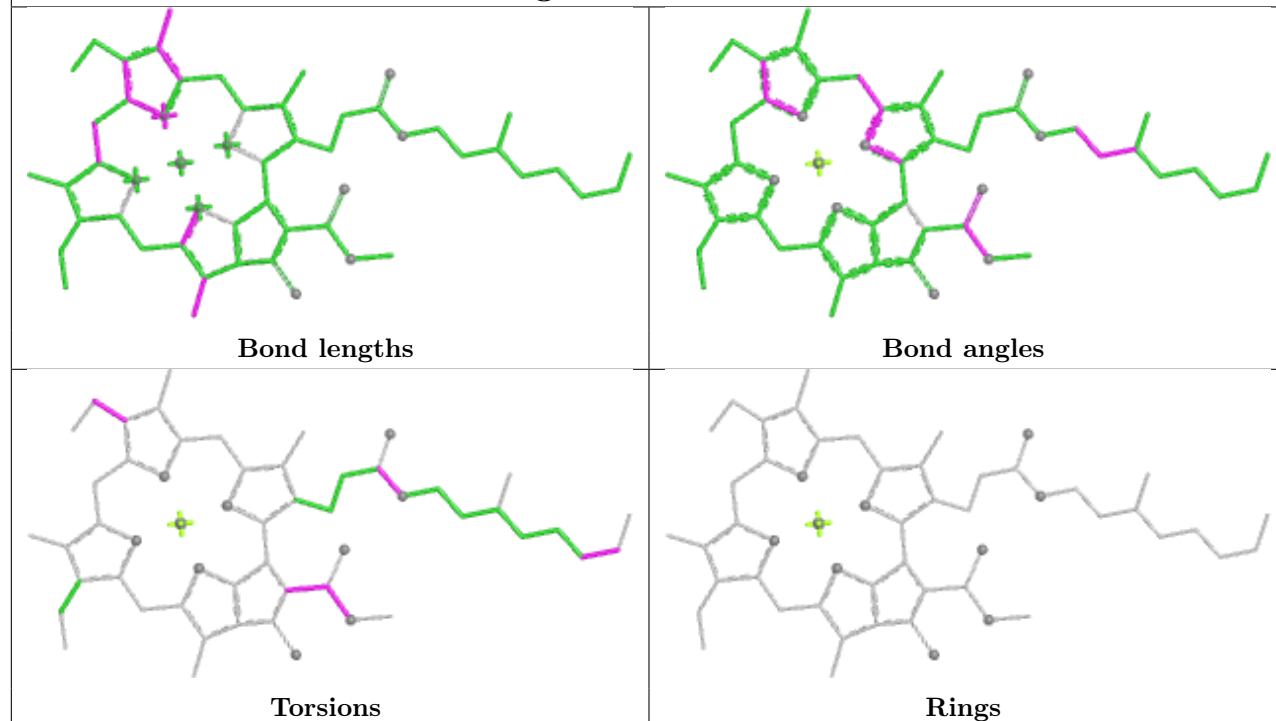
## Ligand CLA A 831

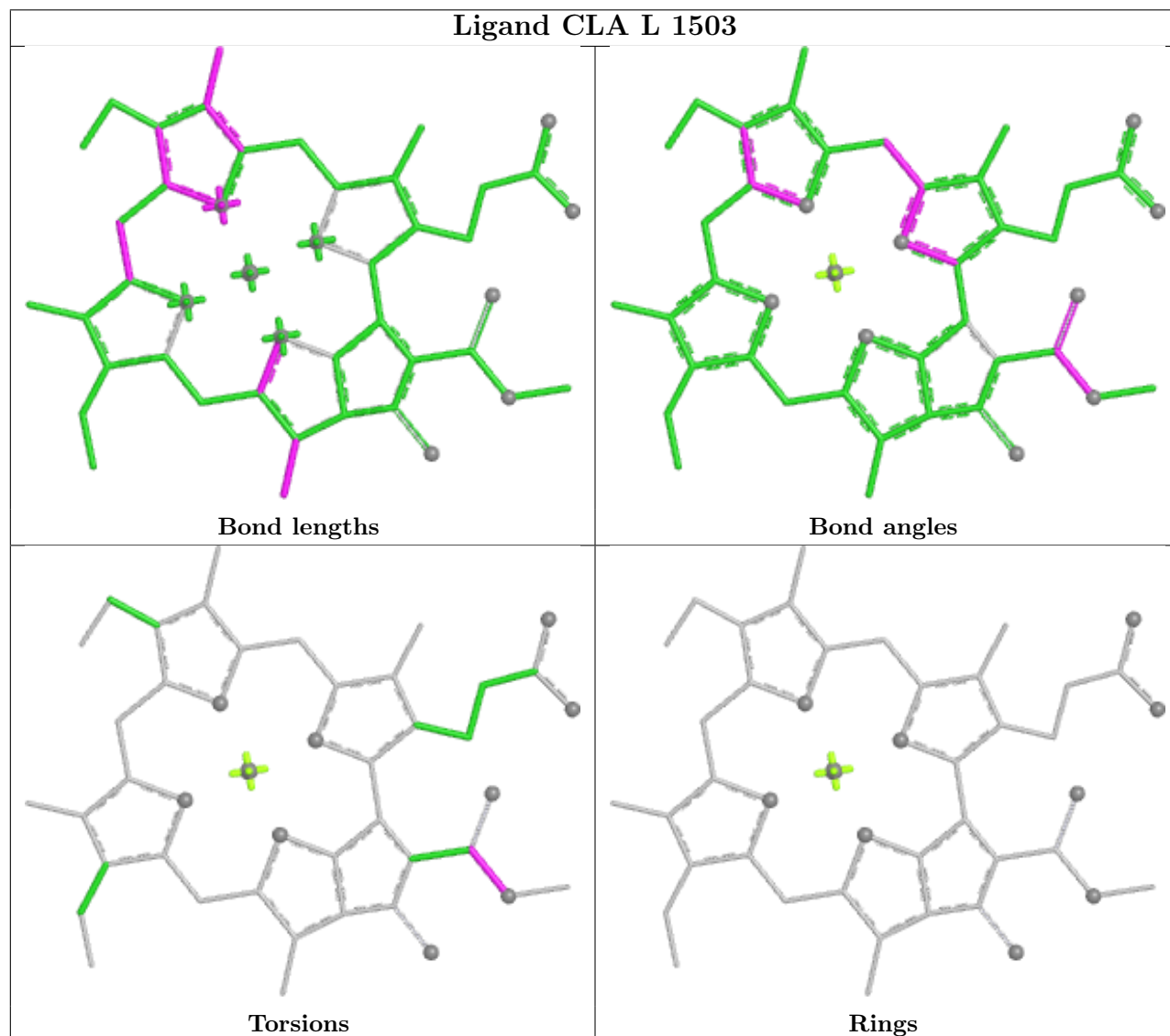
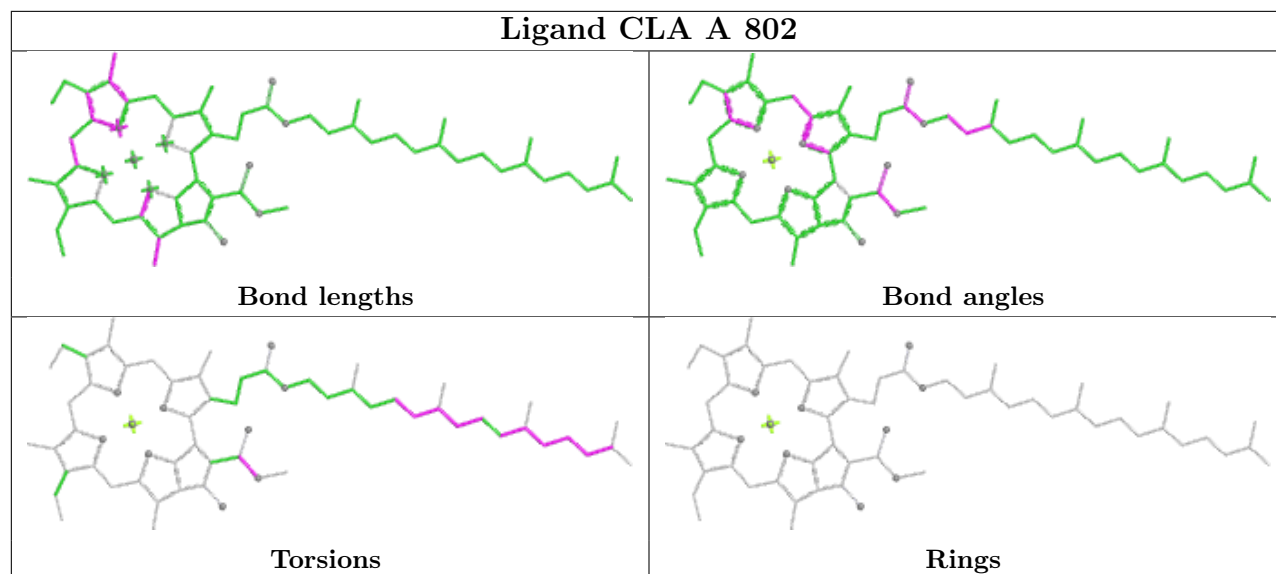


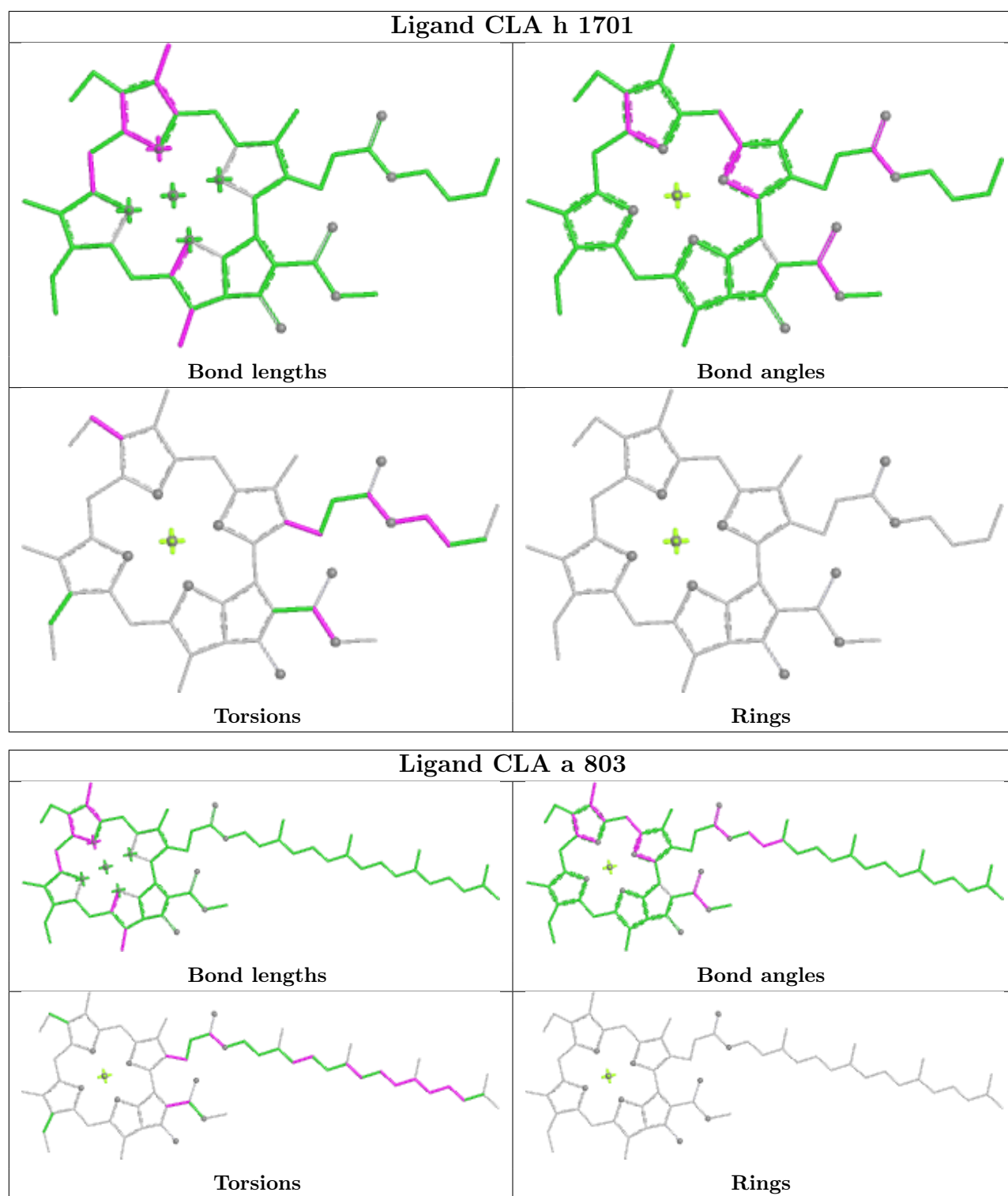
## Ligand BCR G 848



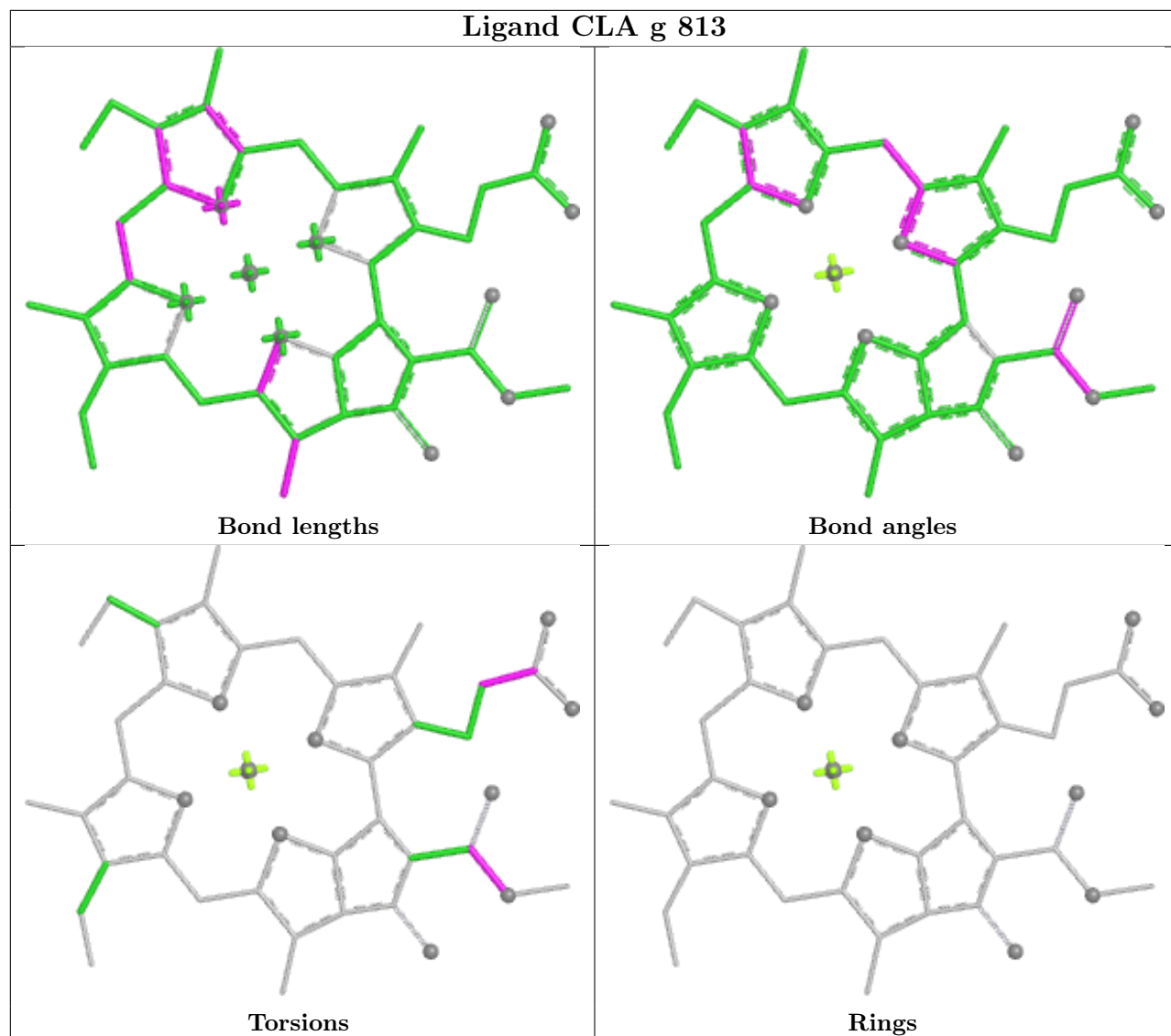
## Ligand CLA n 811



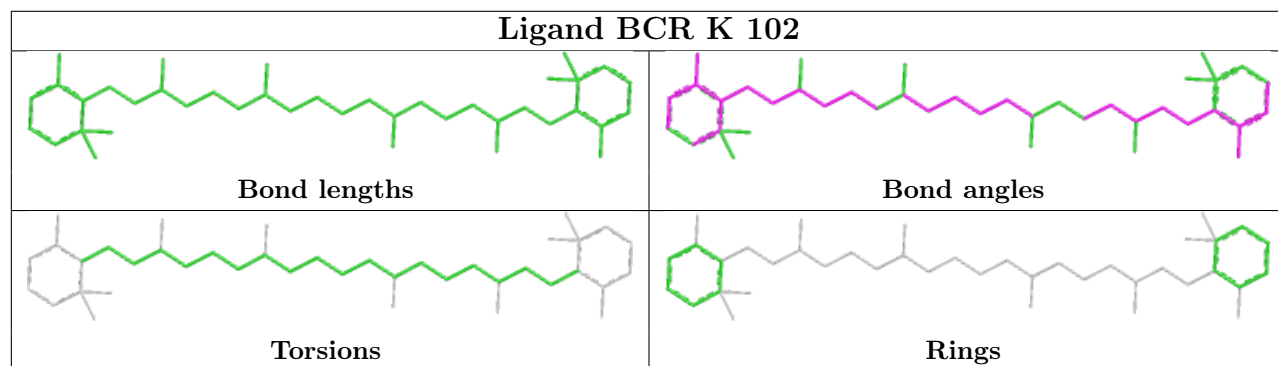


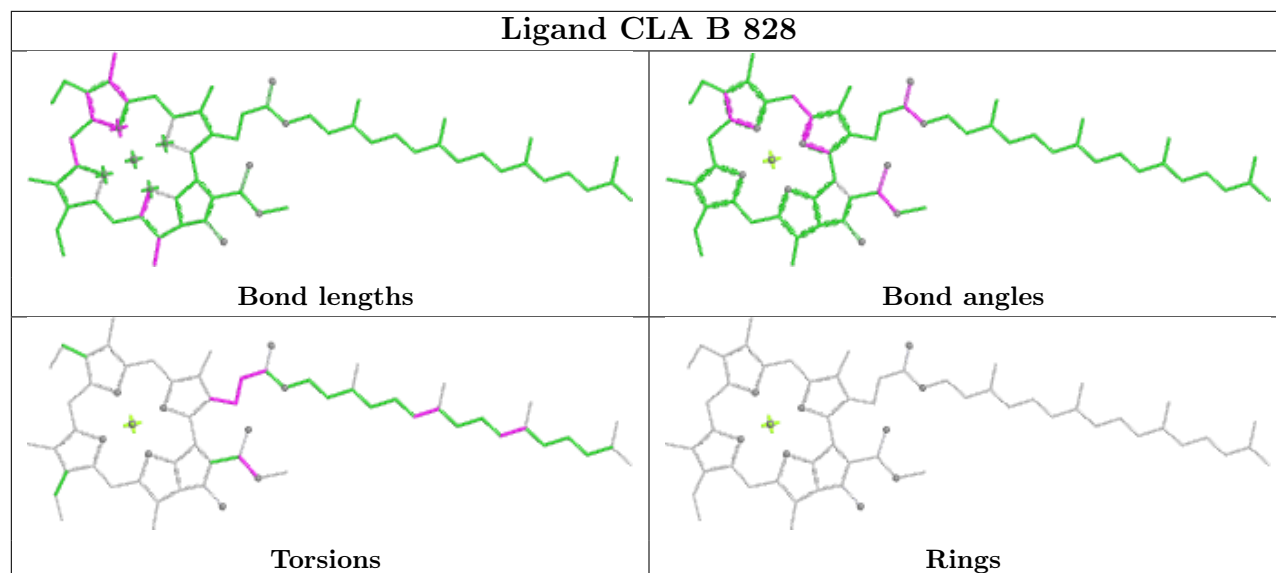
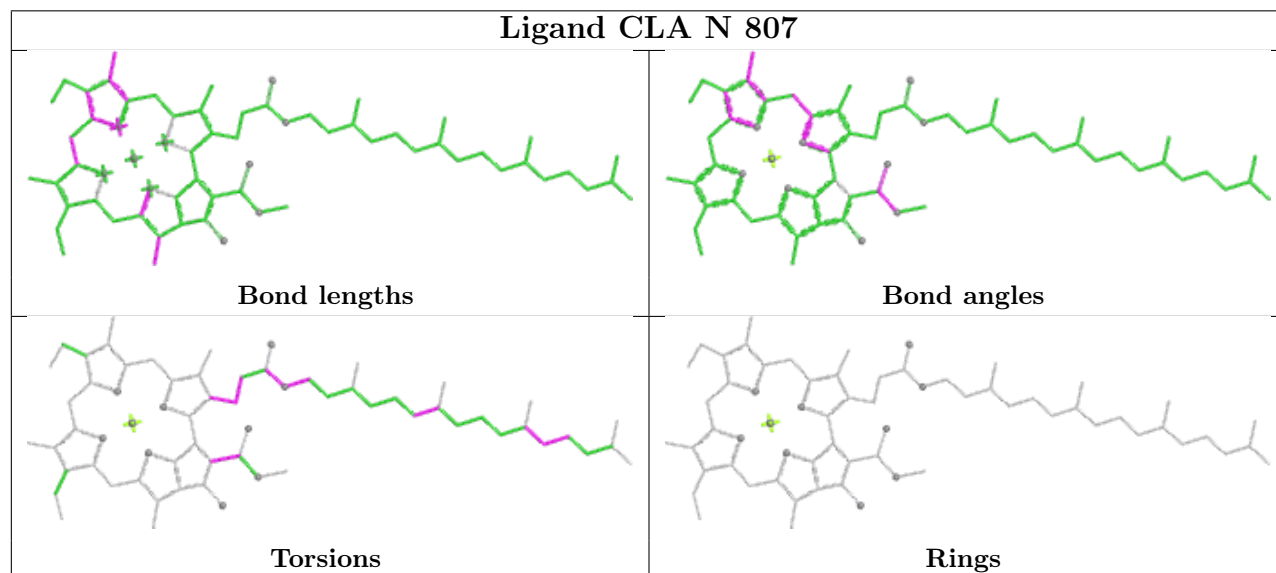
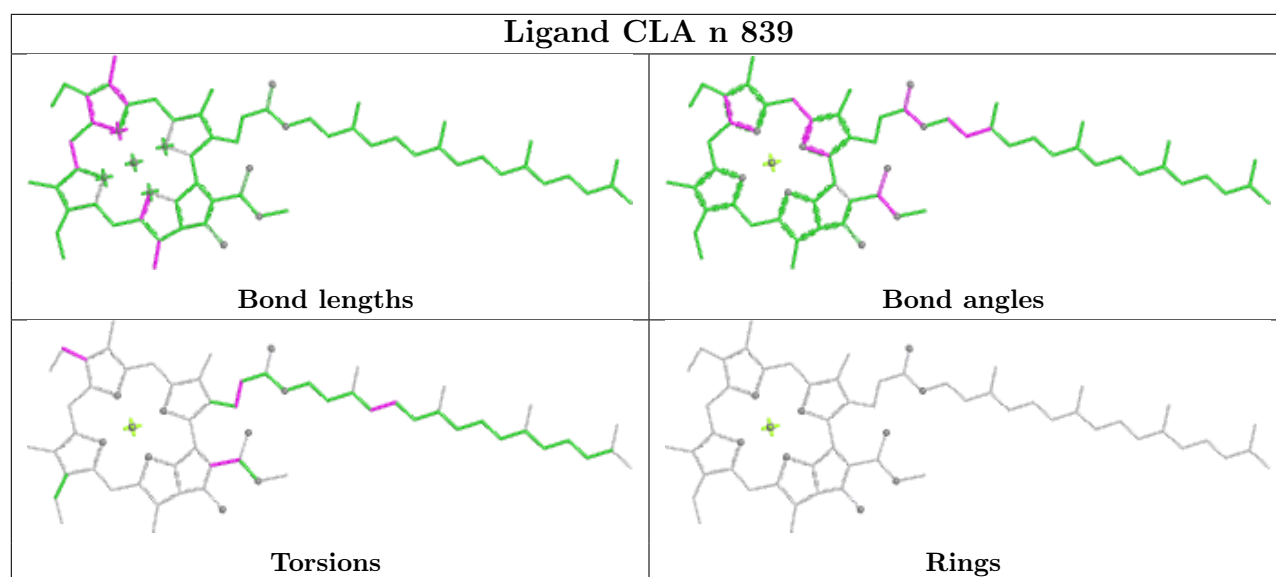


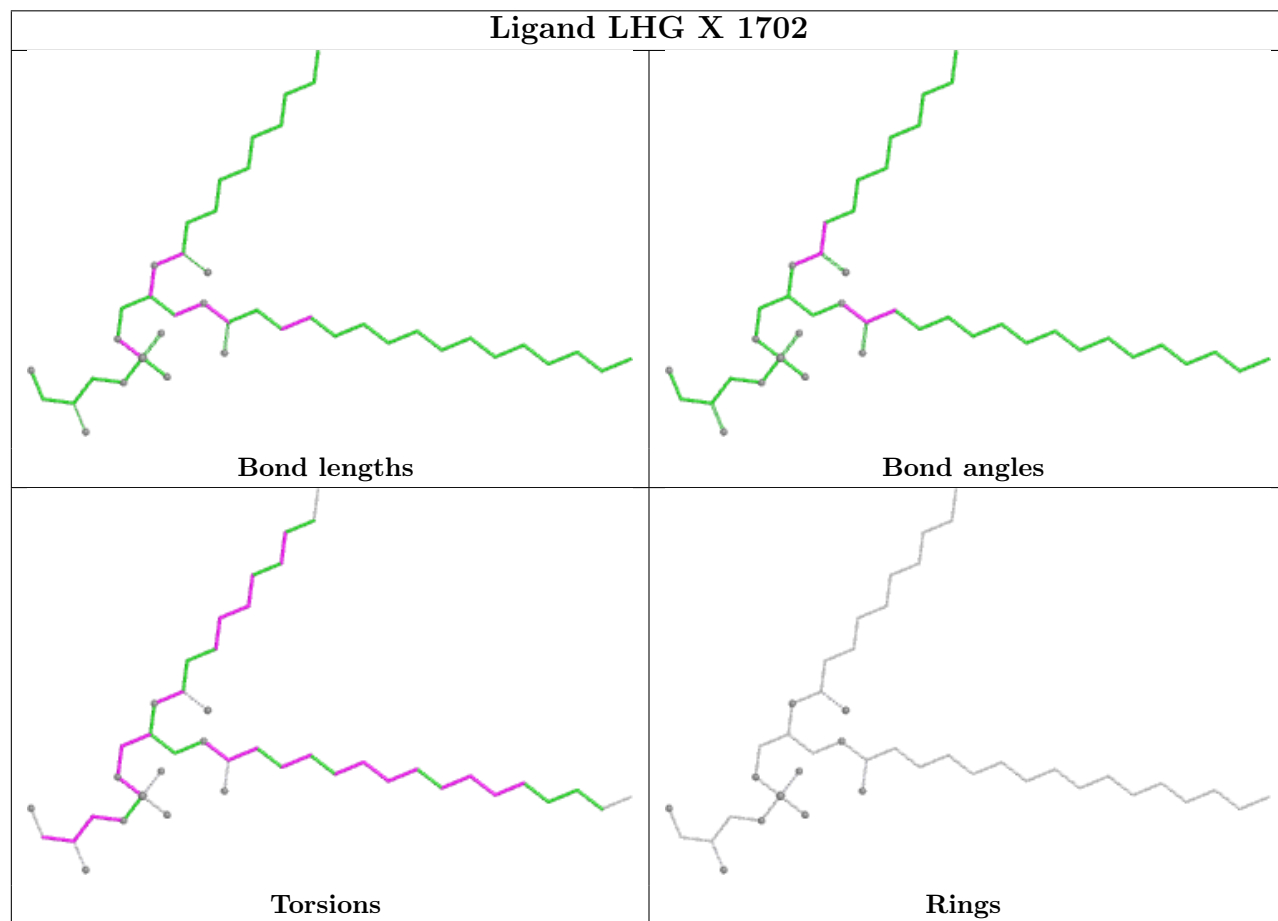
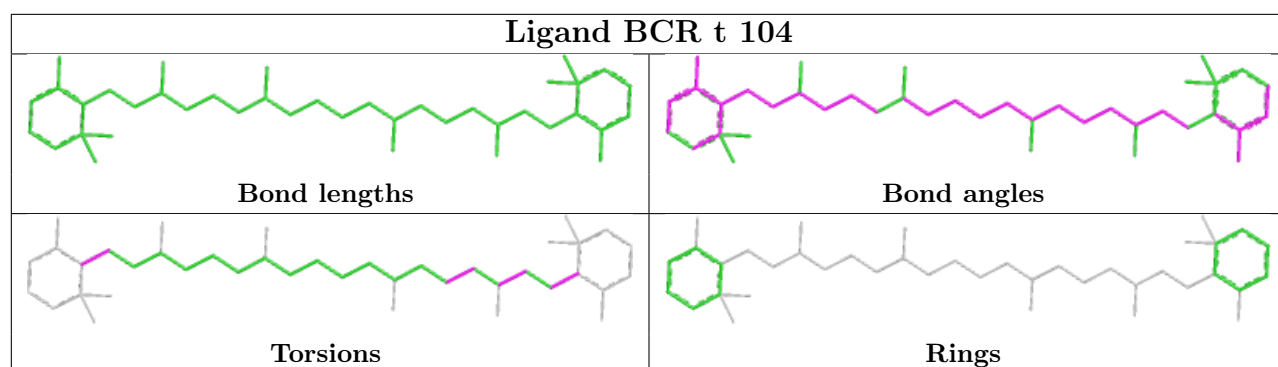
## Ligand CLA g 813



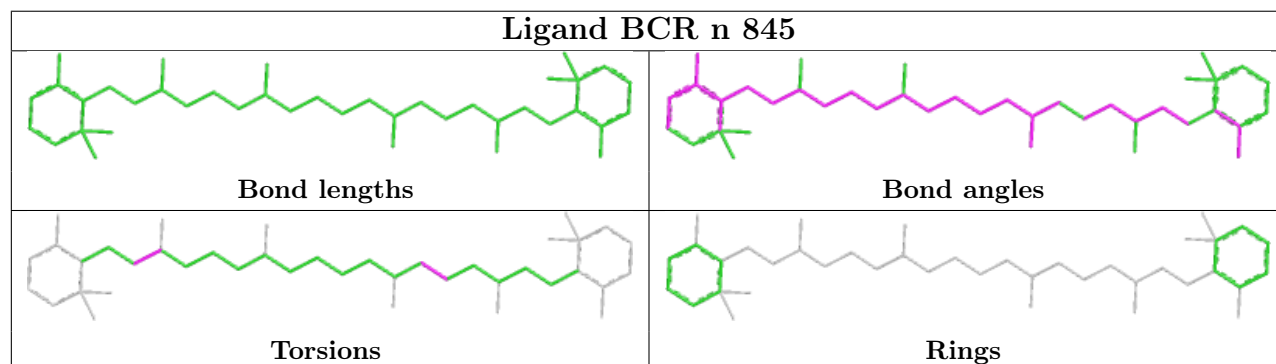
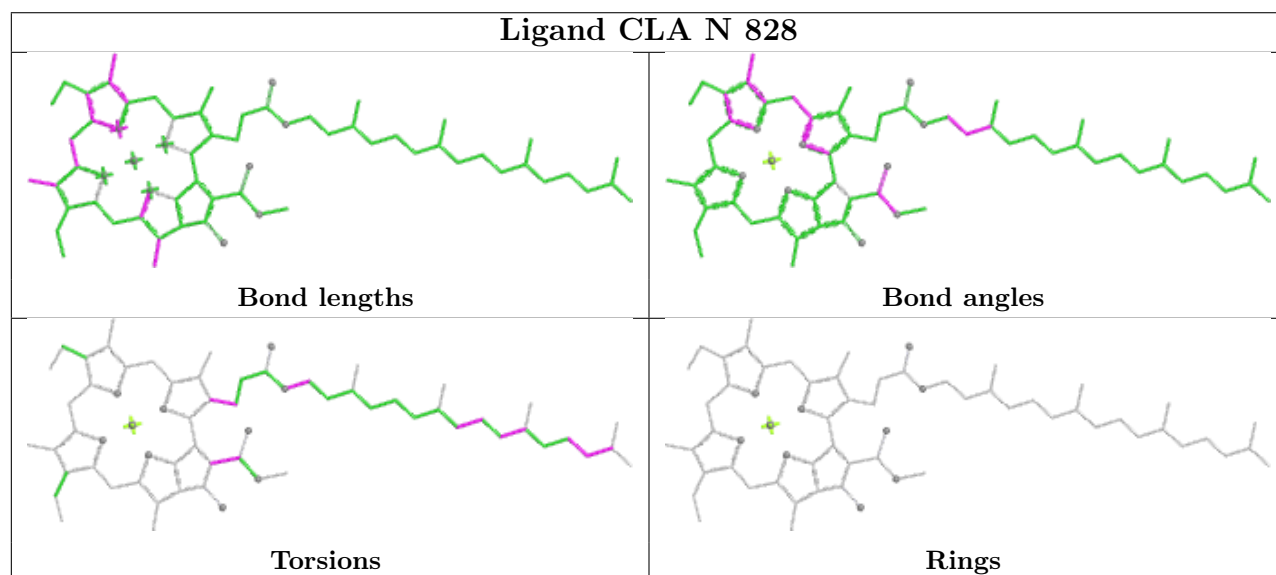
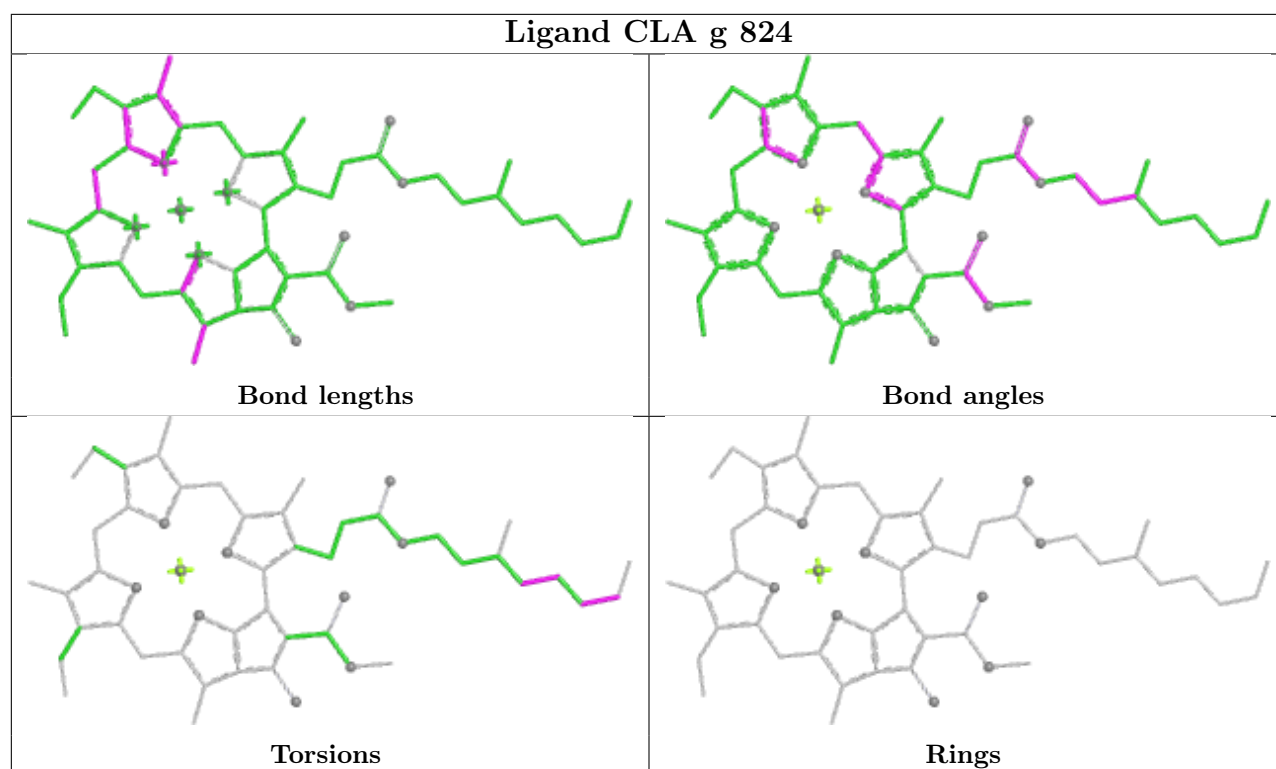
## Ligand BCR K 102



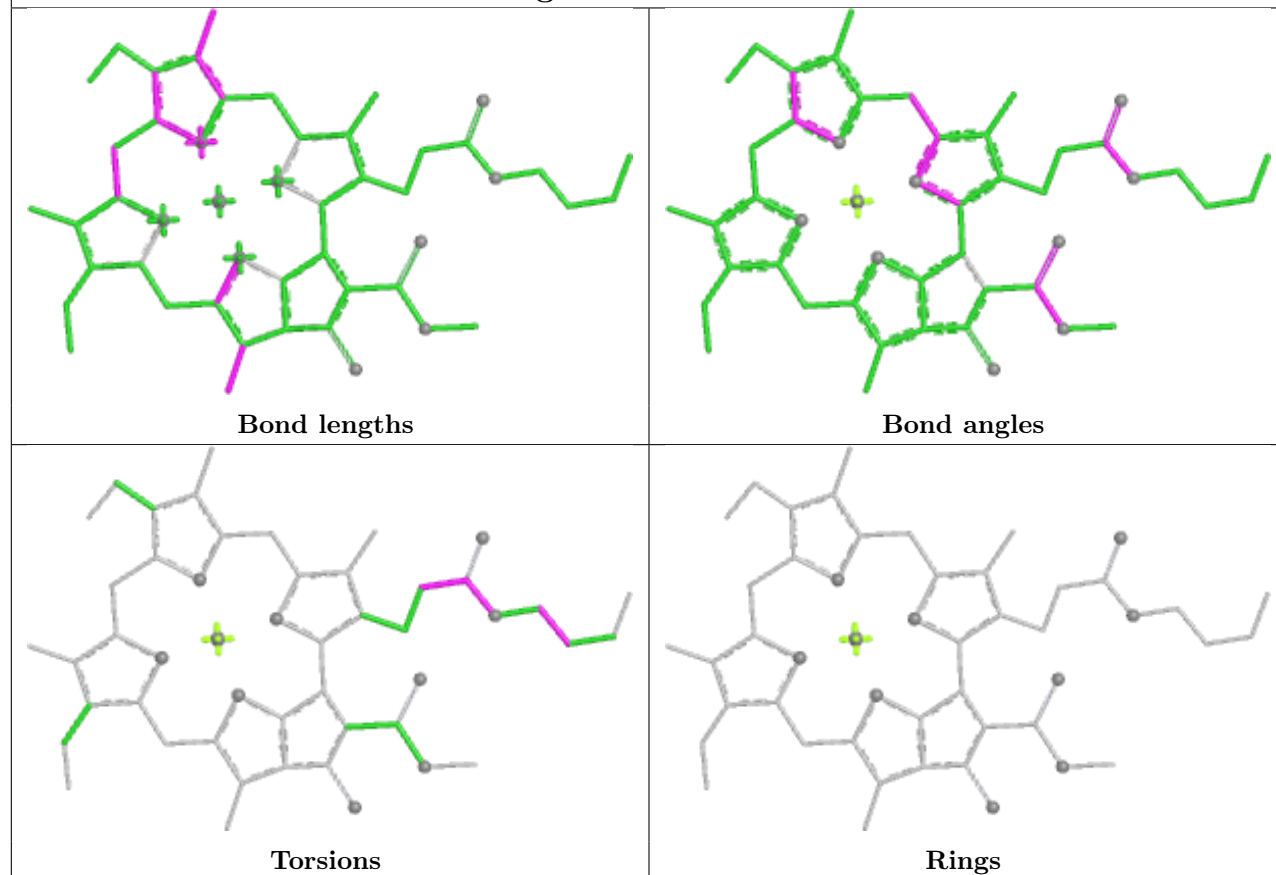




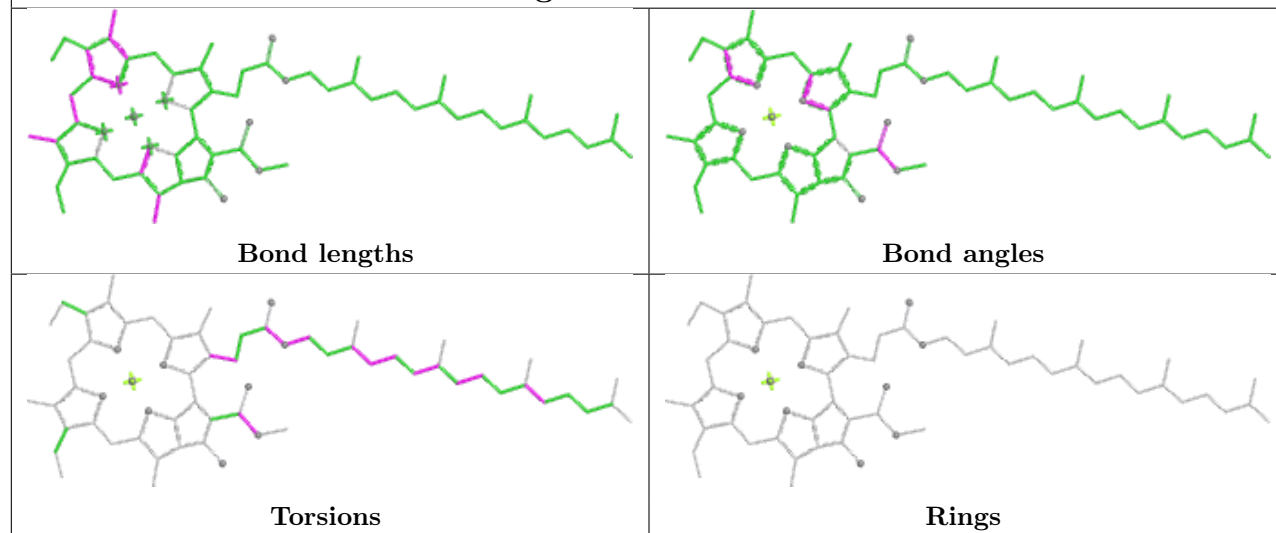




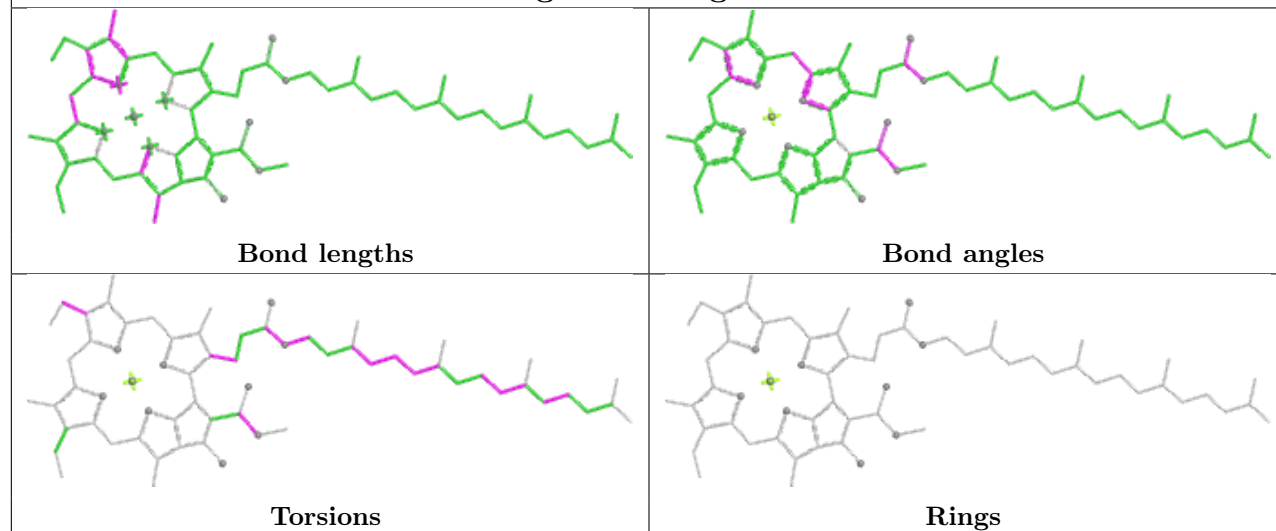
## Ligand CLA a 854



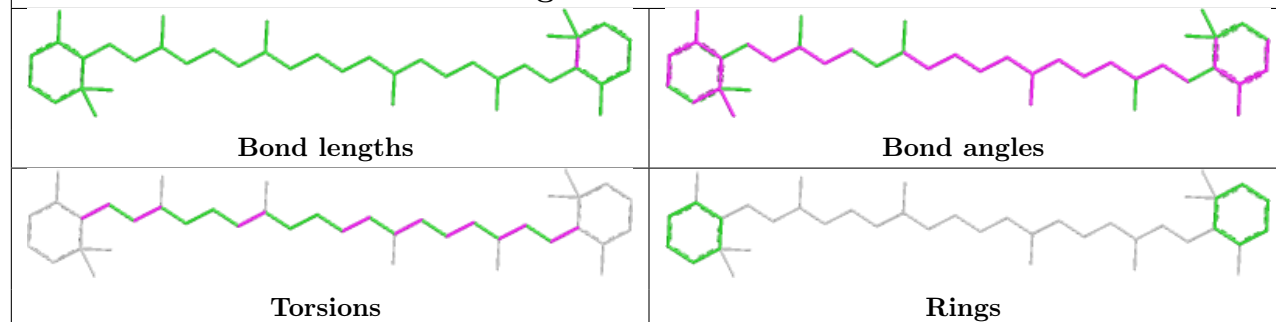
## Ligand CLA n 802



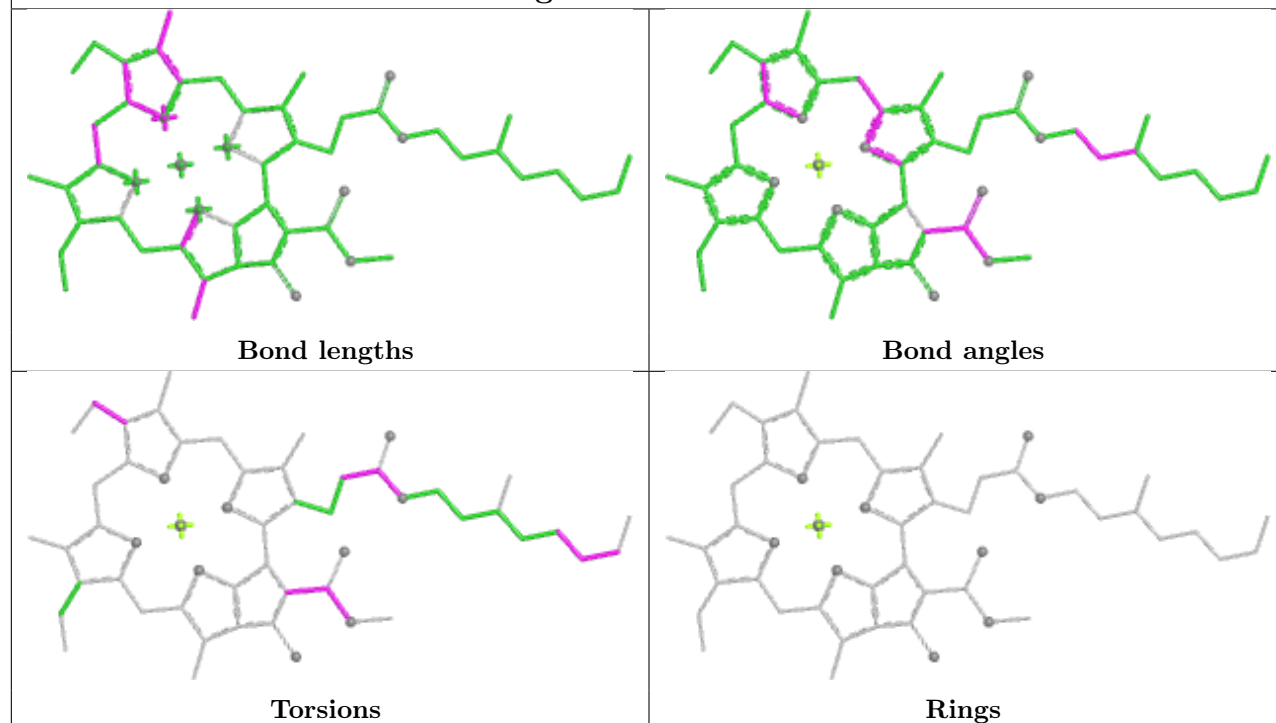
## Ligand CLA g 837

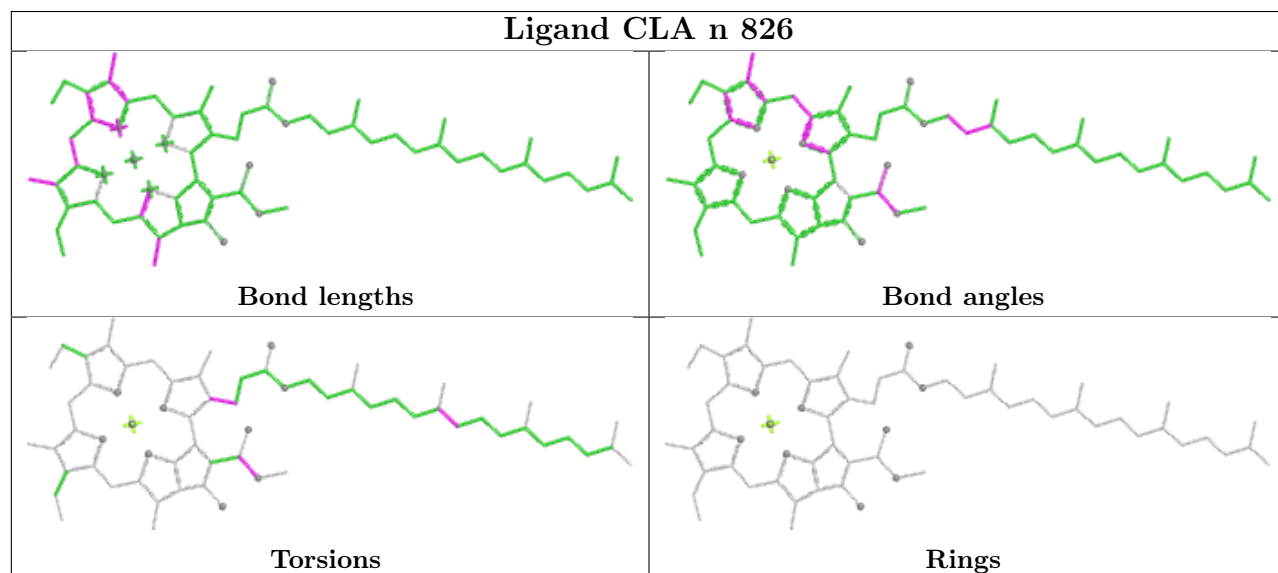
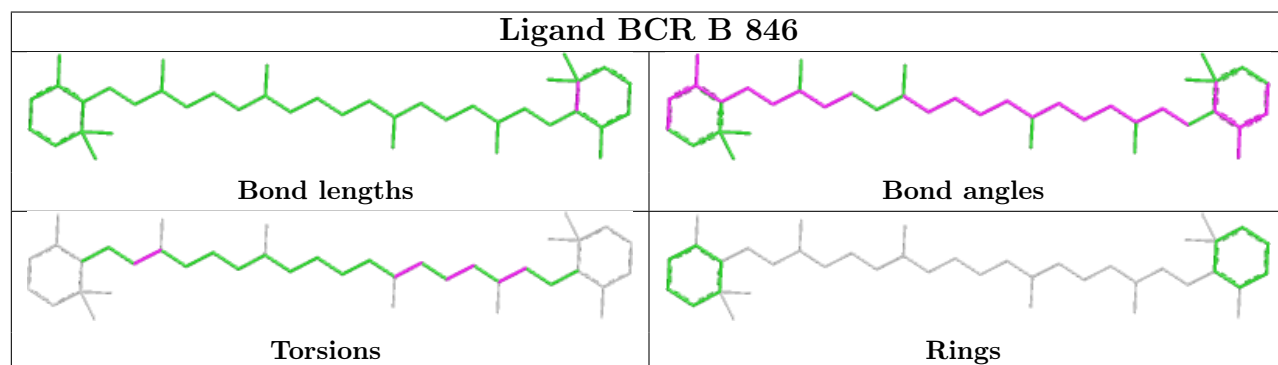
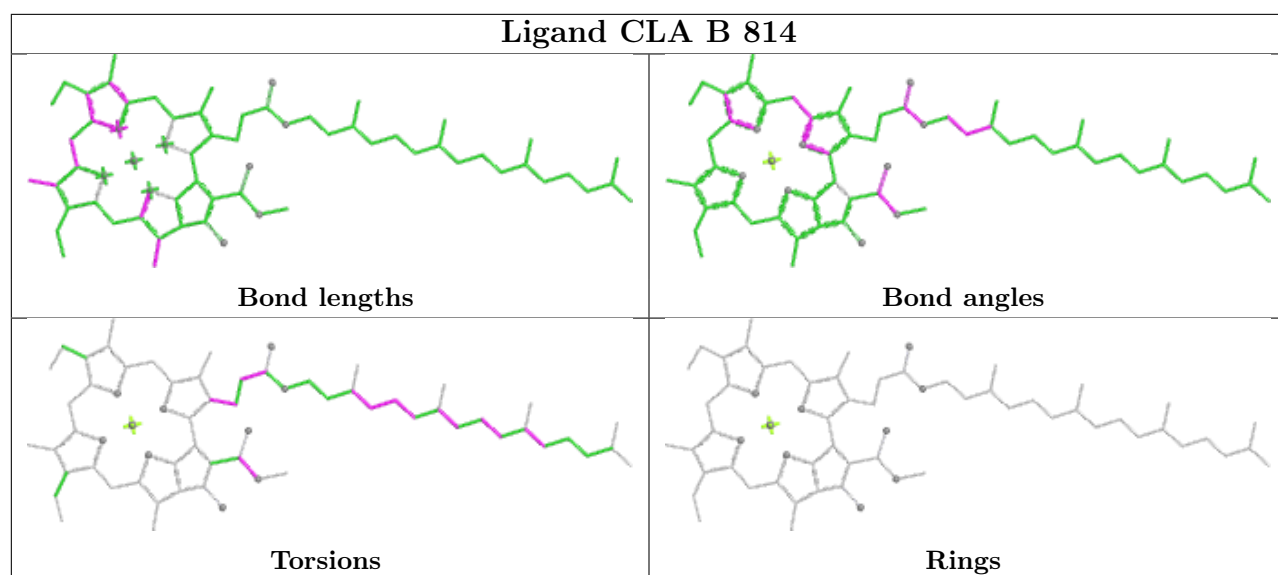


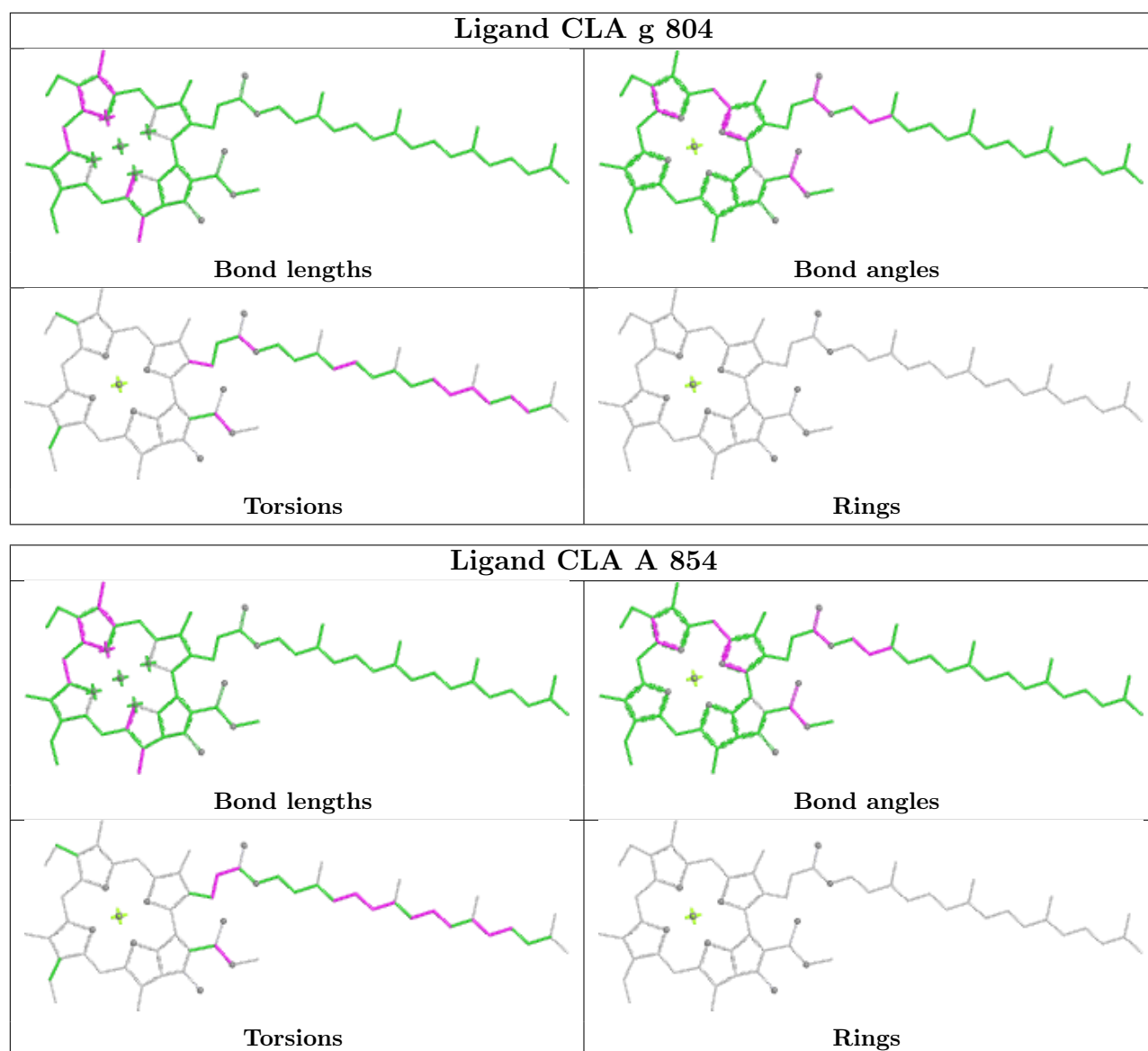
## Ligand BCR I 102

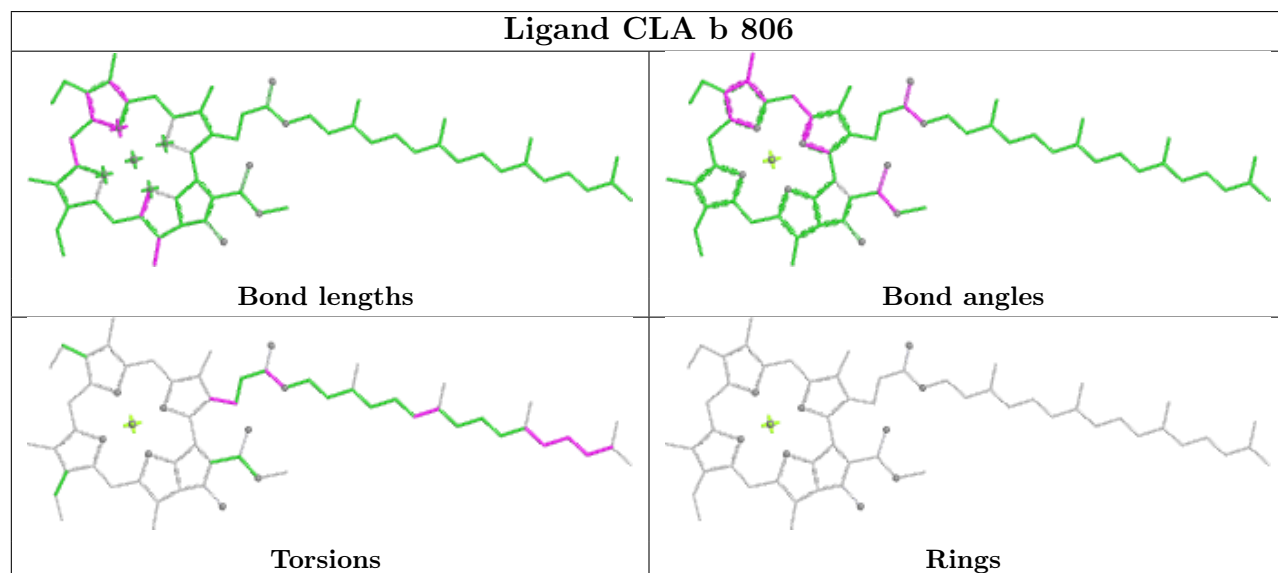
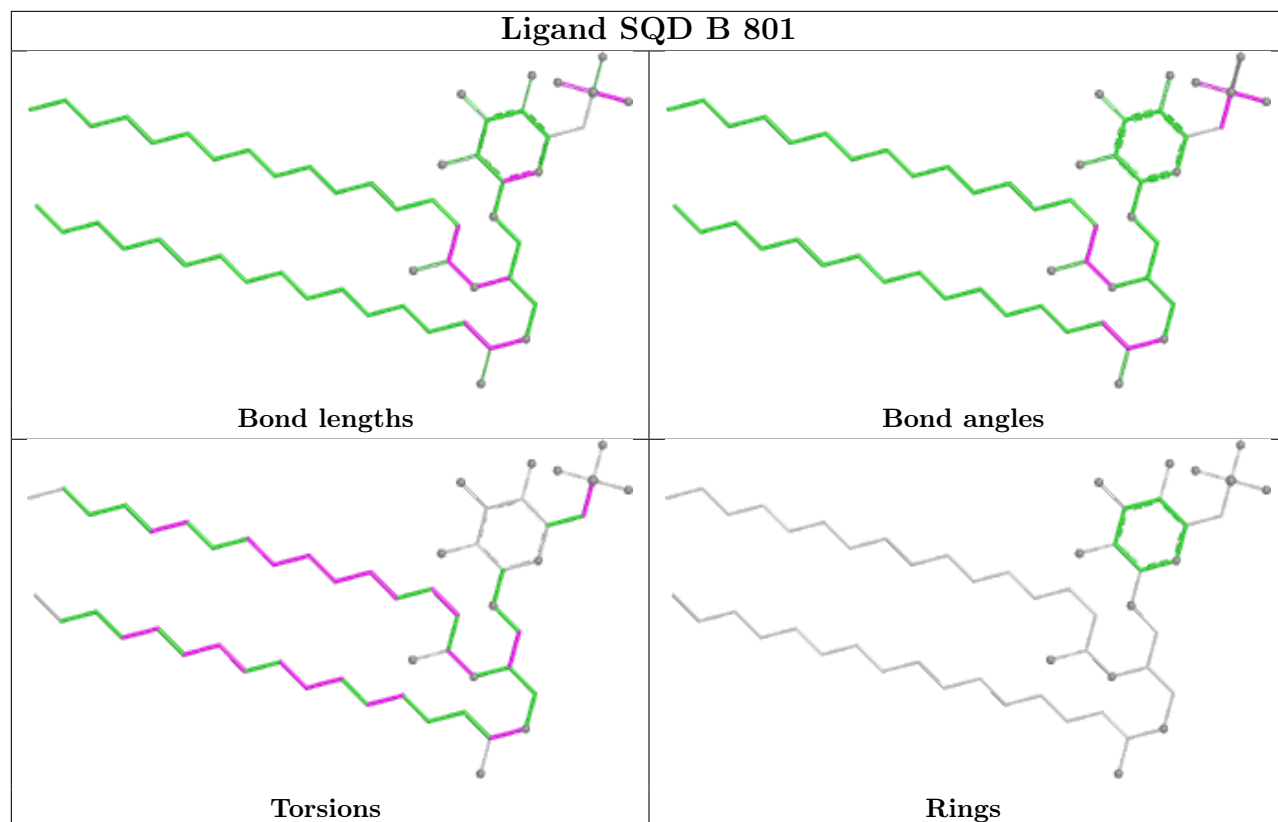


## Ligand CLA b 812

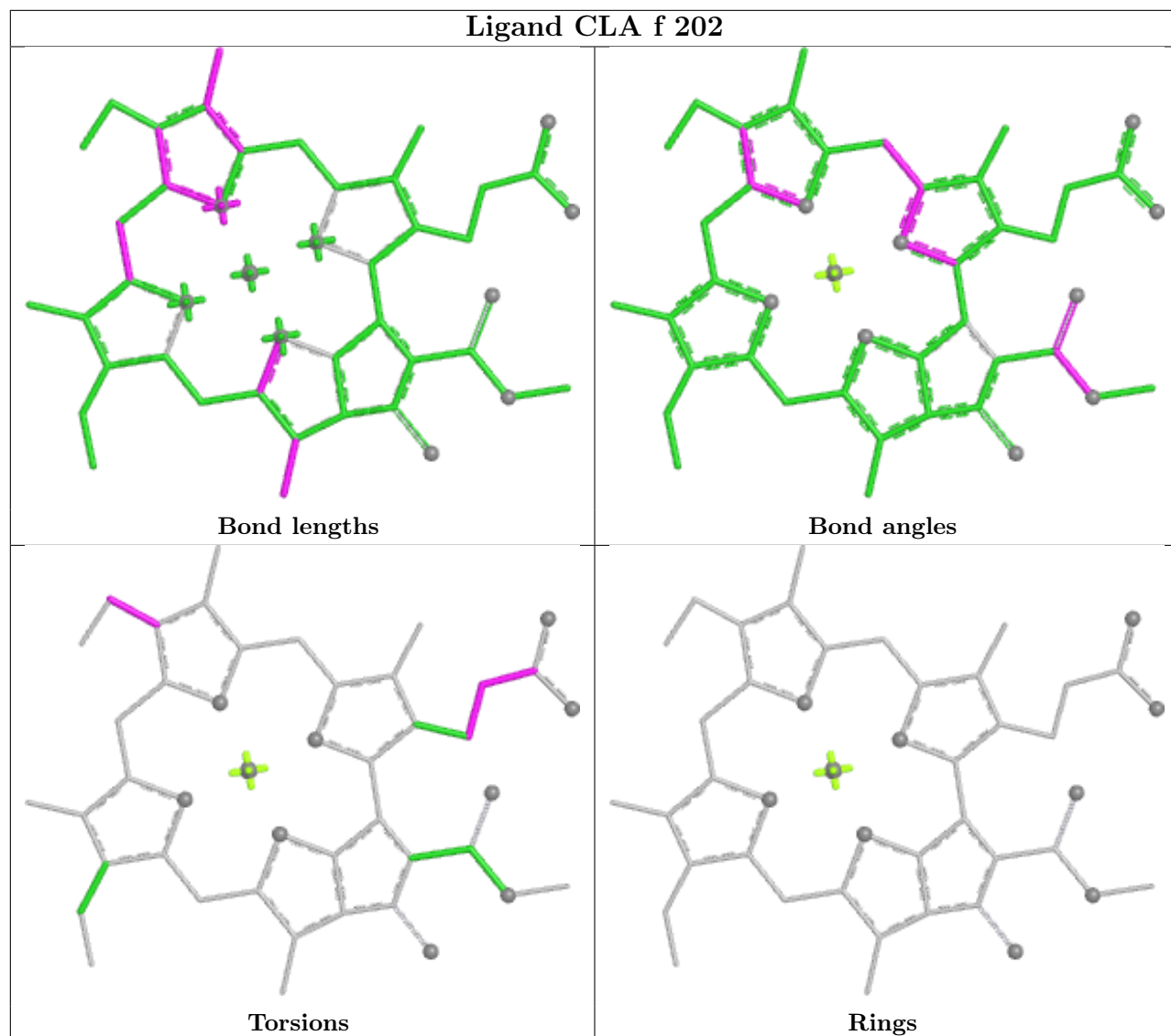




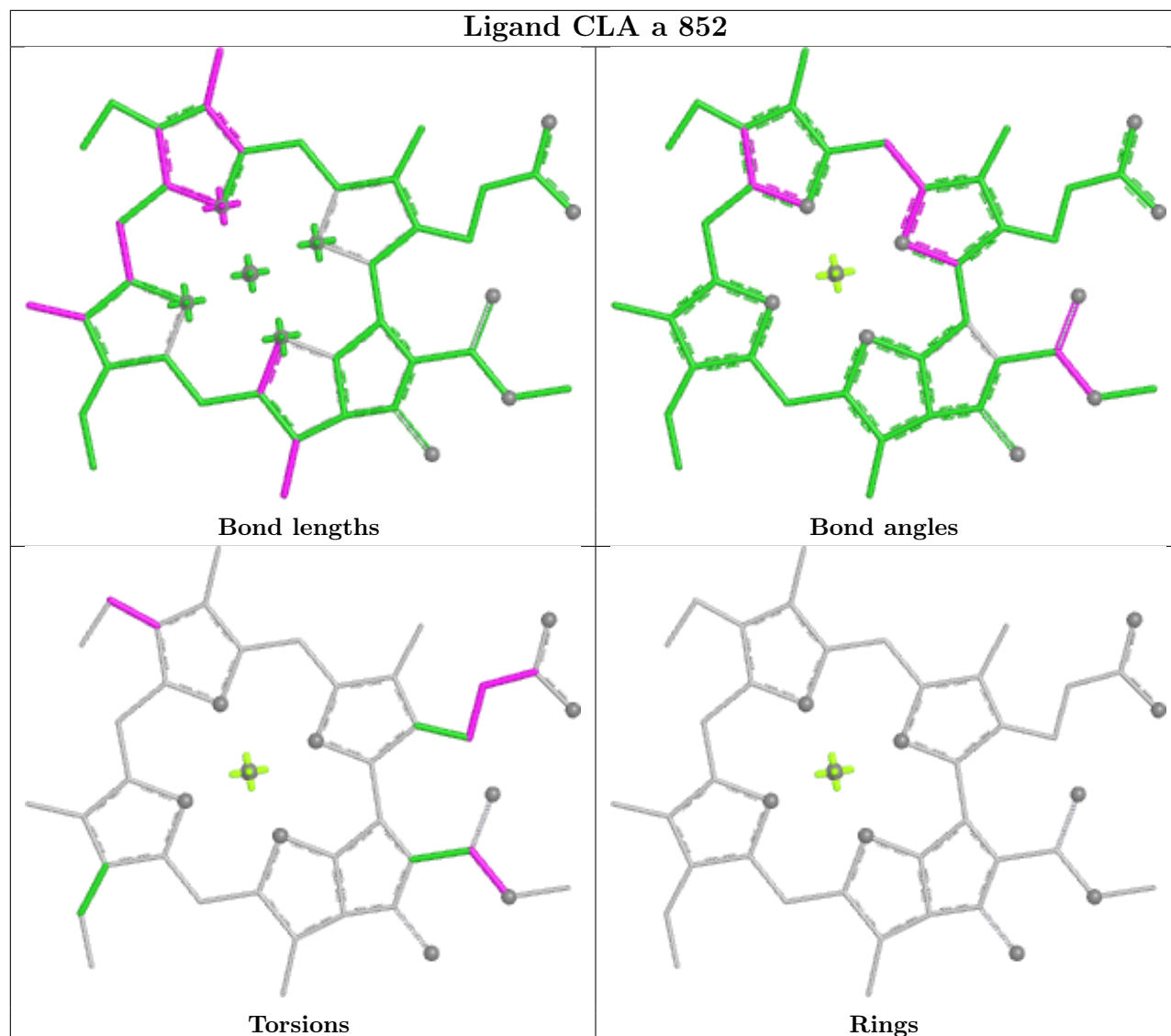




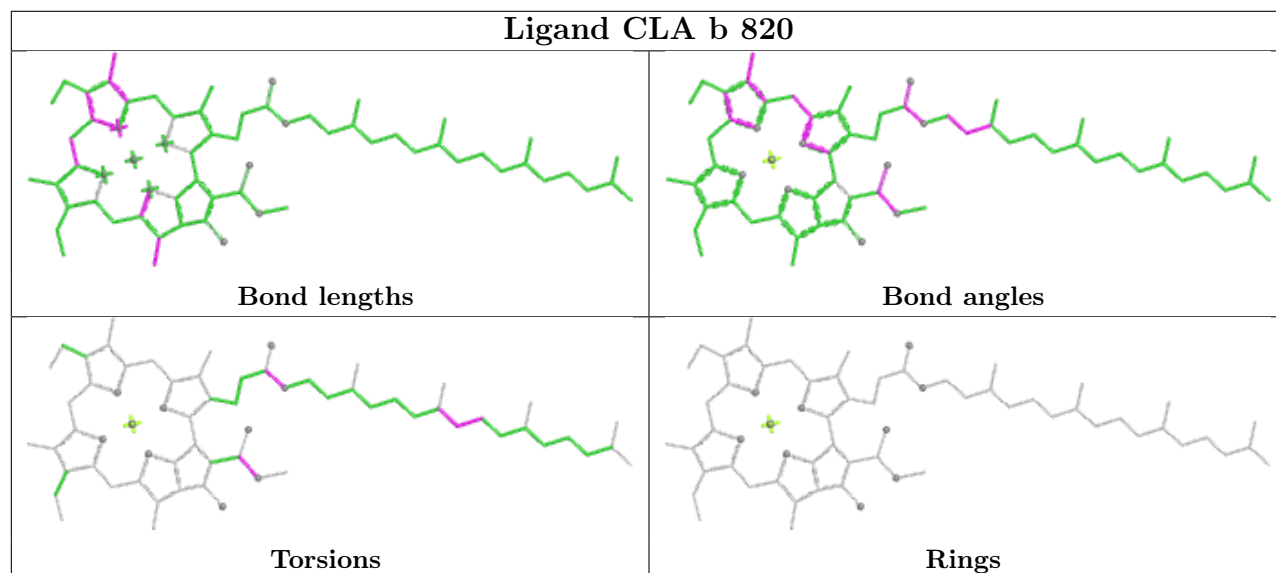
## Ligand CLA f 202



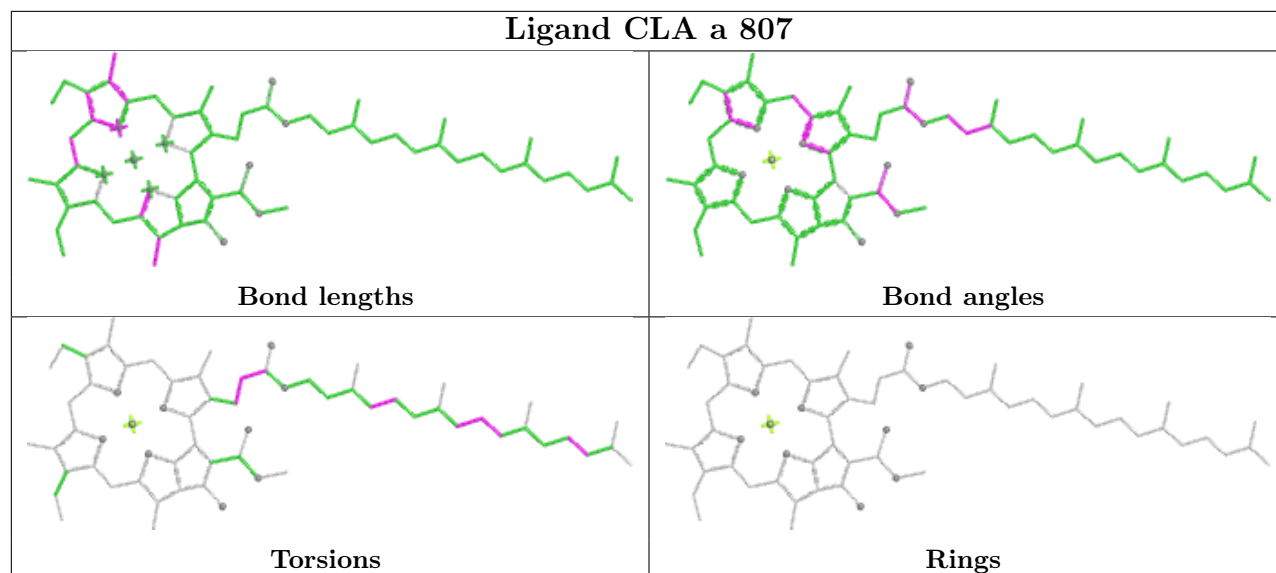
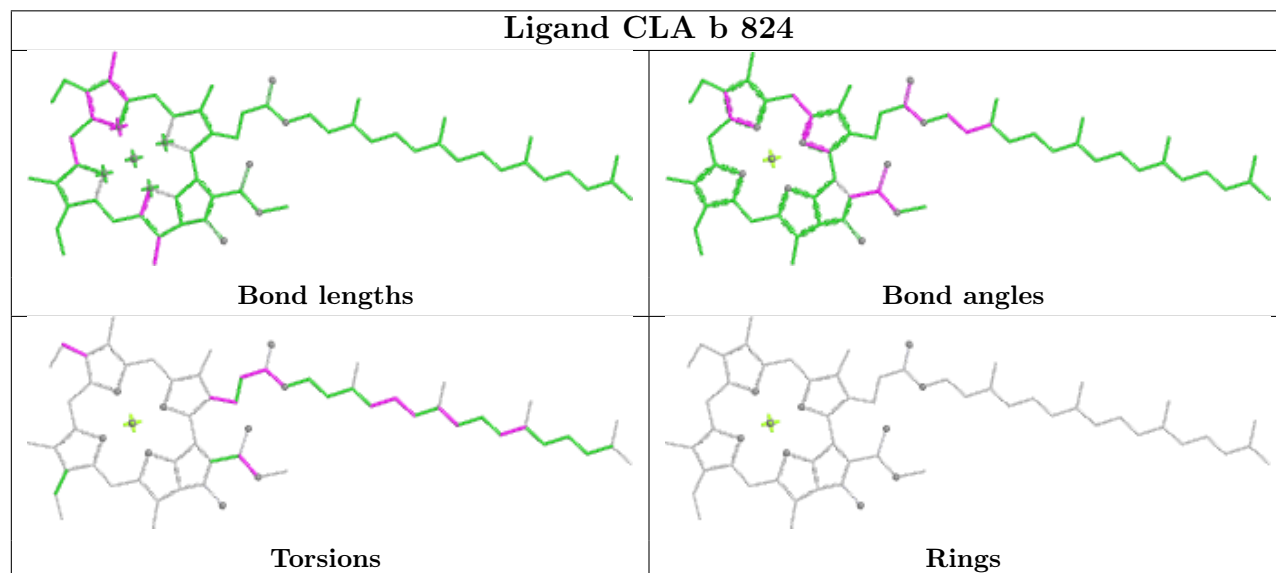
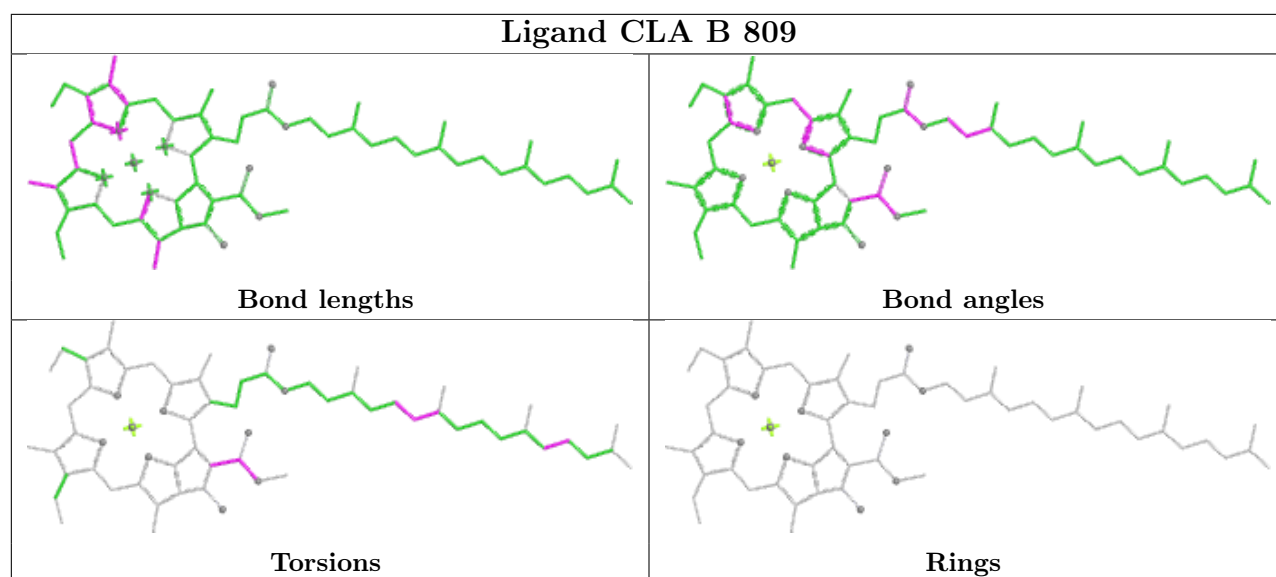
## Ligand CLA a 852

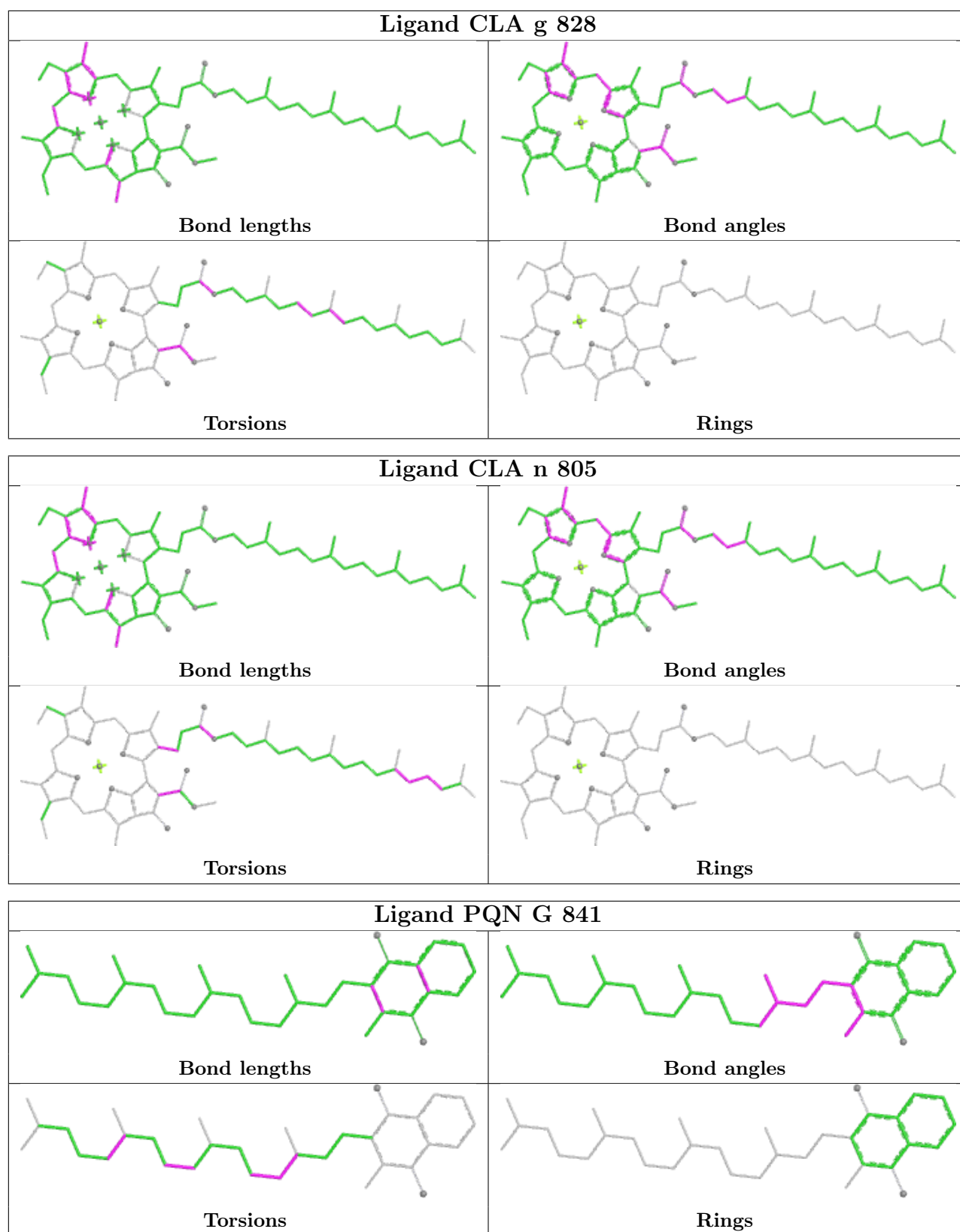


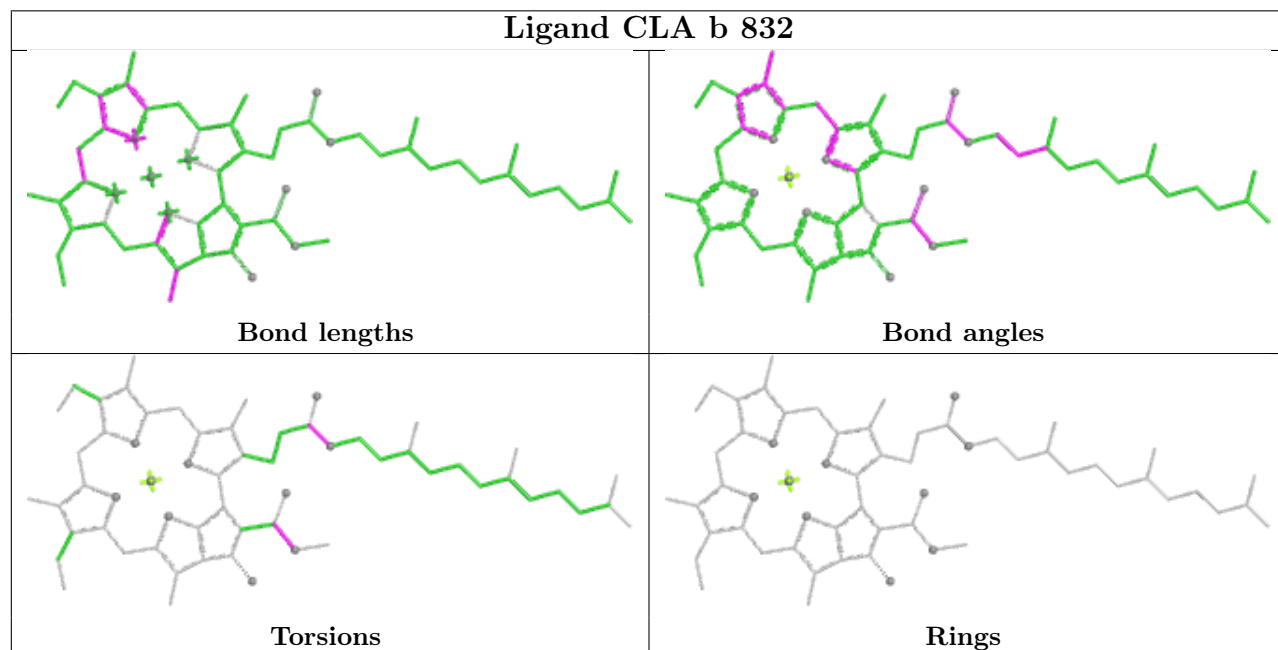
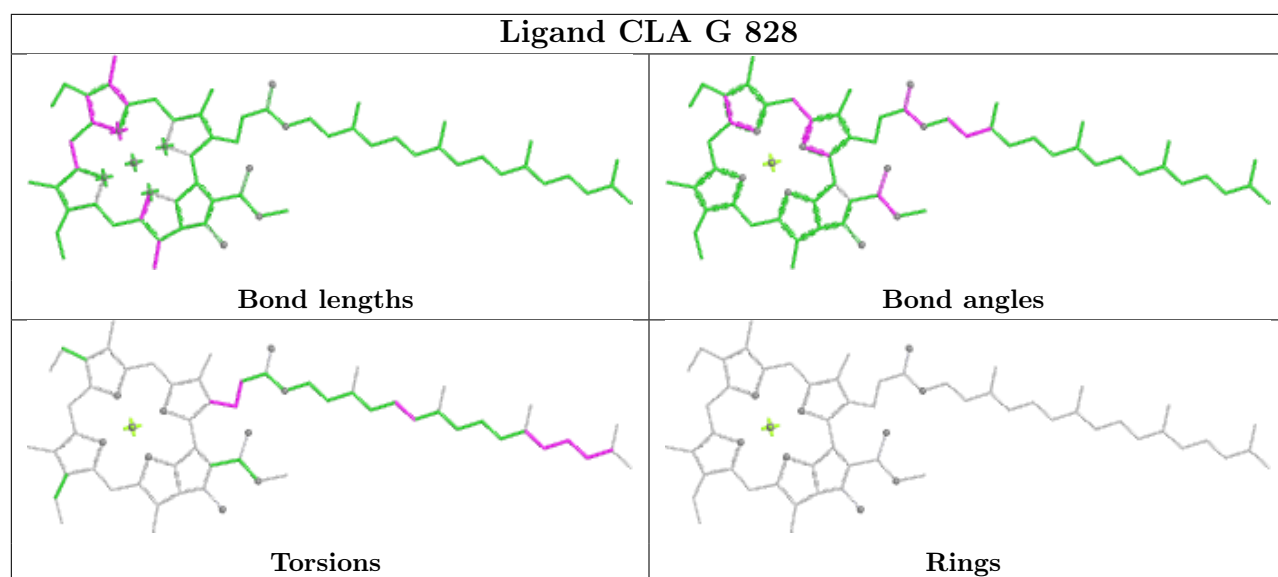
## Ligand CLA b 820



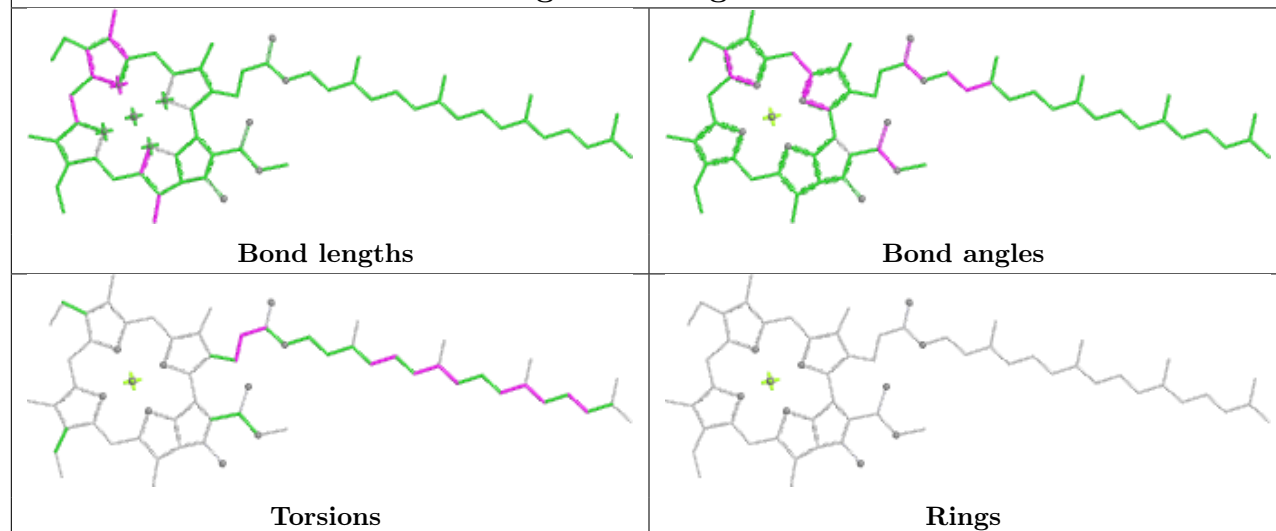




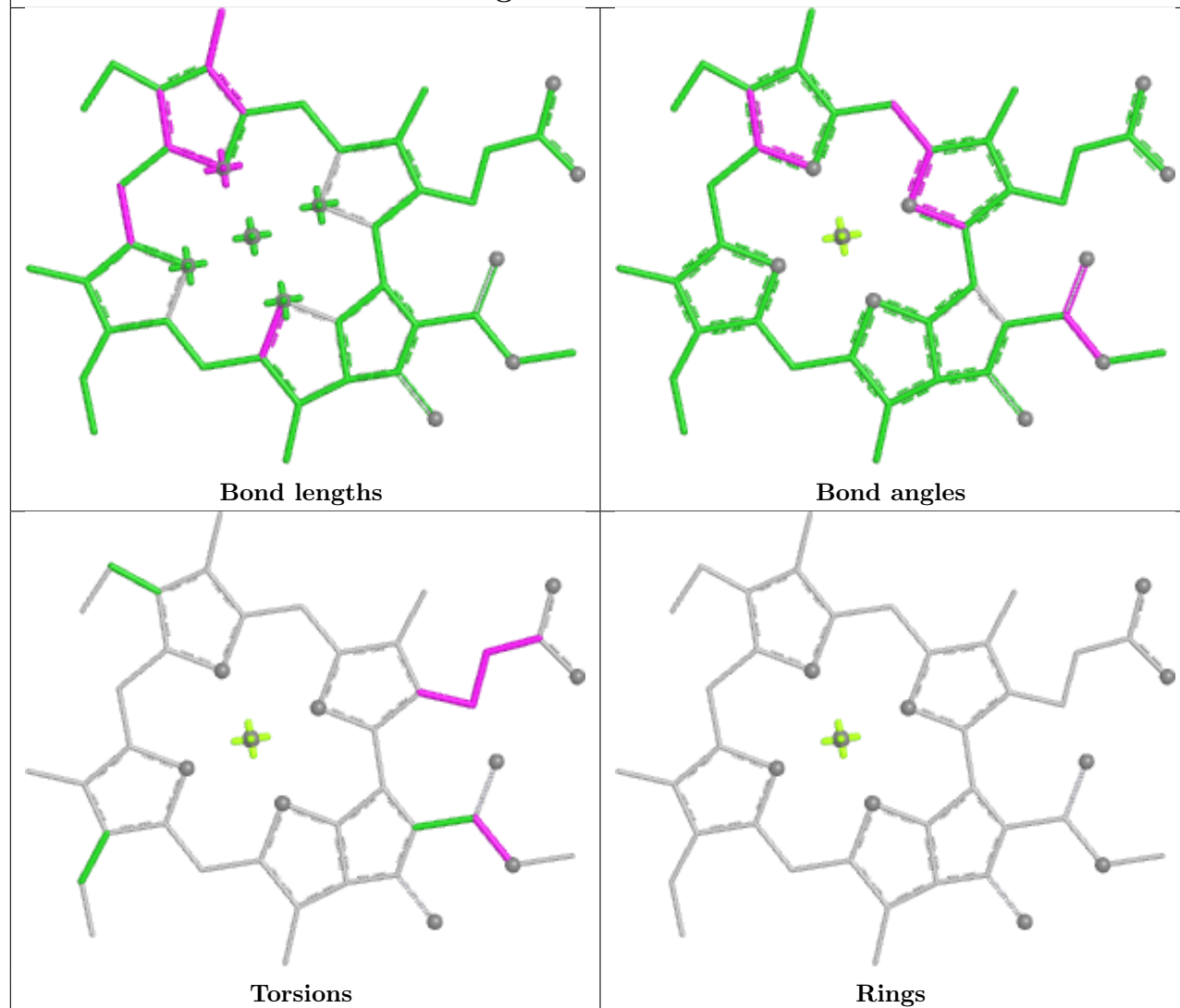


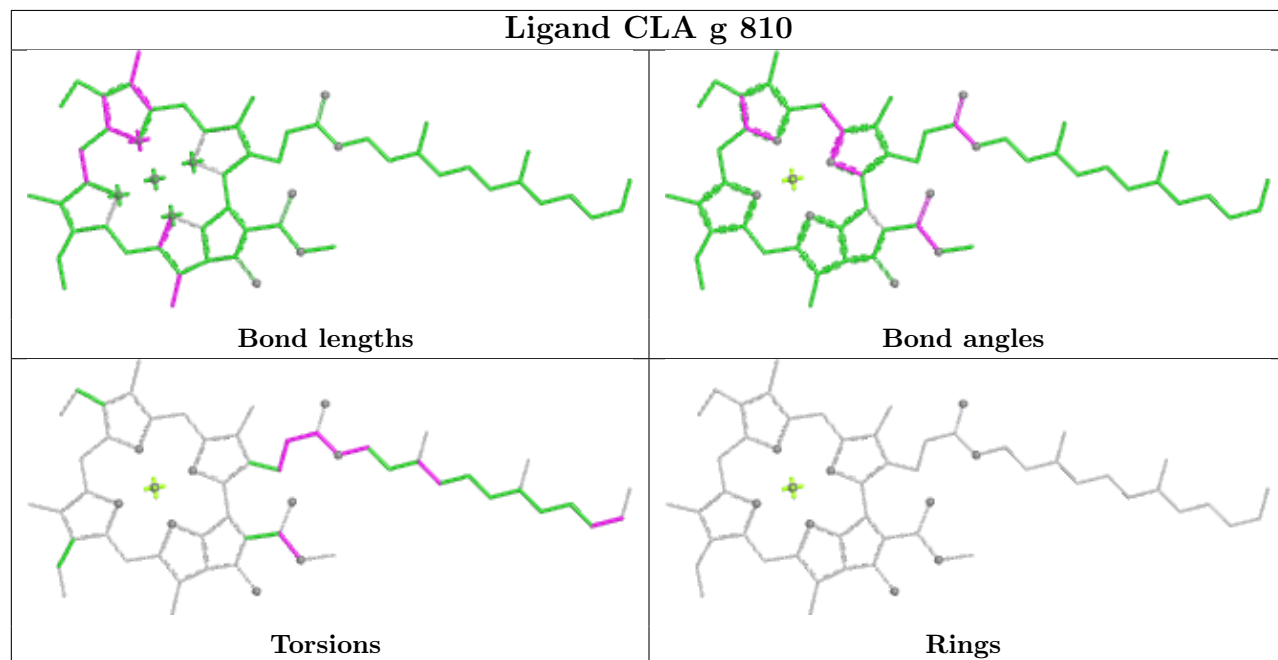
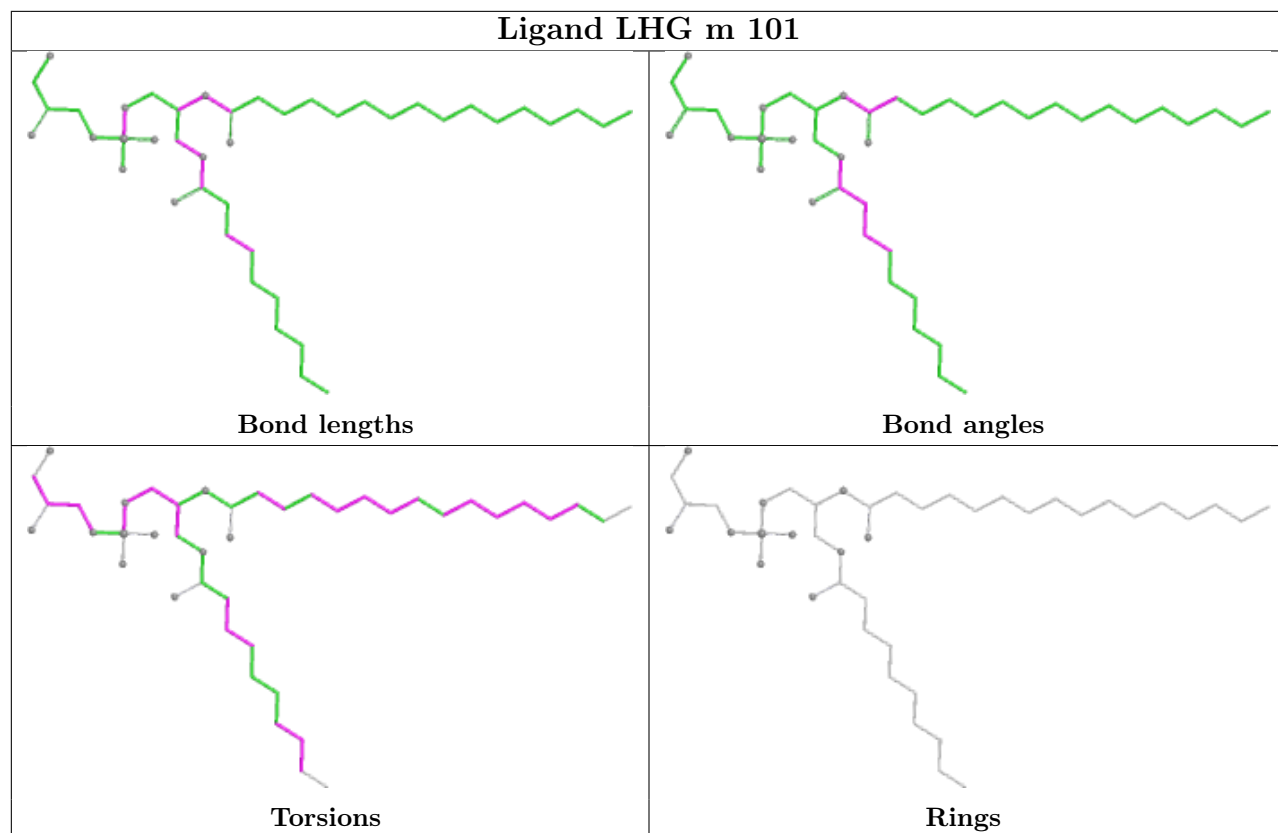


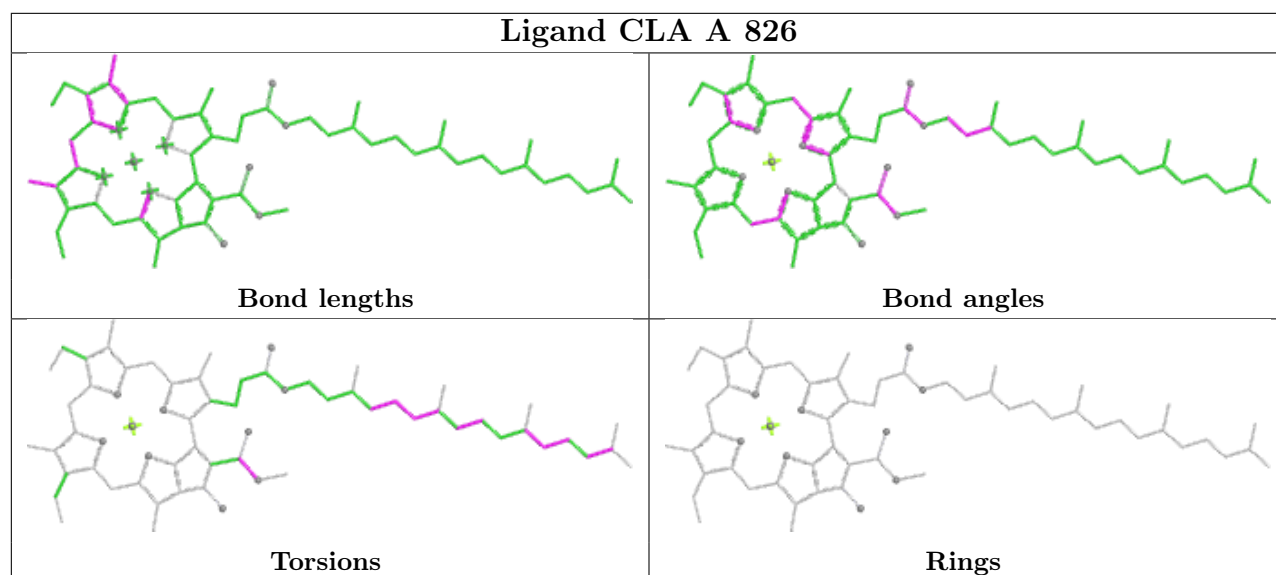
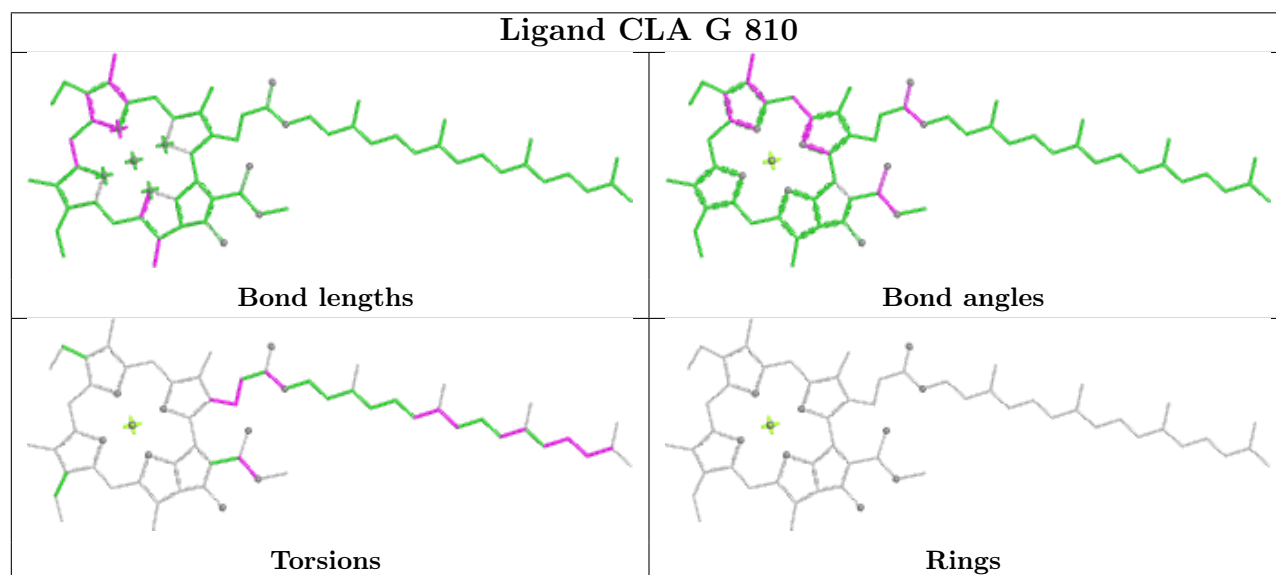
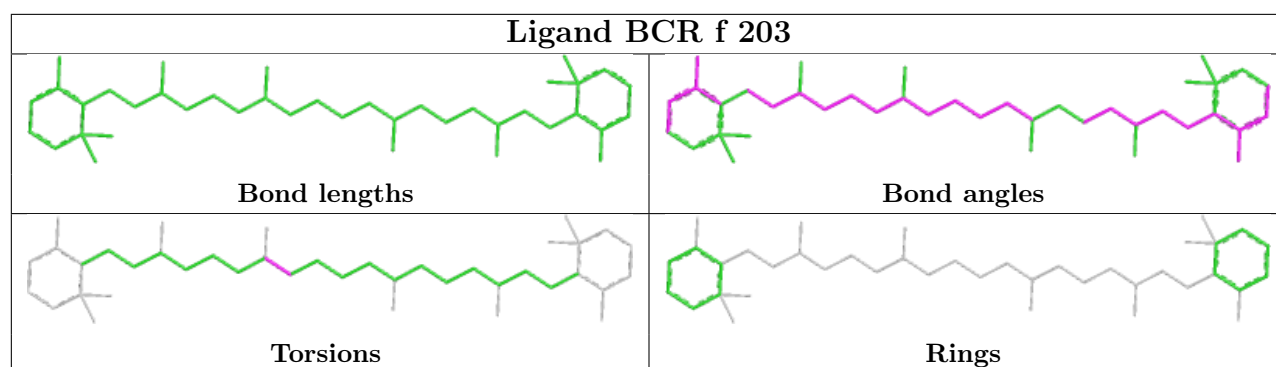
## Ligand CLA g 838

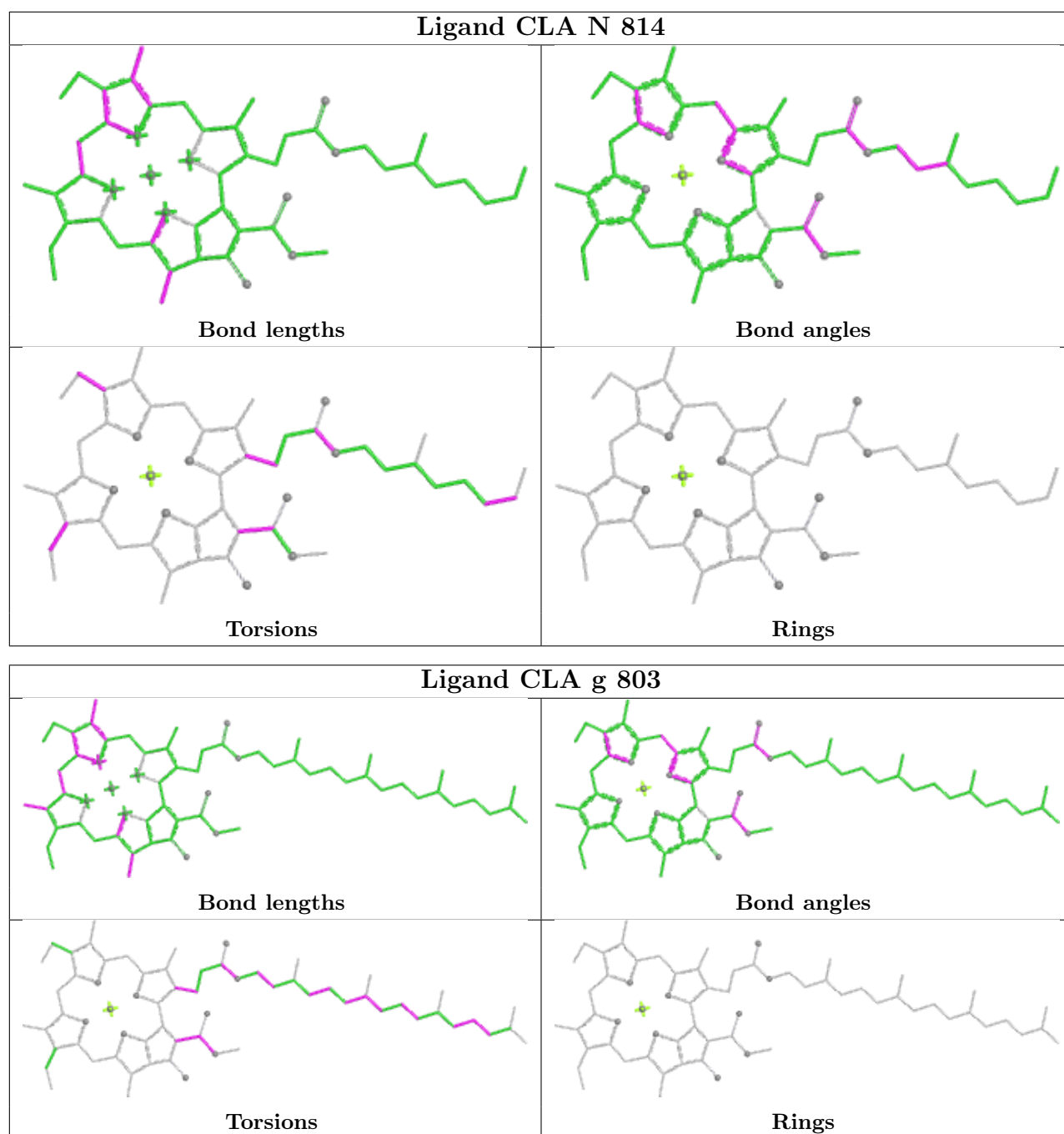


## Ligand CLA a 834

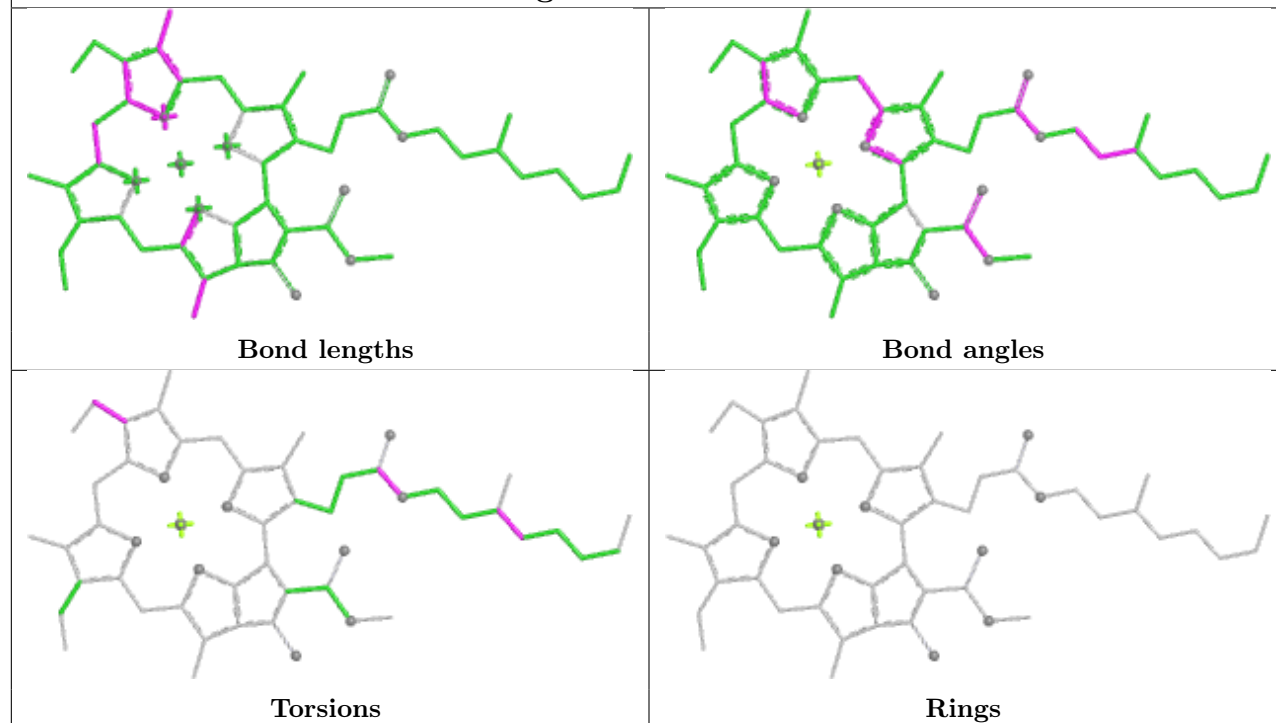




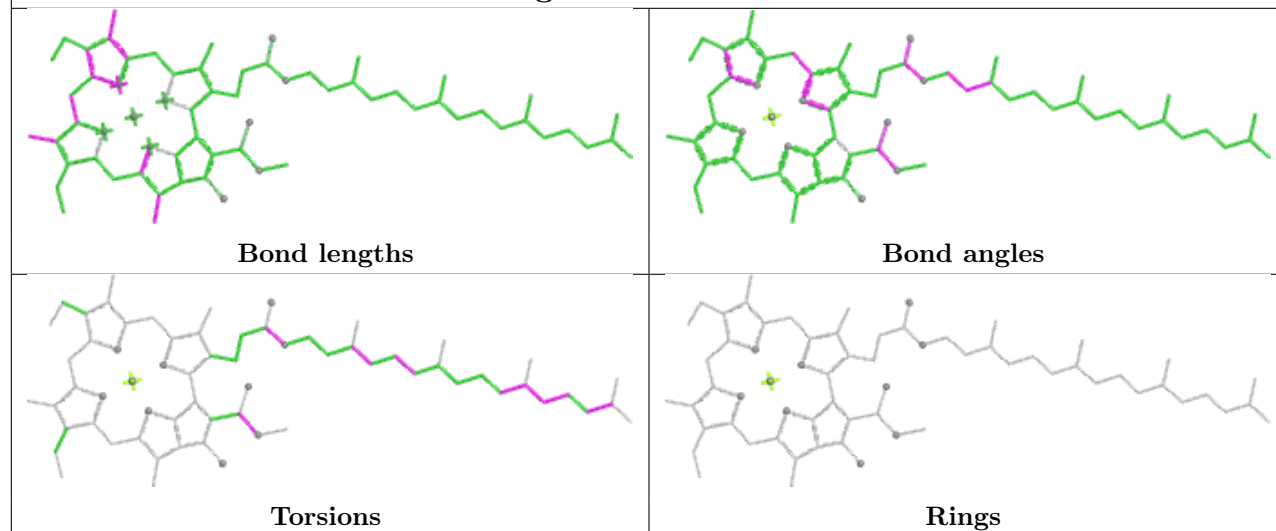




## Ligand CLA a 824

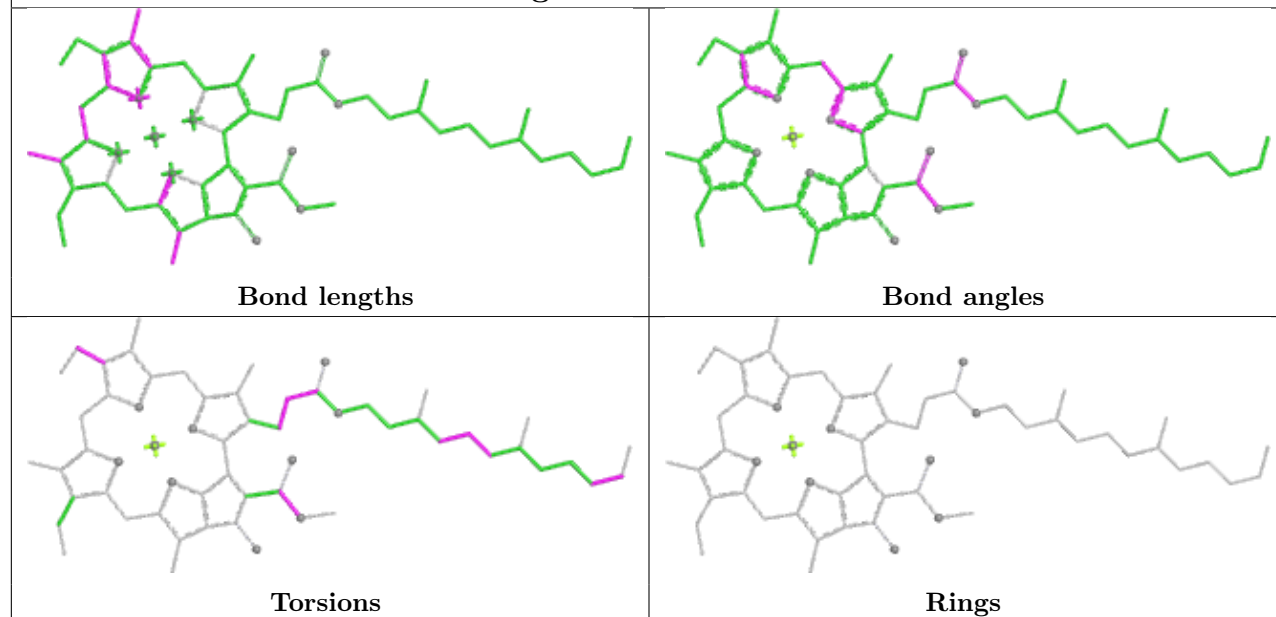


## Ligand CLA n 837

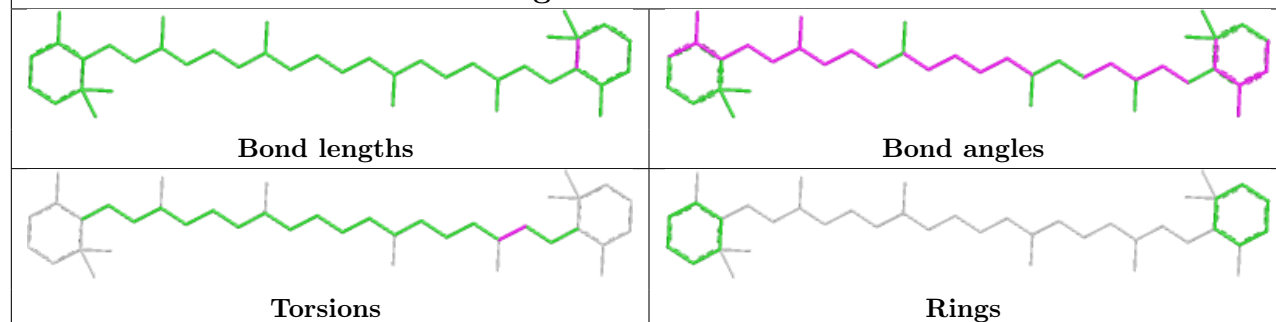




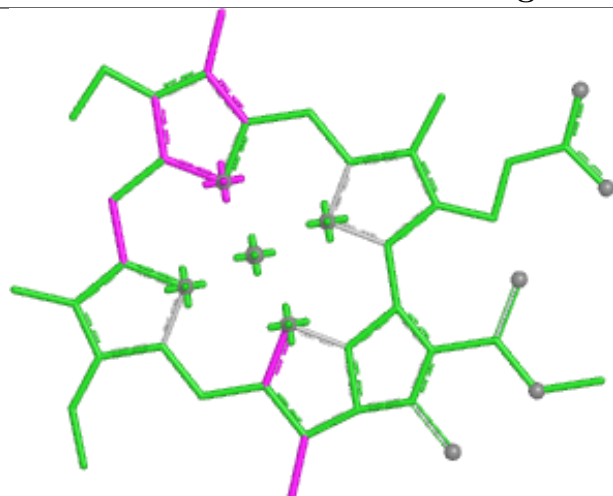
## Ligand CLA A 816



## Ligand BCR n 847



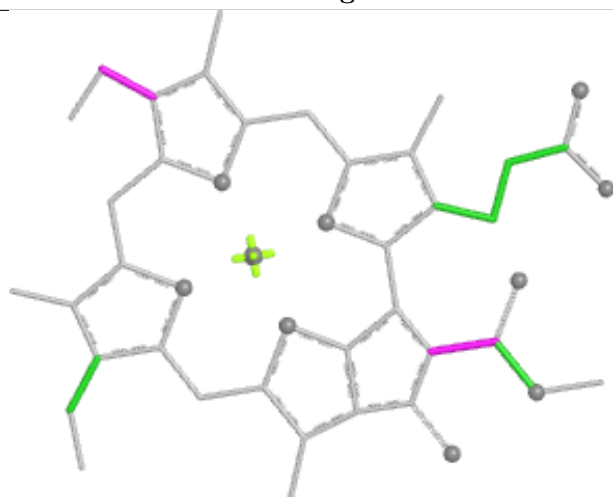
## Ligand CLA n 821



Bond lengths



Bond angles

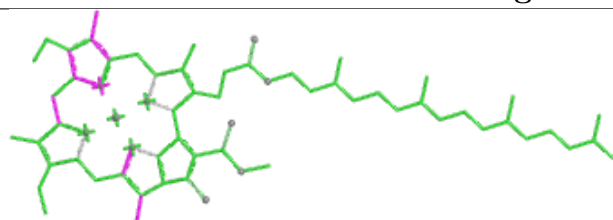


Torsions

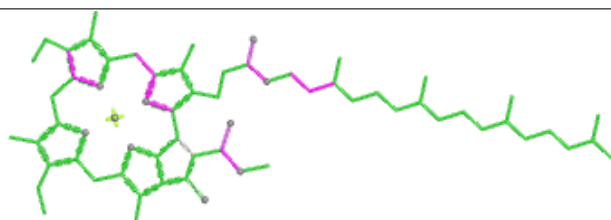


Rings

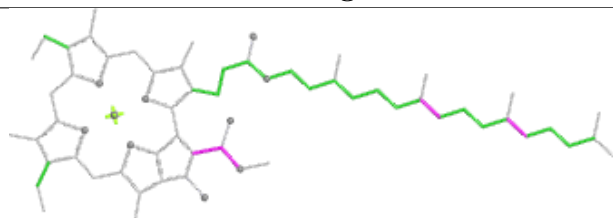
## Ligand CLA B 825



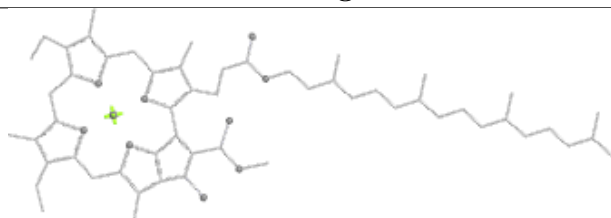
Bond lengths



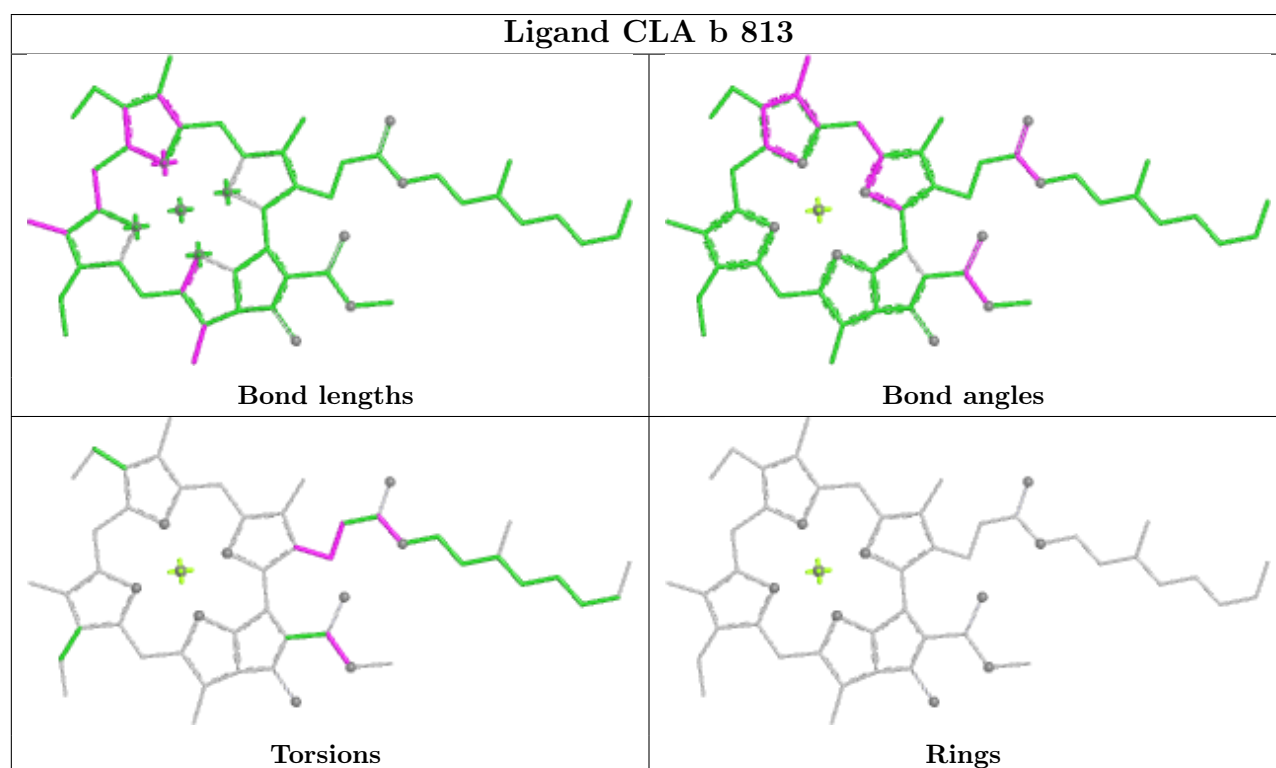
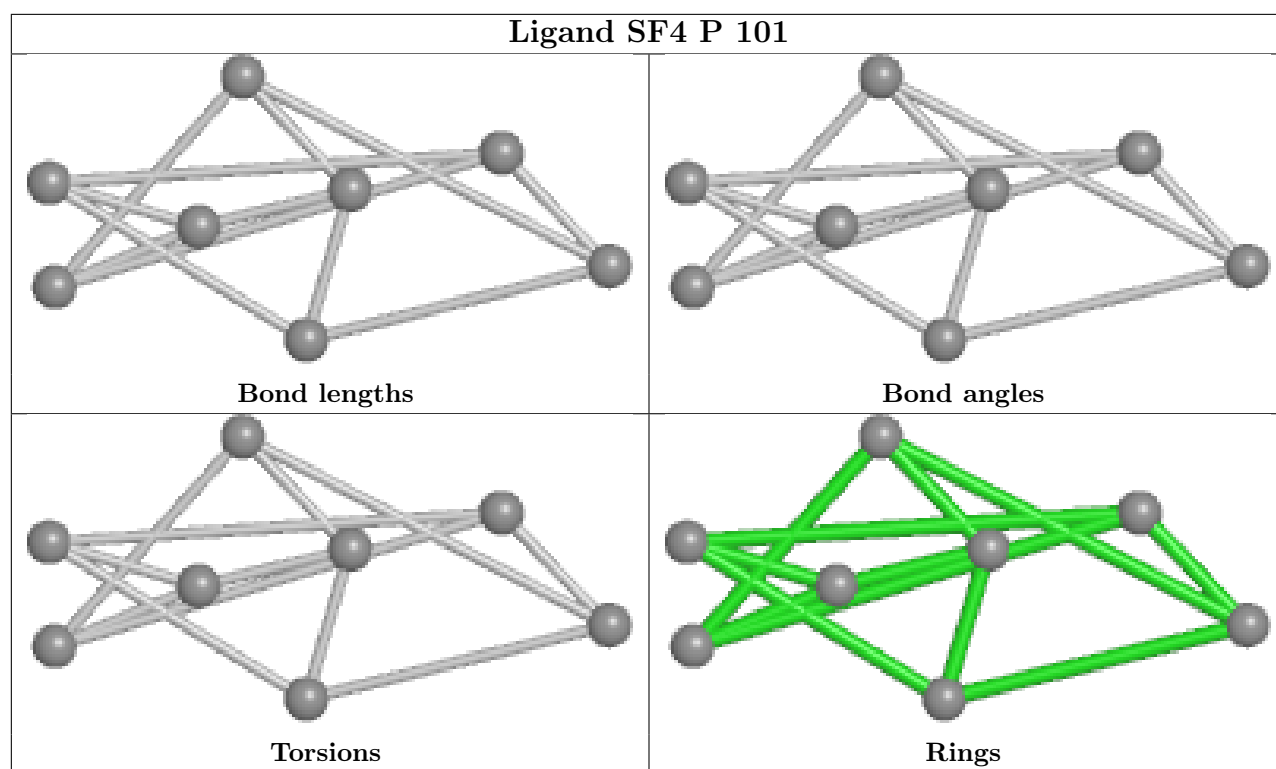
Bond angles



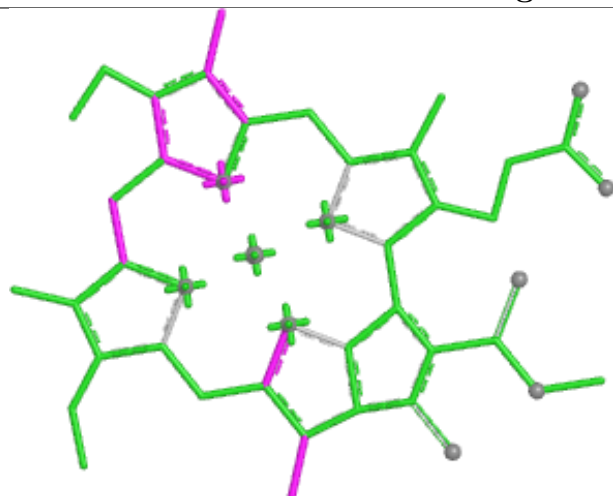
Torsions



Rings



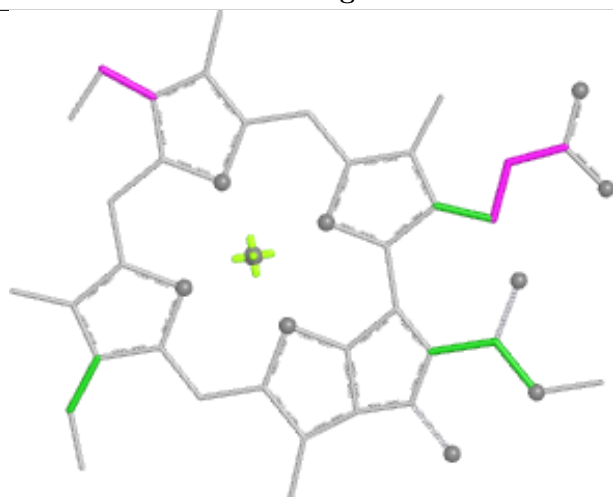
## Ligand CLA F 202



Bond lengths



Bond angles

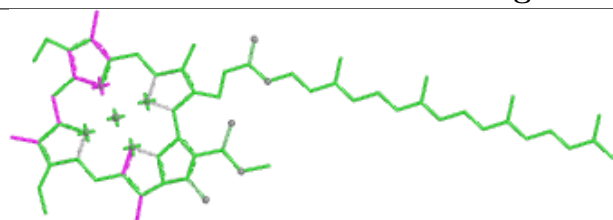


Torsions

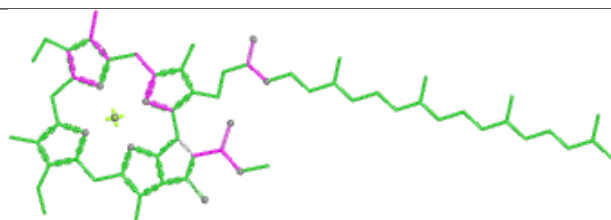


Rings

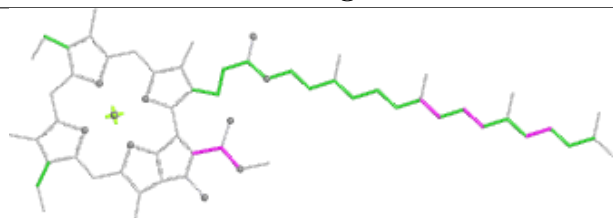
## Ligand CLA A 829



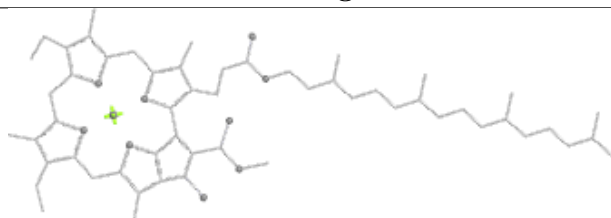
Bond lengths



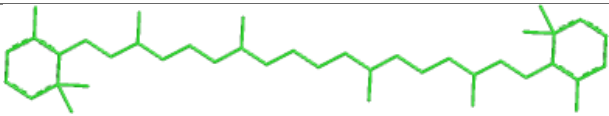
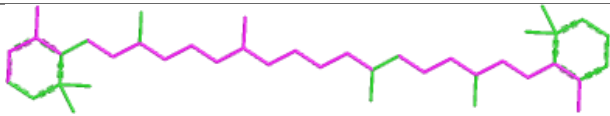
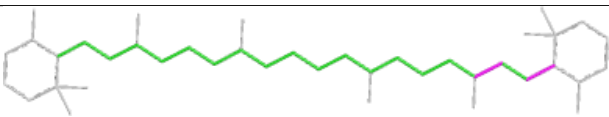
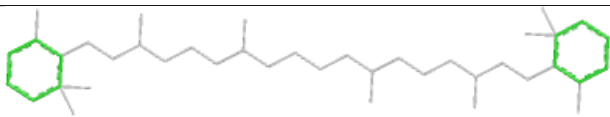
Bond angles

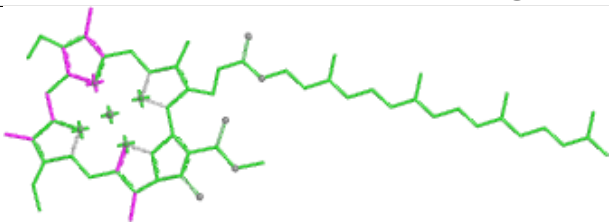
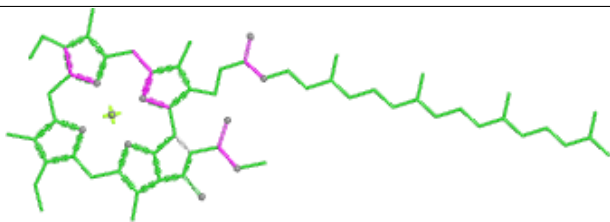
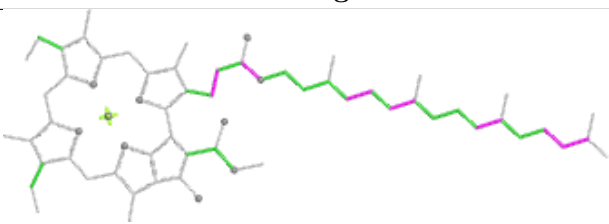
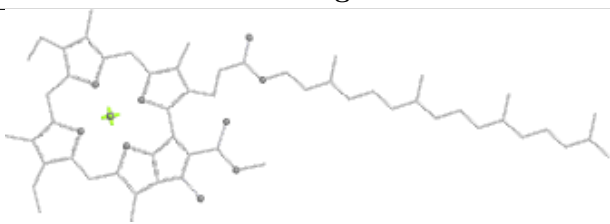


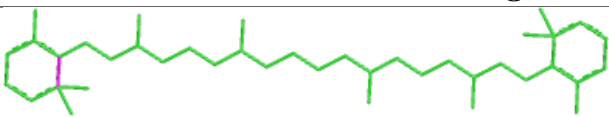
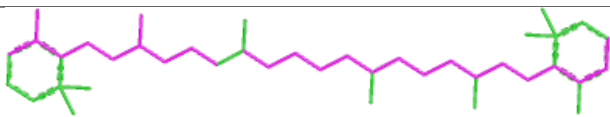
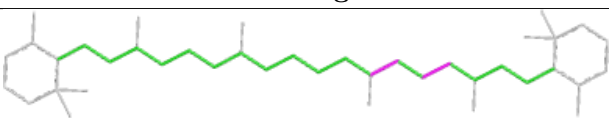
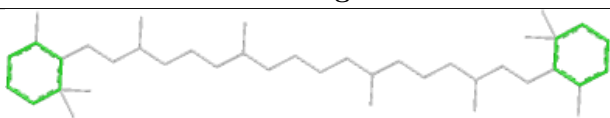
Torsions



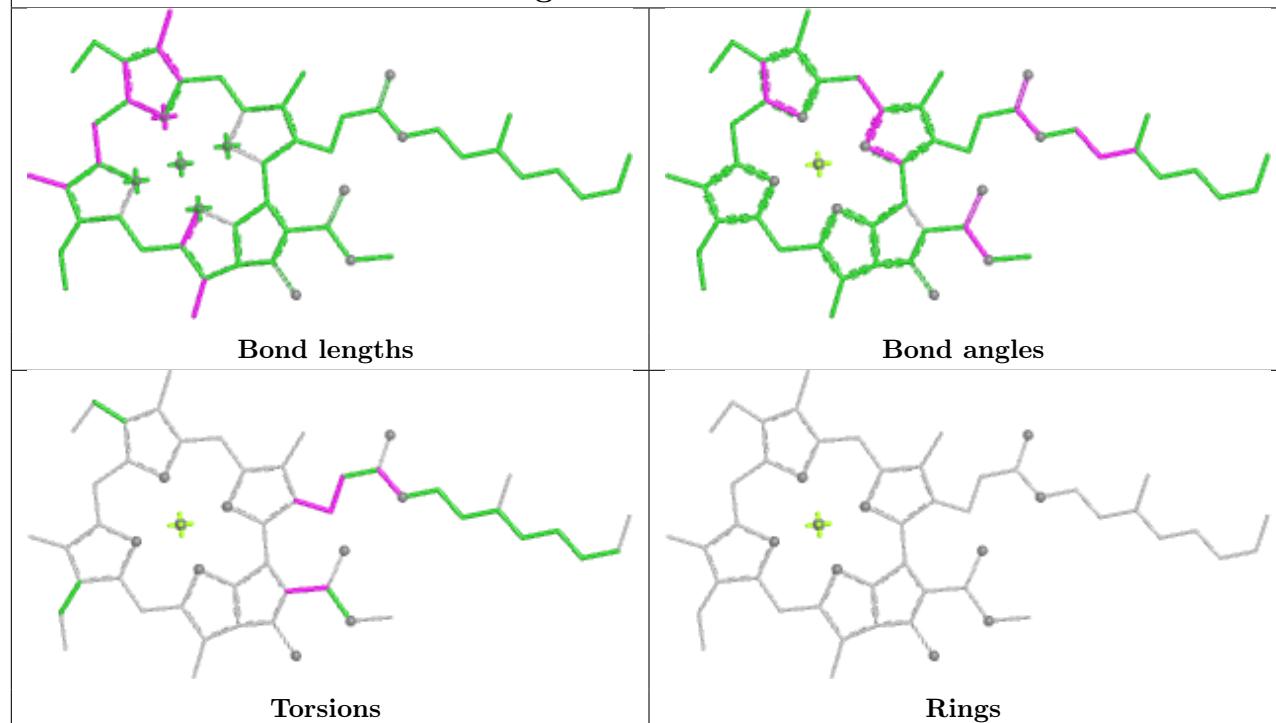
Rings

| Ligand BCR W 205  |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

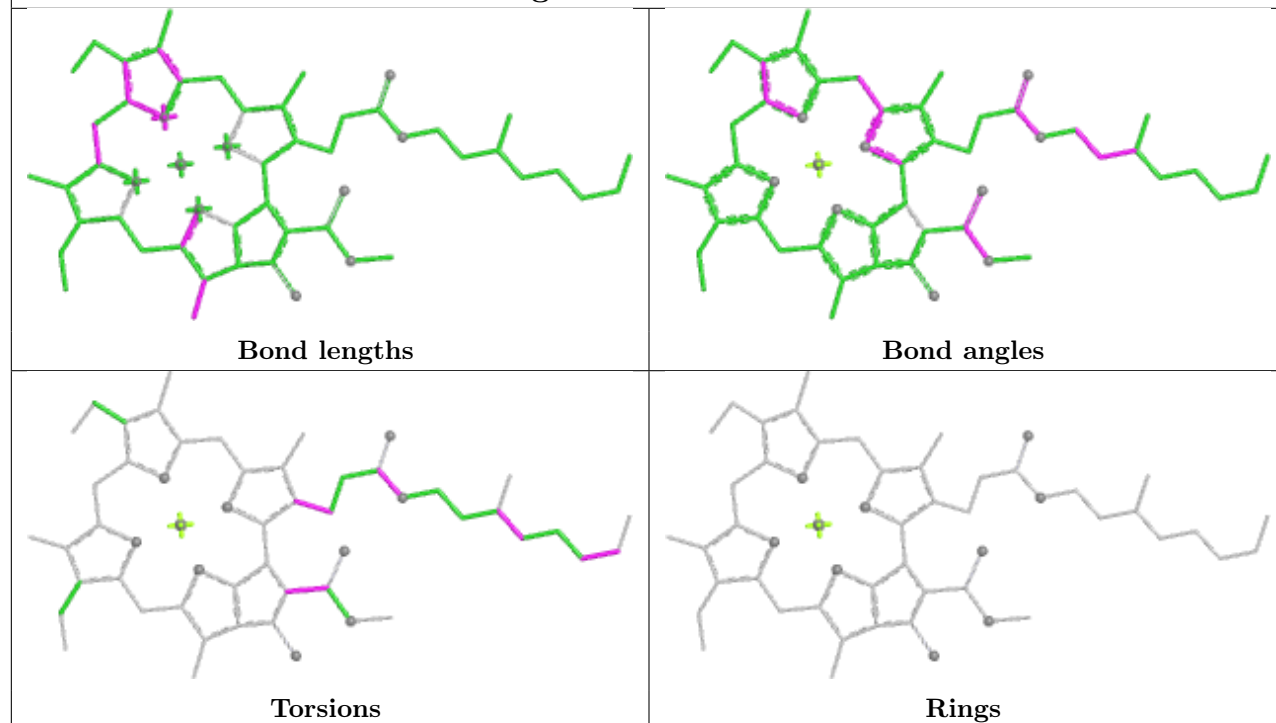
| Ligand CLA B 840   |   |
|--|---|
|   |   |
| Bond lengths   | Bond angles   |
|  |  |
| Torsions   | Rings   |

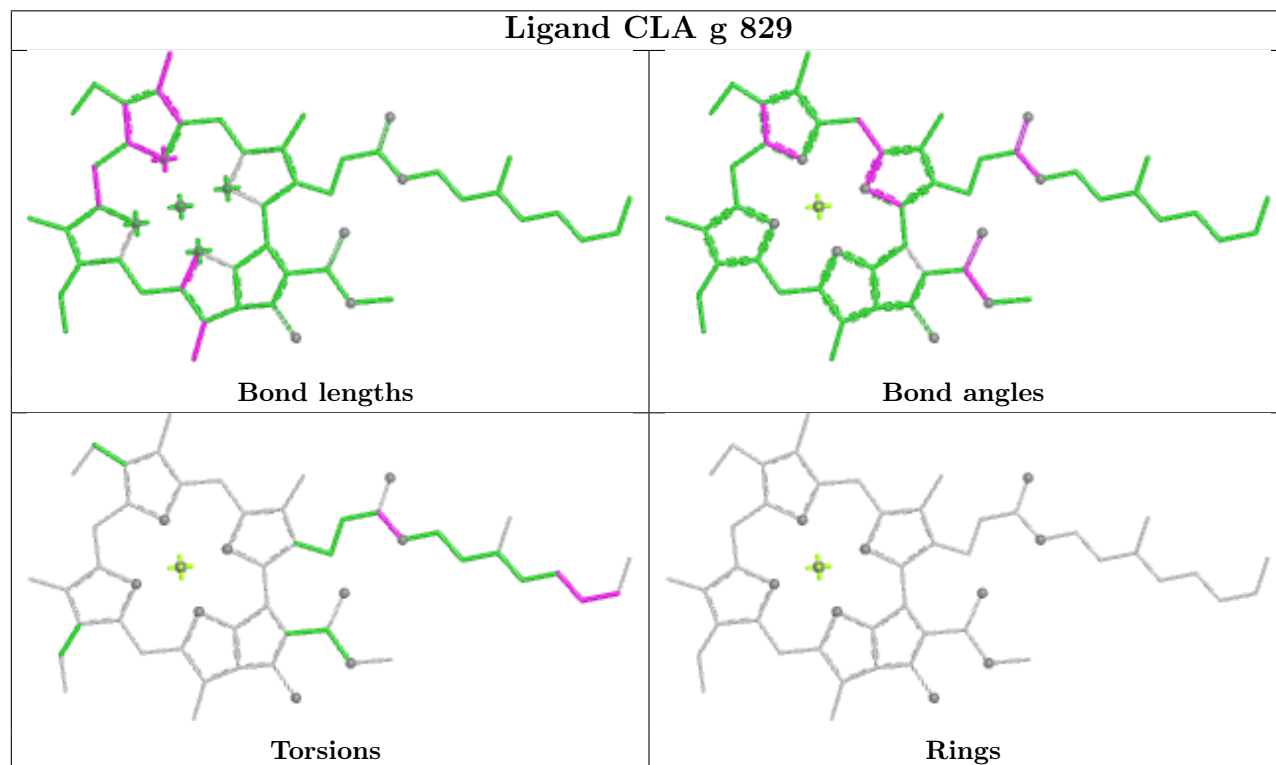
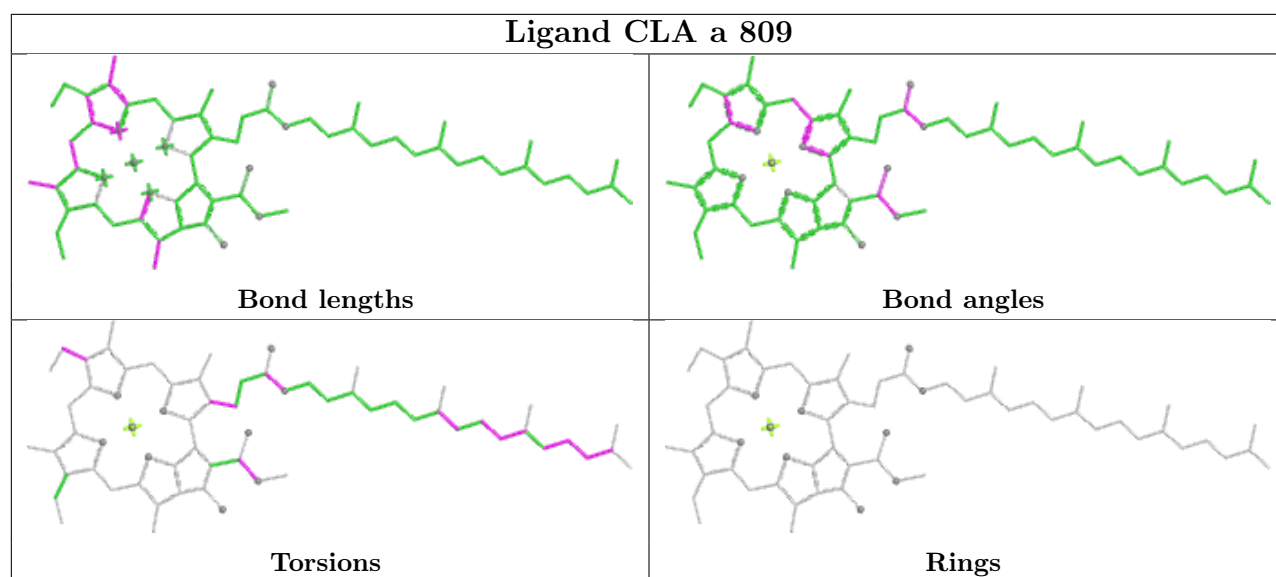
| Ligand BCR N 852  |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

## Ligand CLA n 812

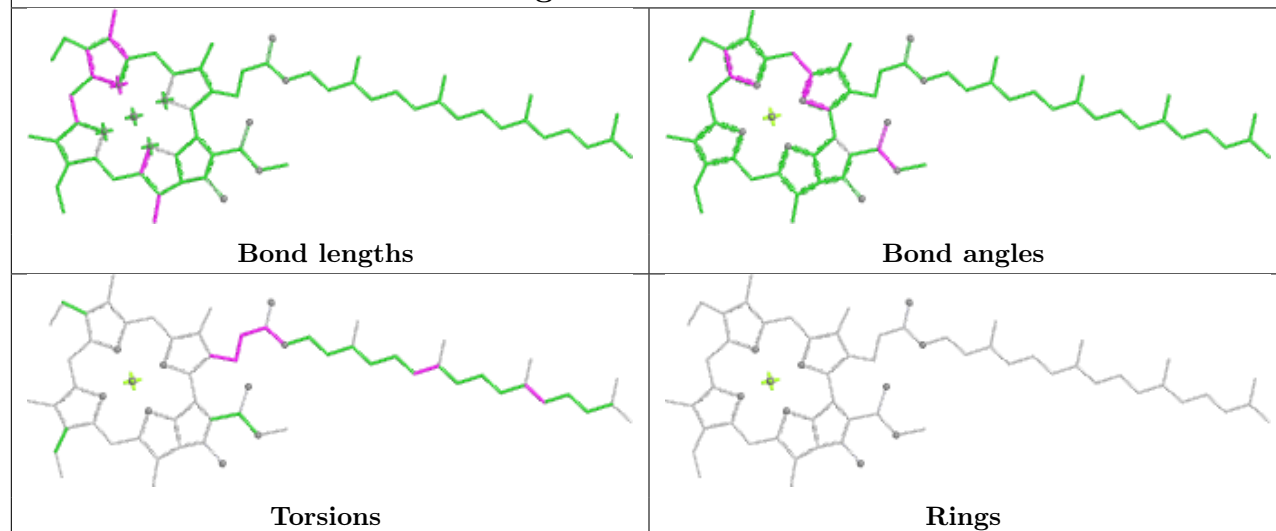


## Ligand CLA A 825

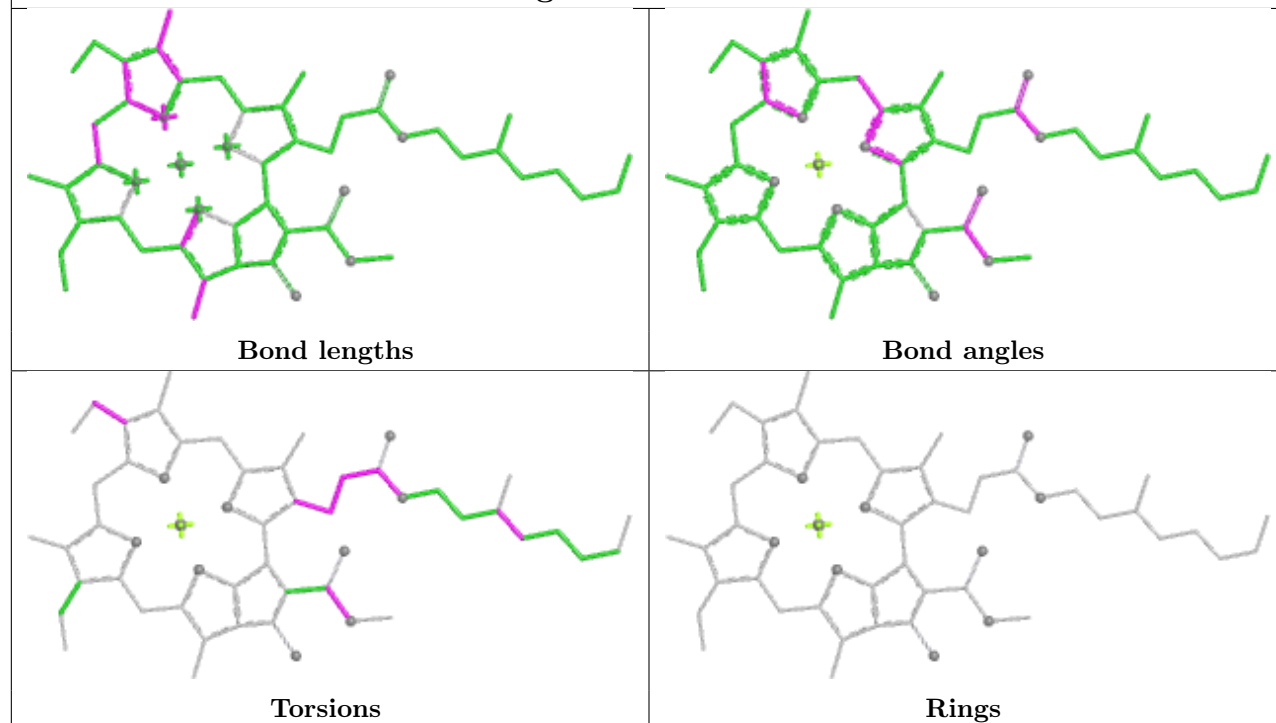




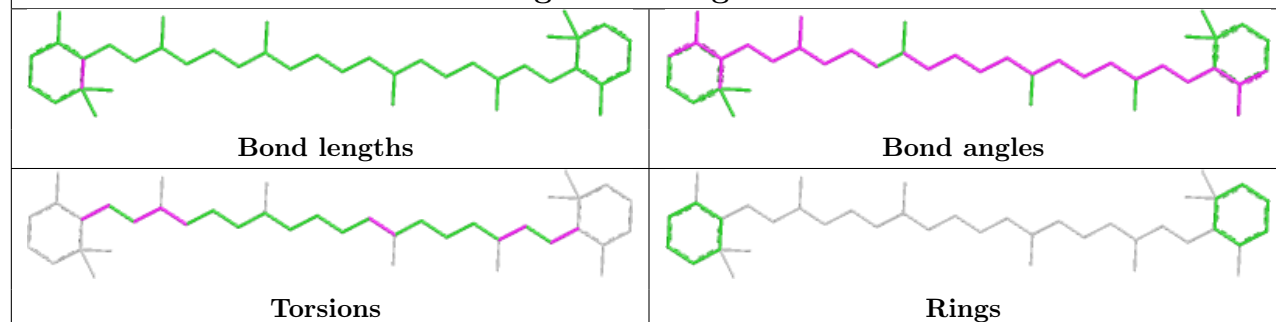
## Ligand CLA b 818



## Ligand CLA a 821

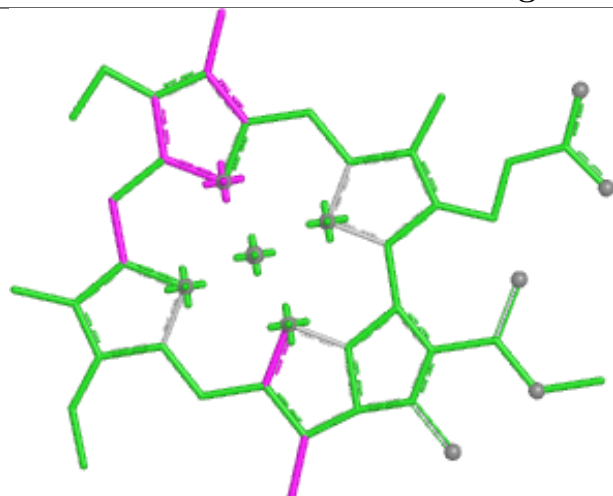


## Ligand BCR g 848

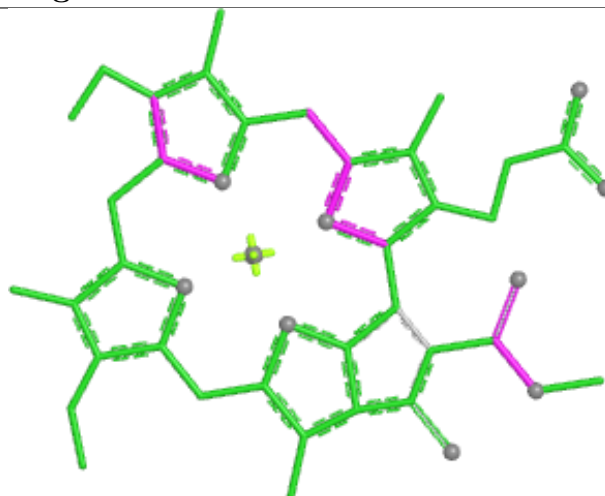




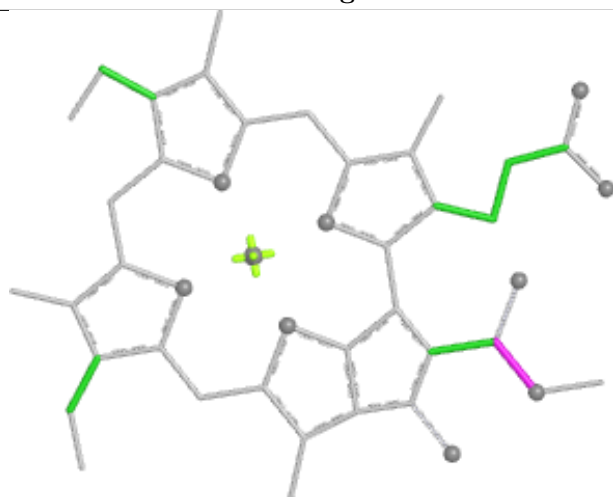
## Ligand CLA g 822



Bond lengths



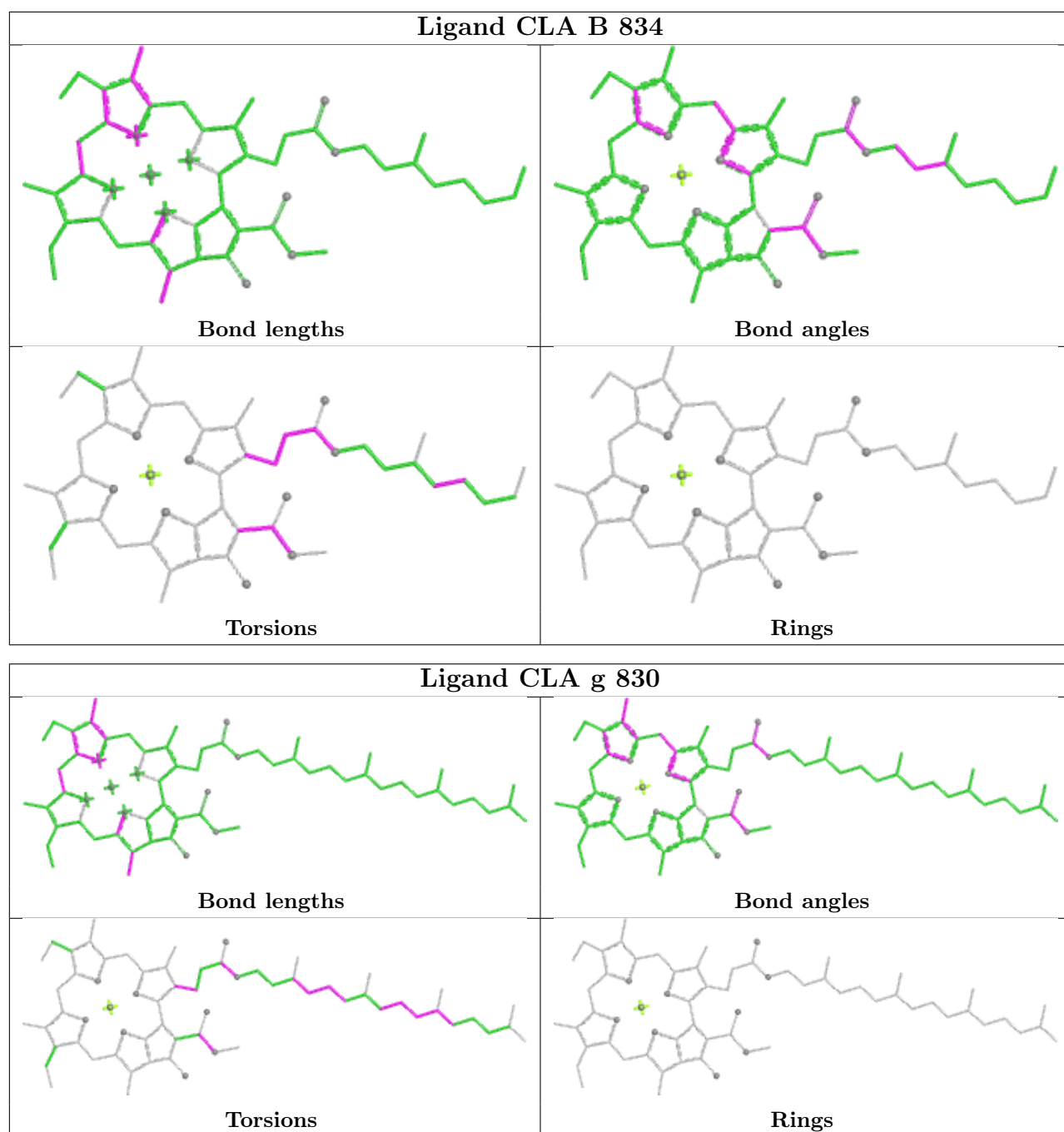
Bond angles



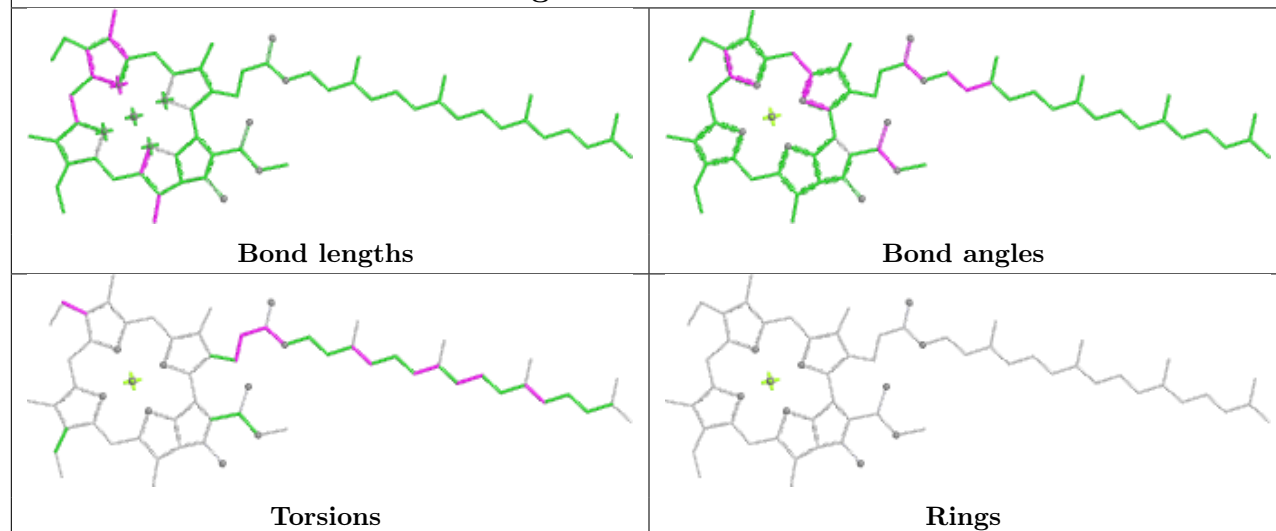
Torsions



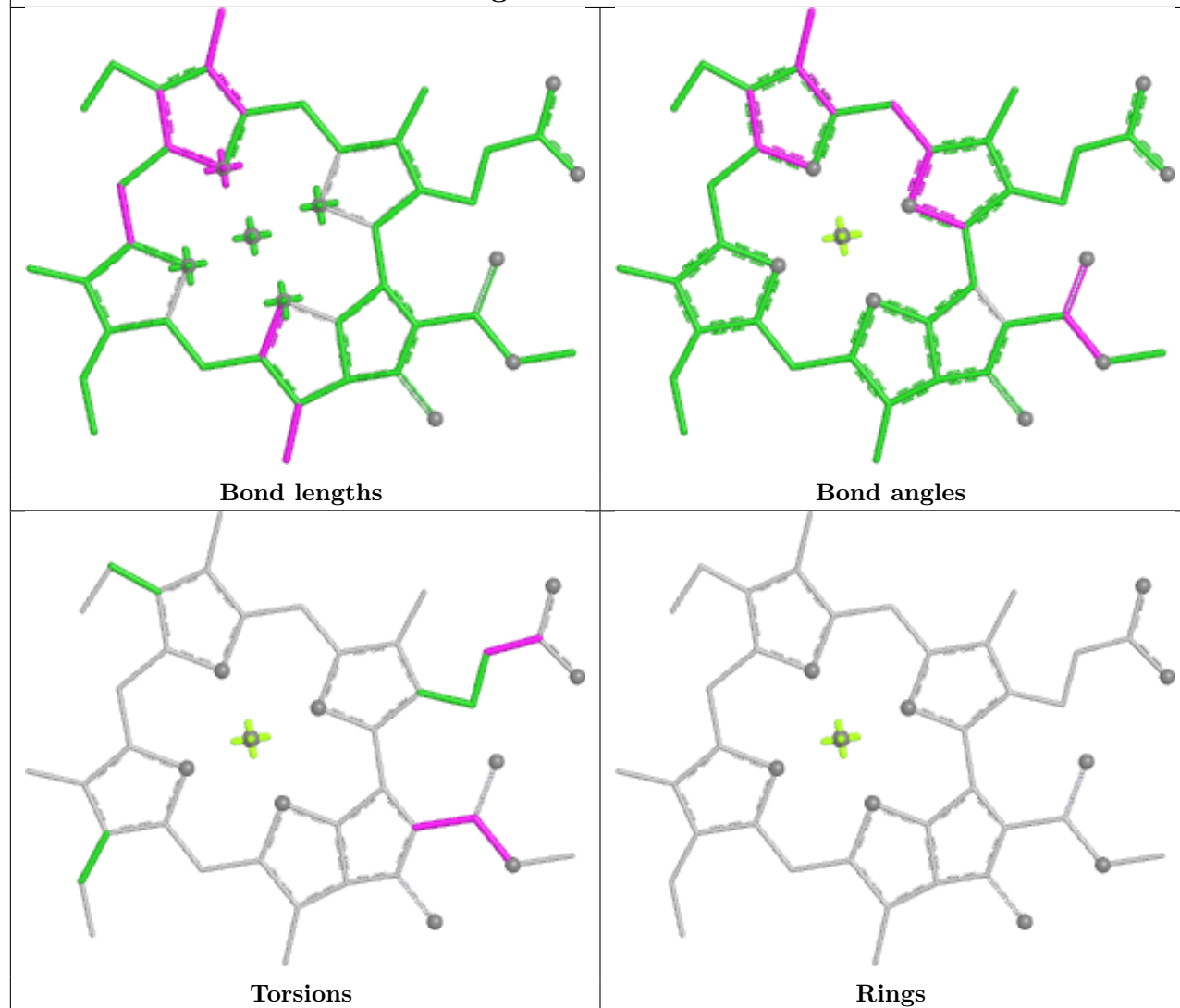
Rings



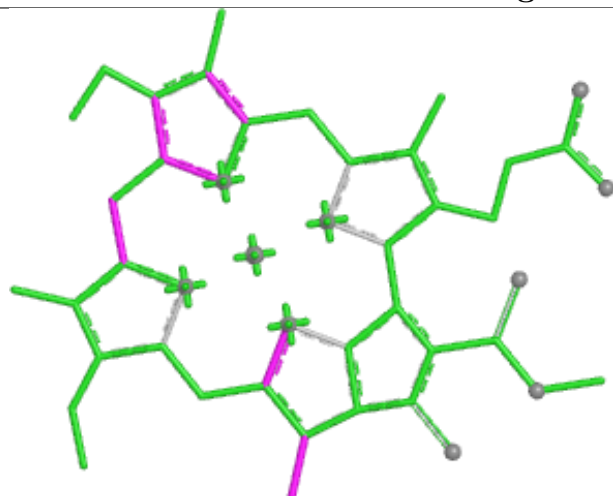
## Ligand CLA A 840



## Ligand CLA G 814



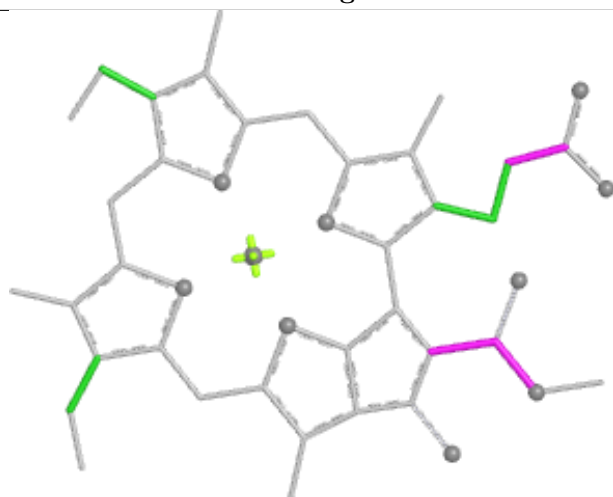
## Ligand CLA n 835



Bond lengths



Bond angles

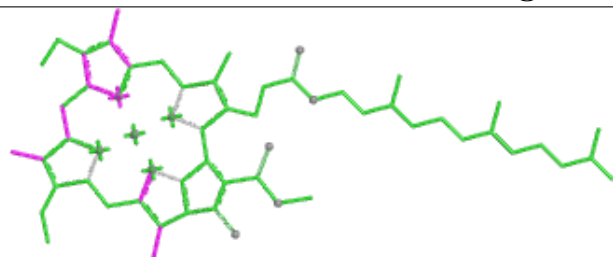


Torsions

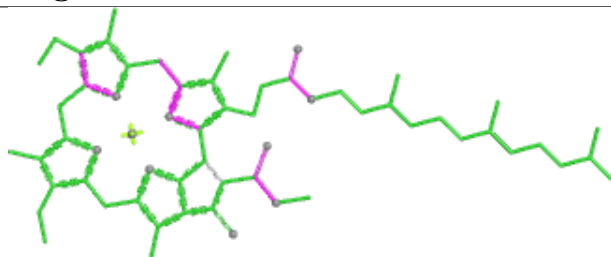


Rings

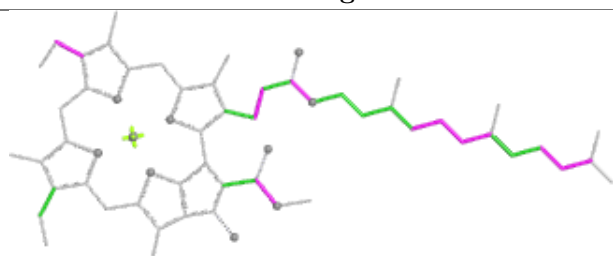
## Ligand CLA g 816



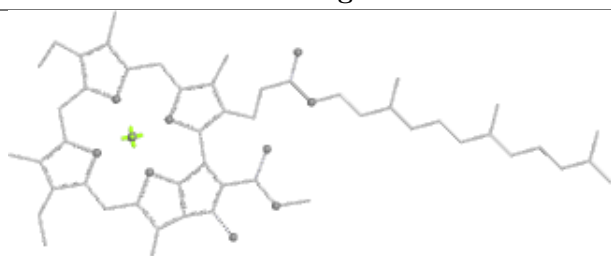
Bond lengths



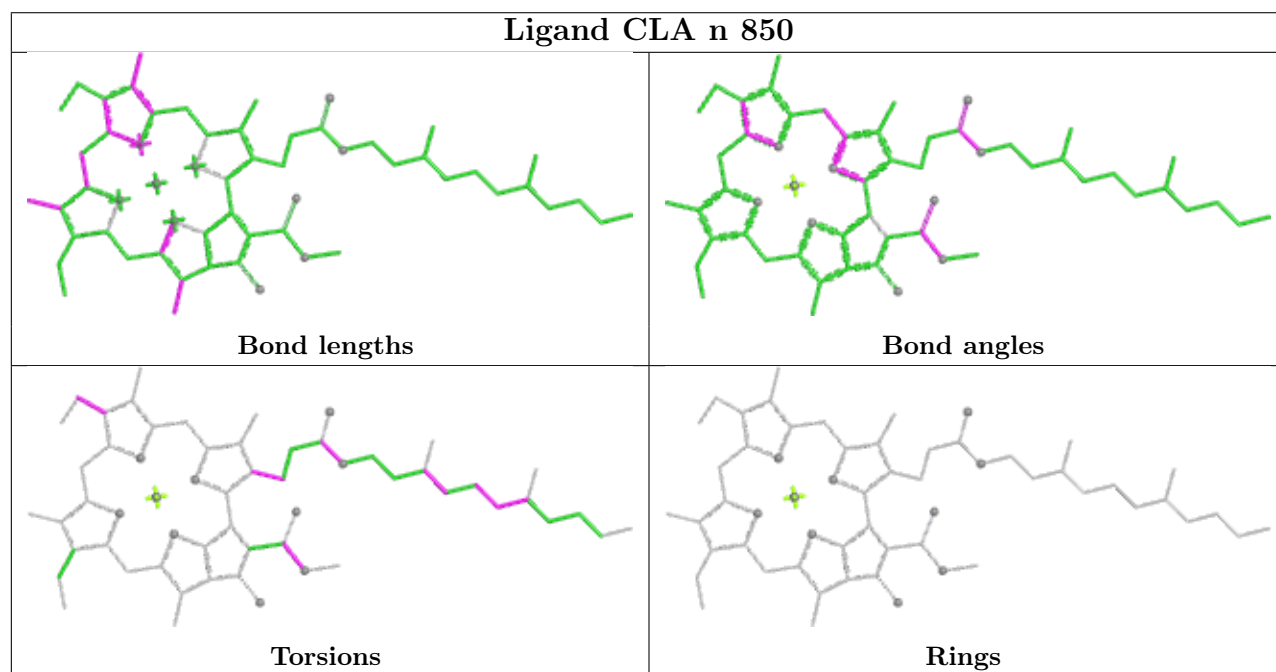
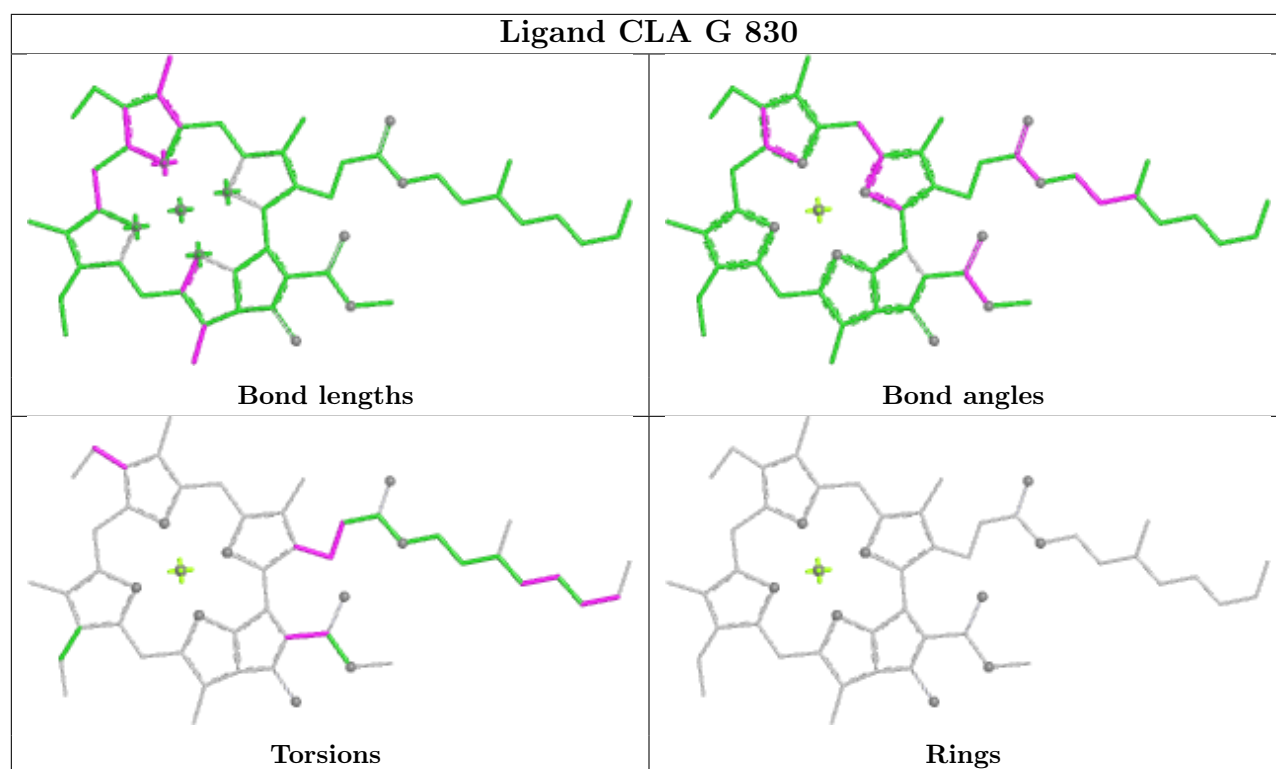
Bond angles

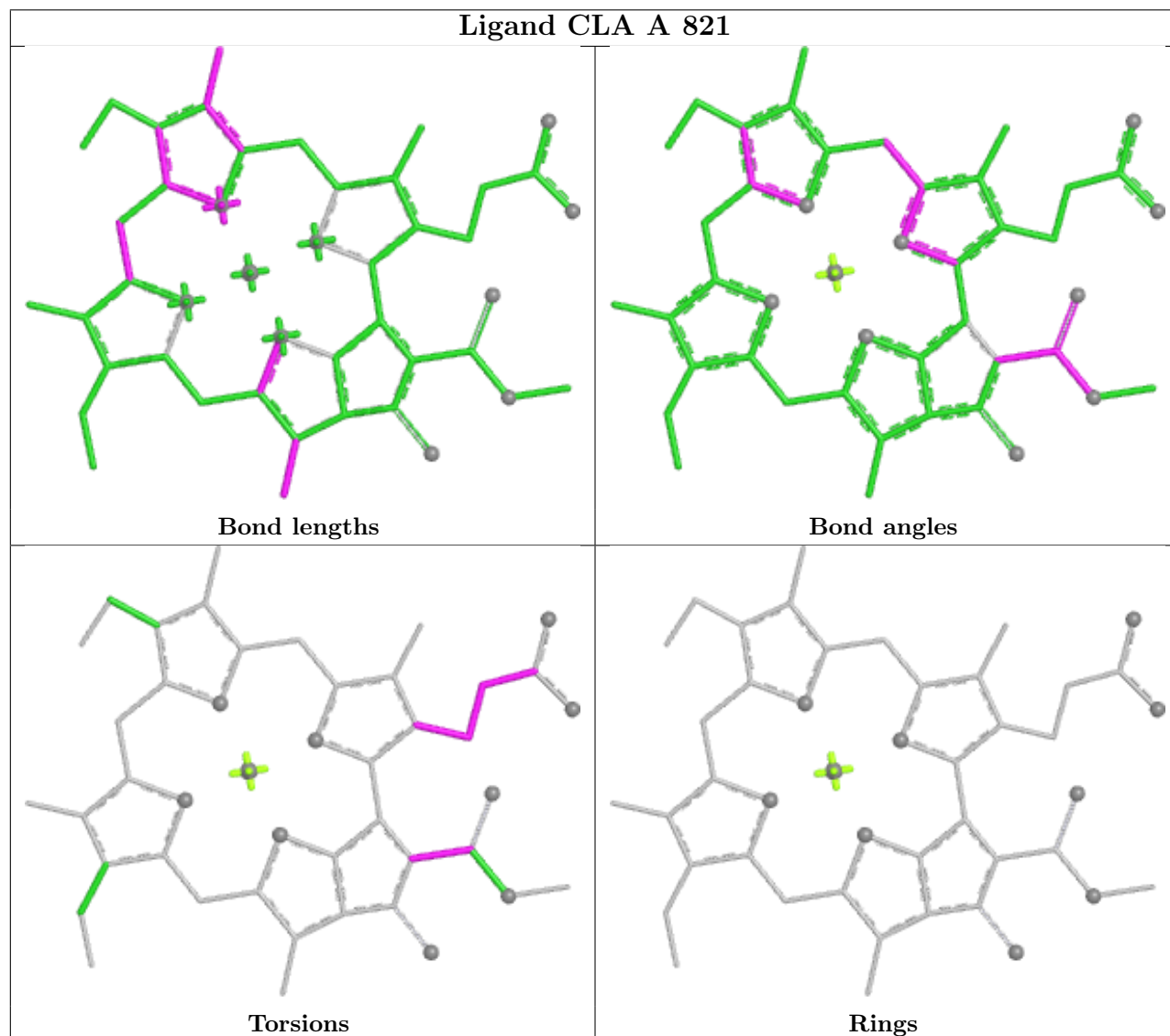
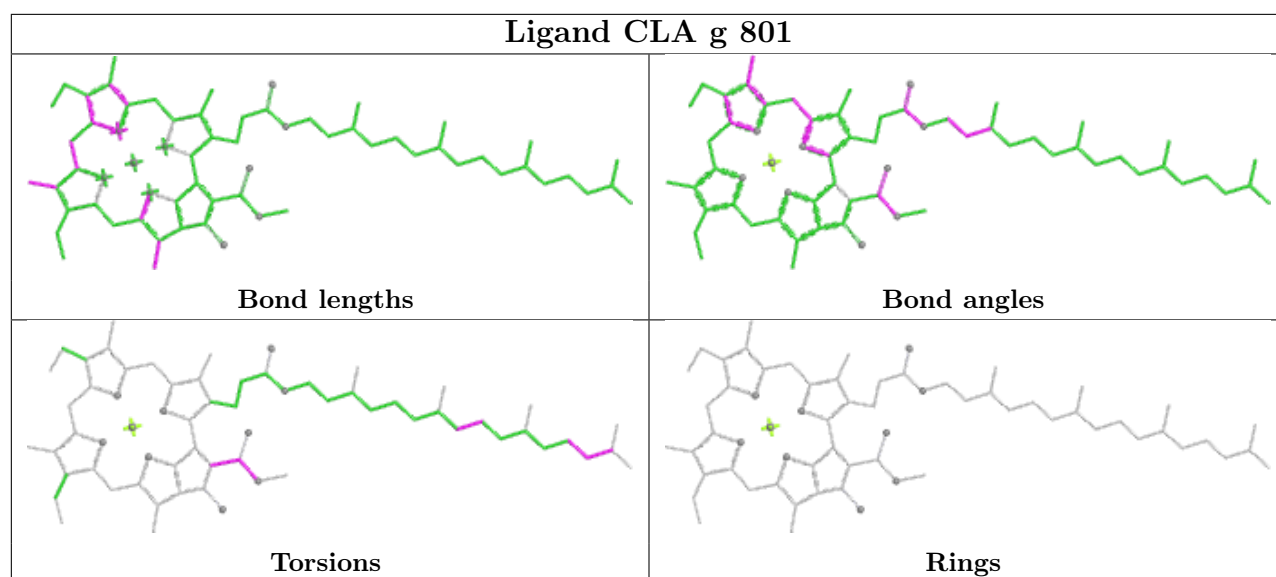


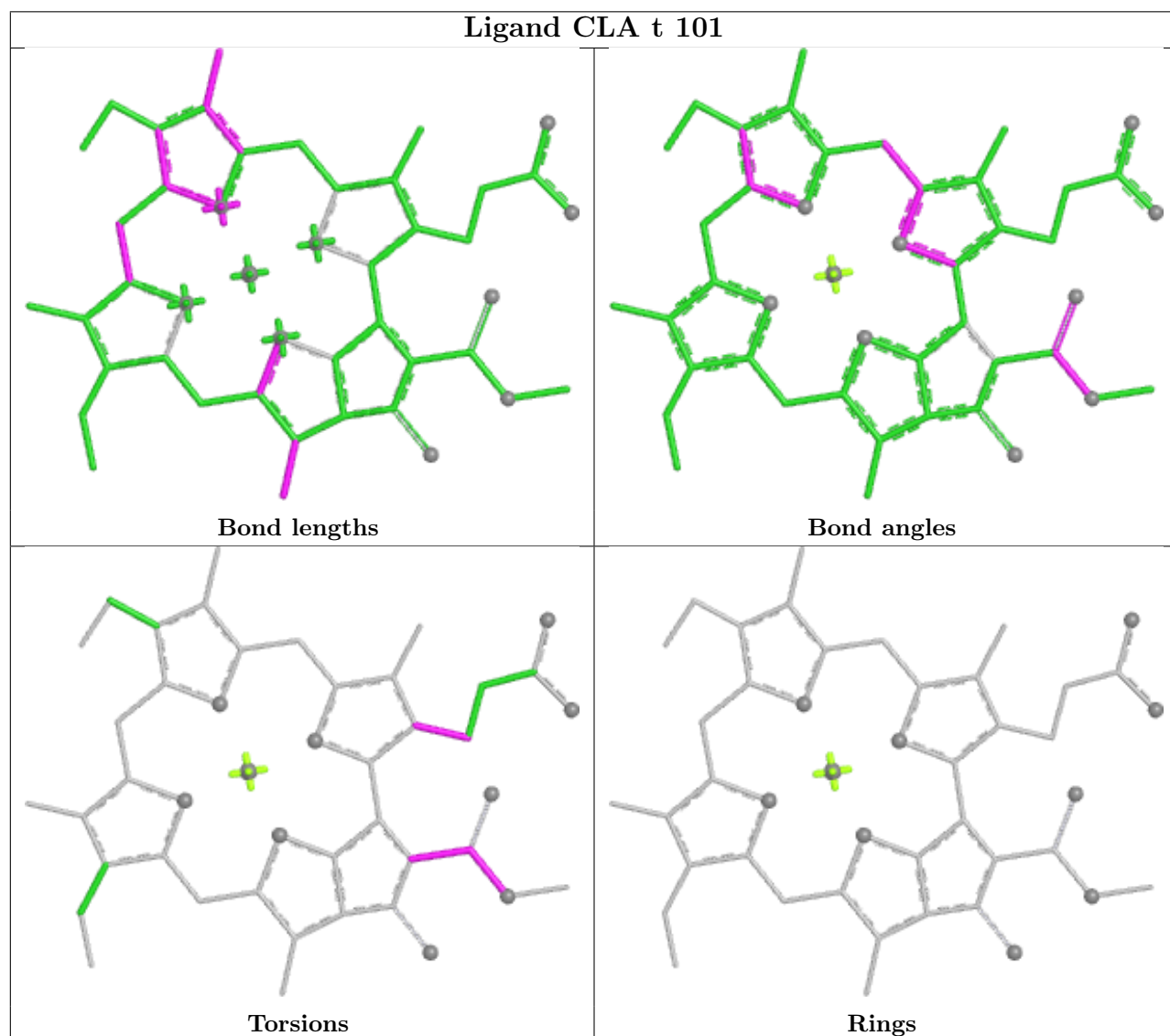
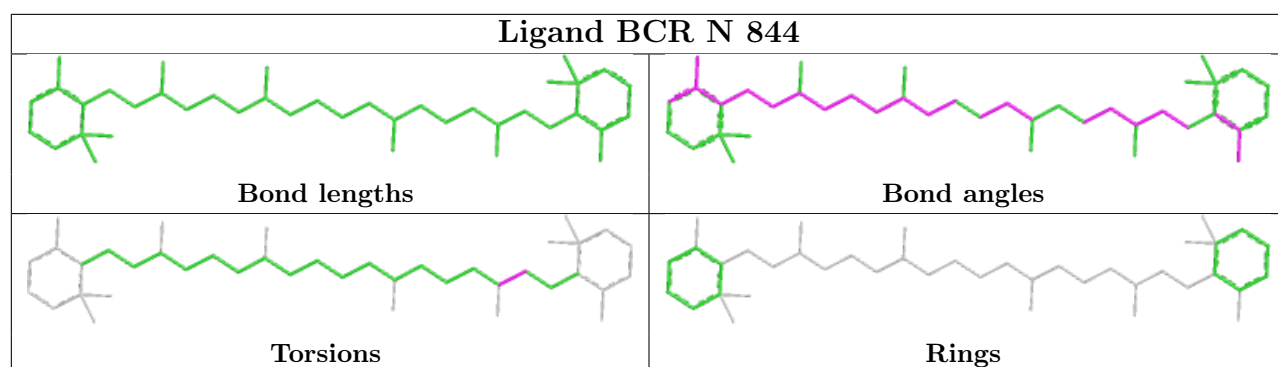
Torsions



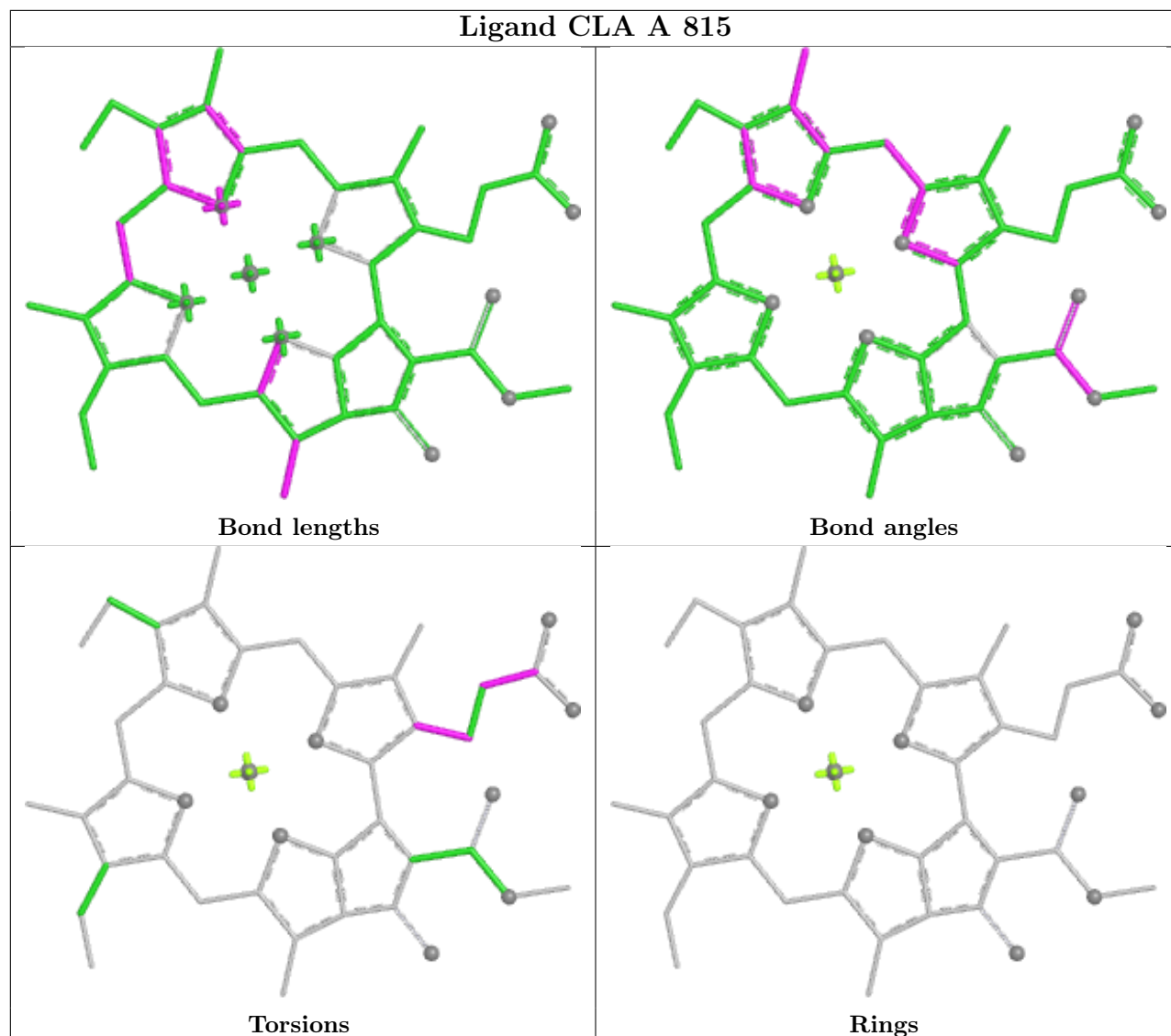
Rings



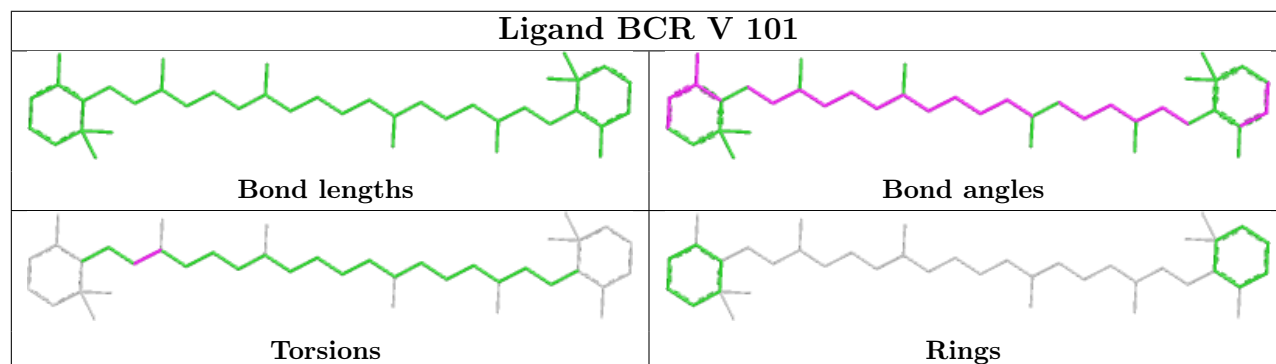




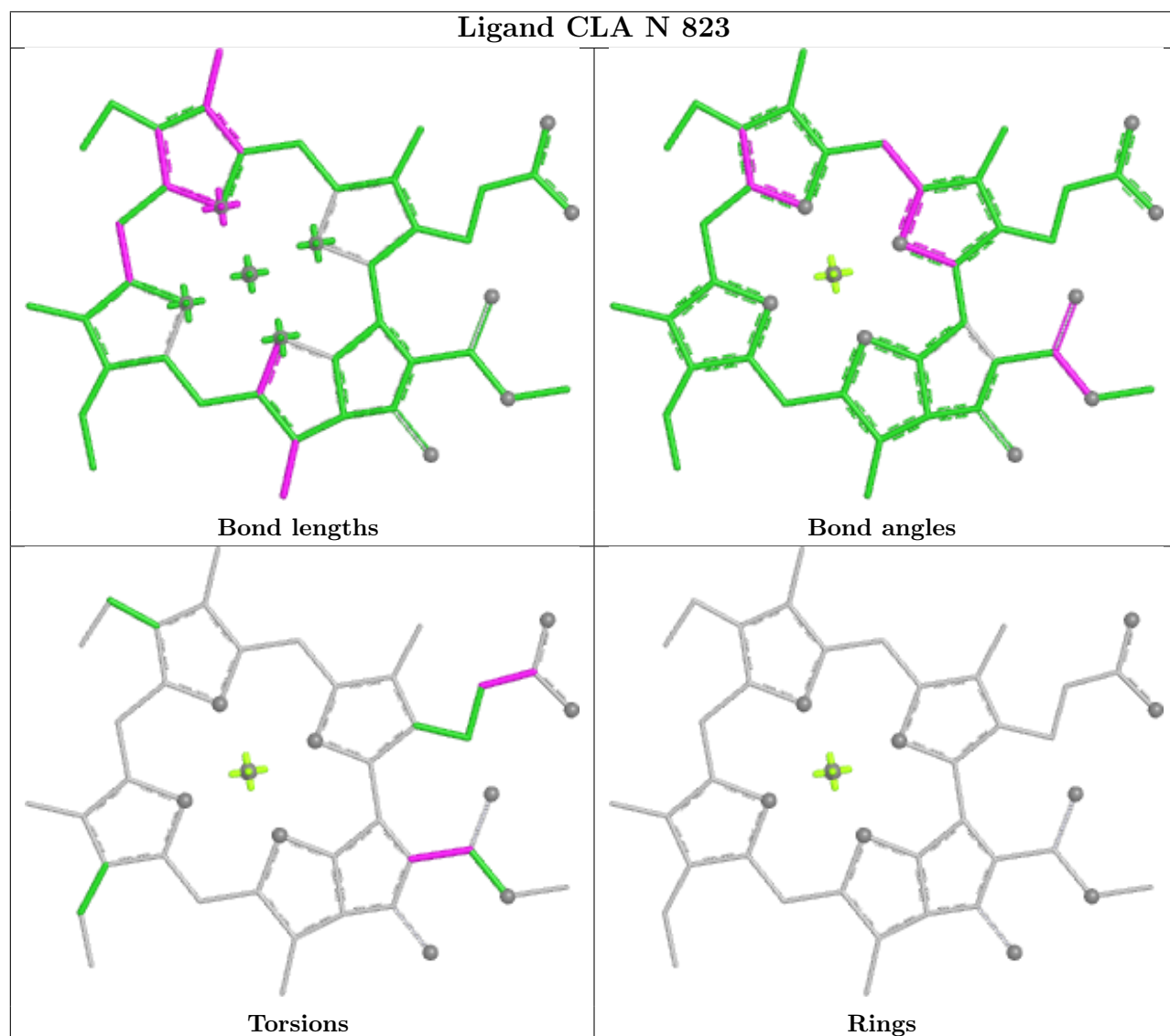
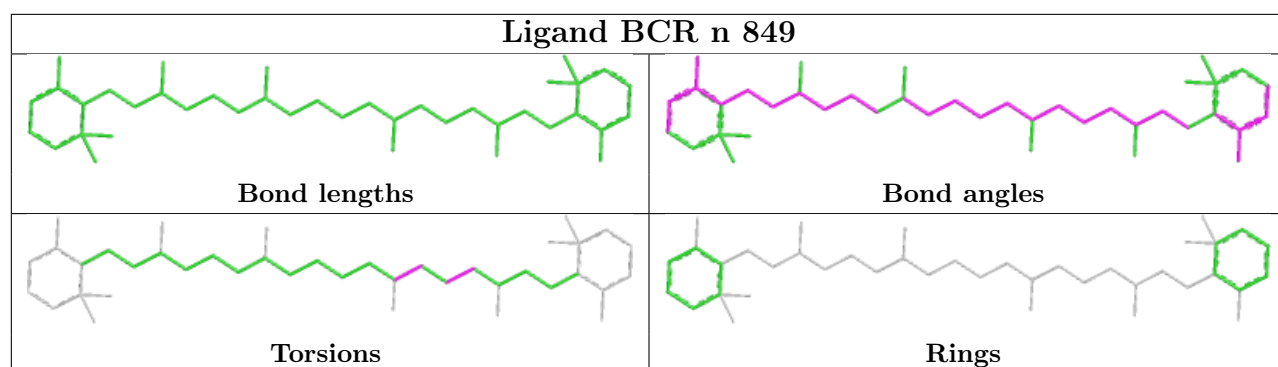
## Ligand CLA A 815

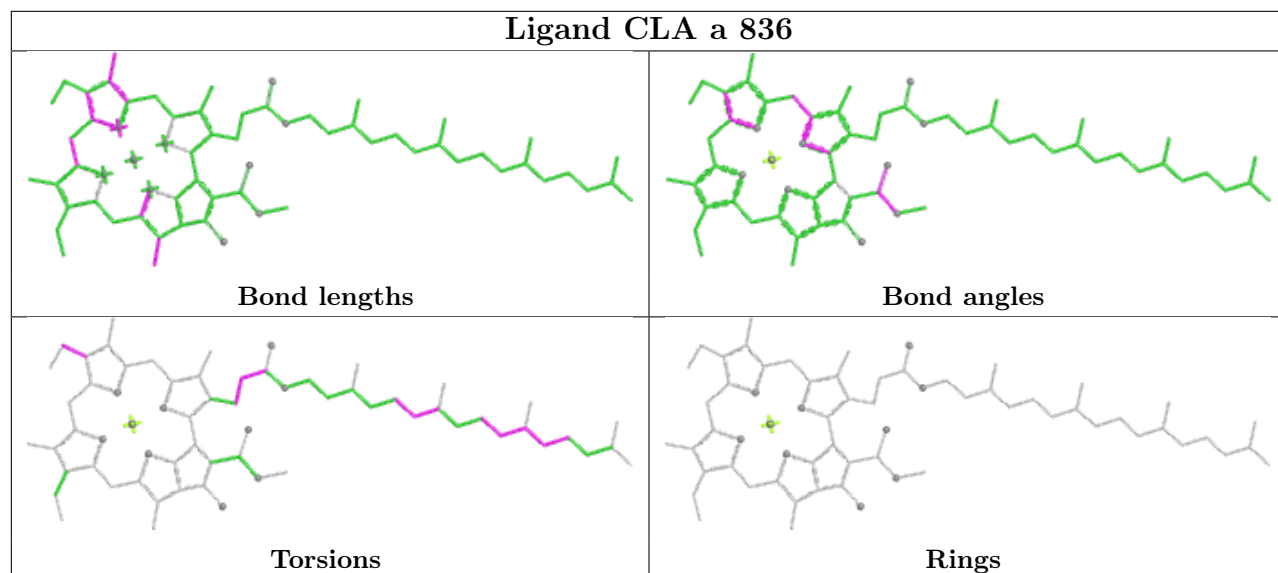
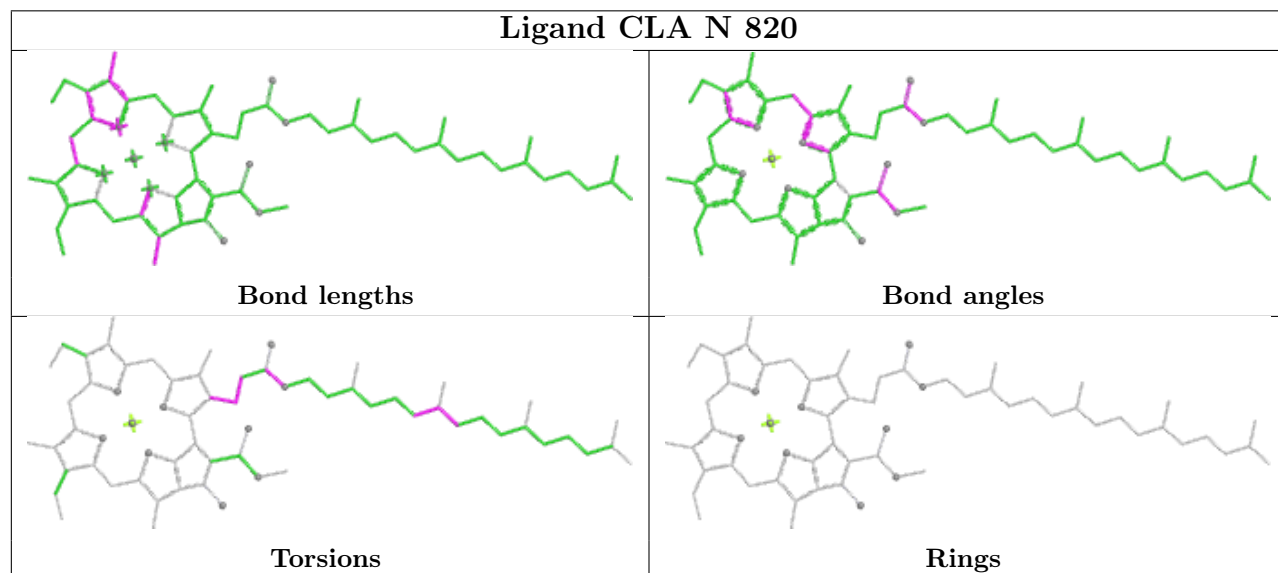
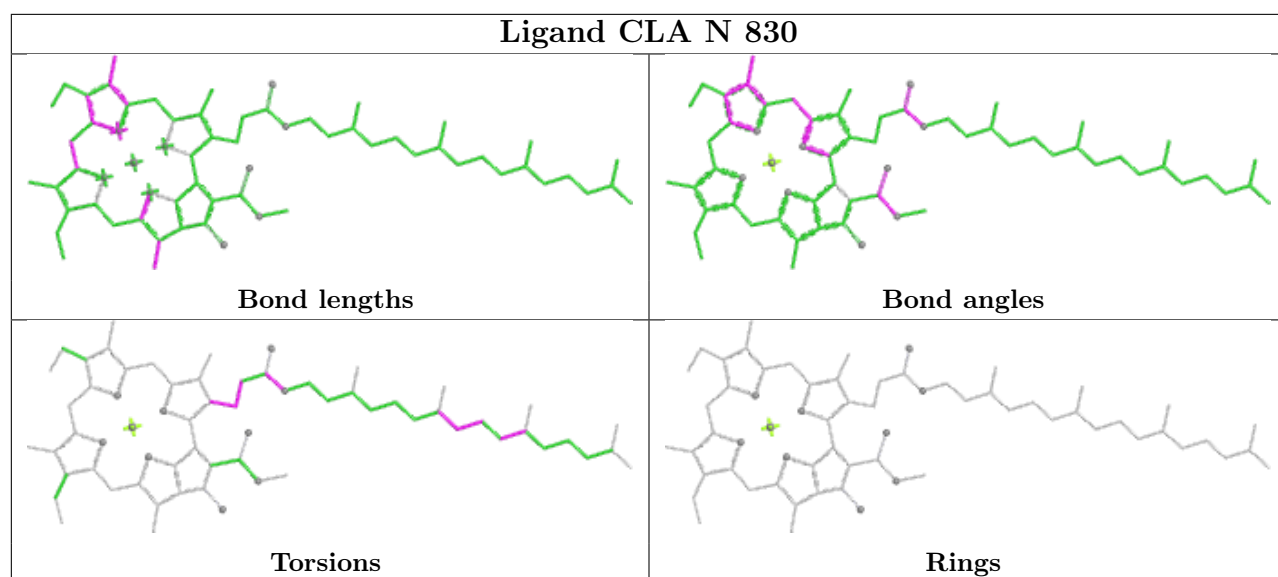


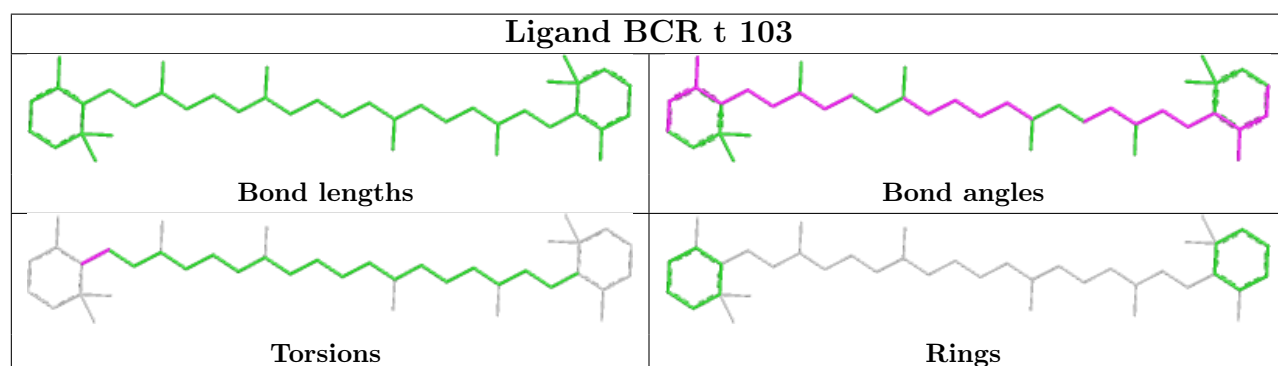
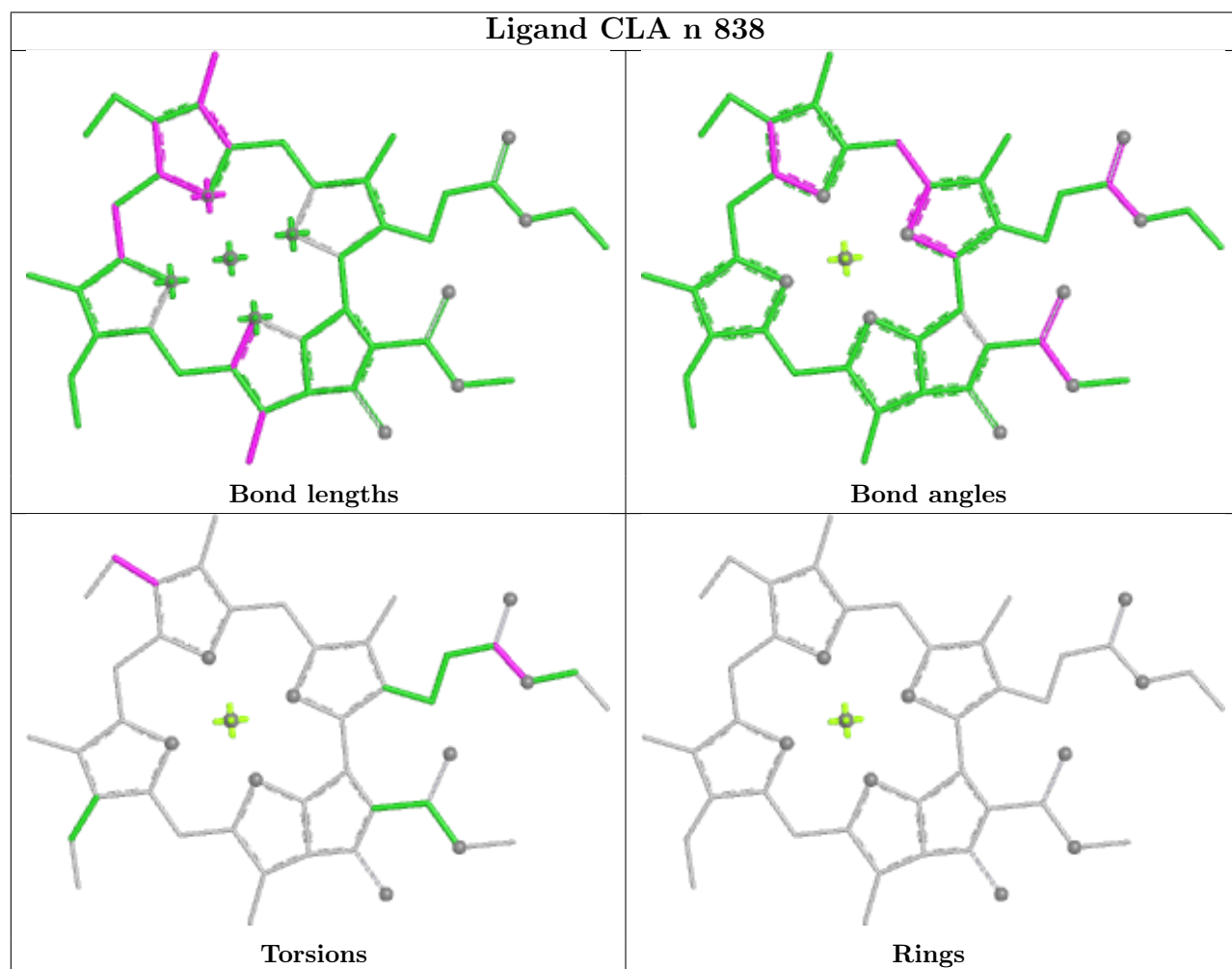
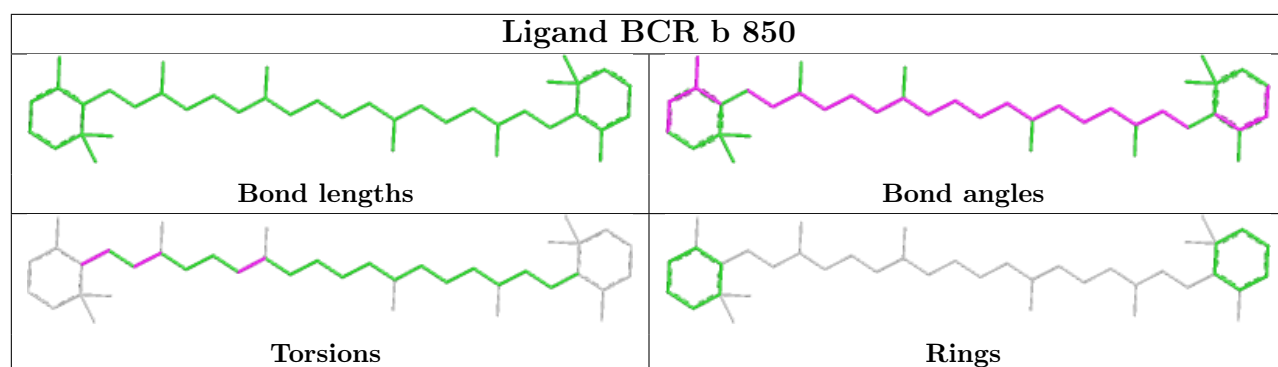
## Ligand BCR V 101

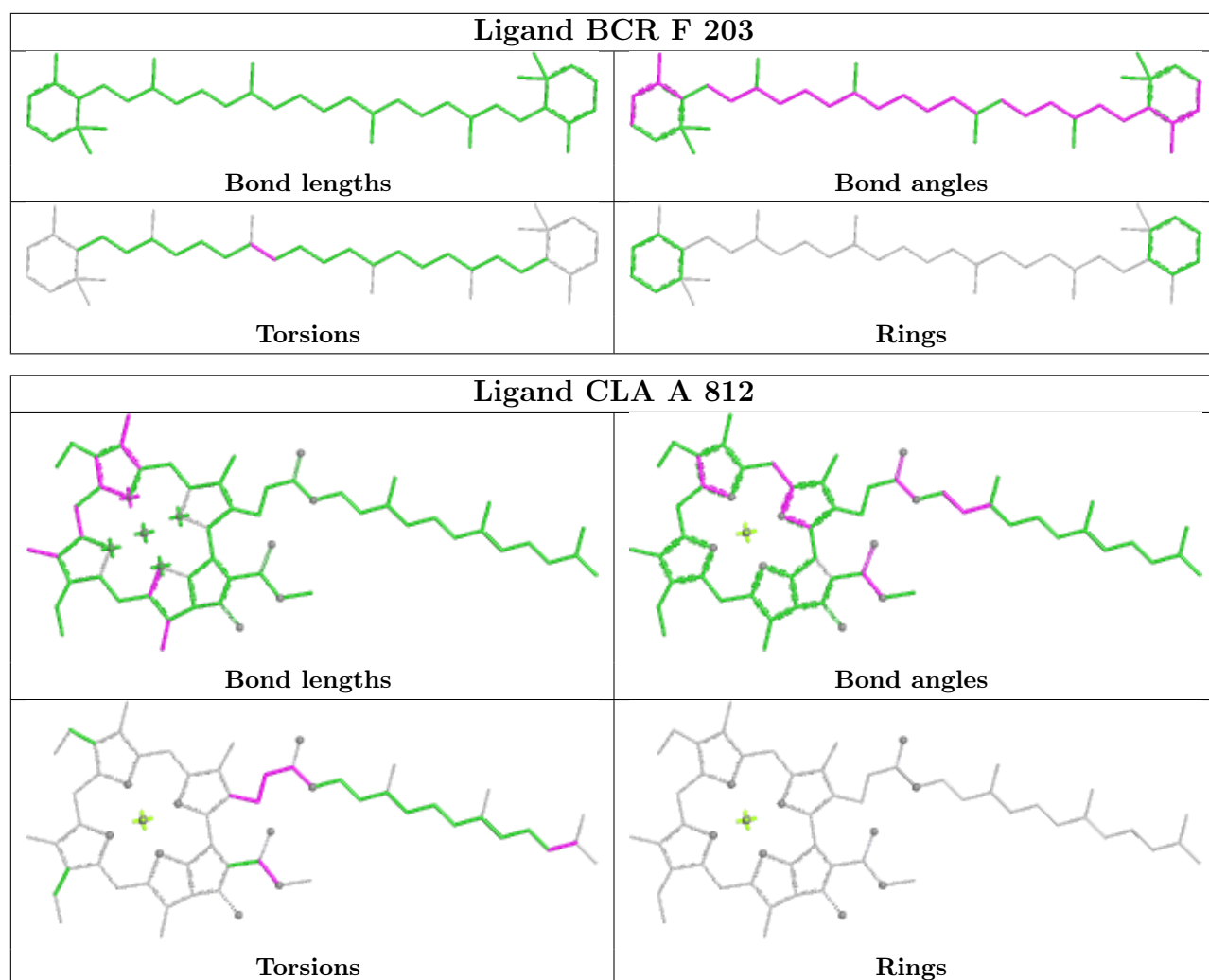




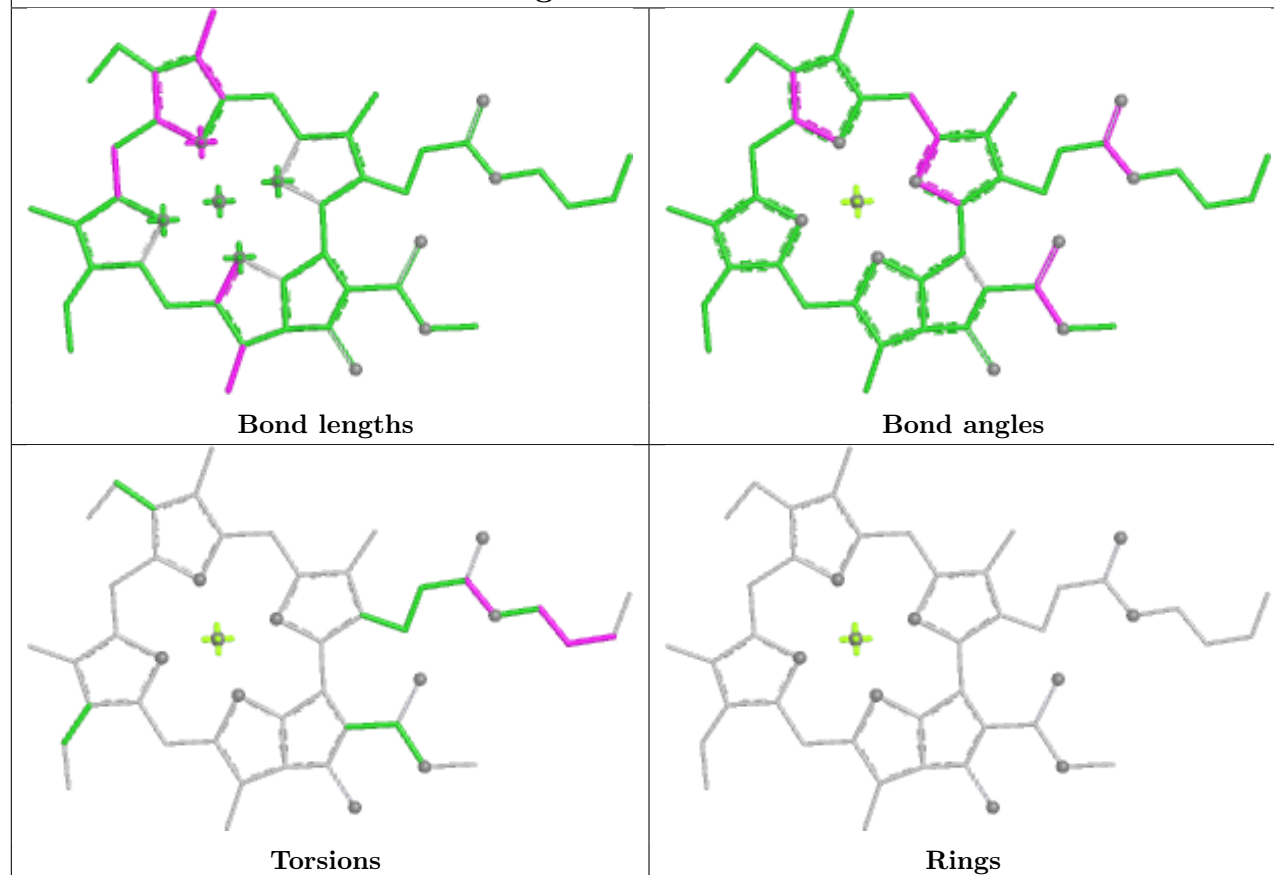




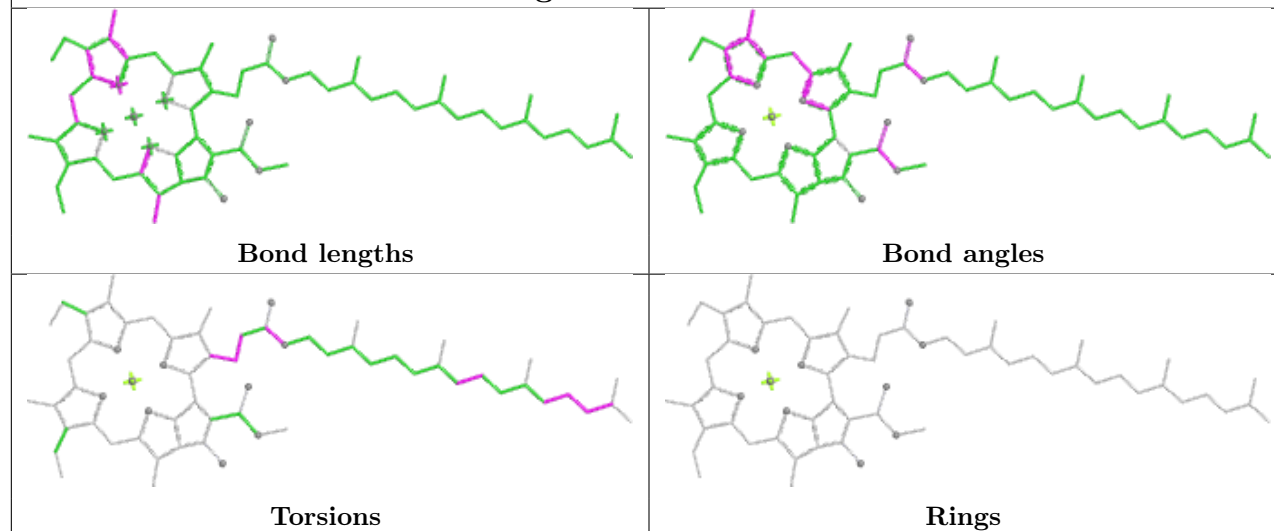




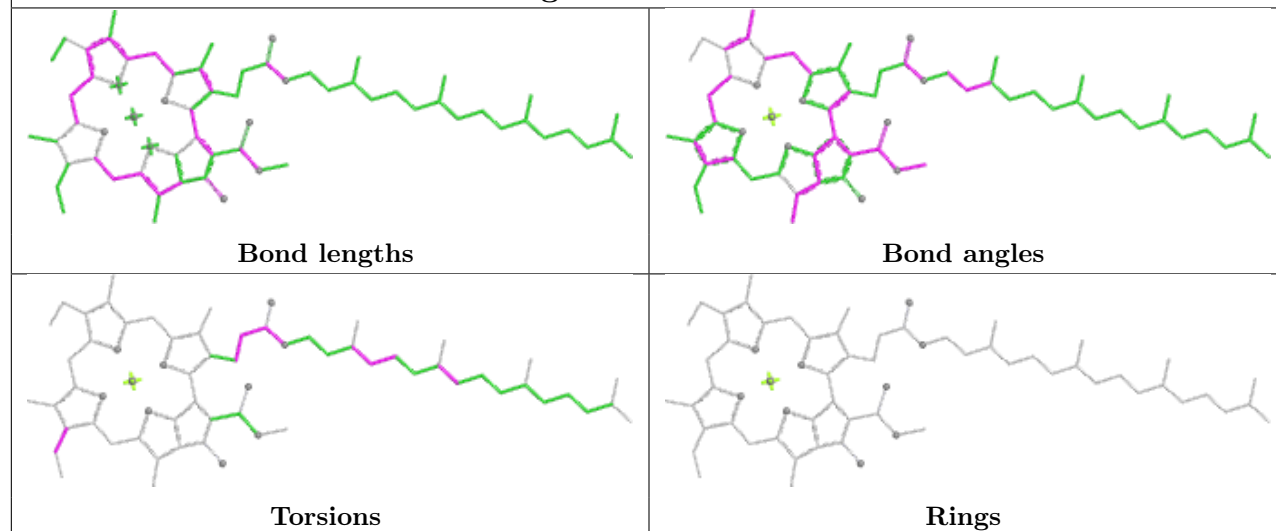
## Ligand CLA b 816



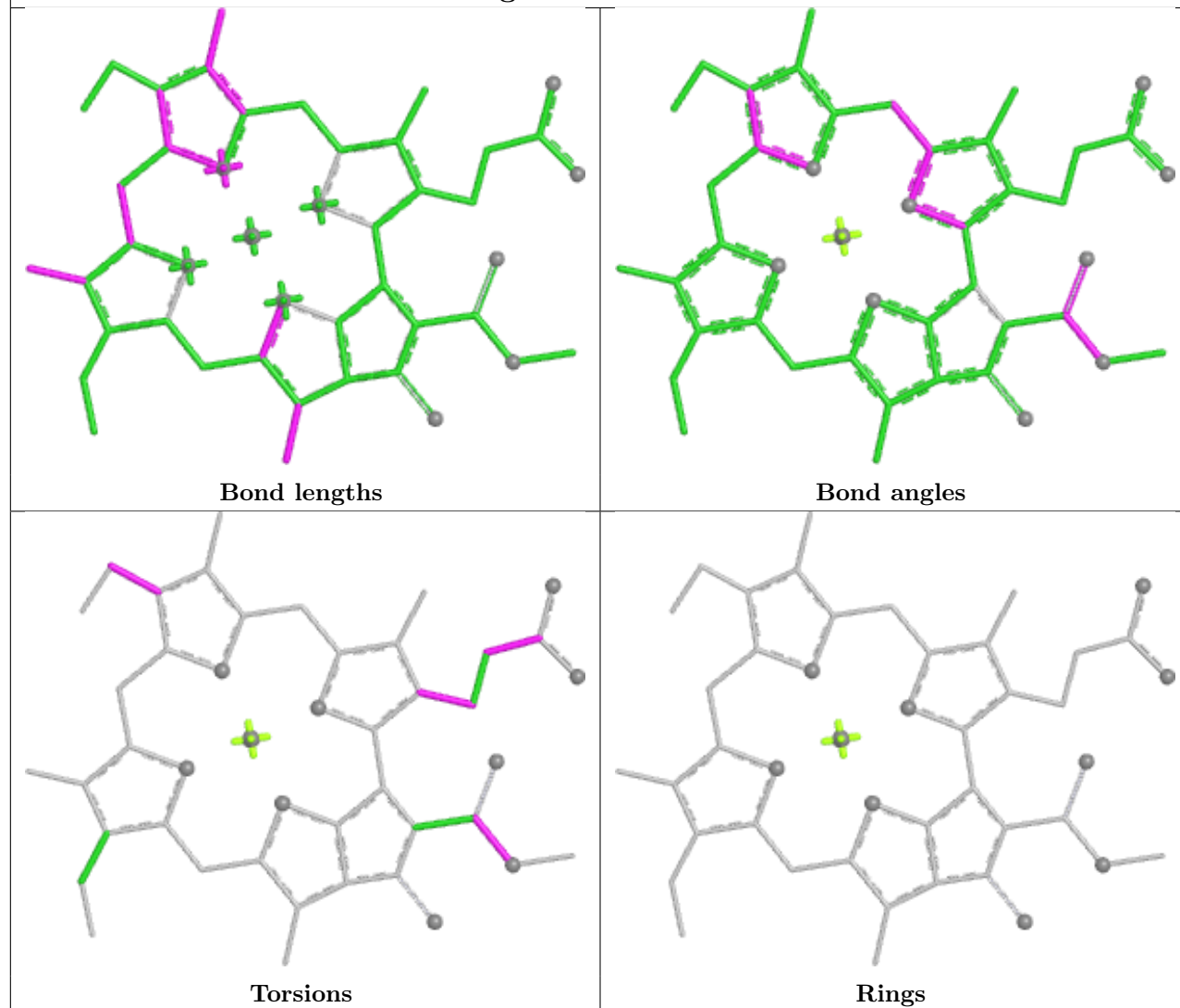
## Ligand CLA b 829

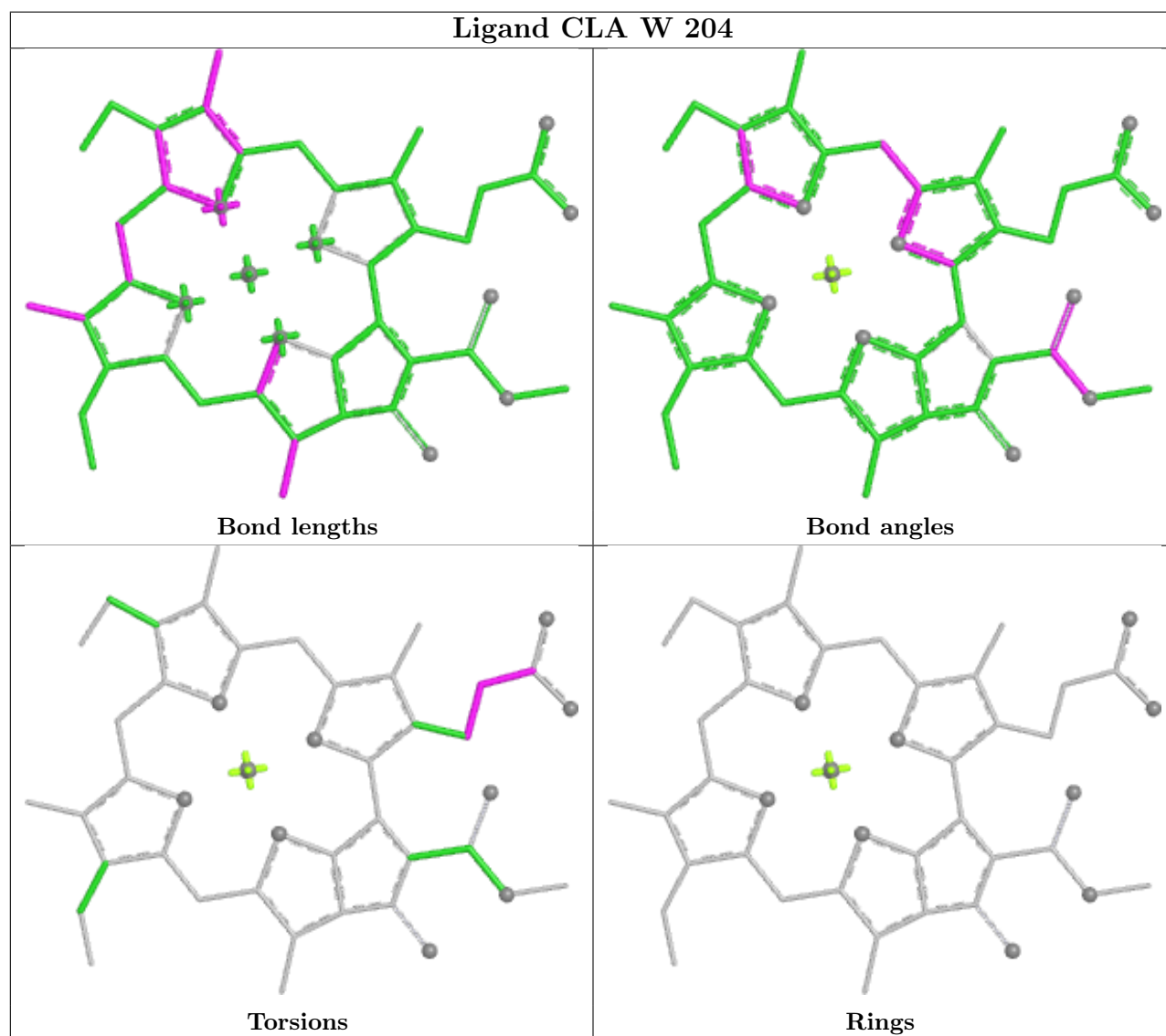
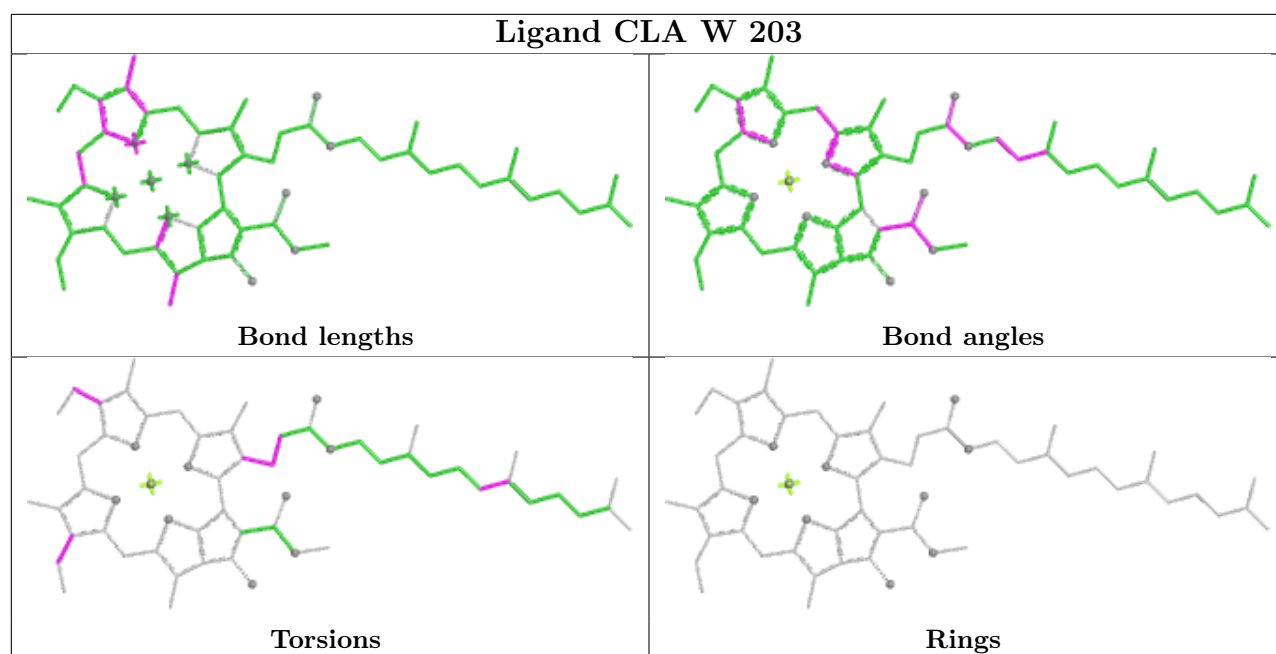


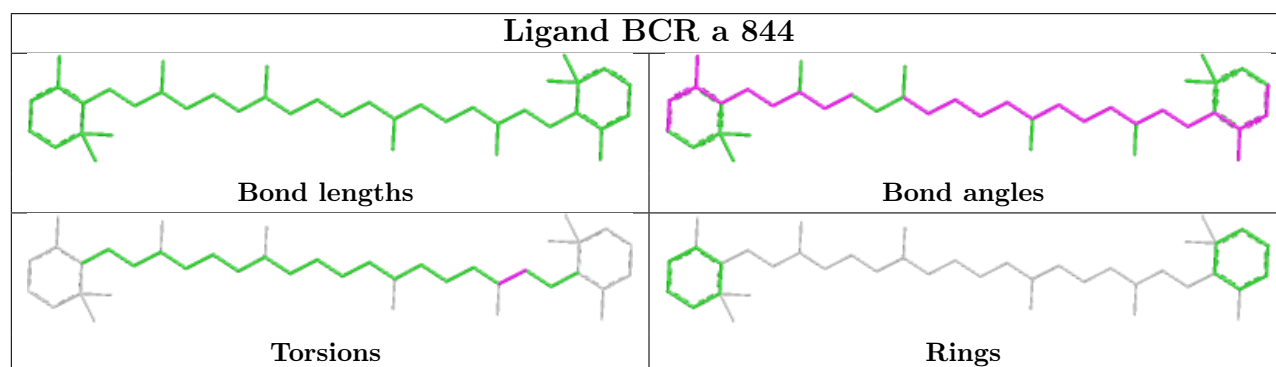
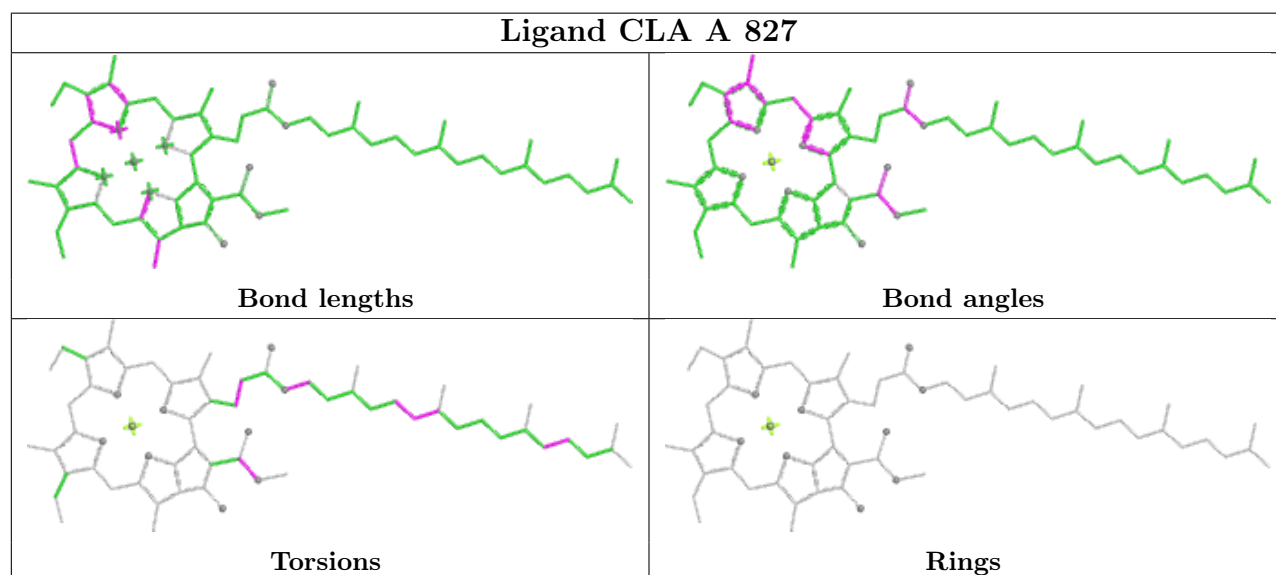
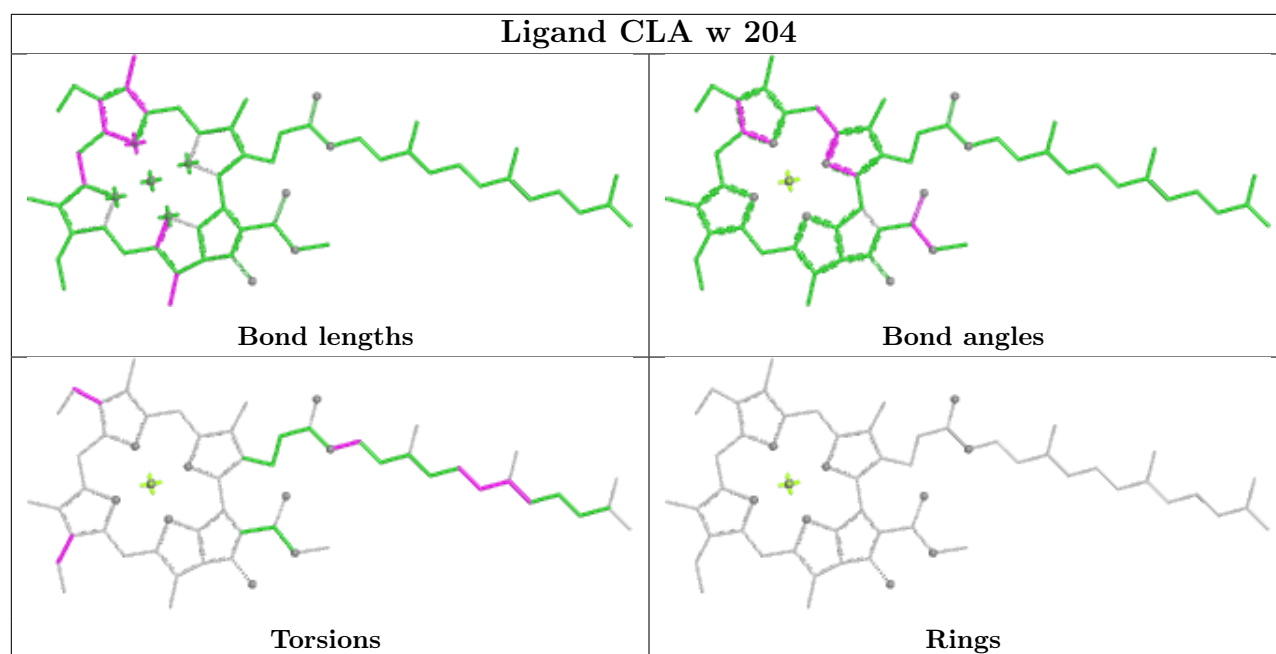
## Ligand CL0 a 851



## Ligand CLA l 204

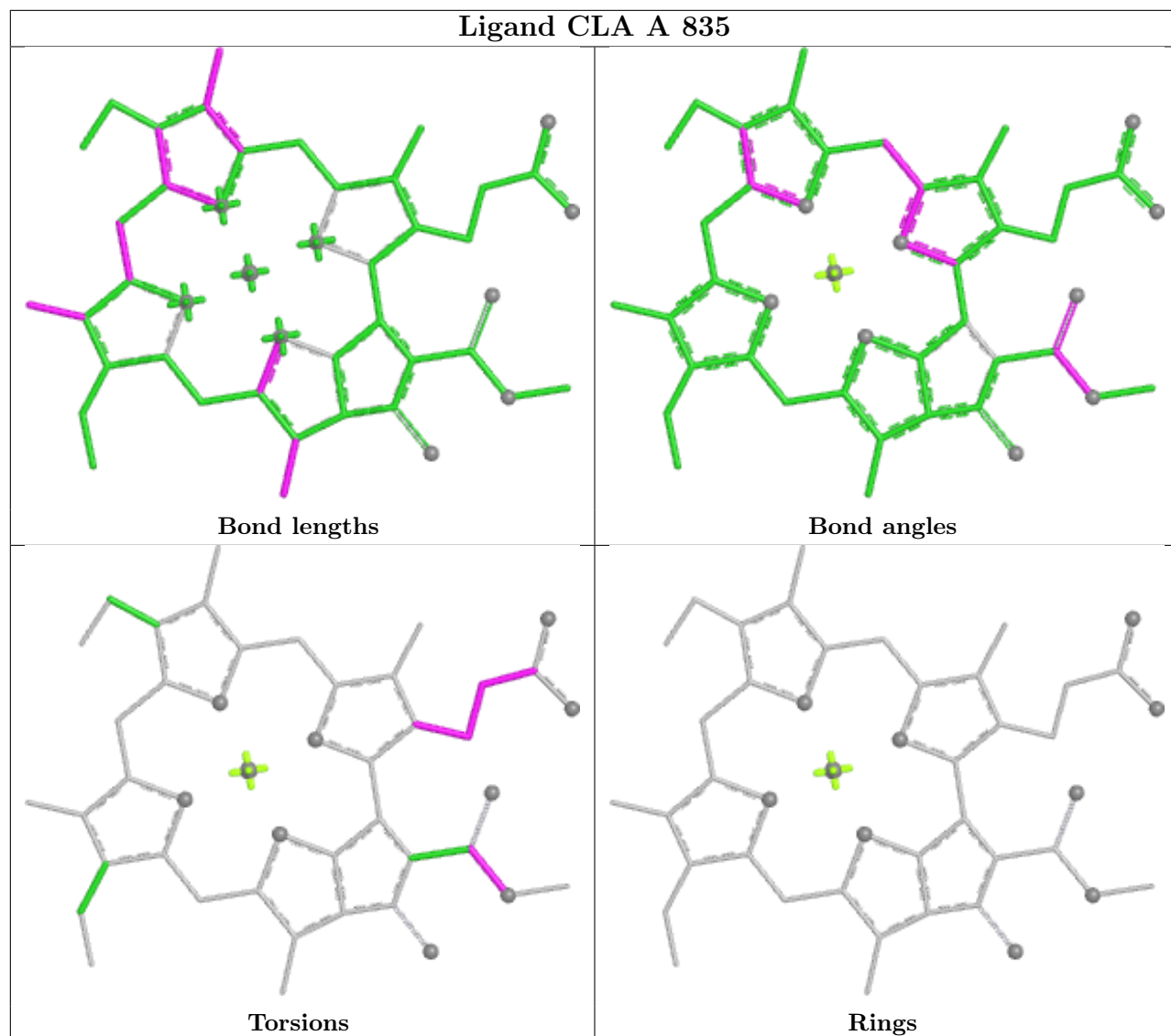




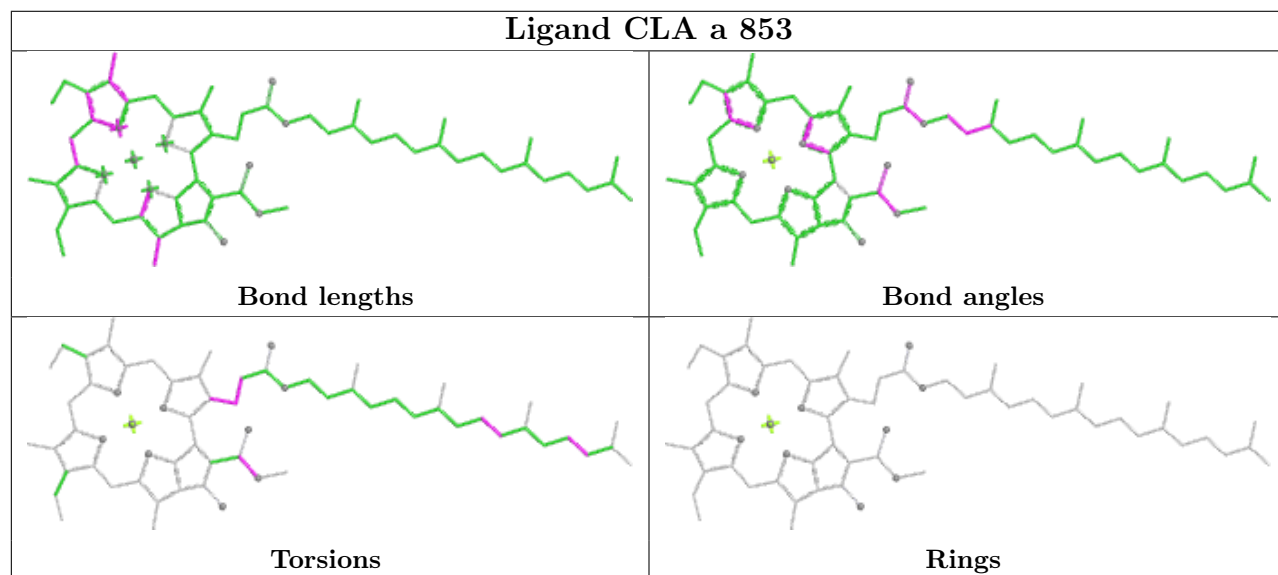




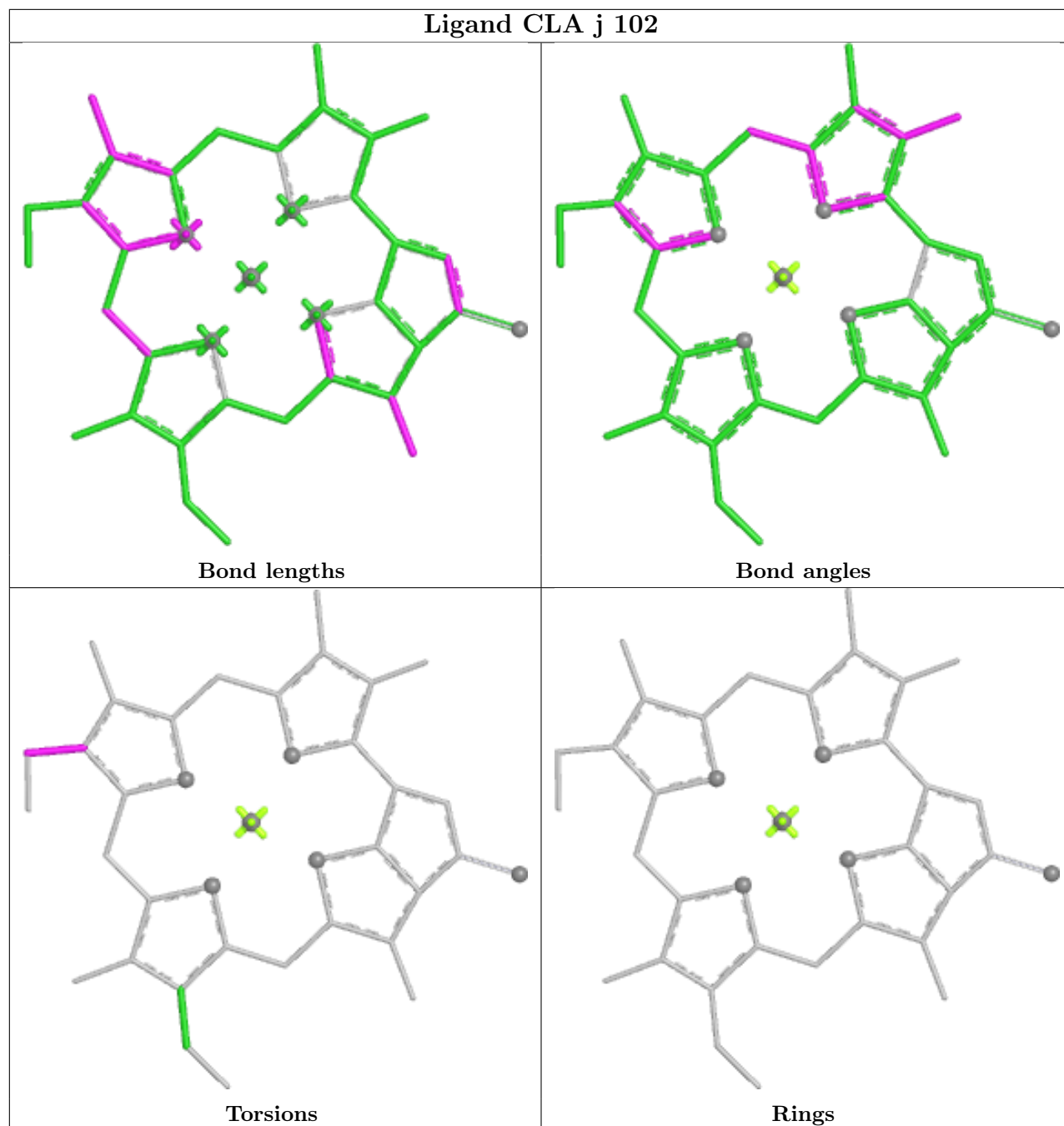
## Ligand CLA A 835



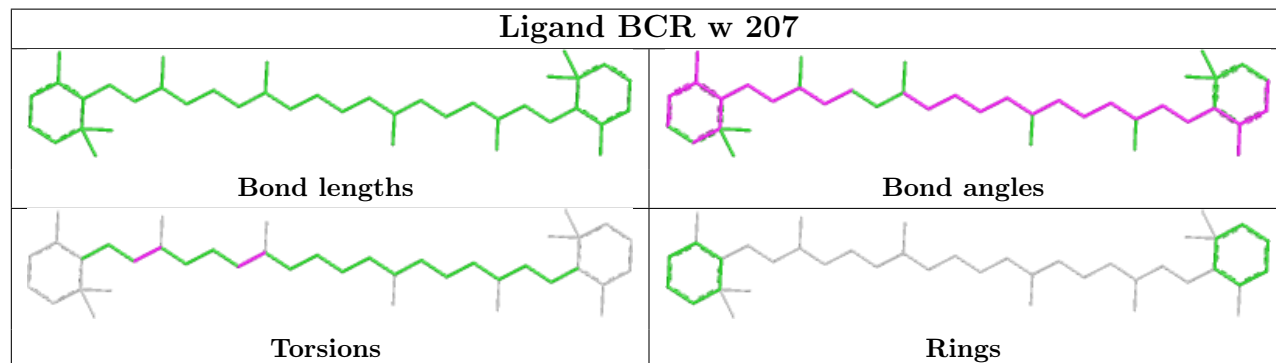
## Ligand CLA a 853

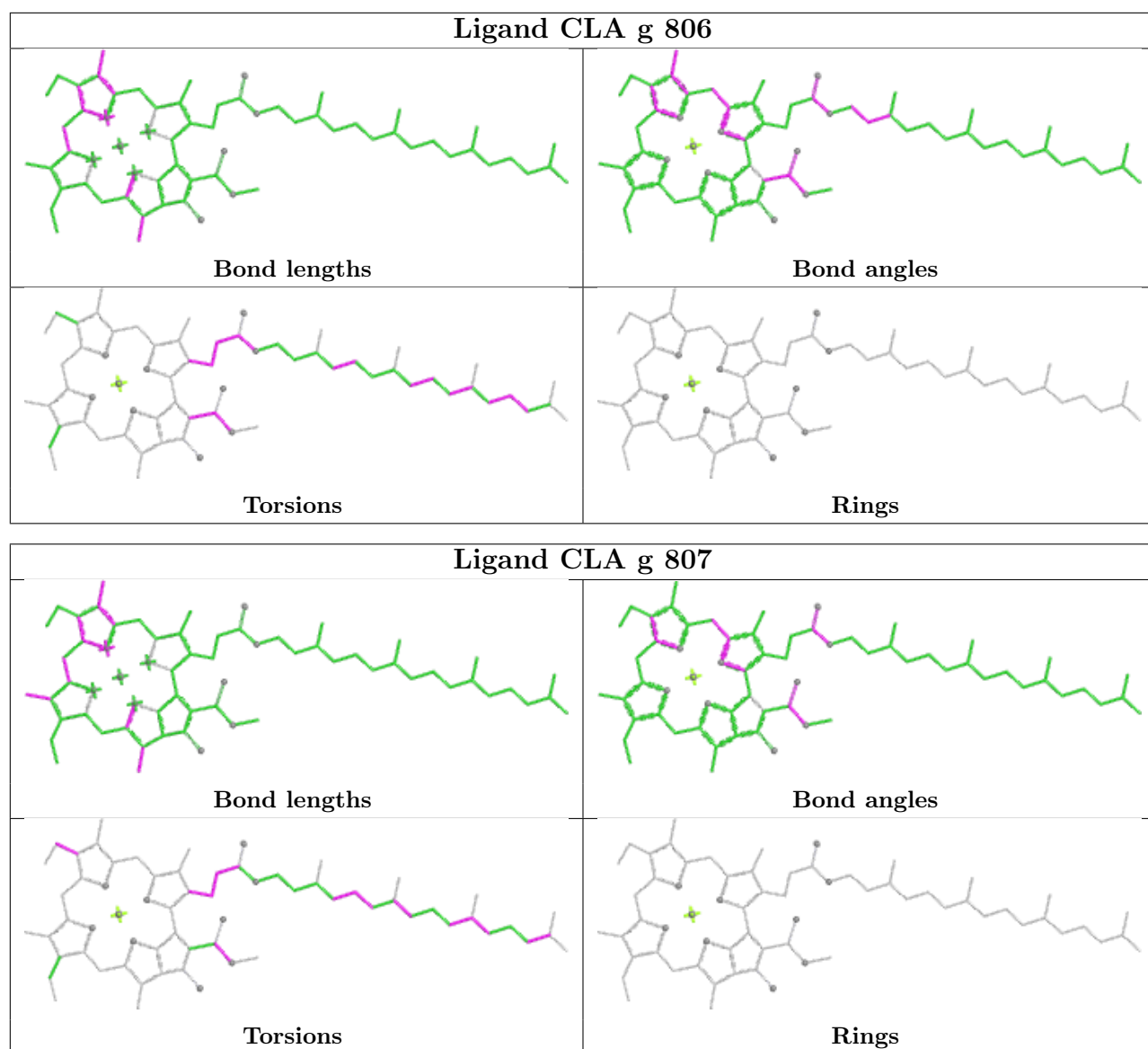


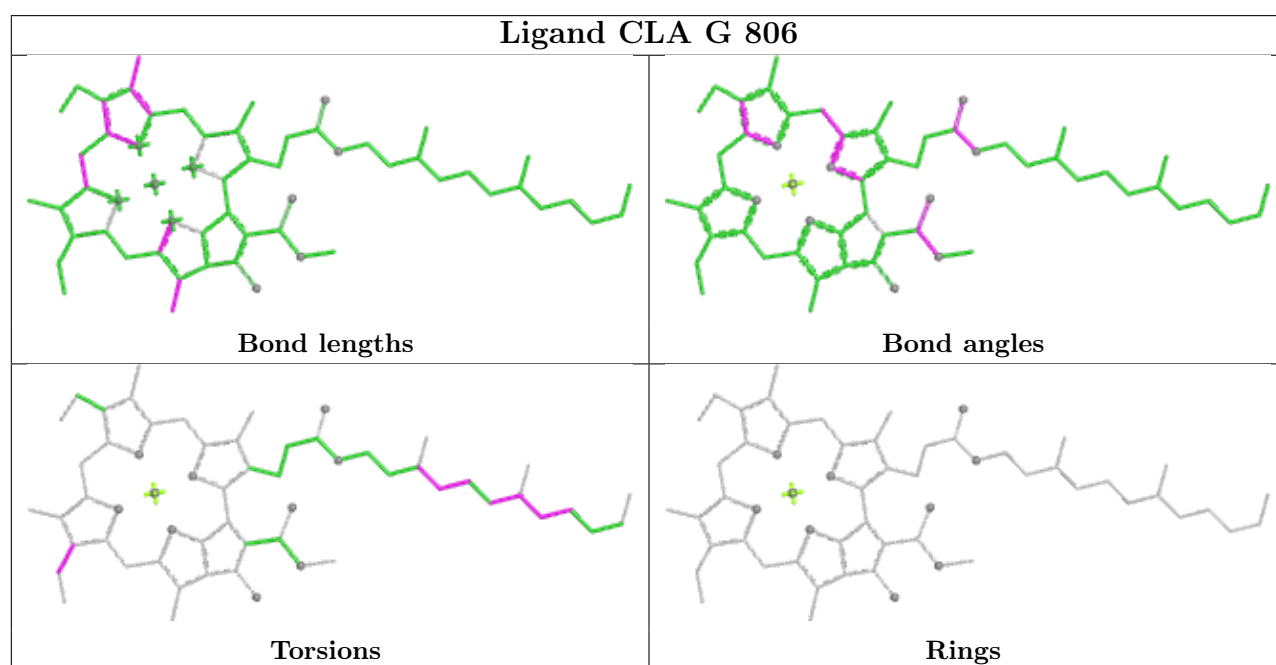
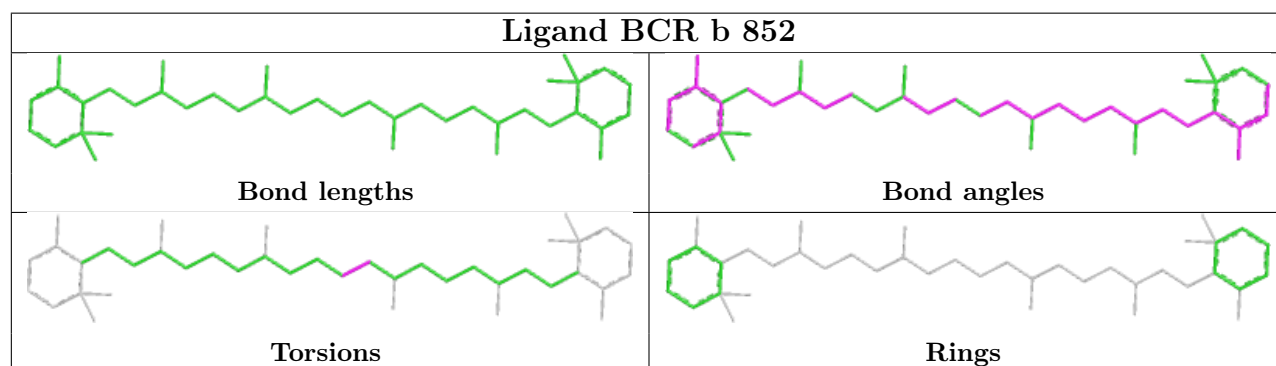
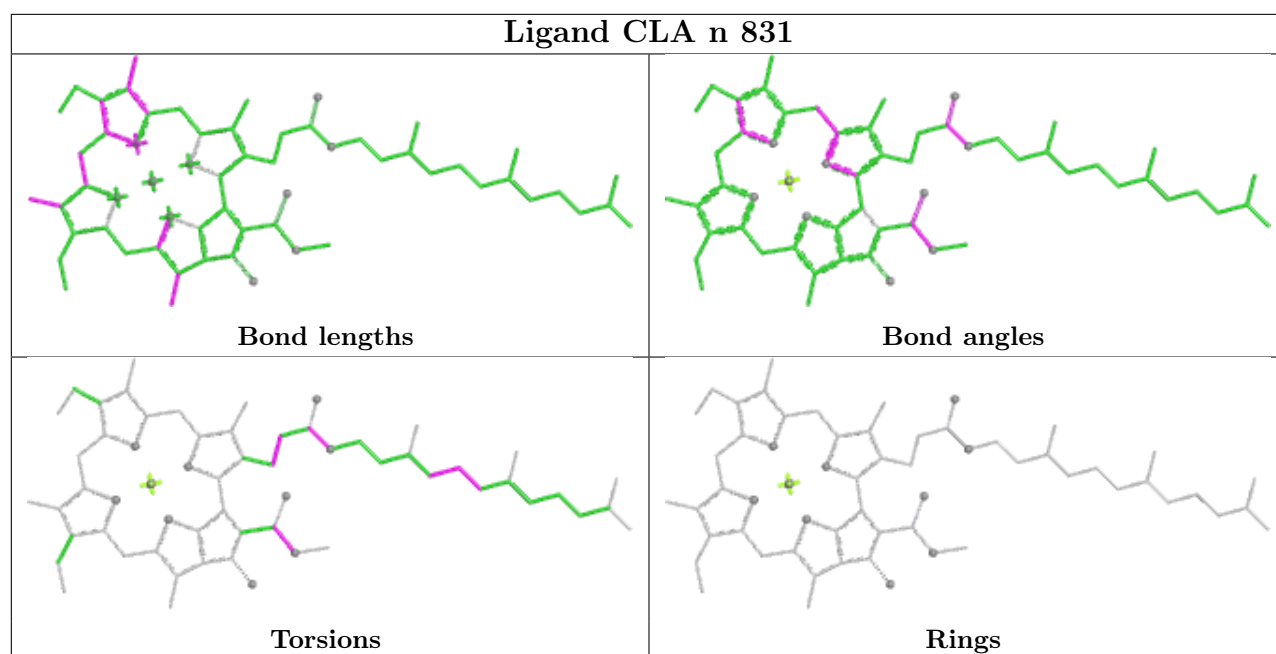
## Ligand CLA j 102

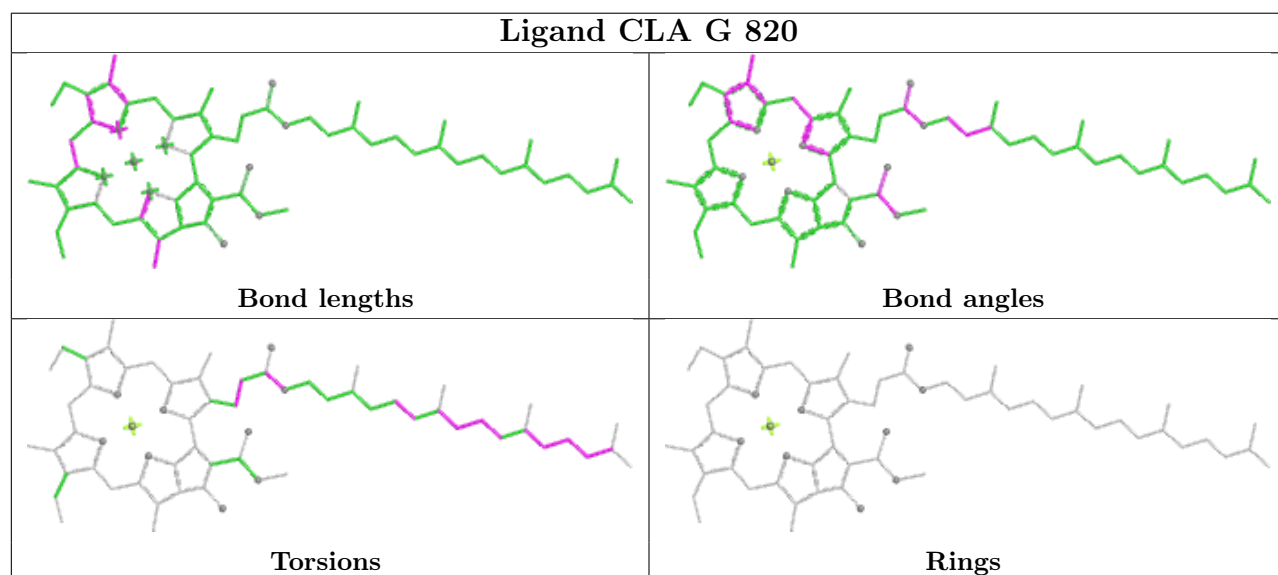
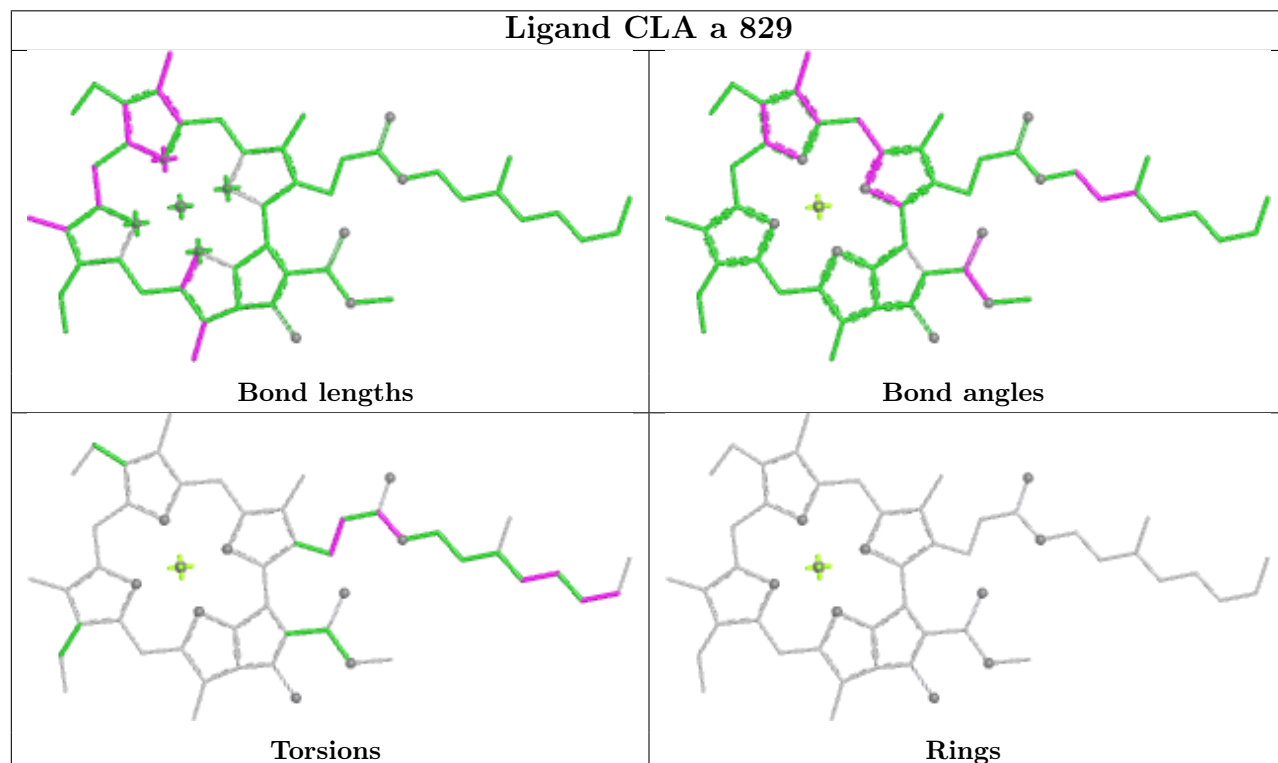
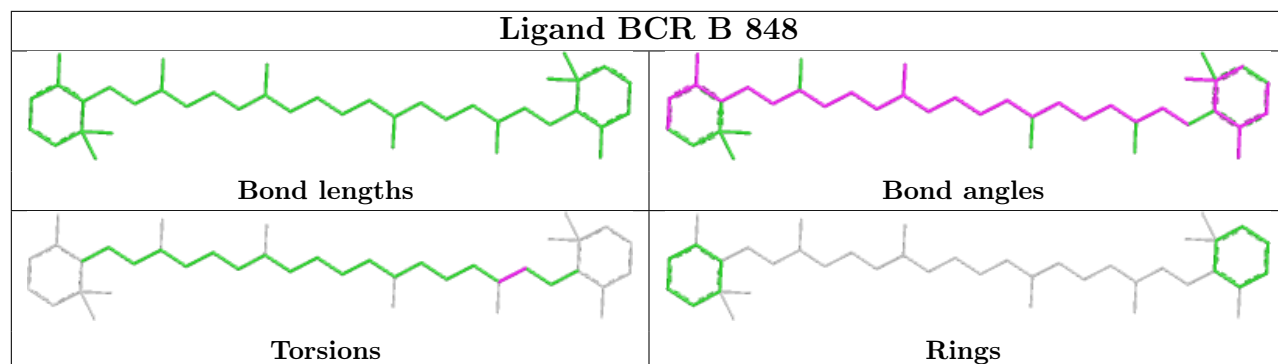


## Ligand BCR w 207

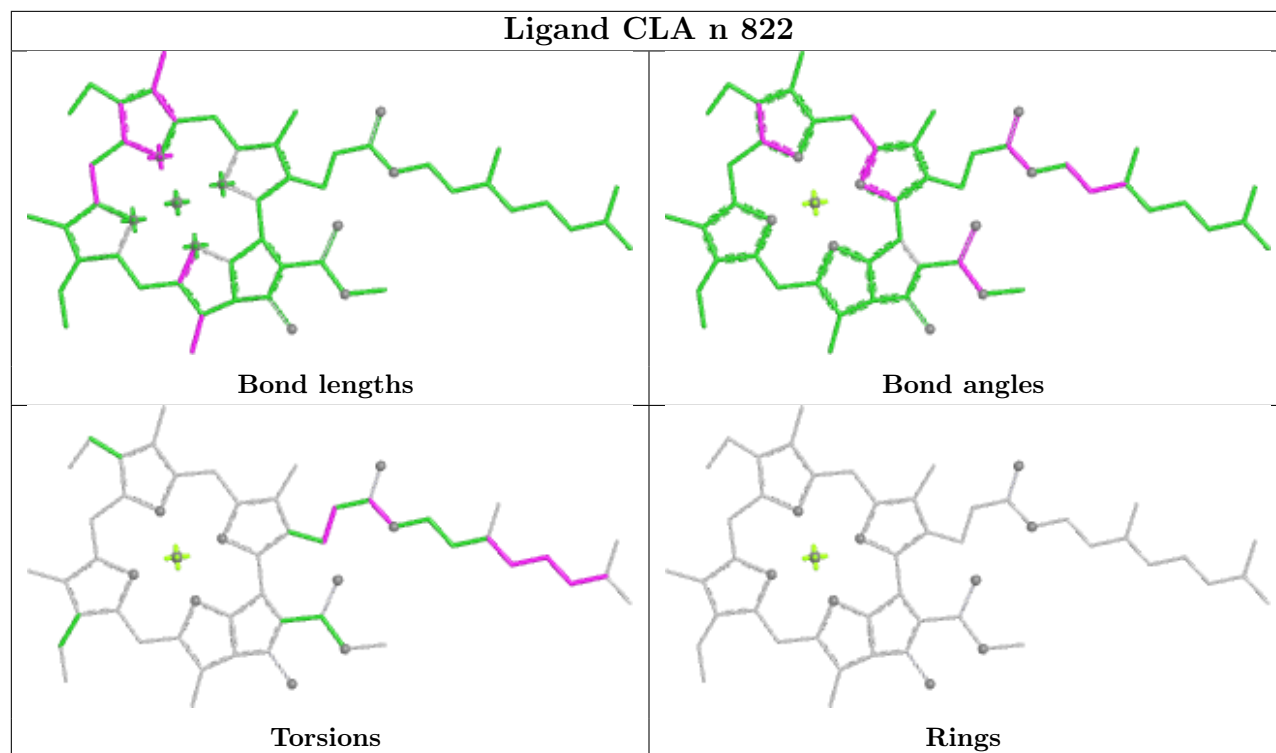




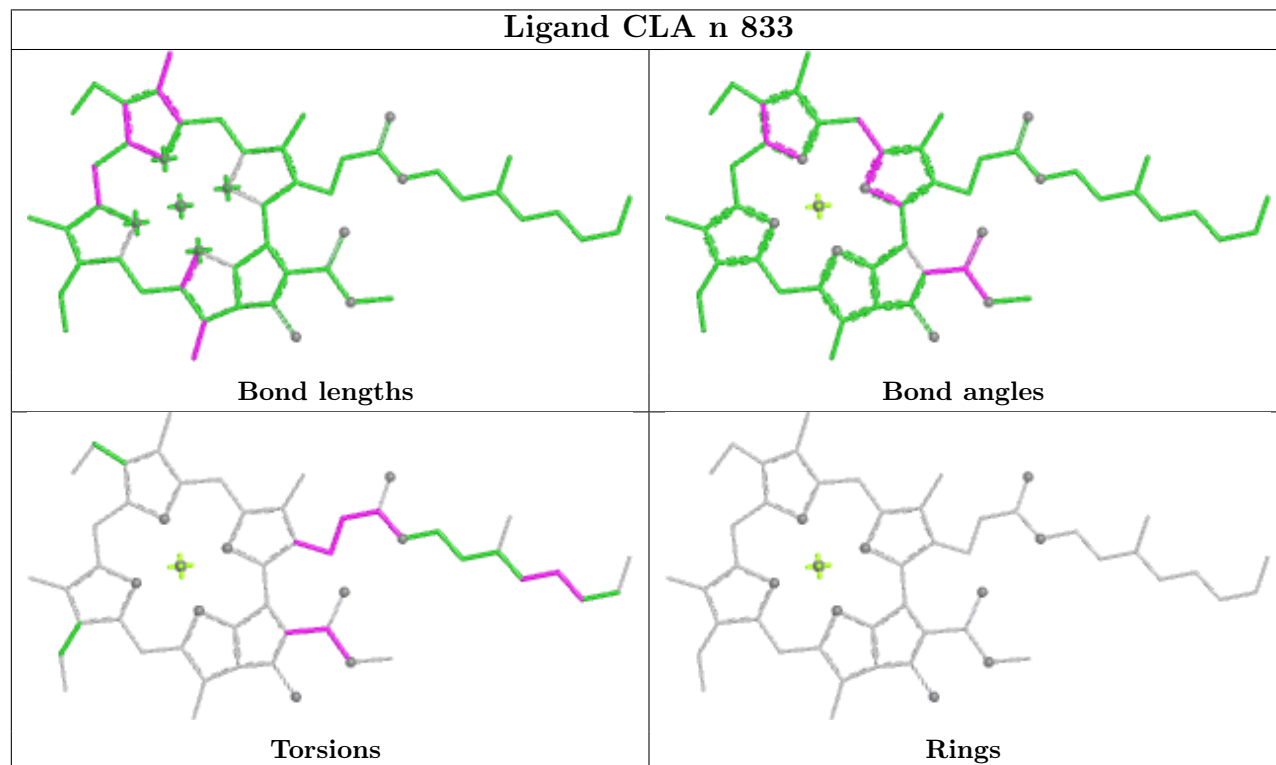




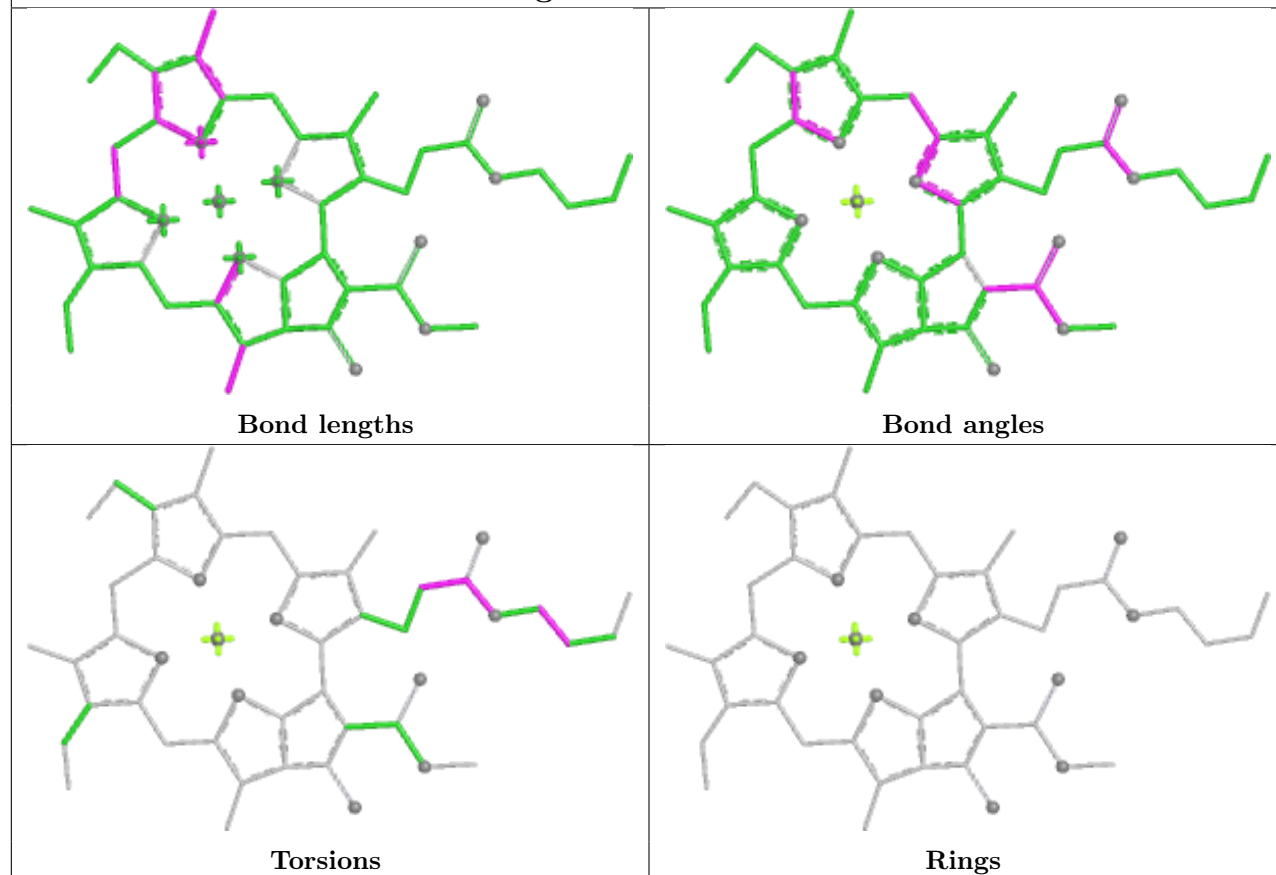
## Ligand CLA n 822



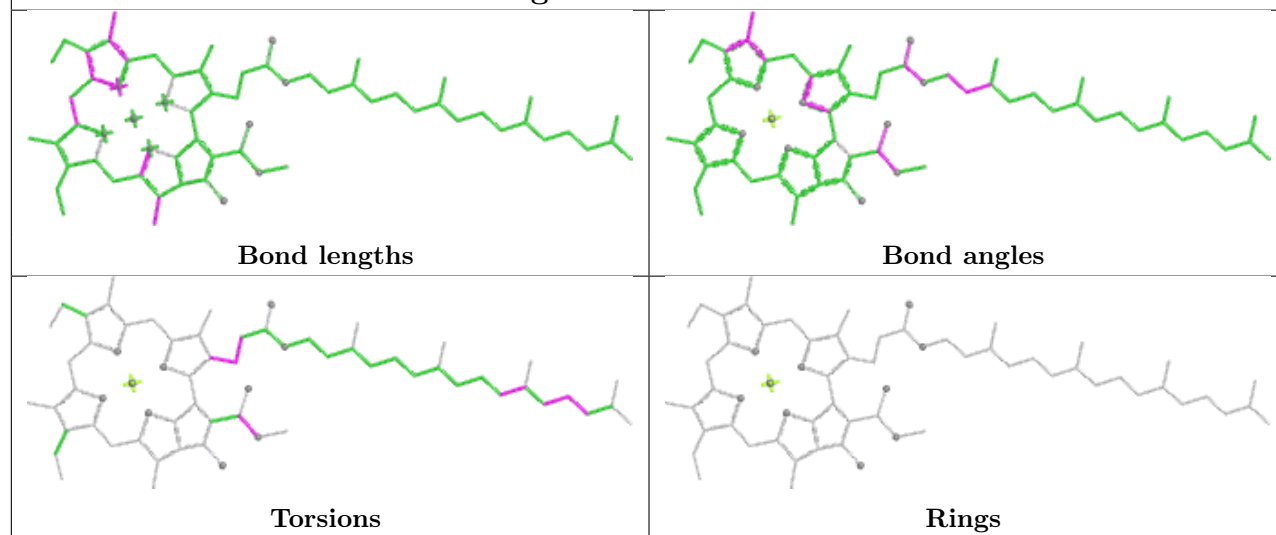
## Ligand CLA n 833

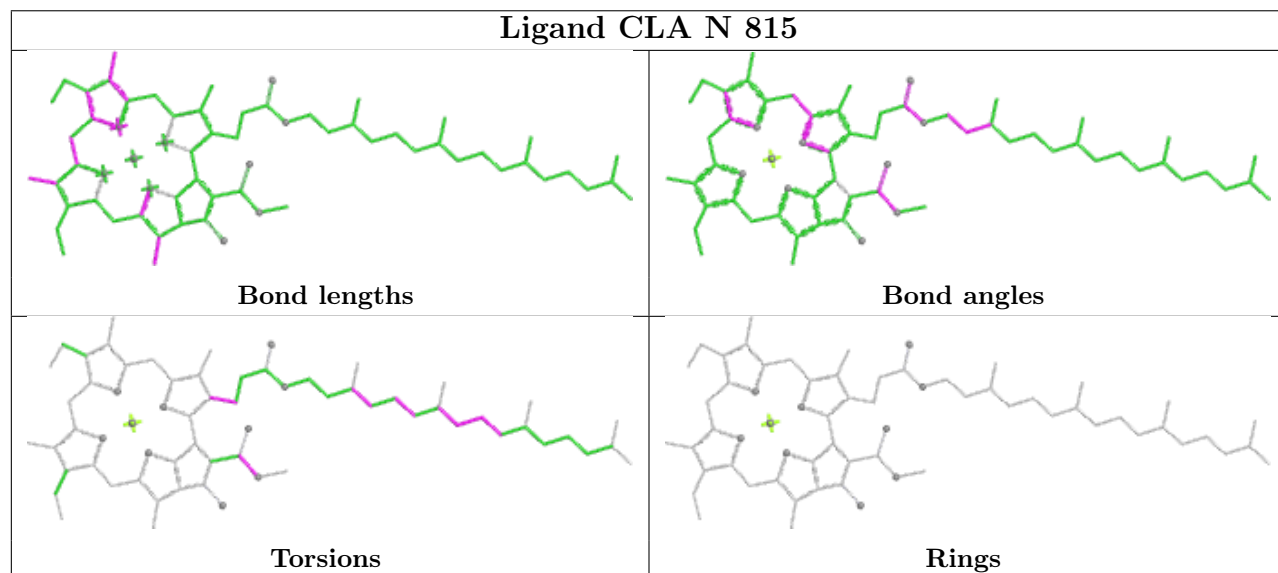
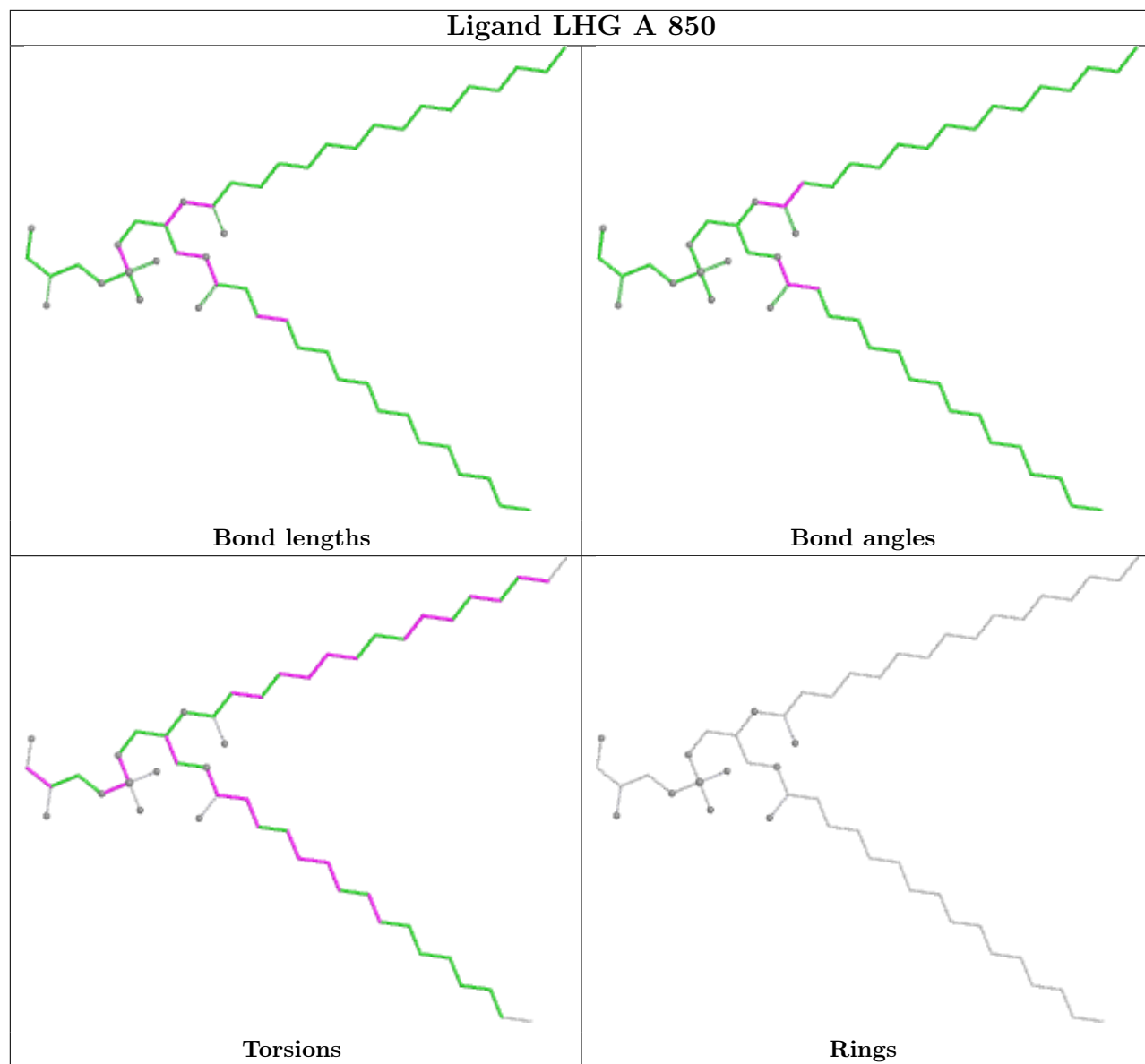


## Ligand CLA u 102



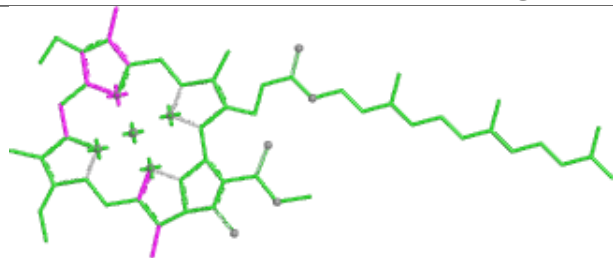
## Ligand CLA G 801



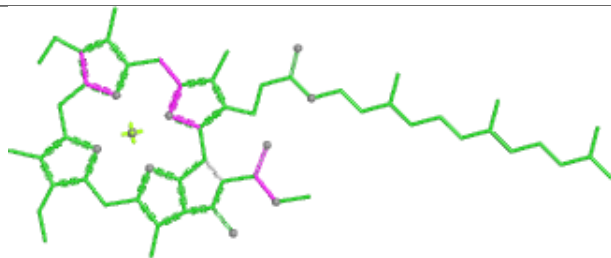




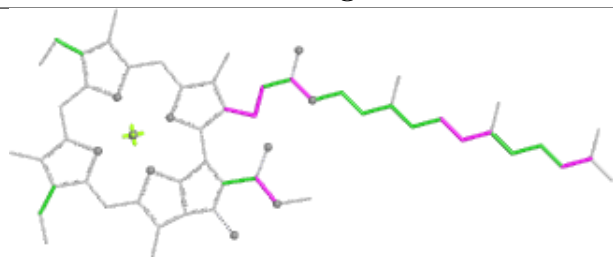
## Ligand CLA B 832



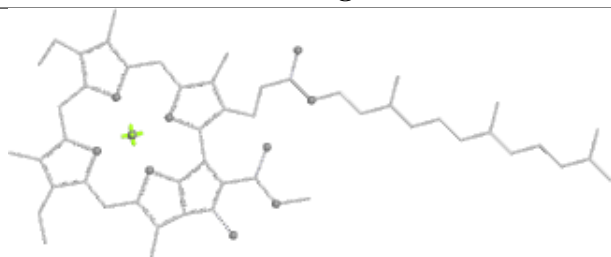
Bond lengths



Bond angles

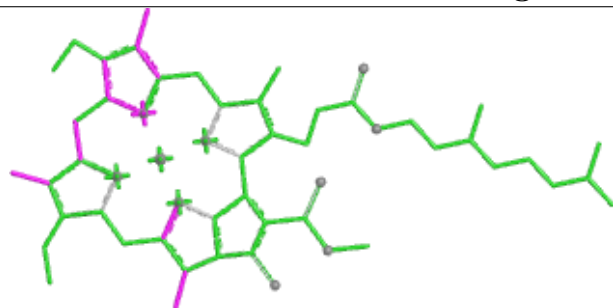


Torsions

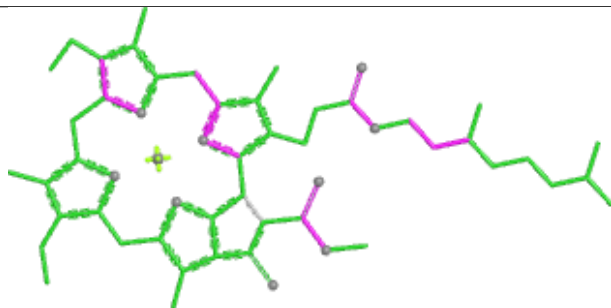


Rings

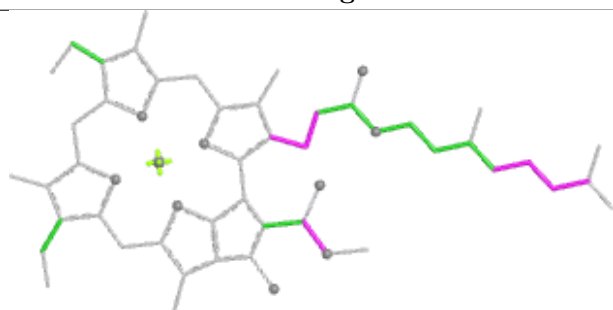
## Ligand CLA N 806



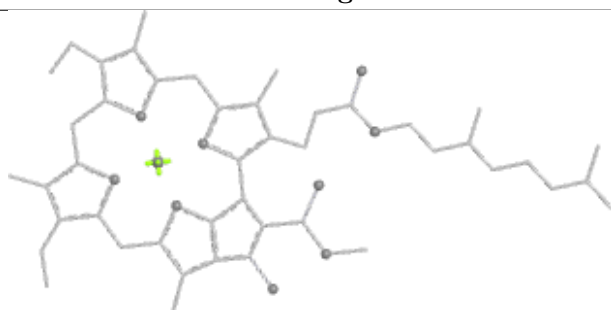
Bond lengths



Bond angles

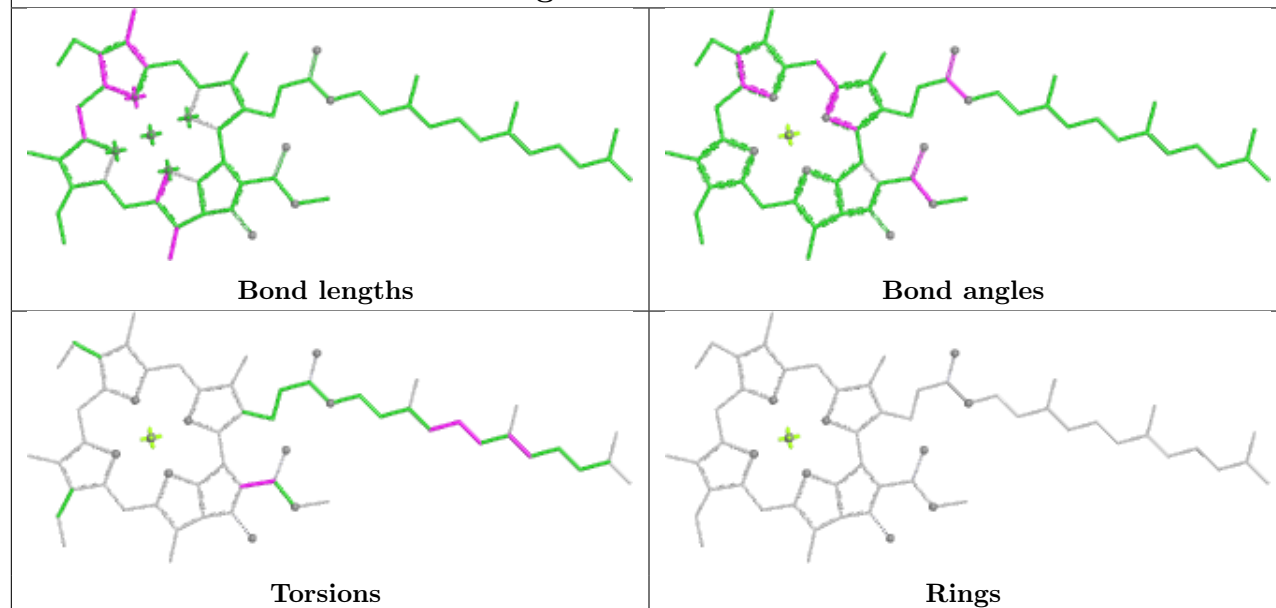


Torsions

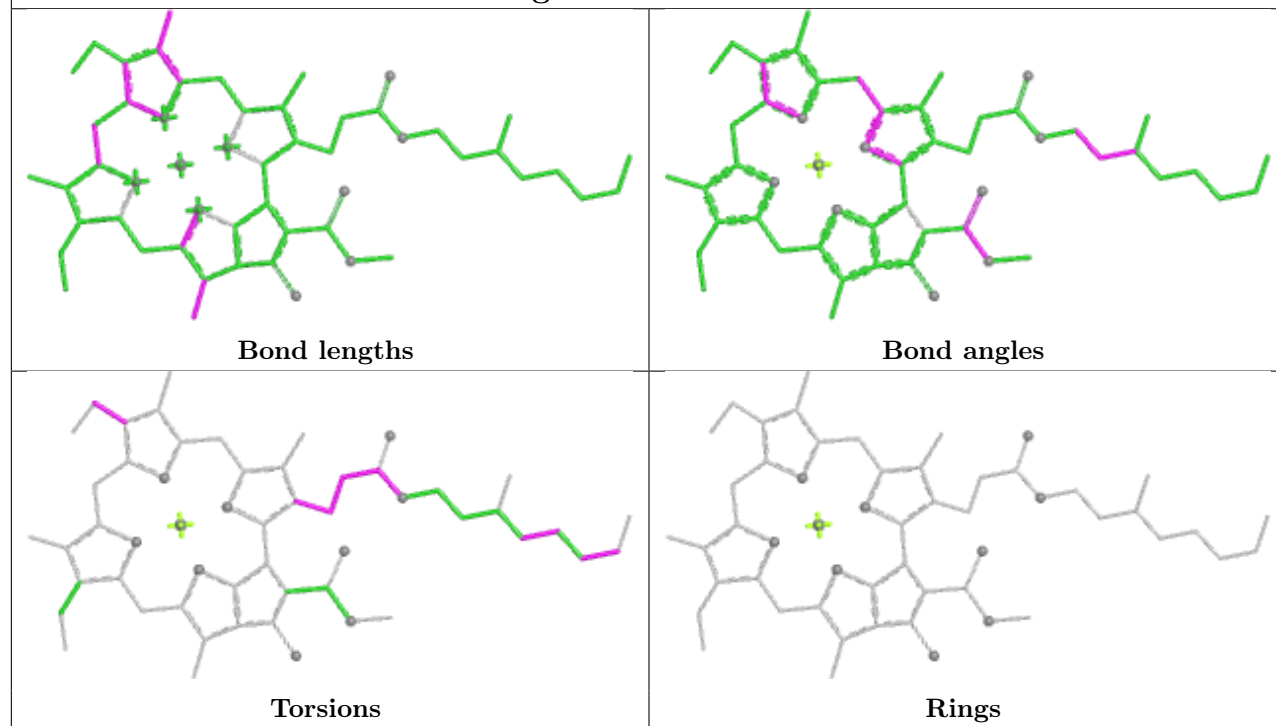


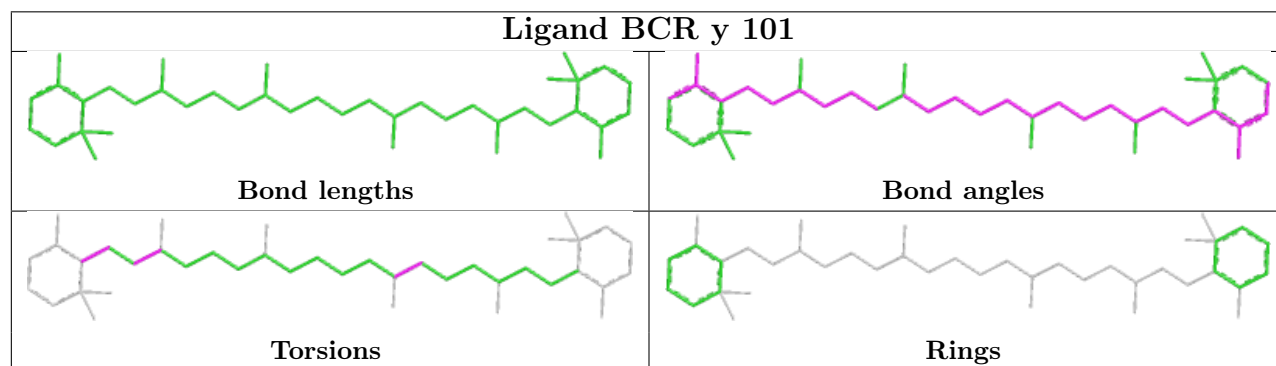
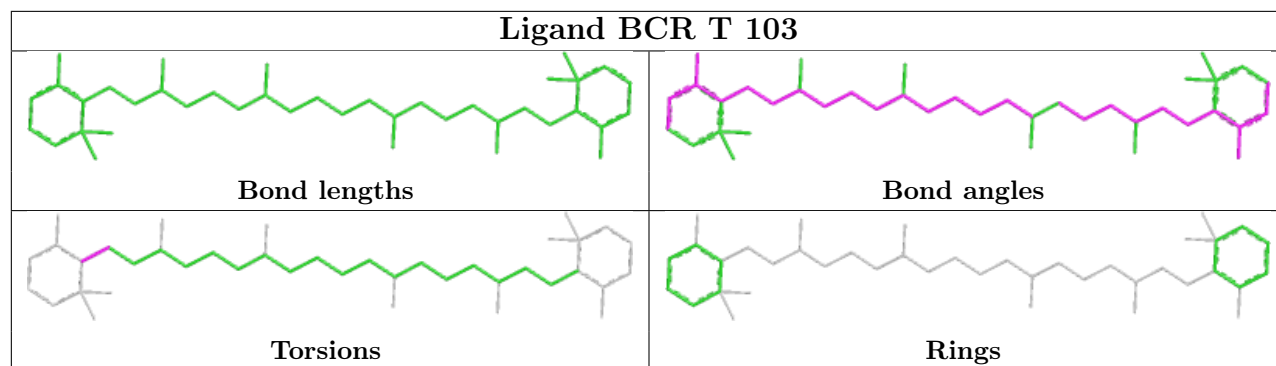
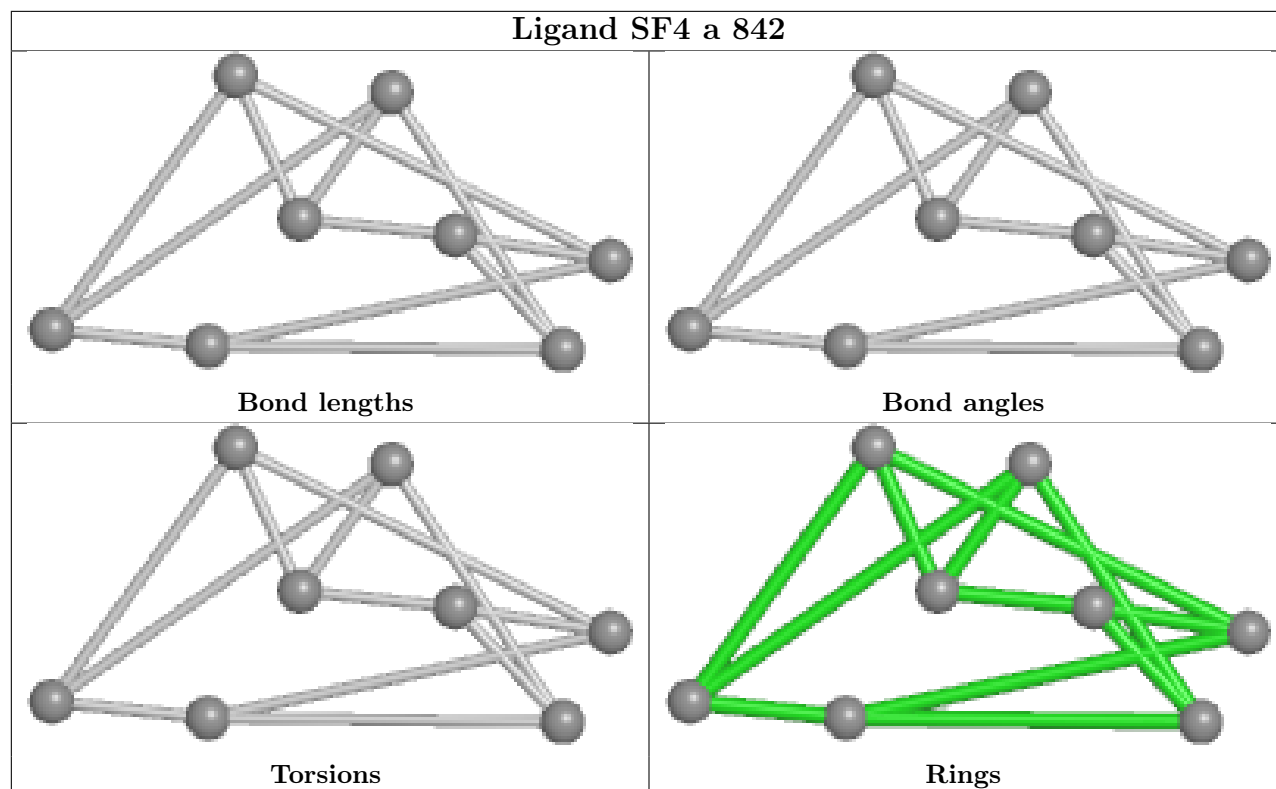
Rings

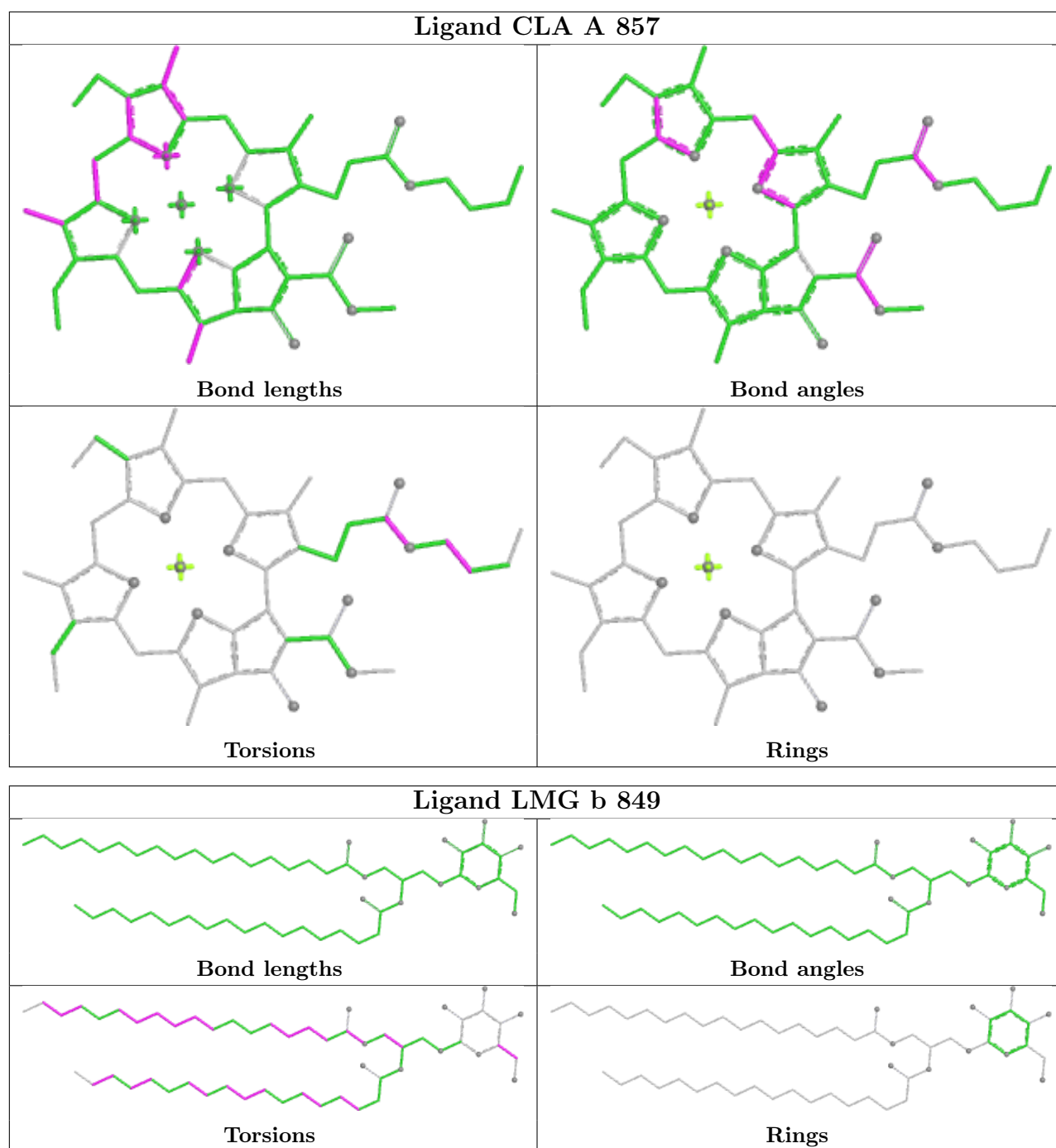
## Ligand CLA a 805



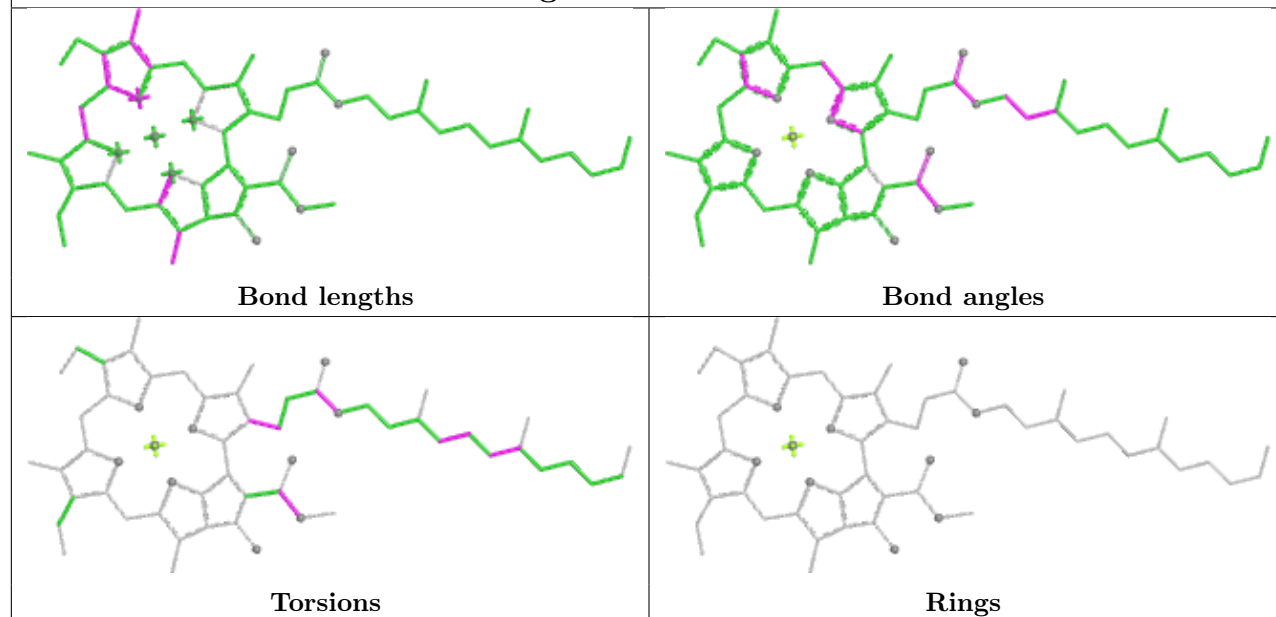
## Ligand CLA B 813



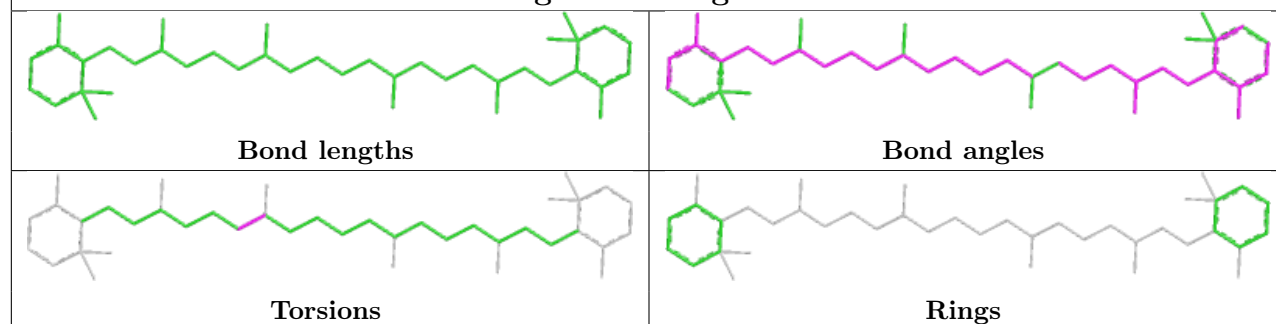




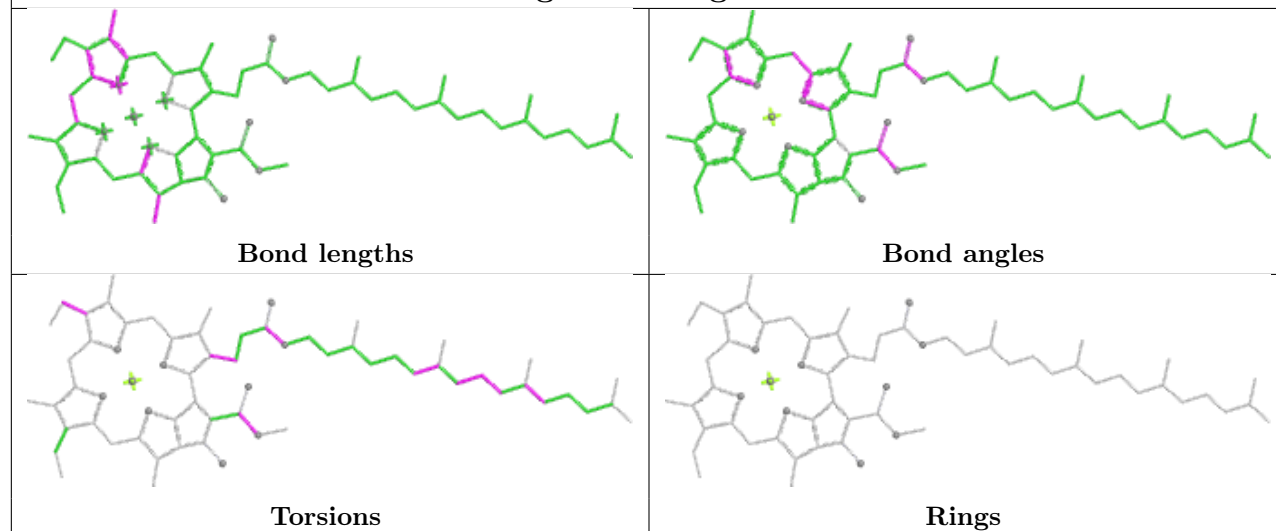
## Ligand CLA f 201

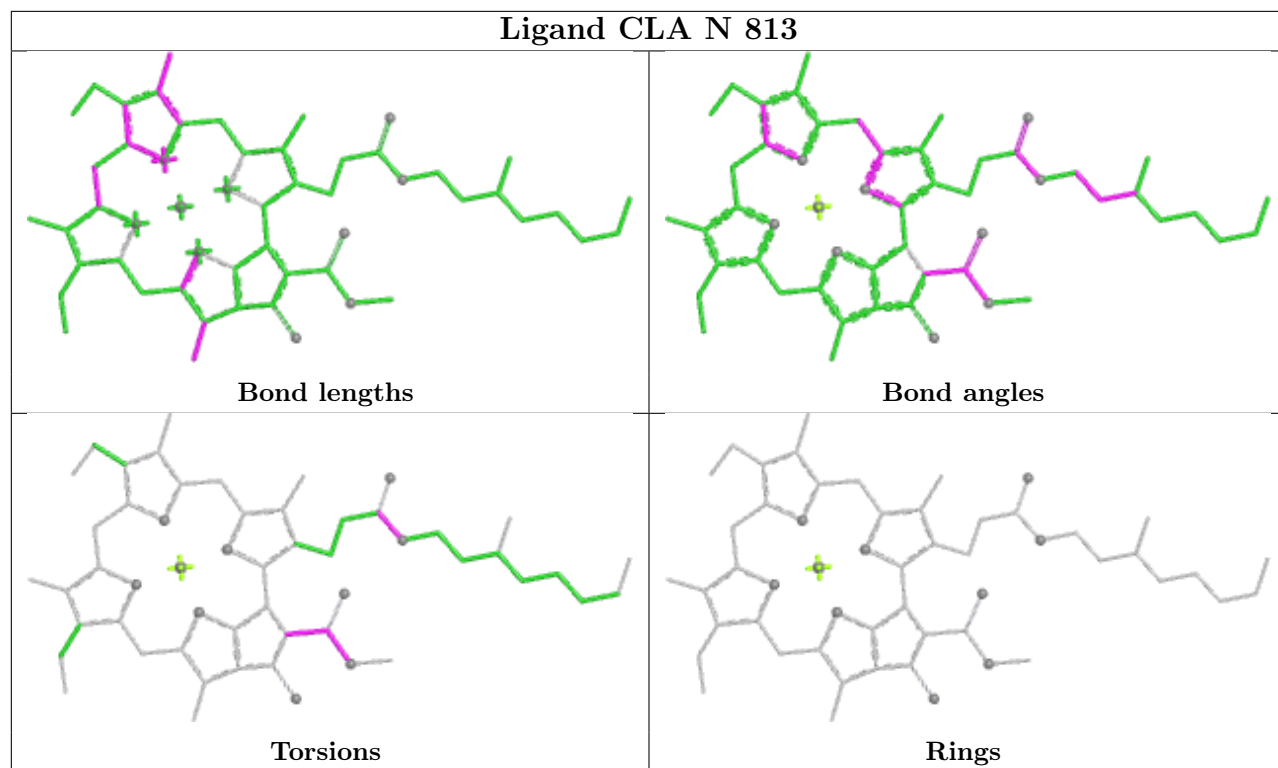


## Ligand BCR g 843

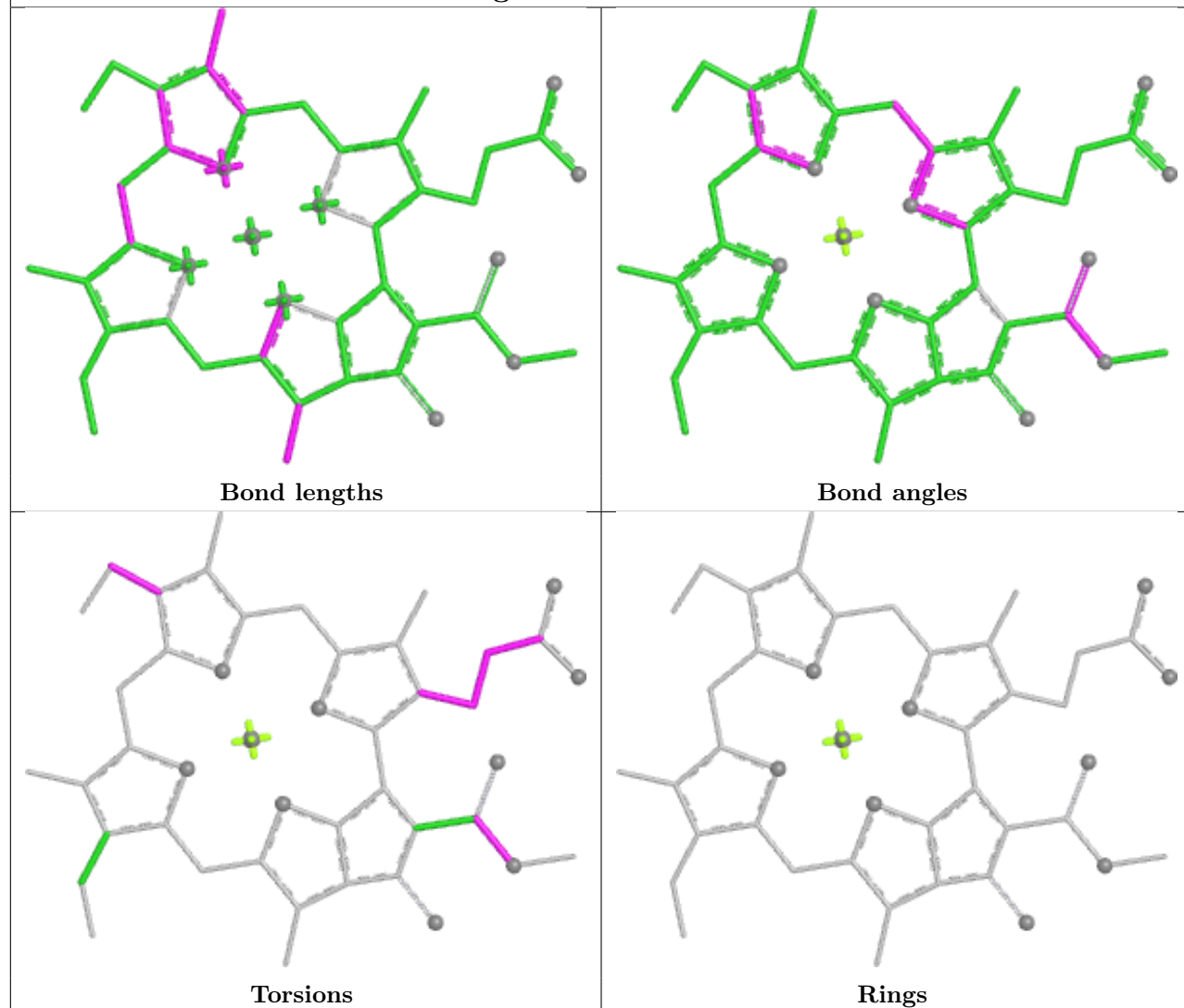


## Ligand CLA g 809

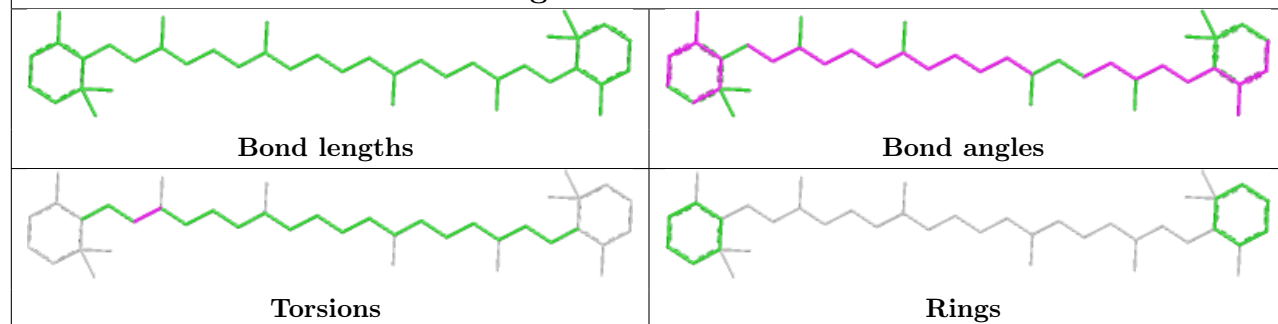


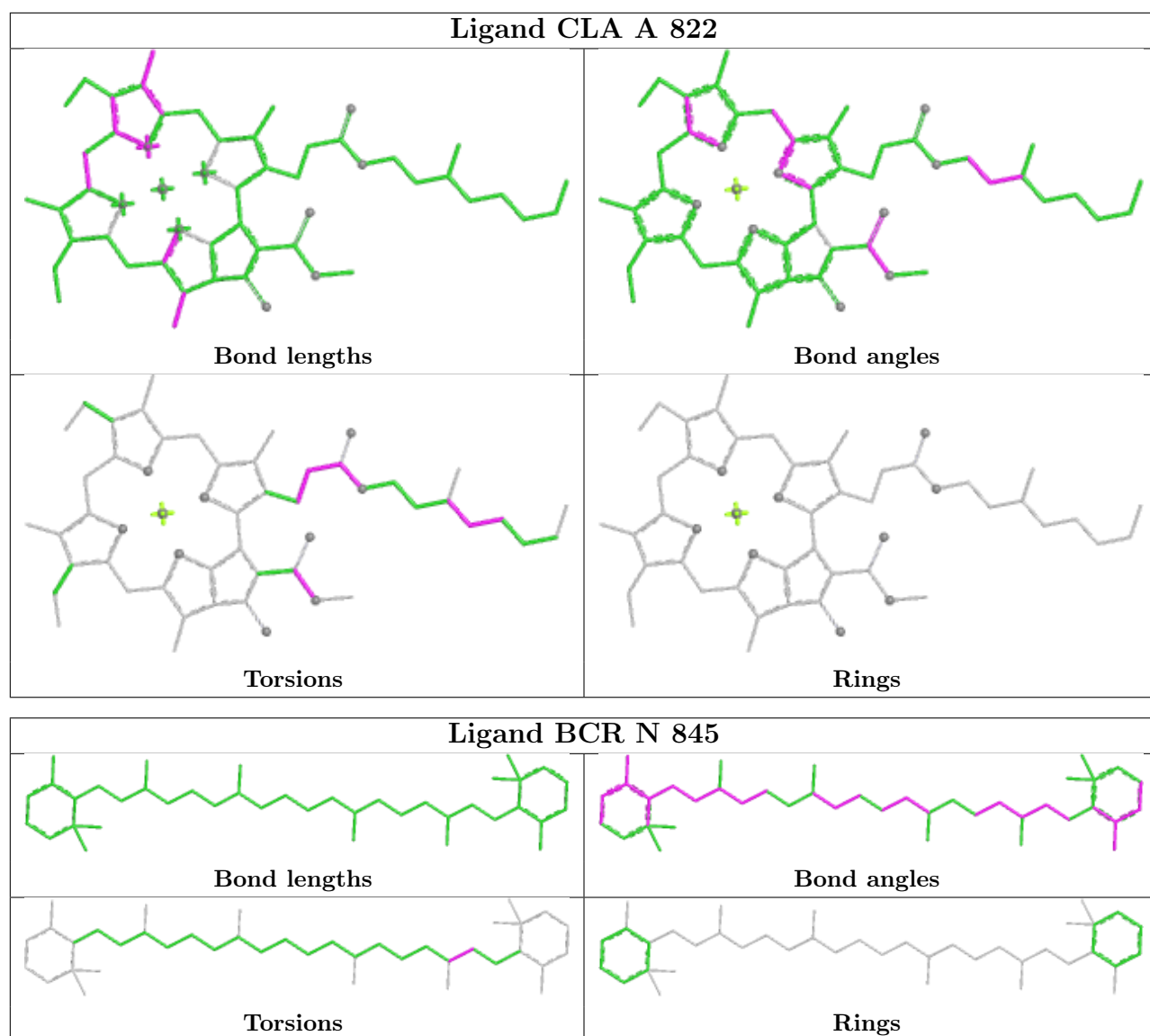


## Ligand CLA B 821

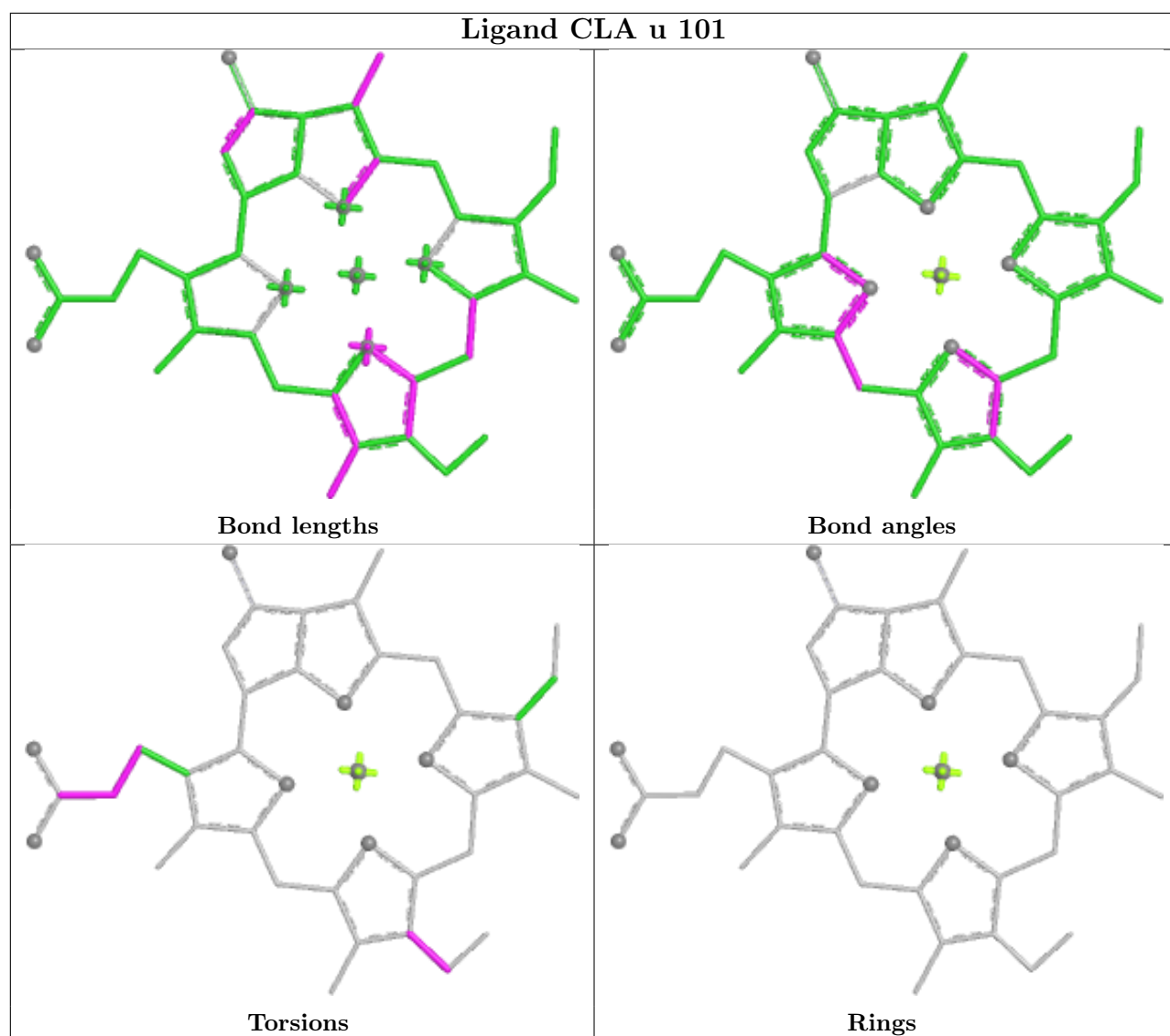


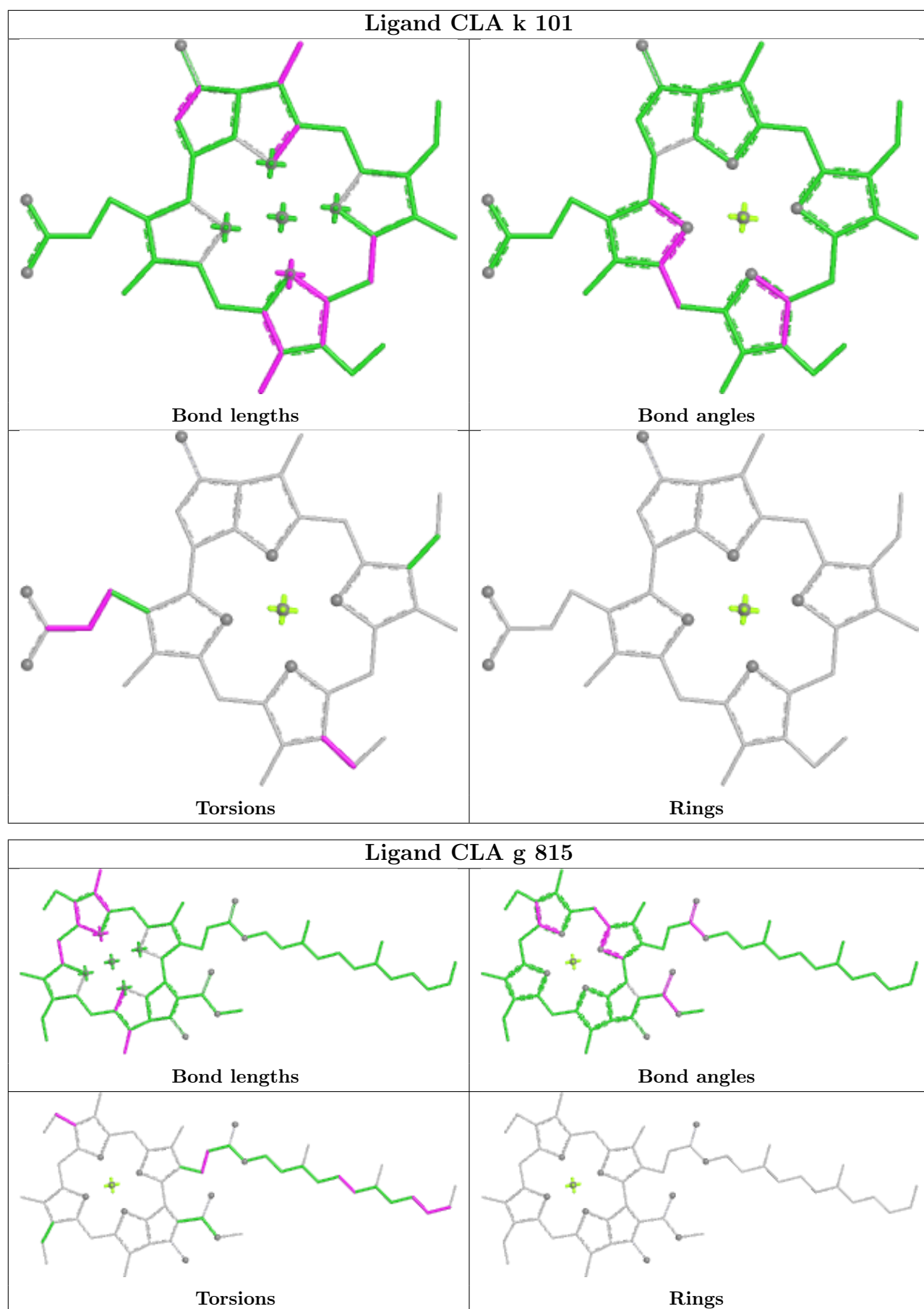
## Ligand BCR A 846



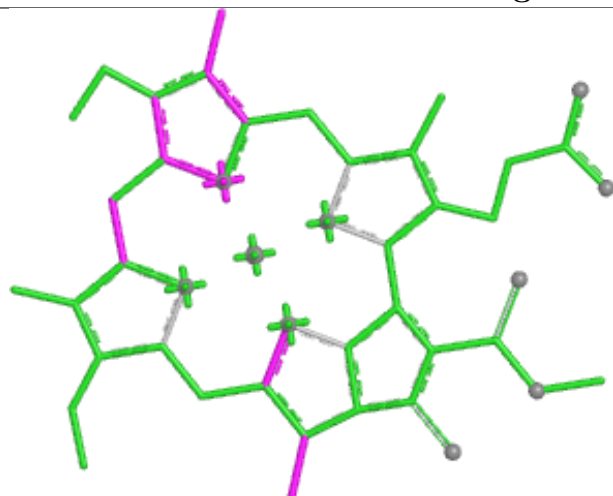




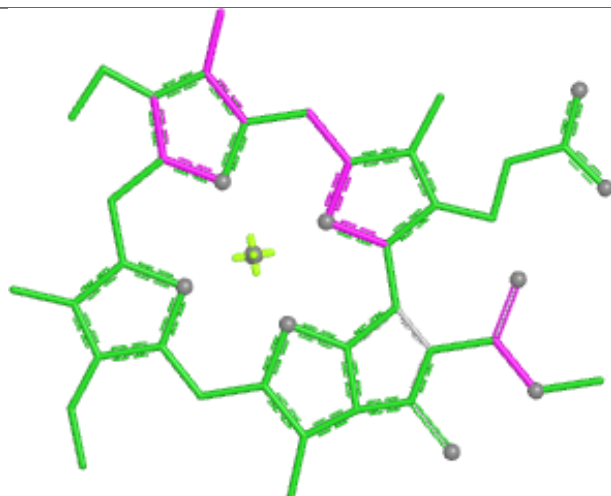




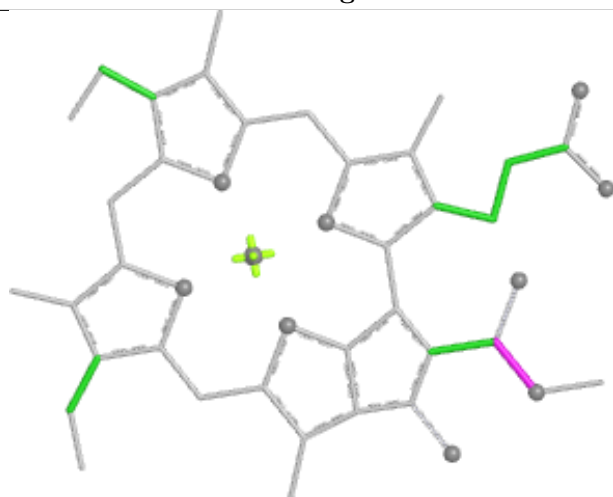
## Ligand CLA N 836



Bond lengths



Bond angles

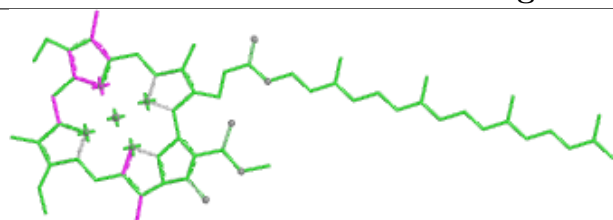


Torsions

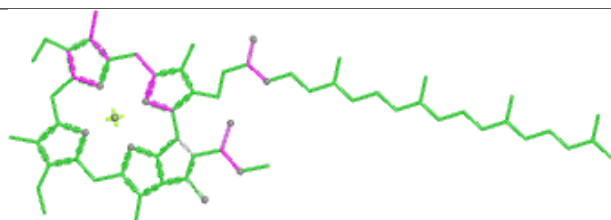


Rings

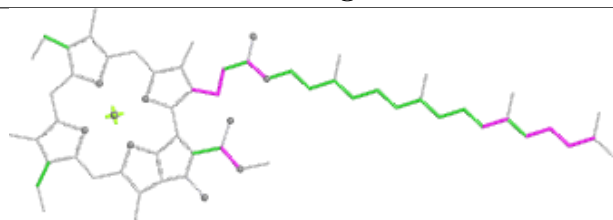
## Ligand CLA n 828



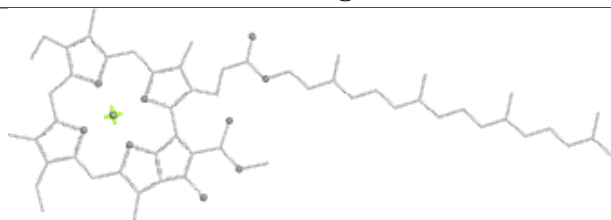
Bond lengths



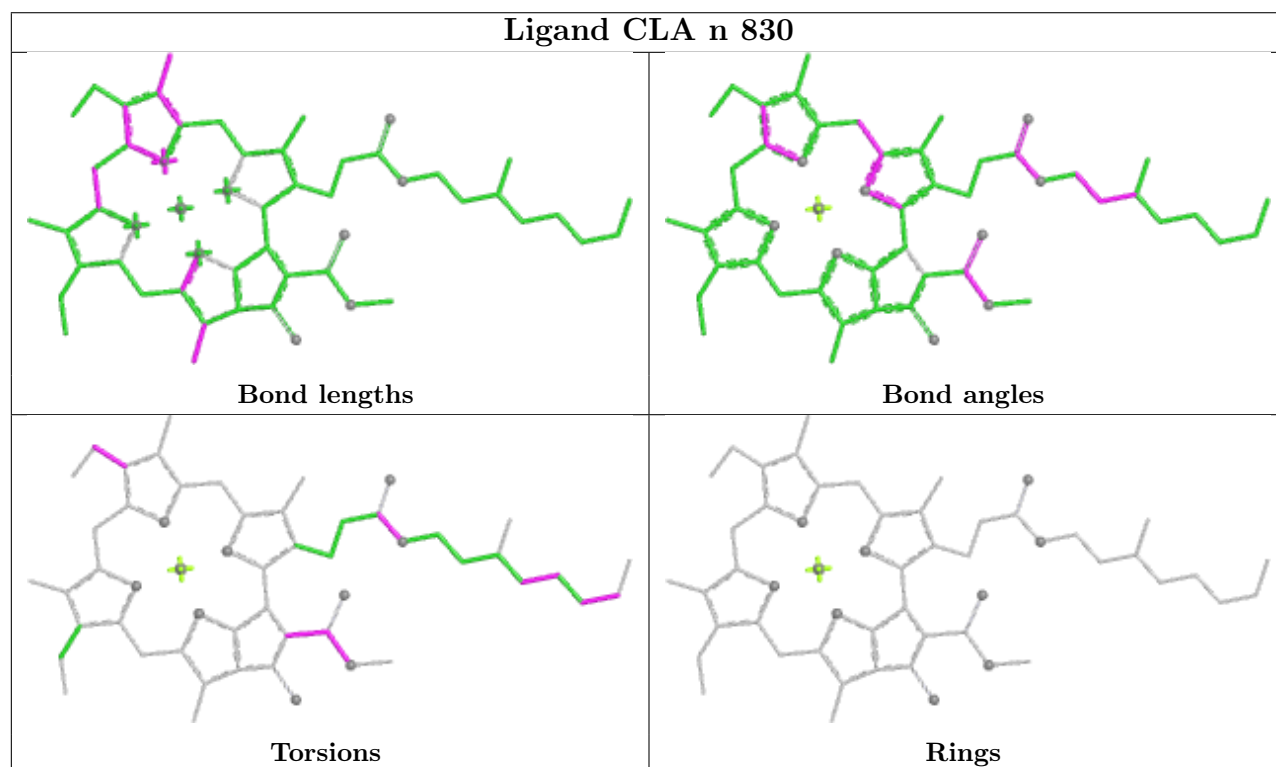
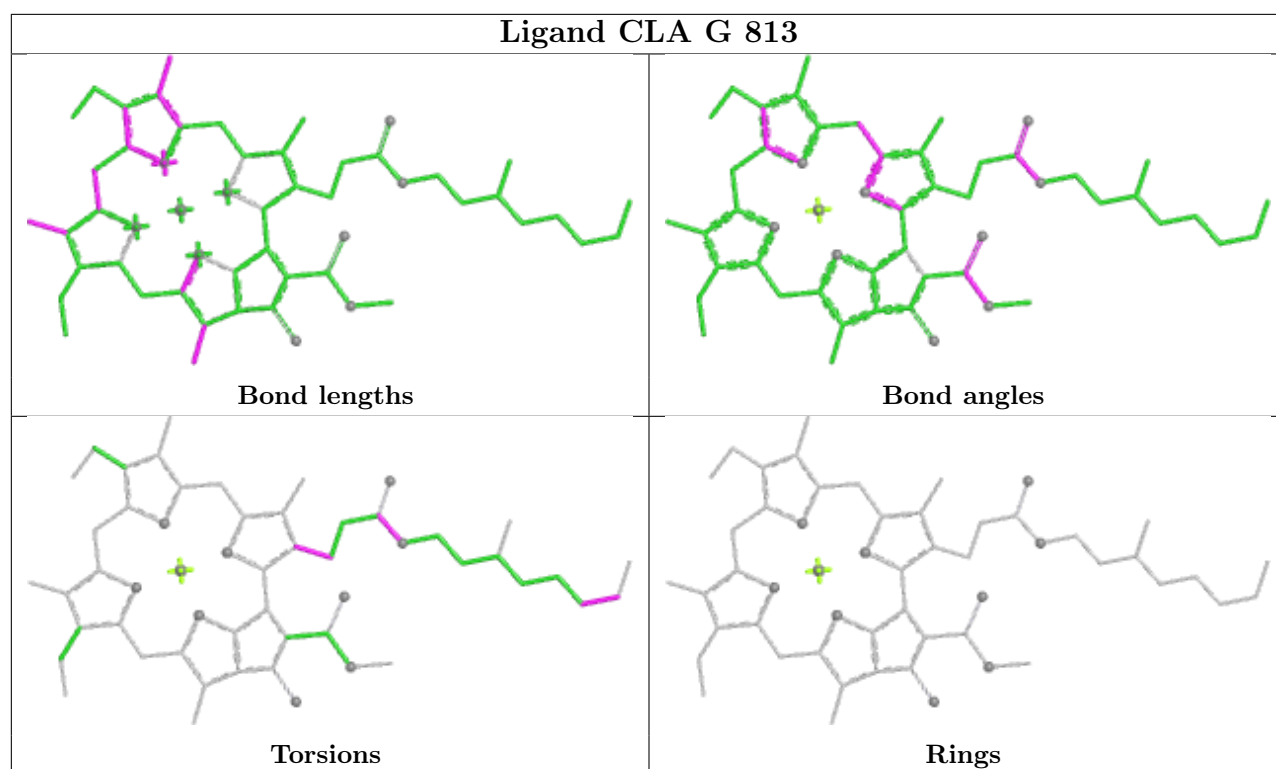
Bond angles



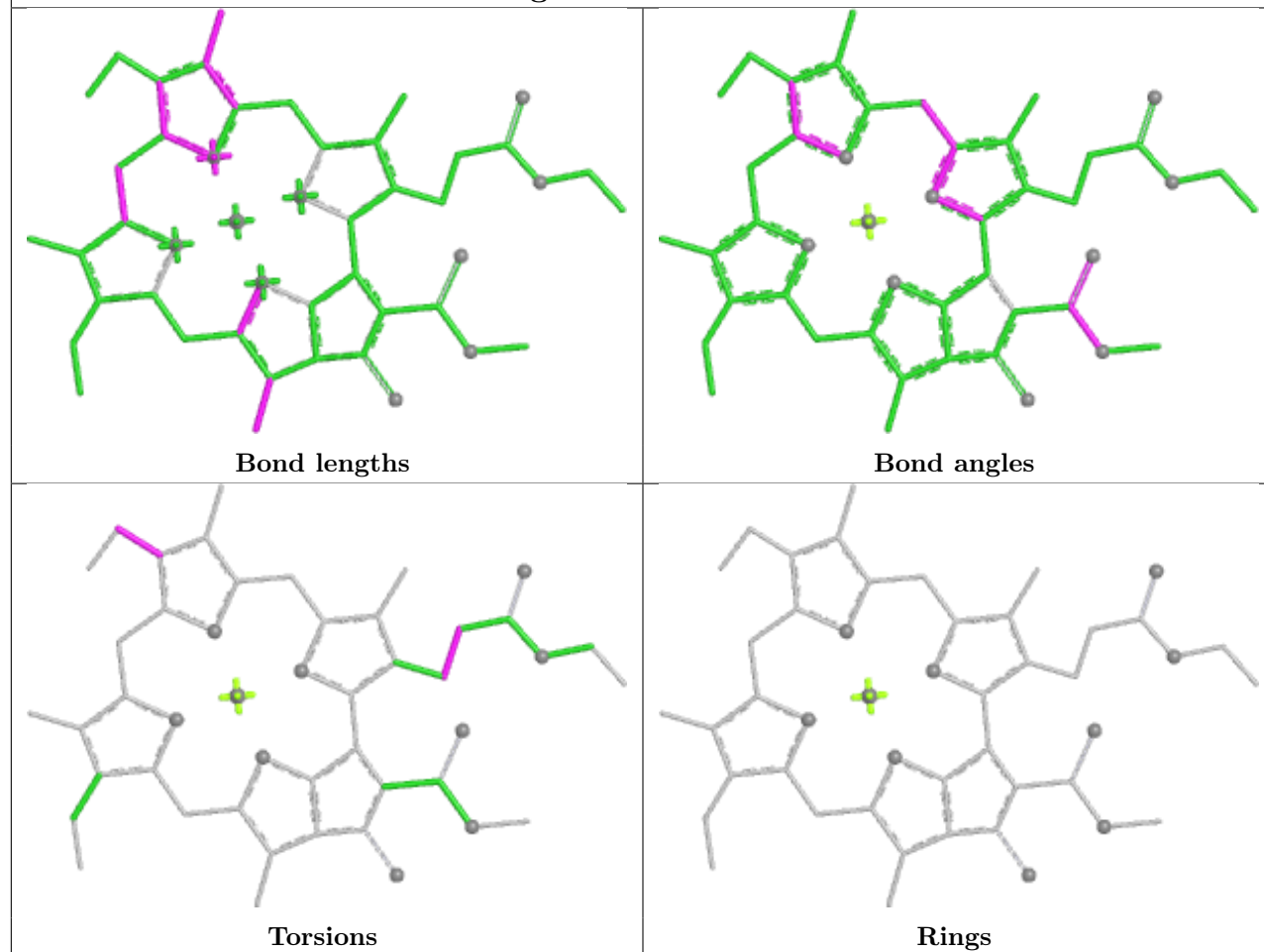
Torsions



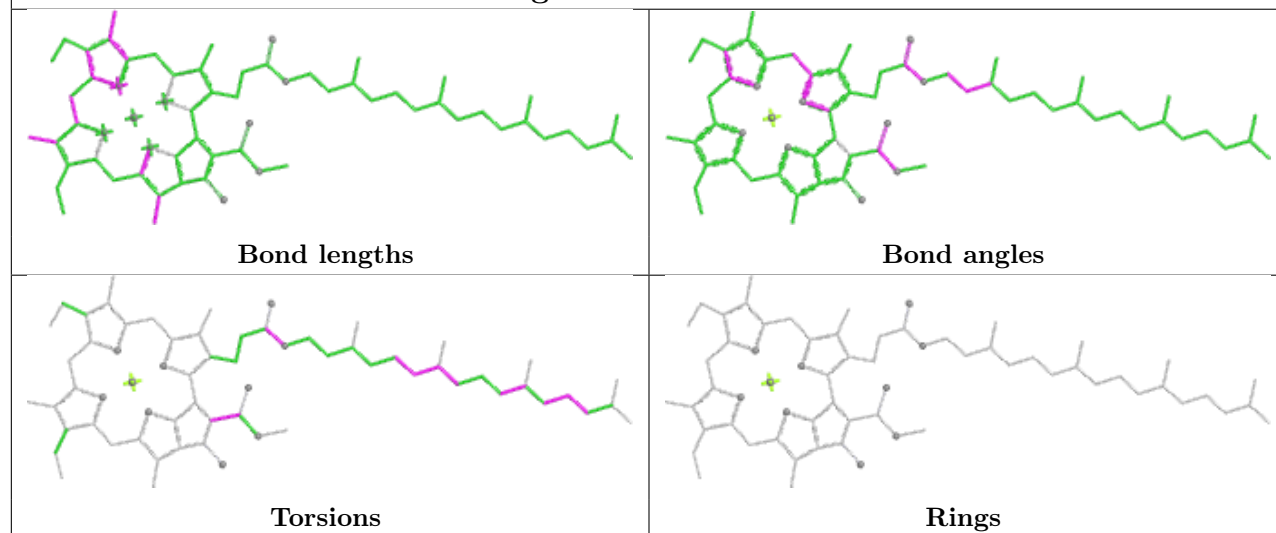
Rings

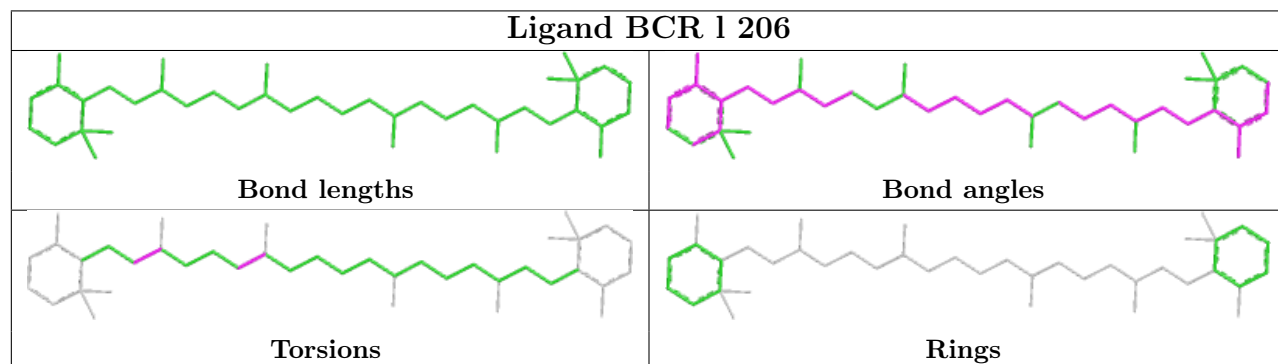
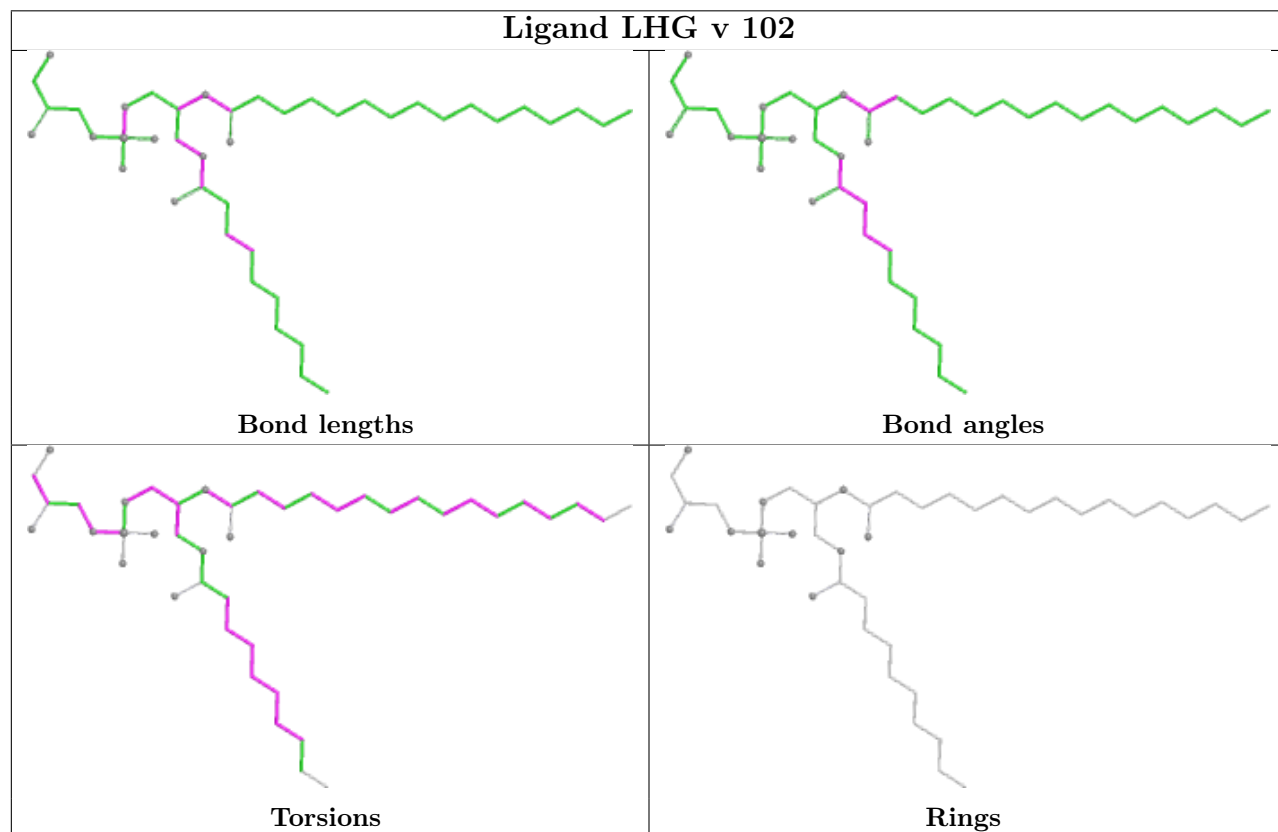
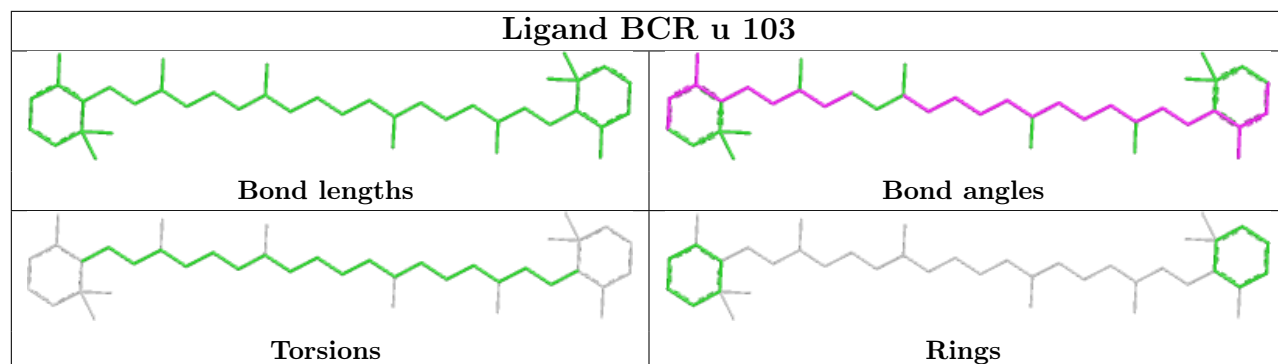


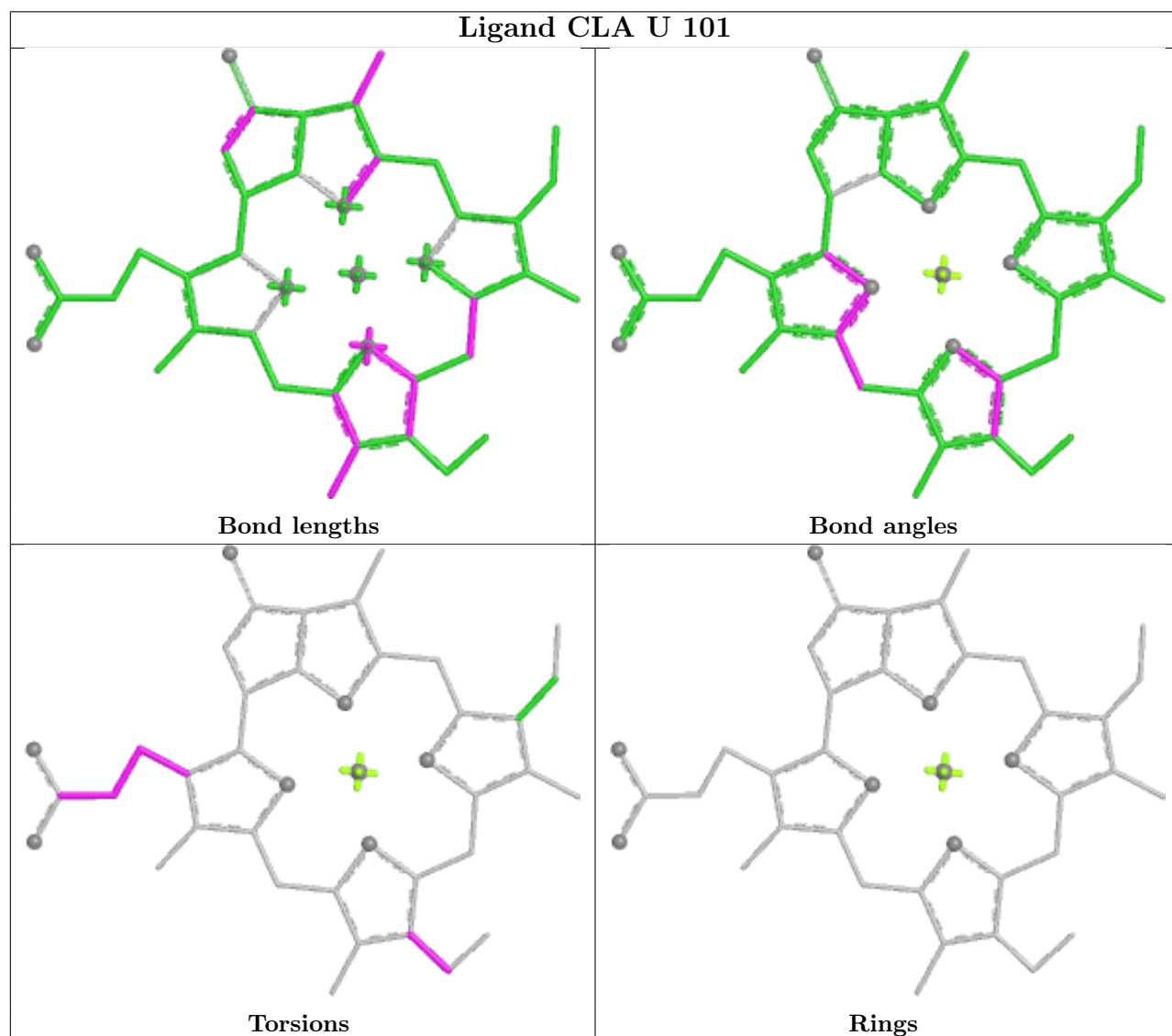
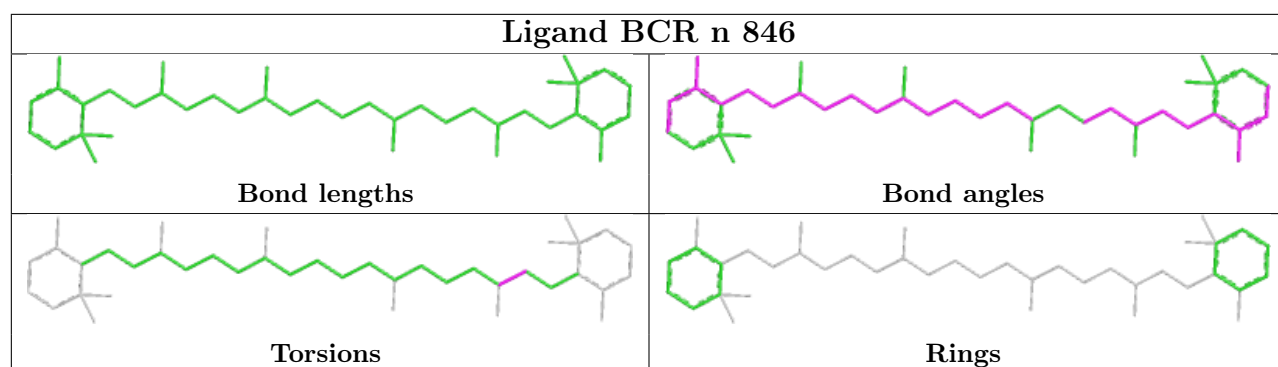
## Ligand CLA b 839

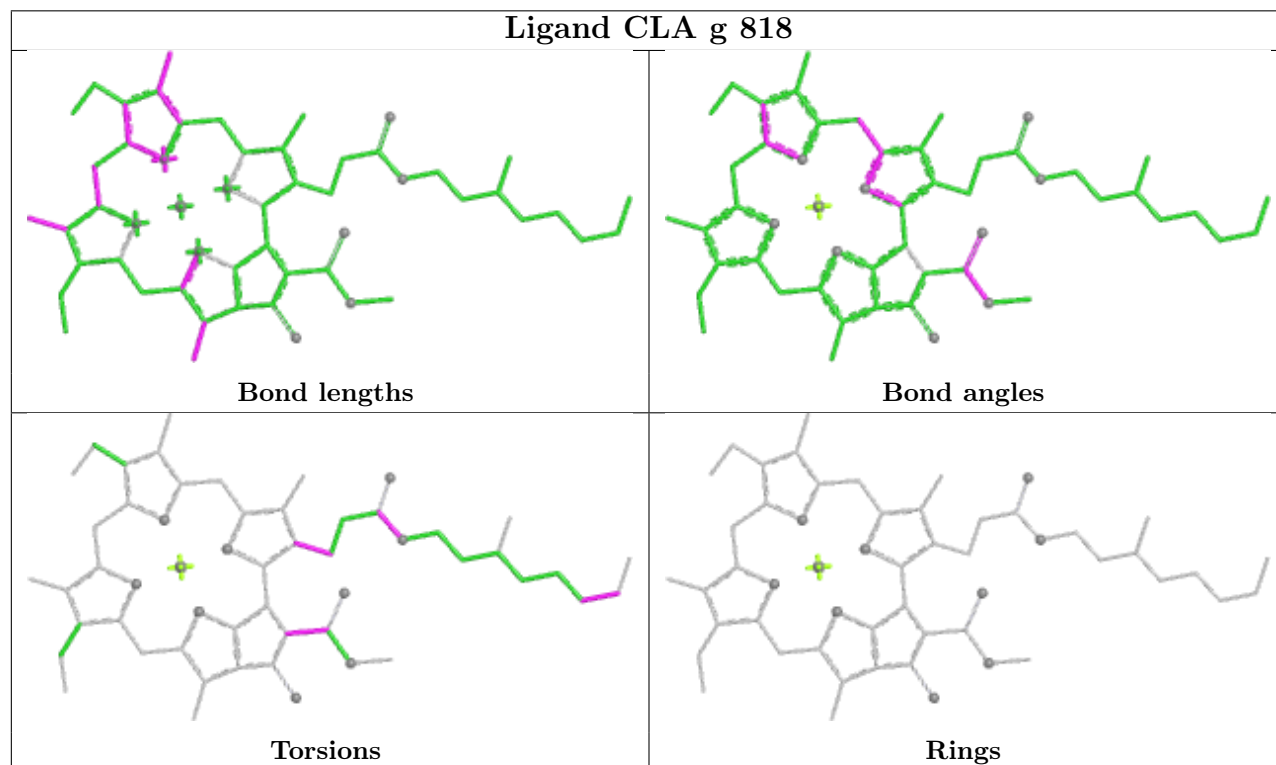
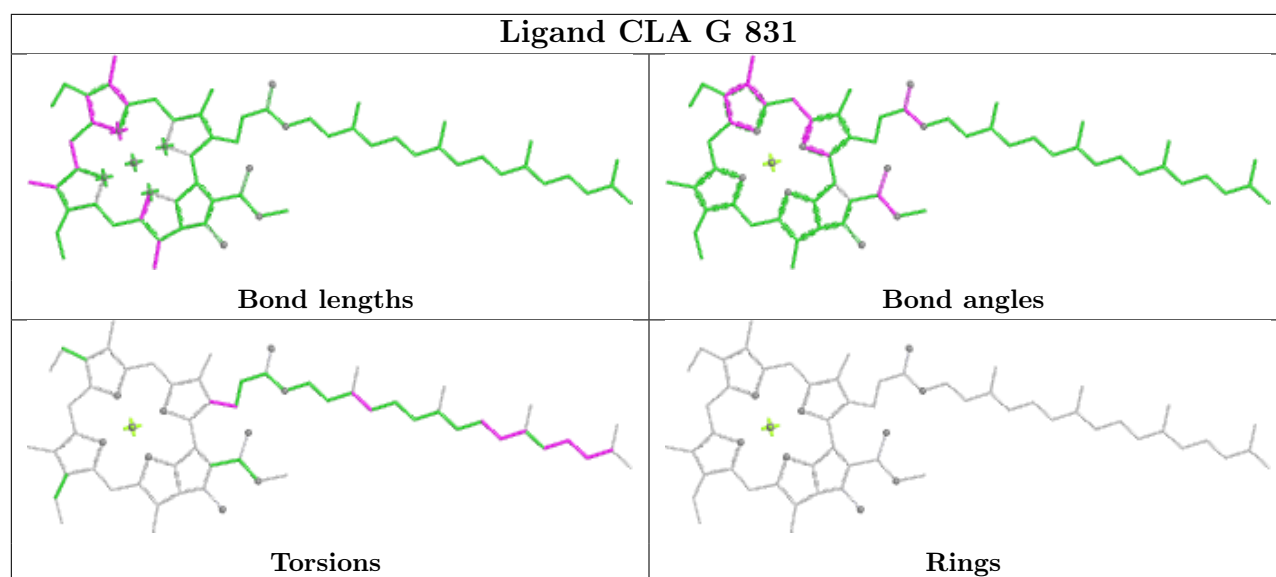


## Ligand CLA N 826

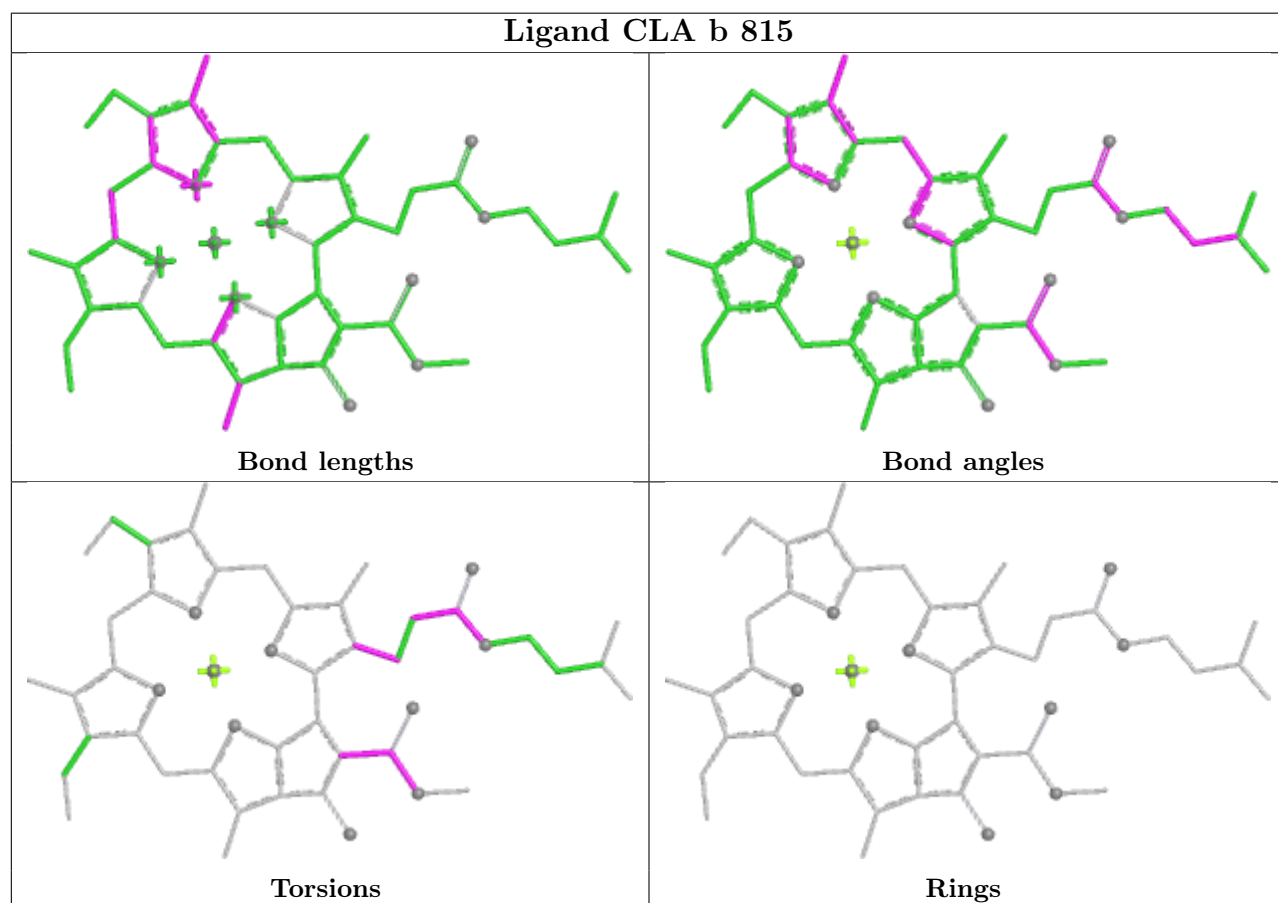
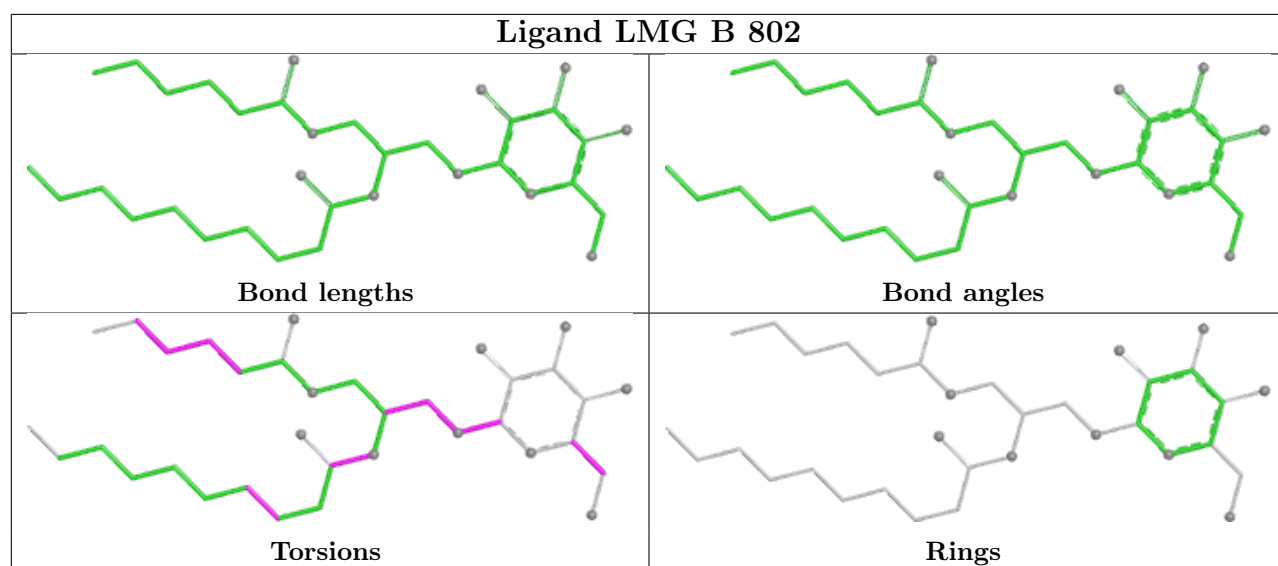


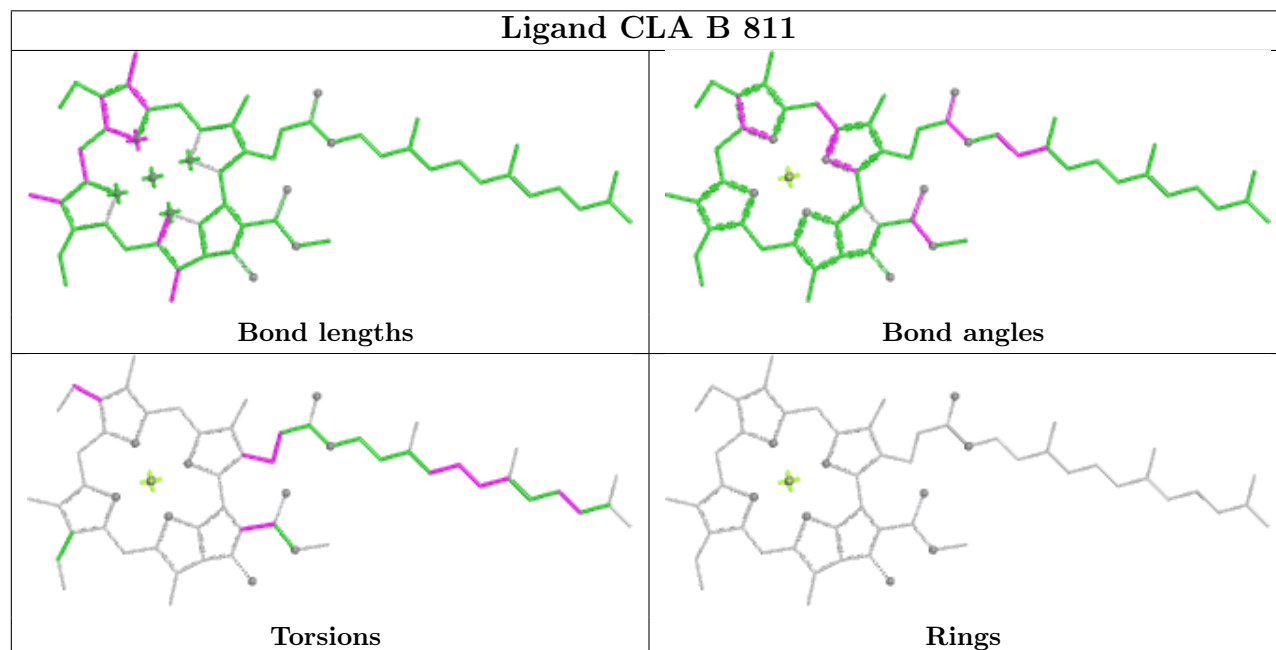
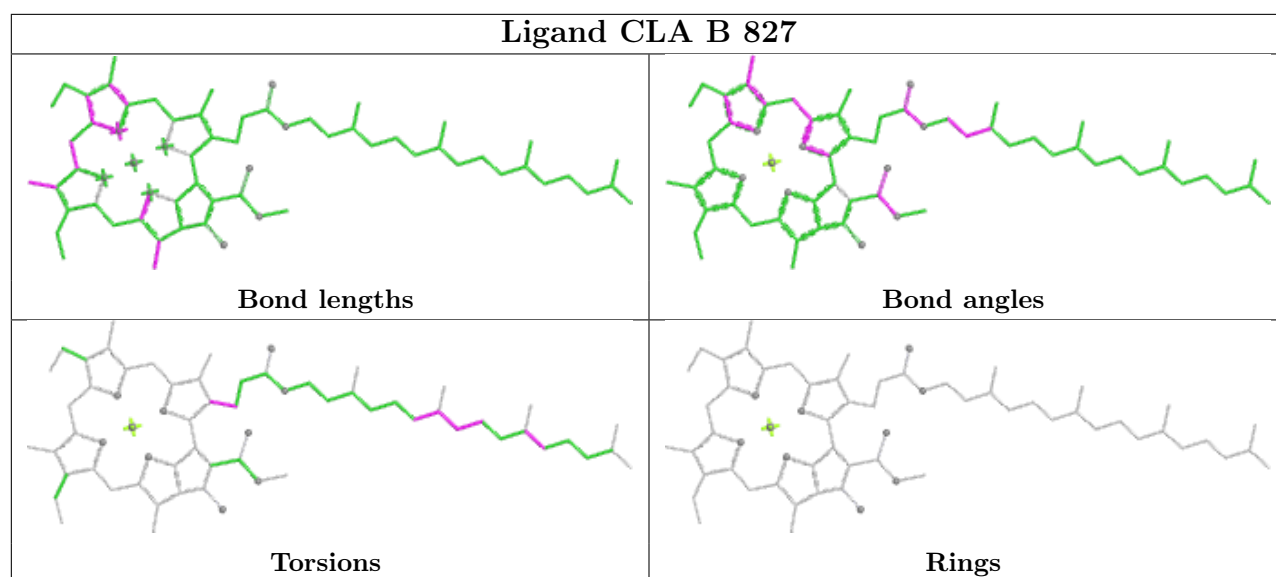


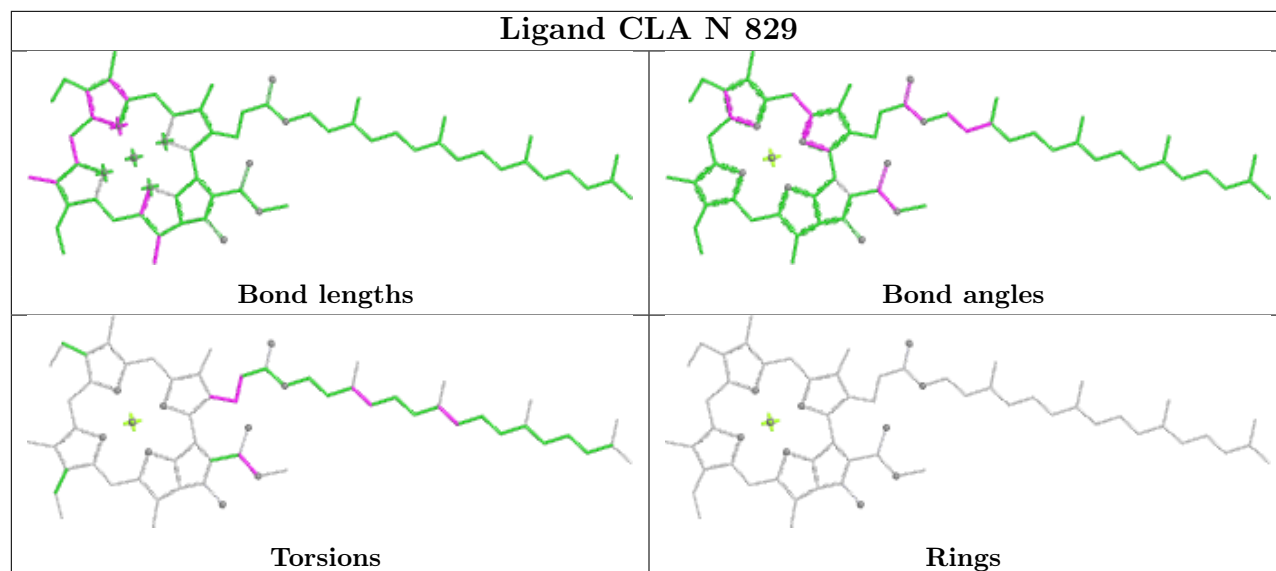
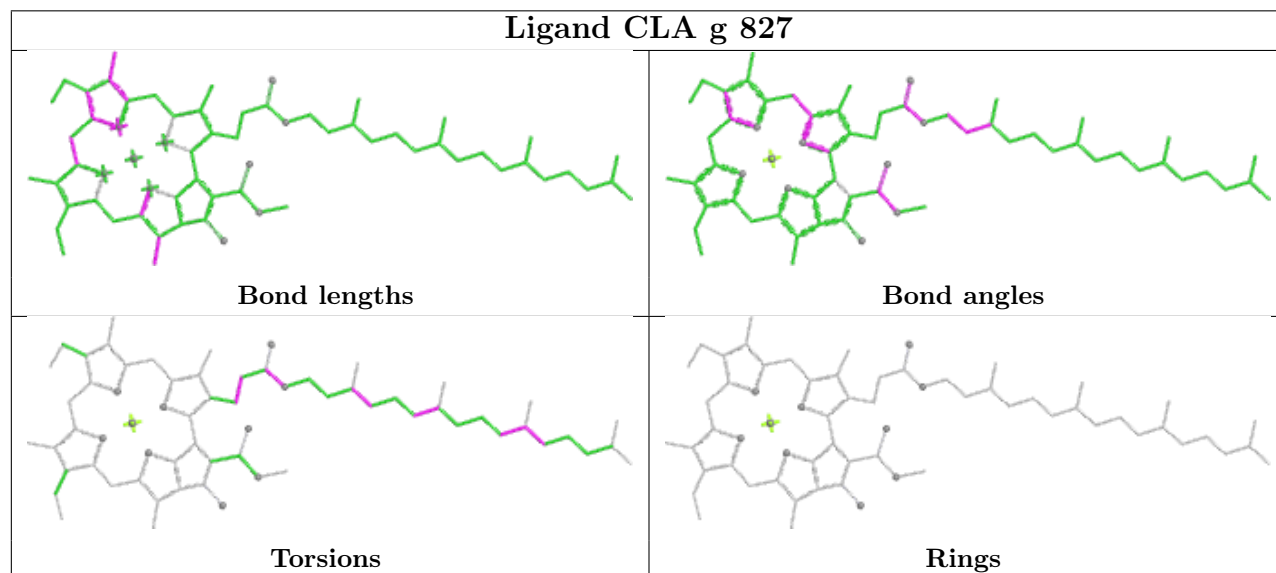
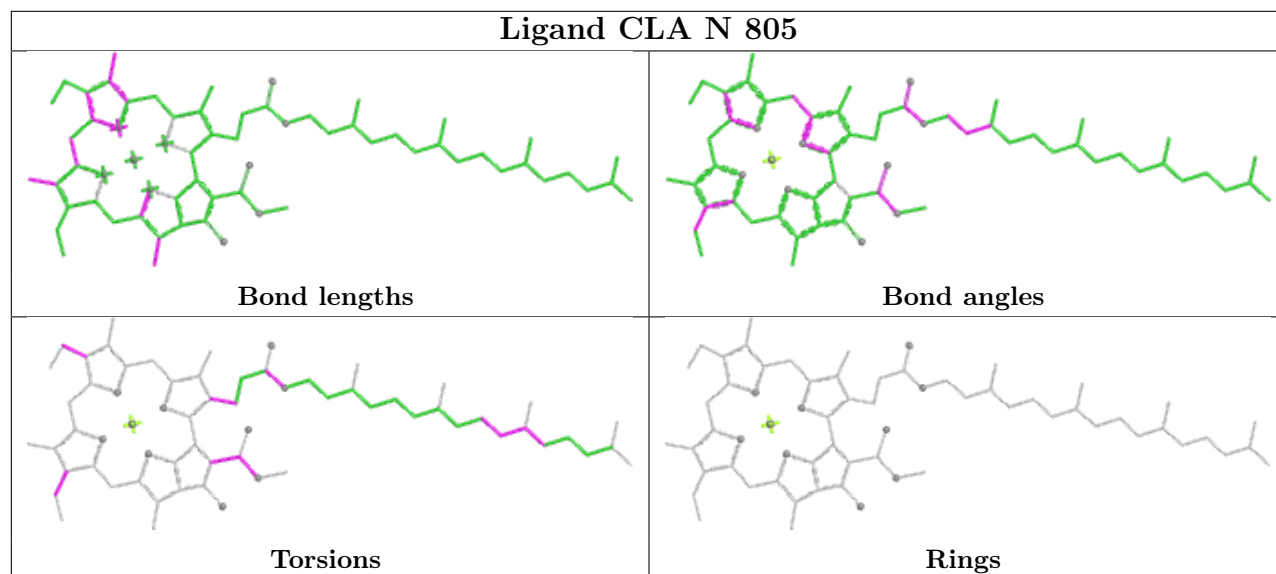


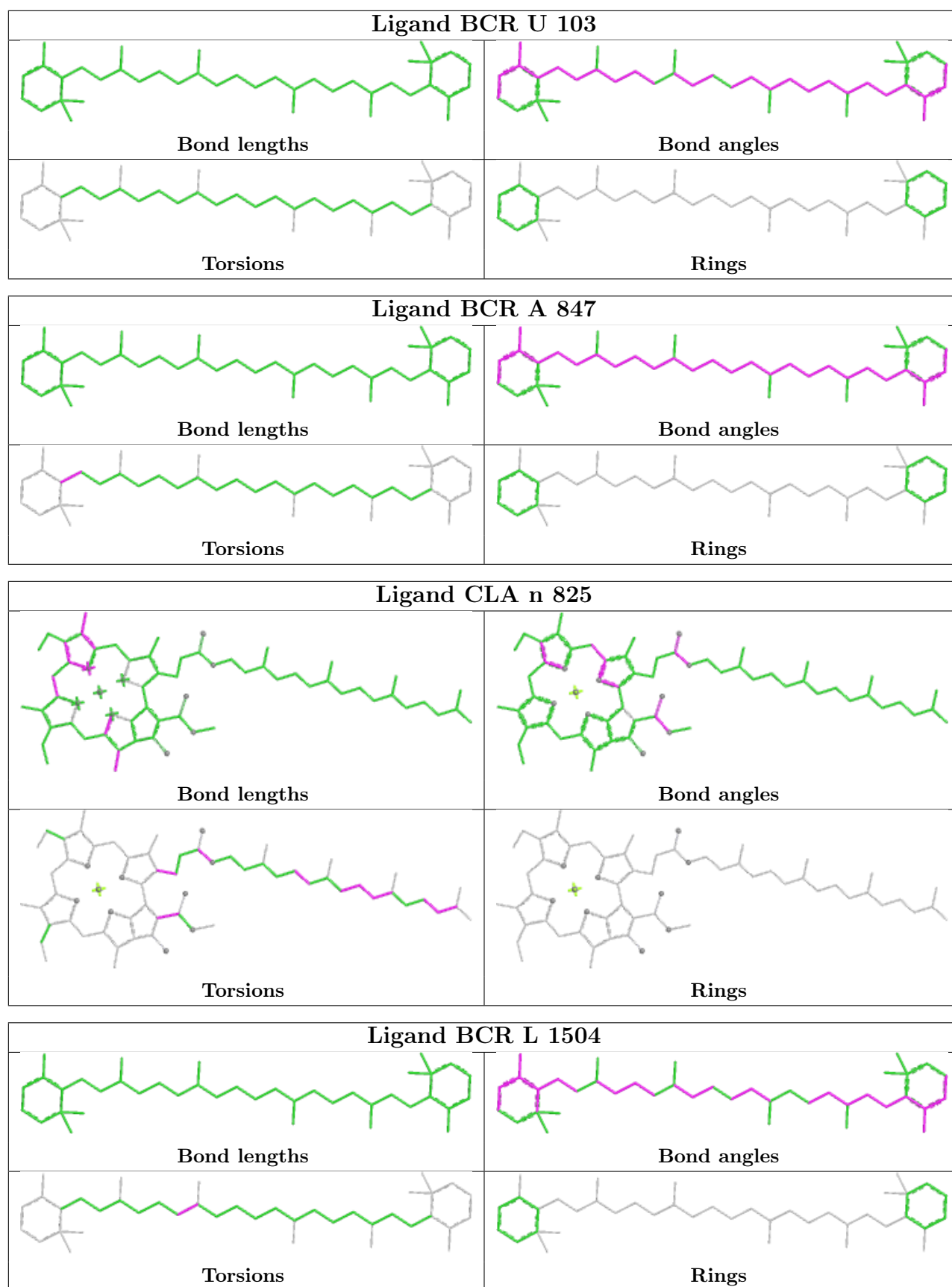


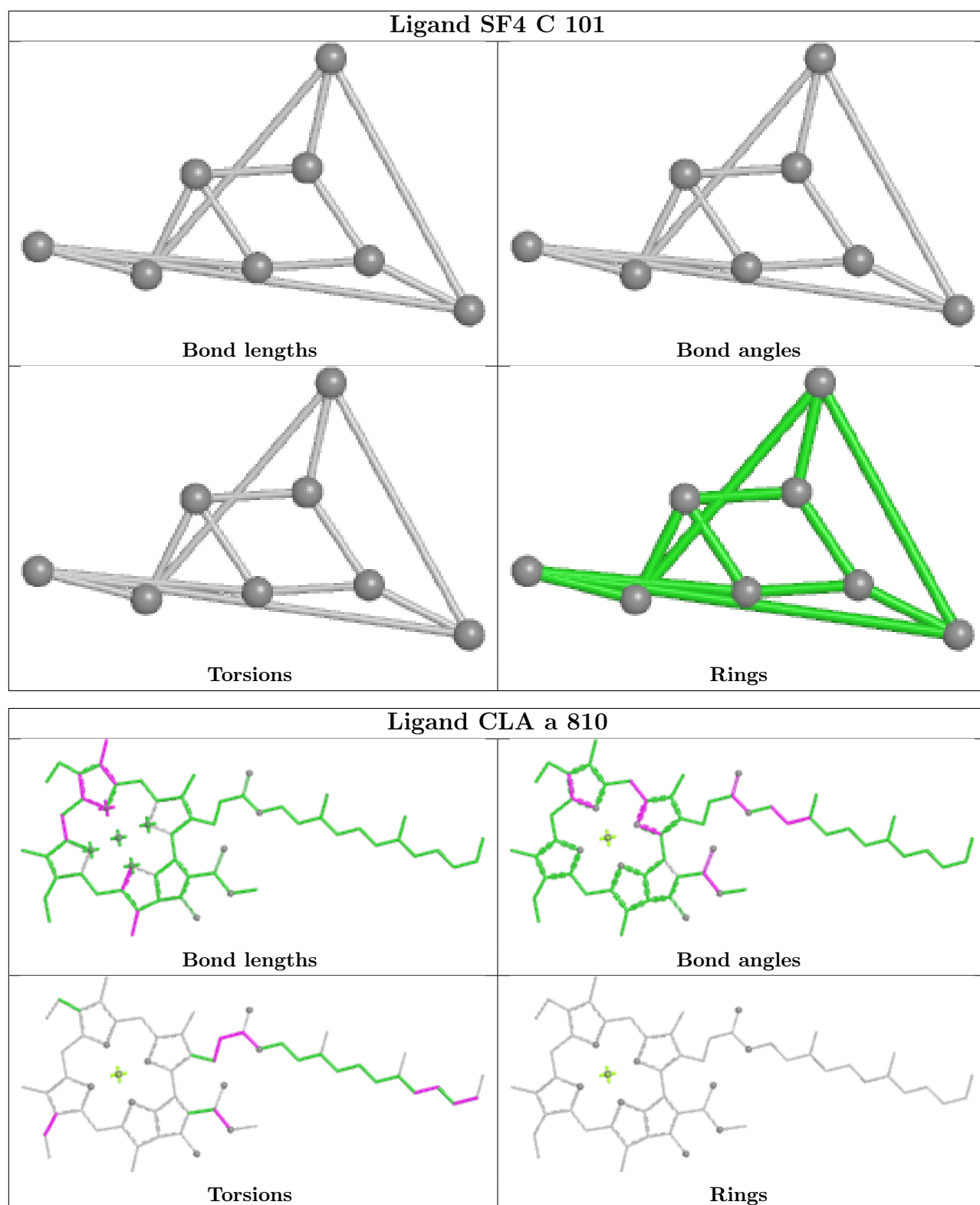


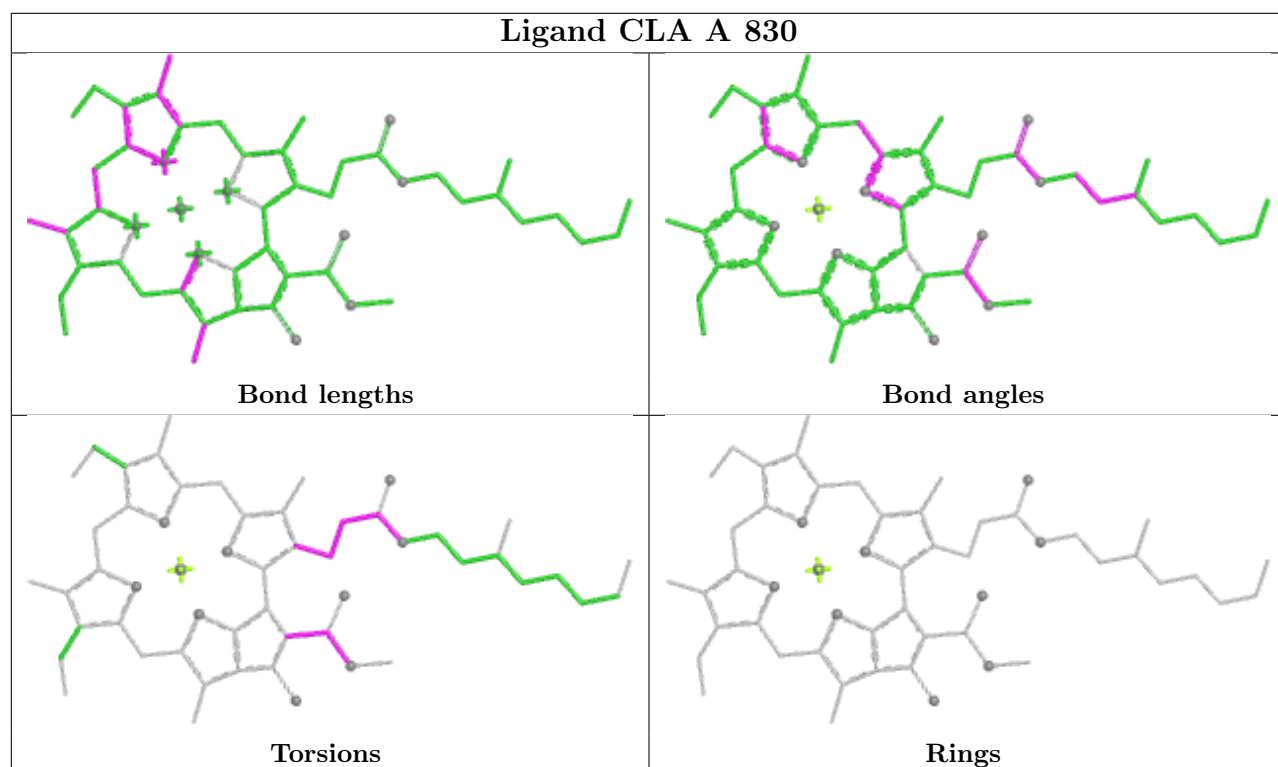
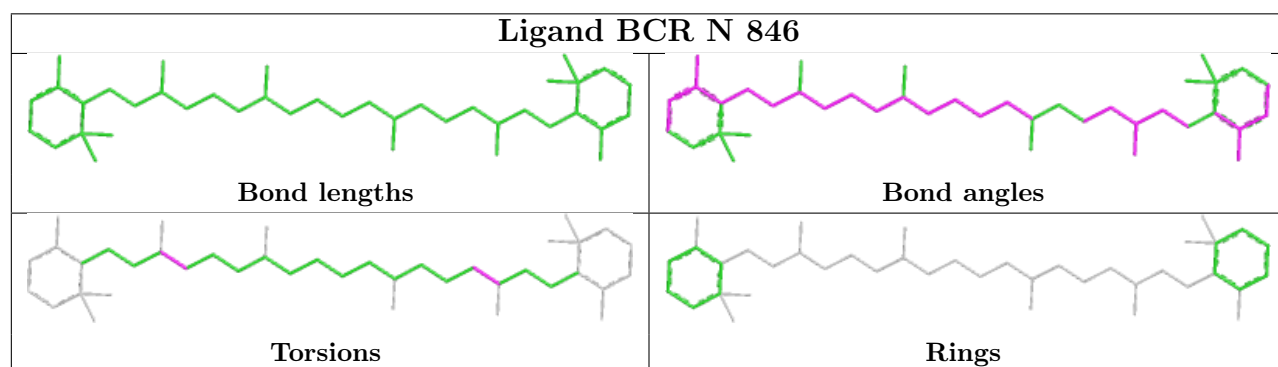
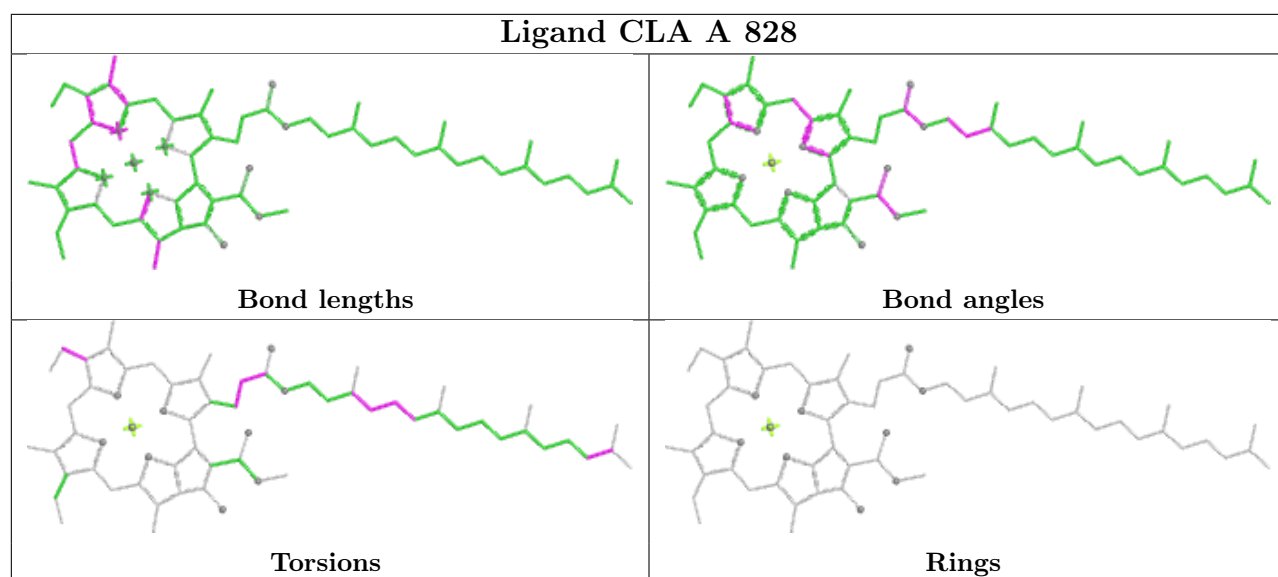


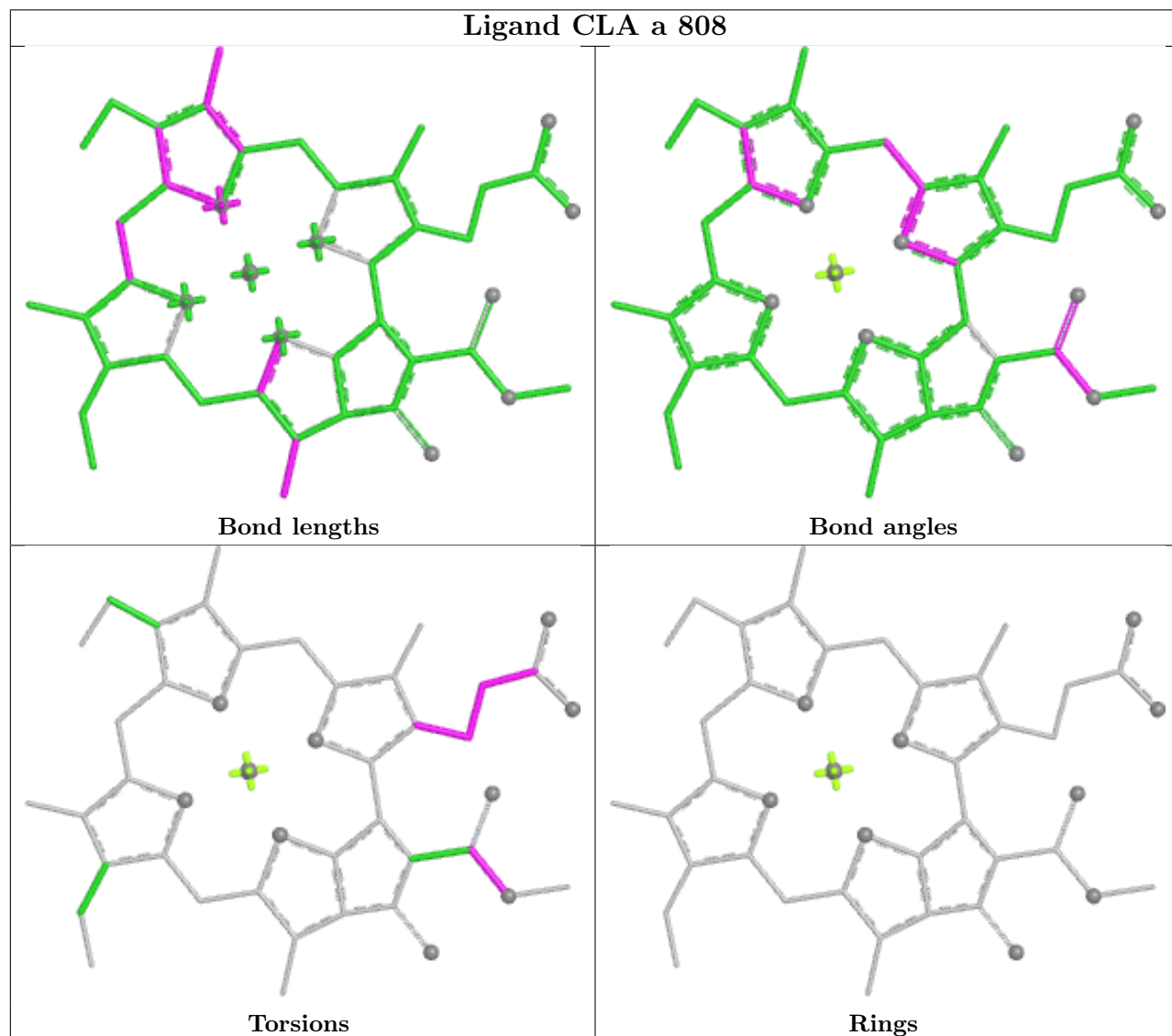
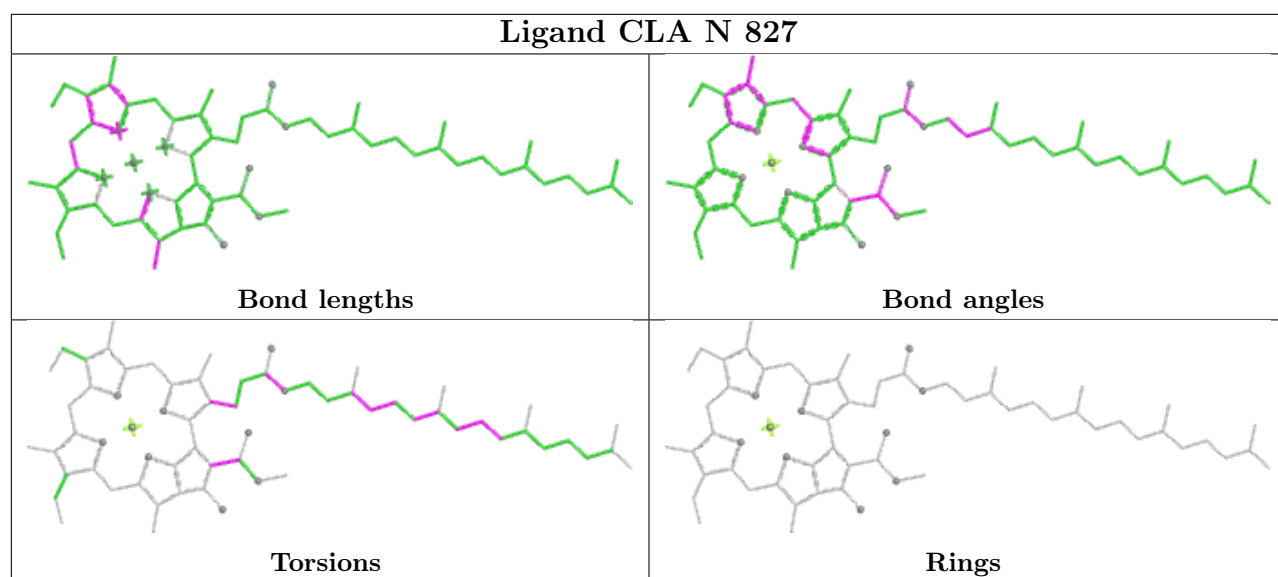


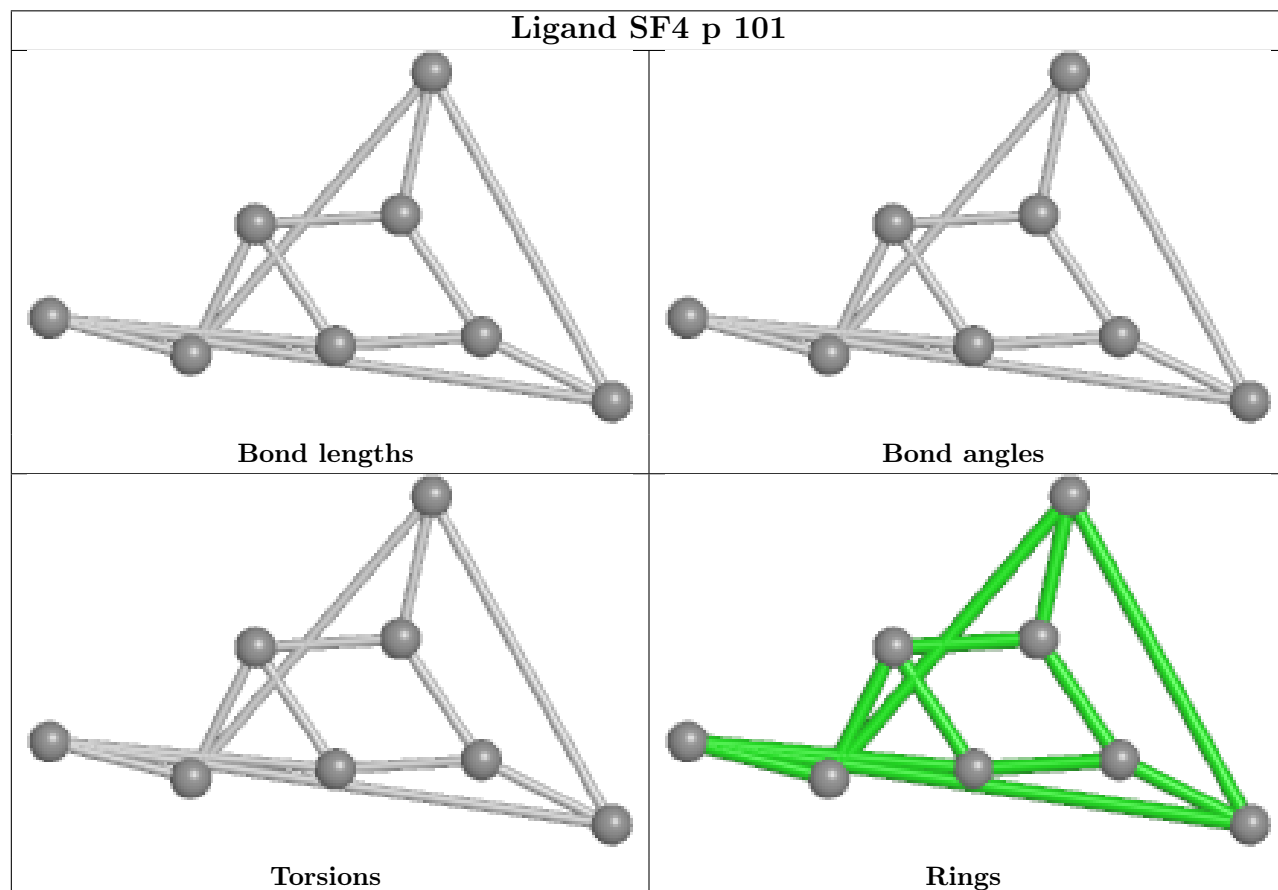
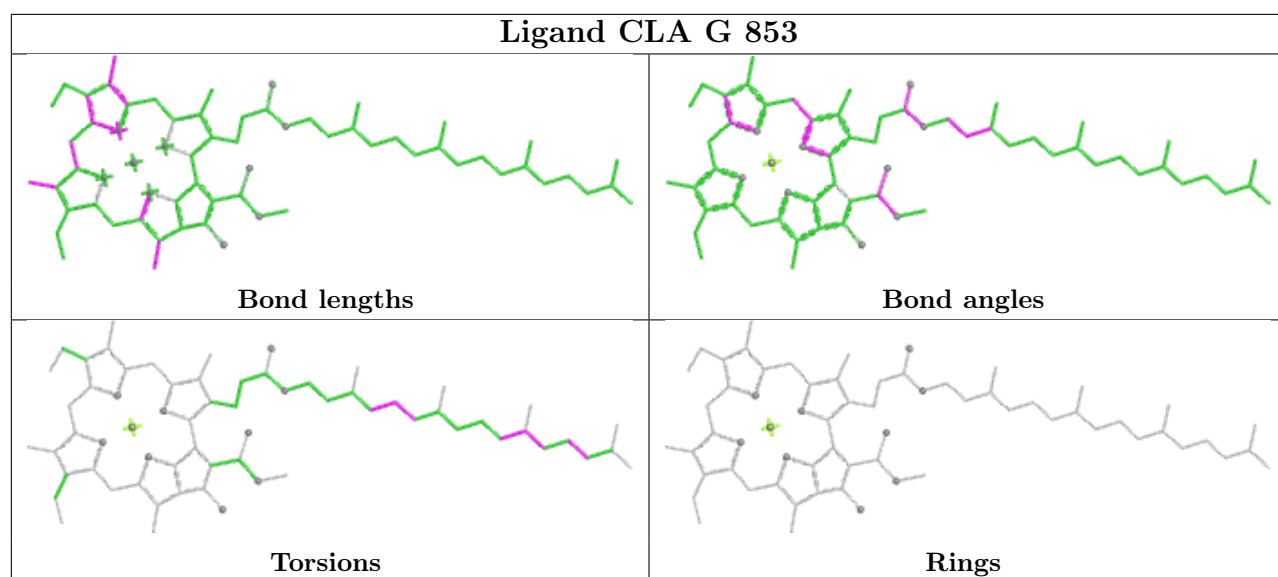




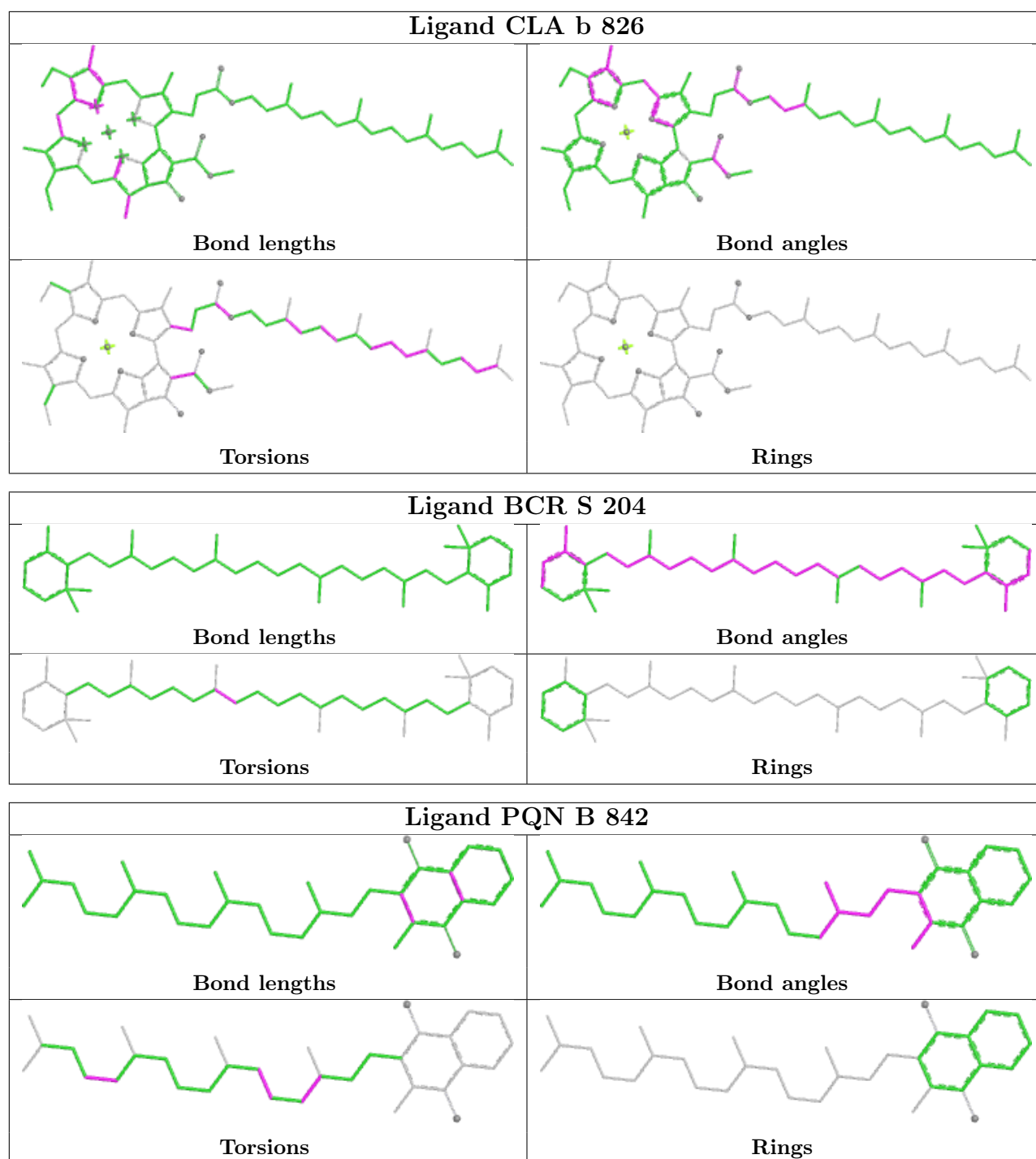


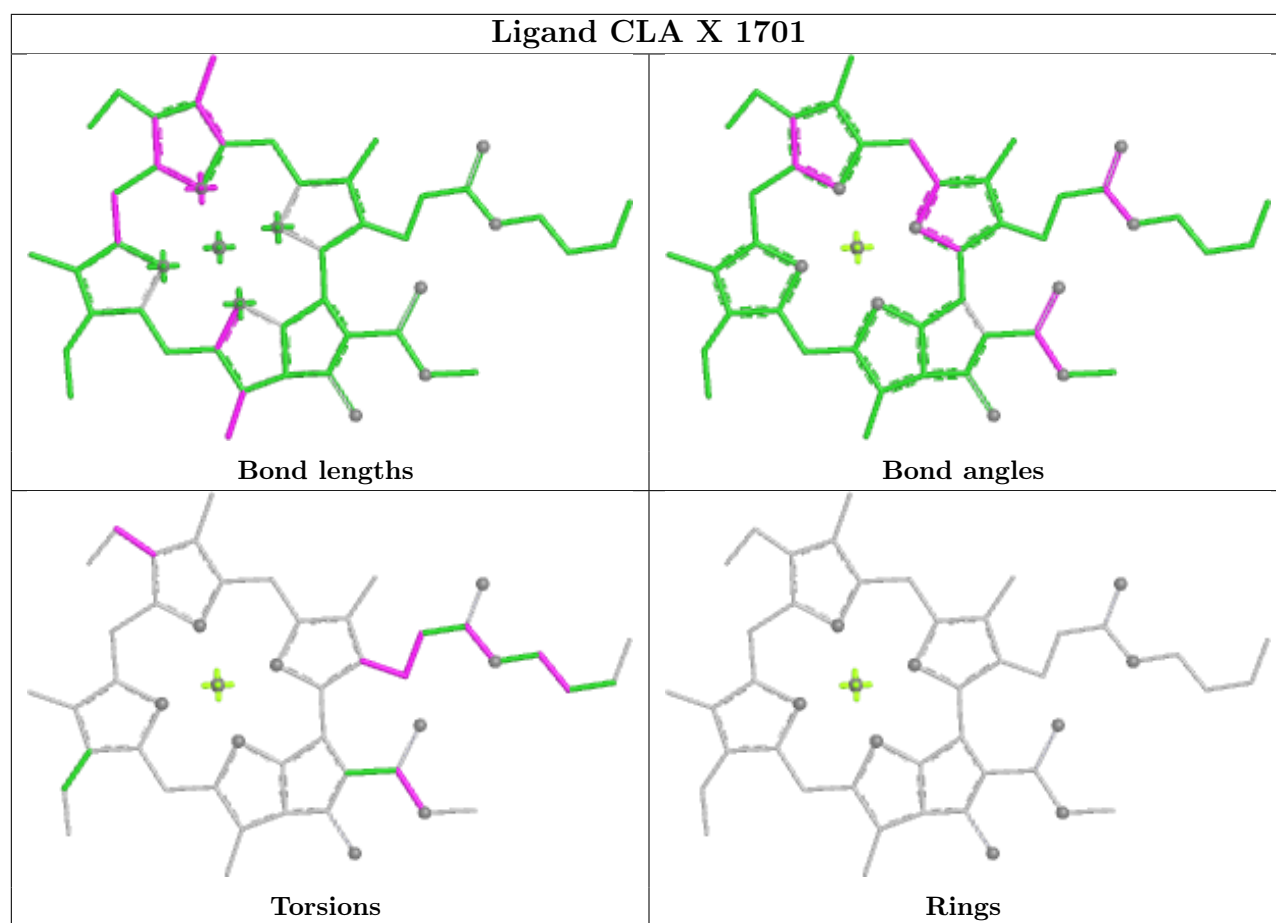




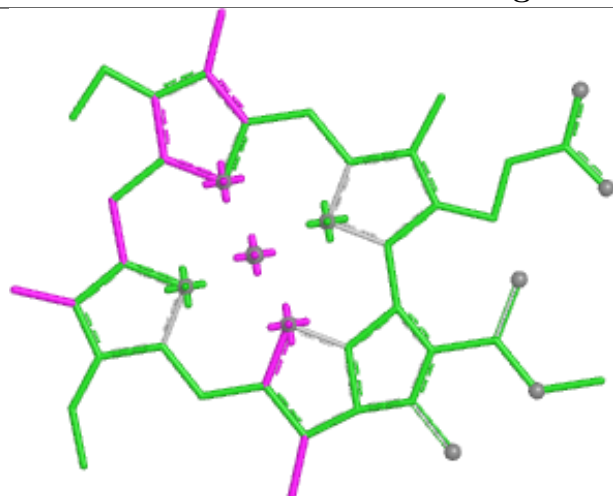








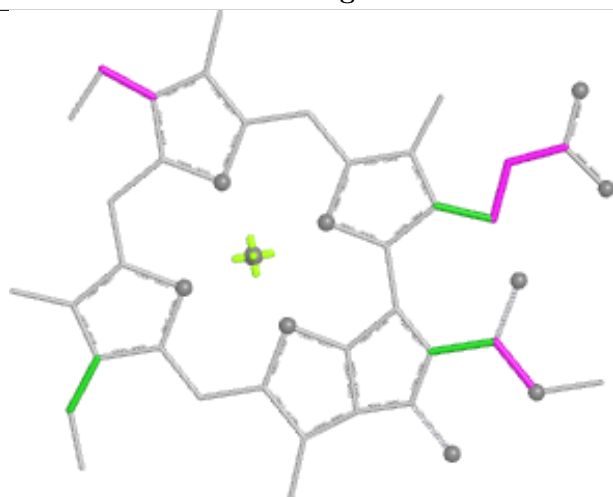
## Ligand CLA G 852



Bond lengths



Bond angles

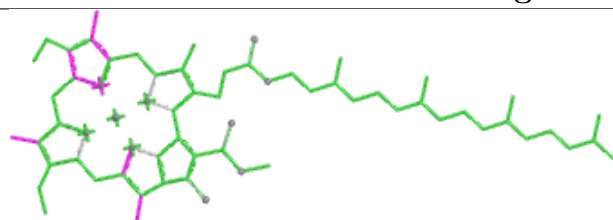


Torsions

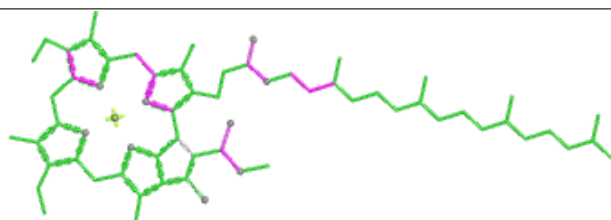


Rings

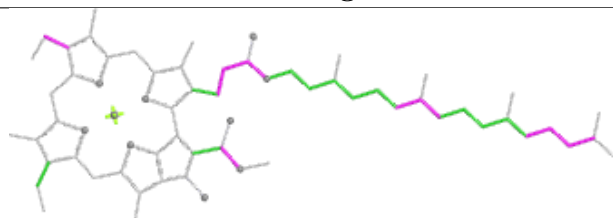
## Ligand CLA B 841



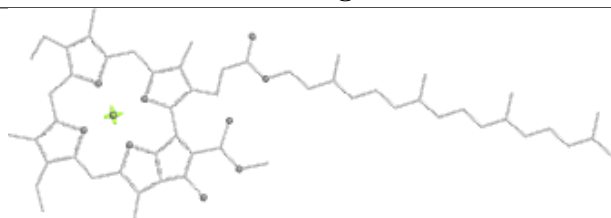
Bond lengths



Bond angles

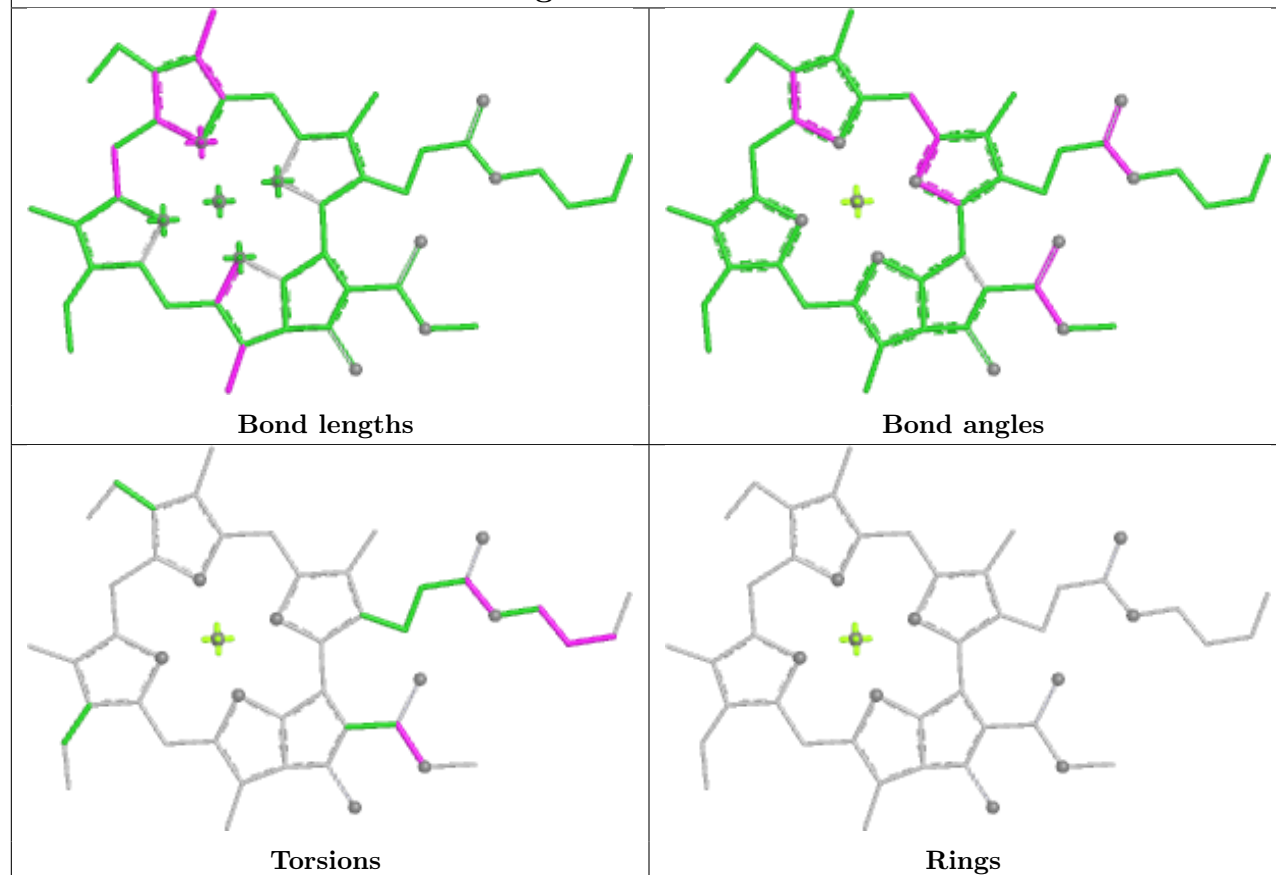


Torsions

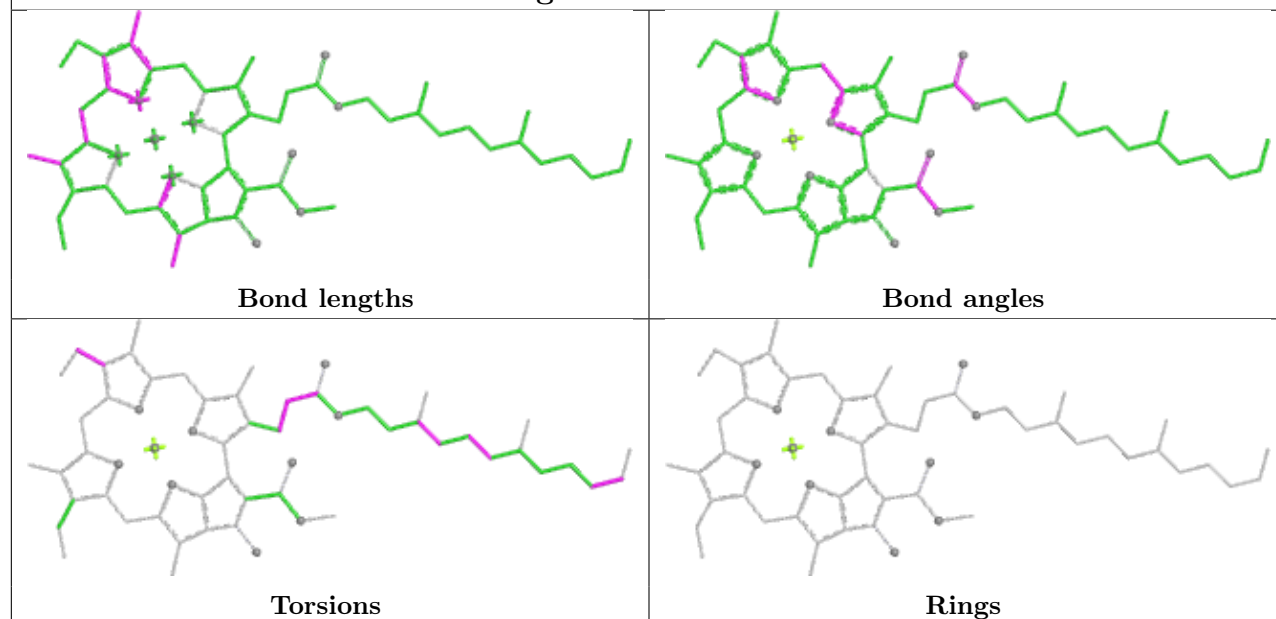


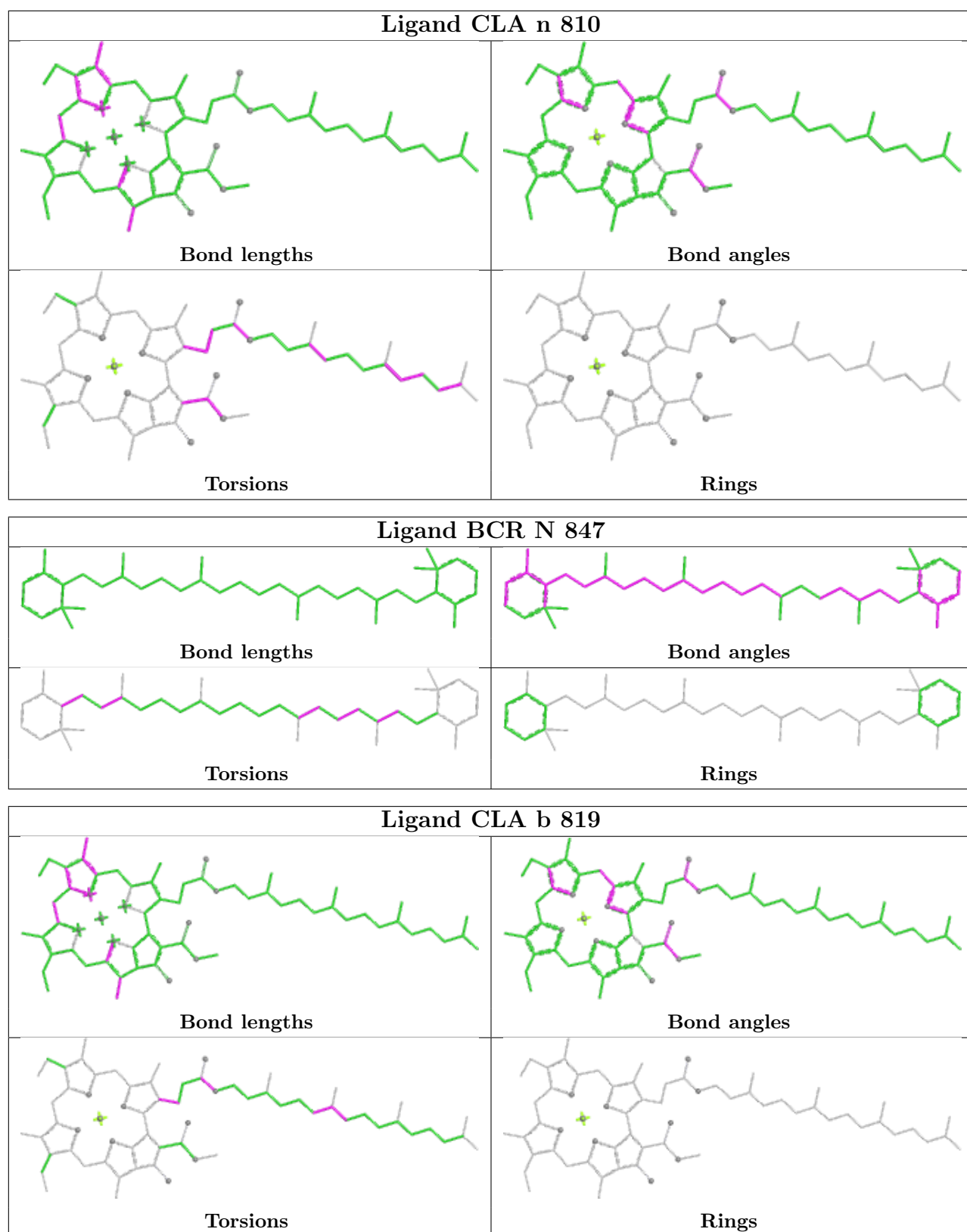
Rings

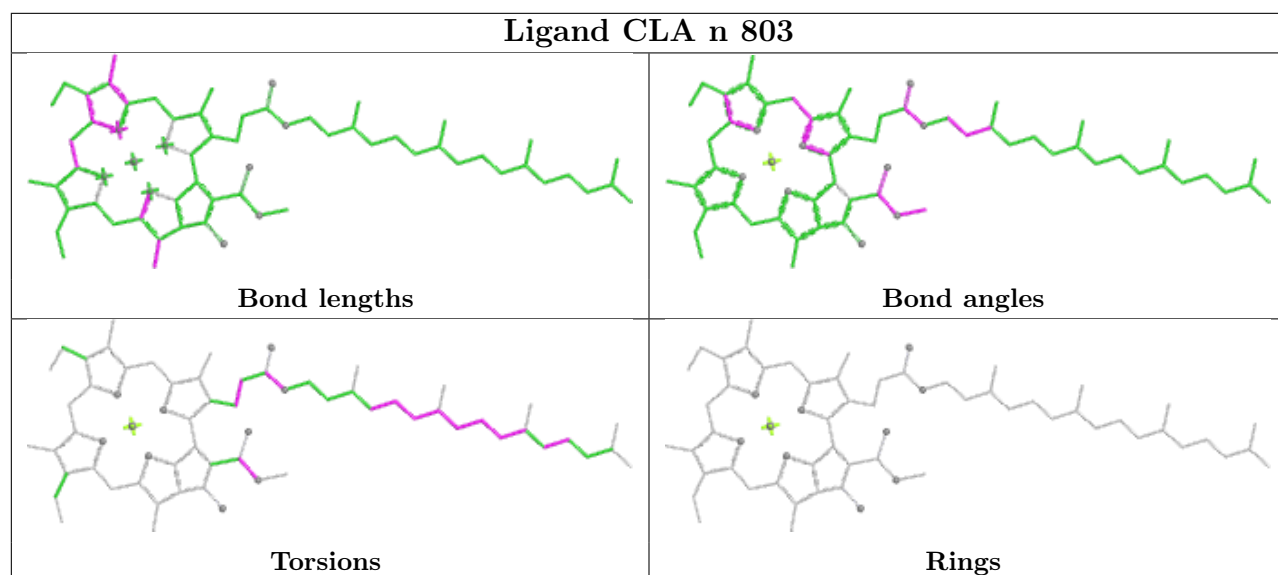
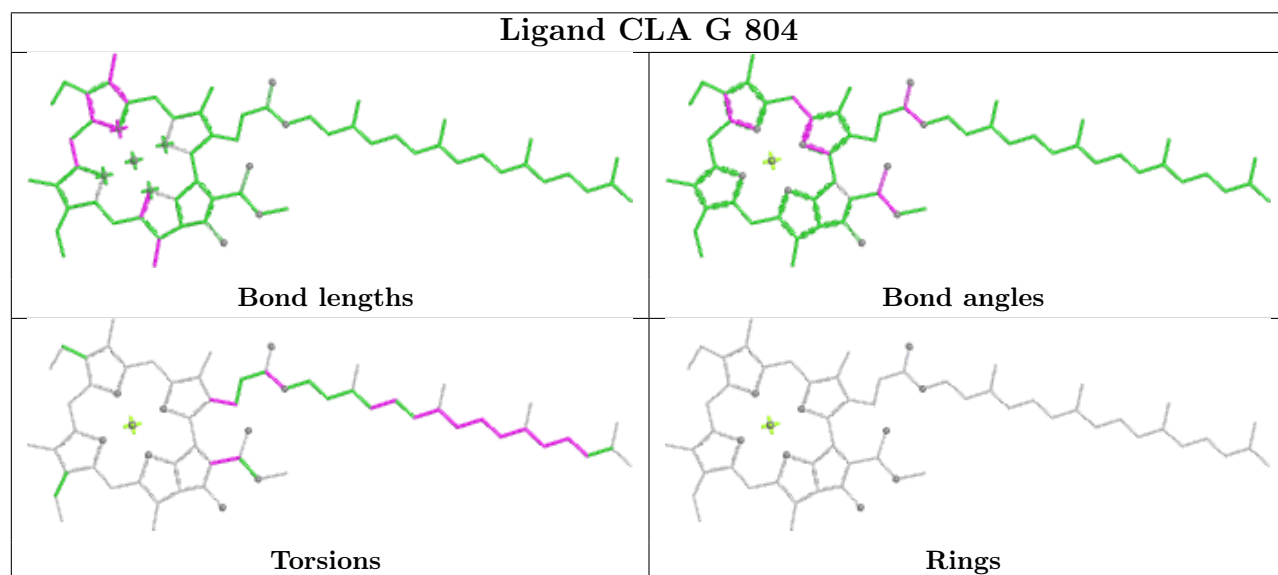
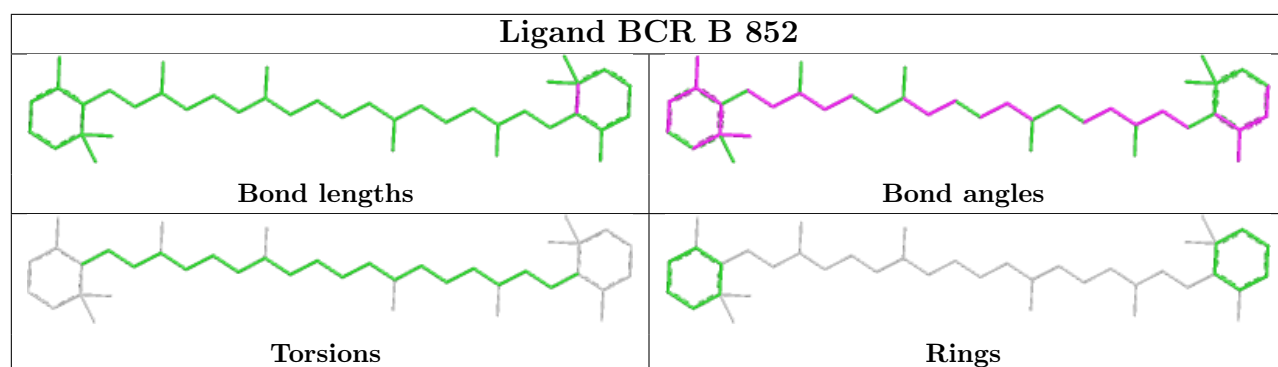
## Ligand CLA n 815



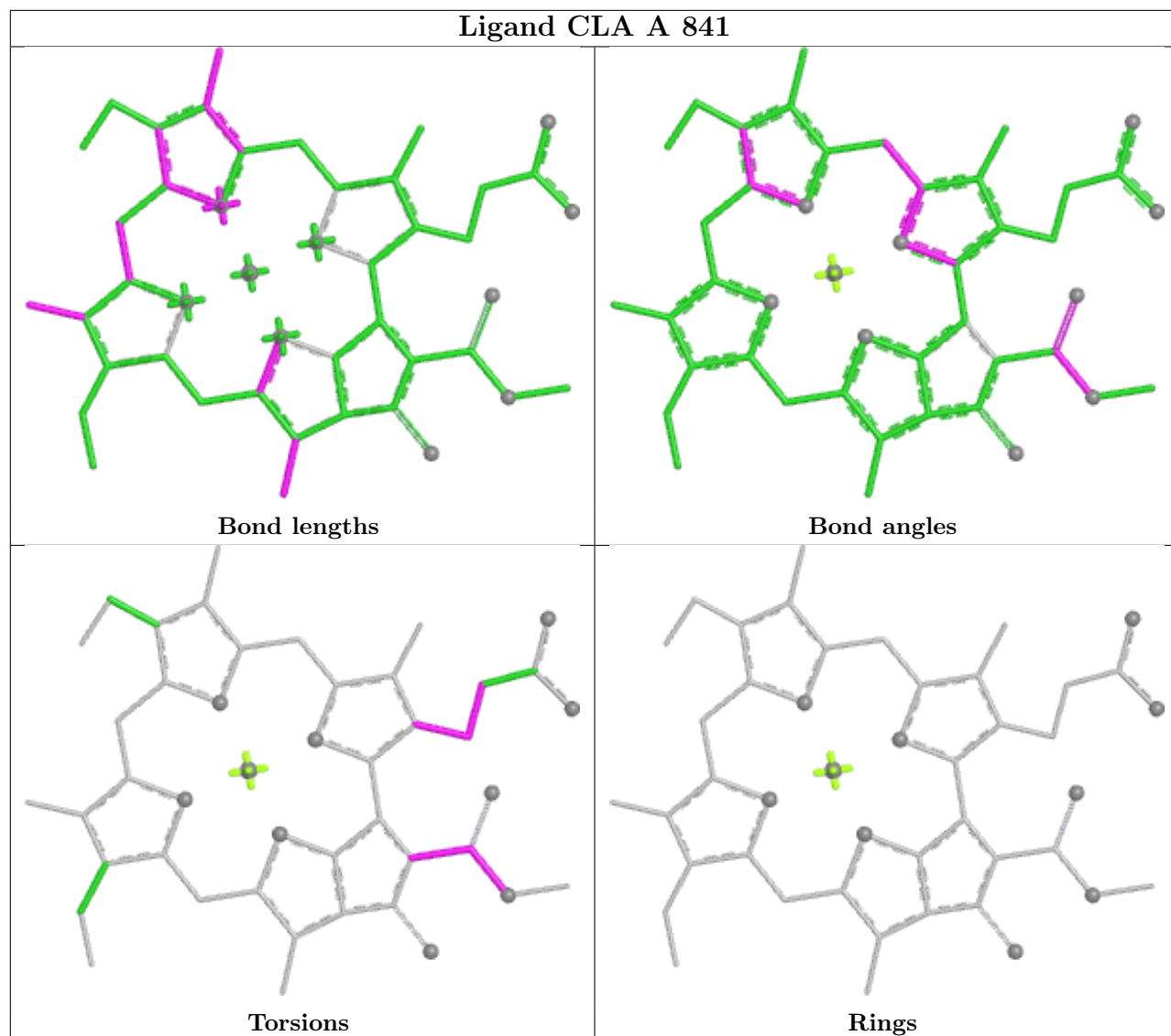
## Ligand CLA a 815



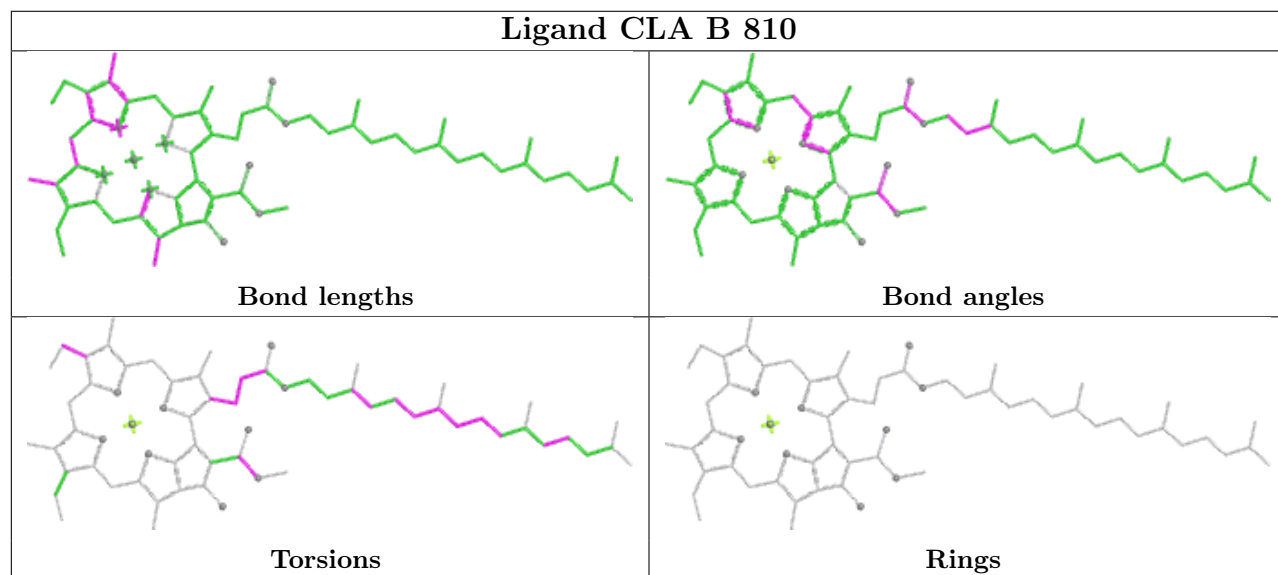


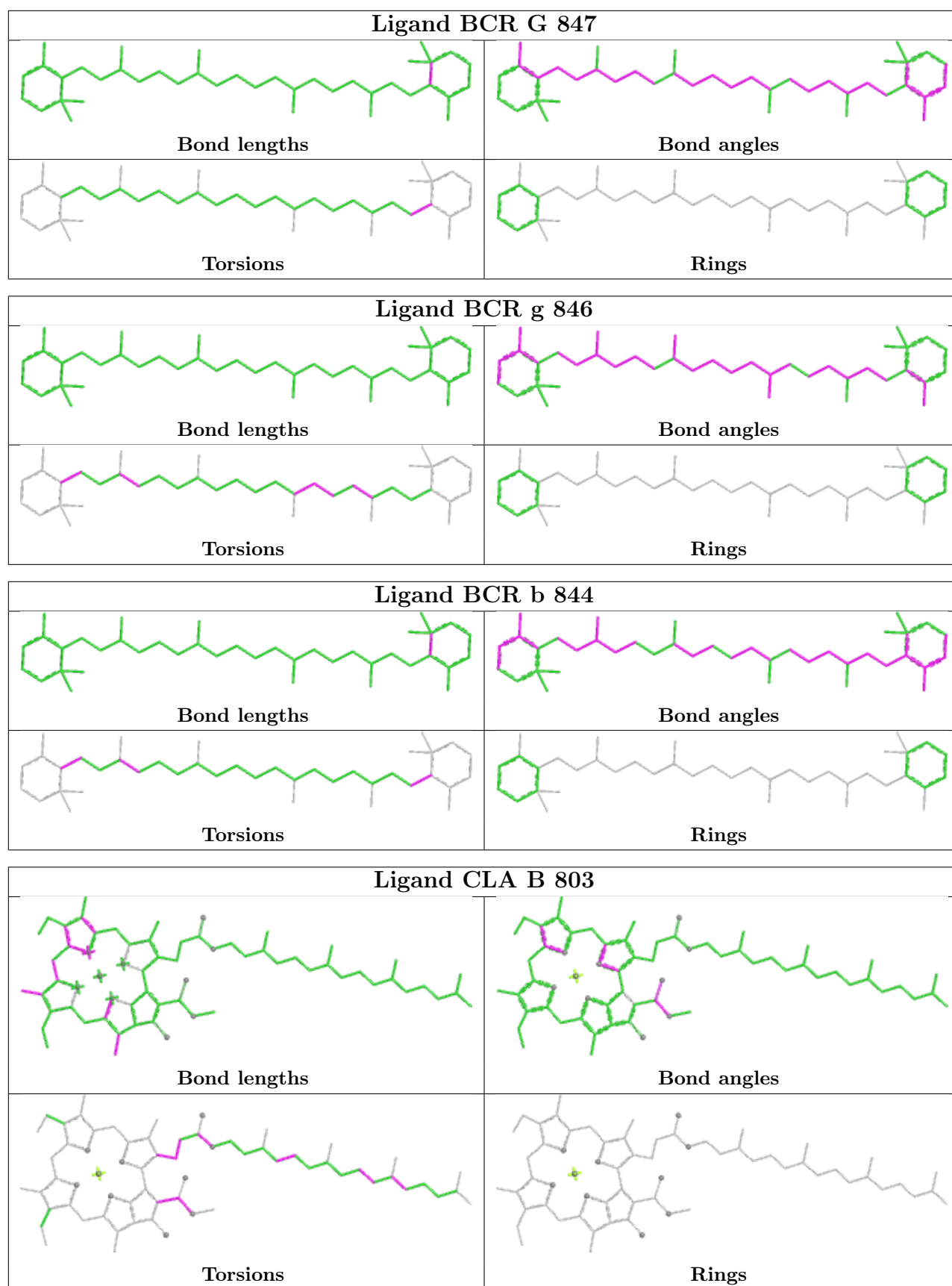


## Ligand CLA A 841

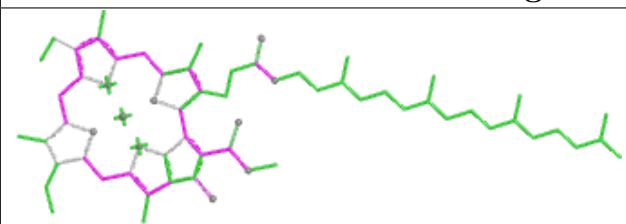
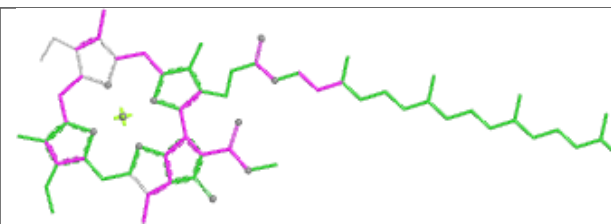
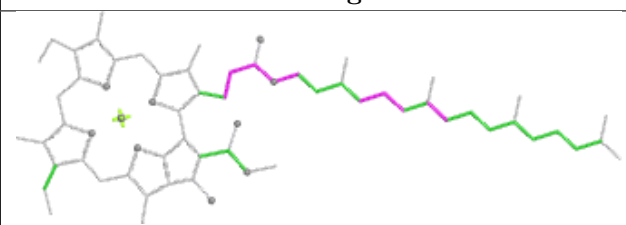
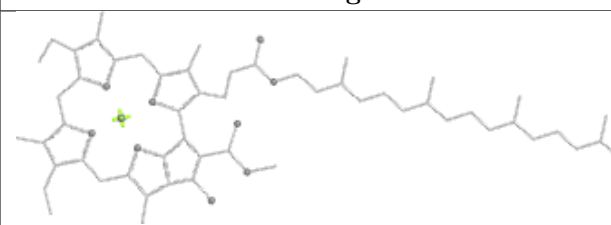


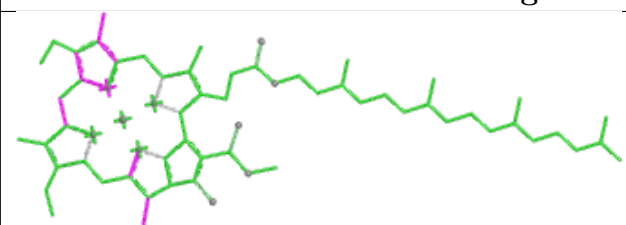
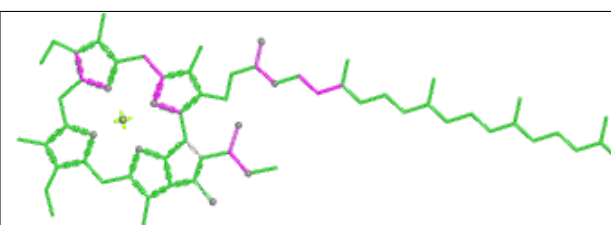
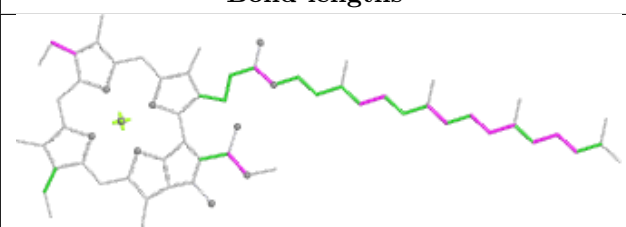
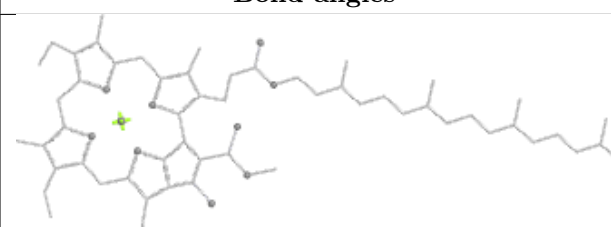
## Ligand CLA B 810


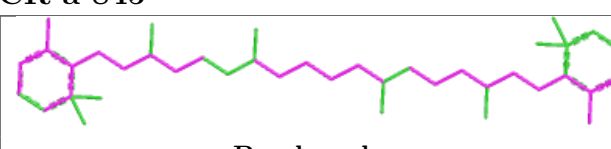
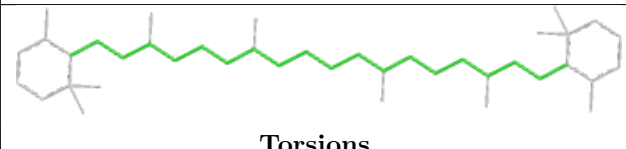
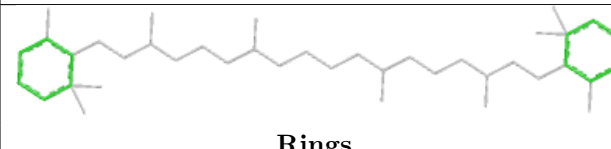




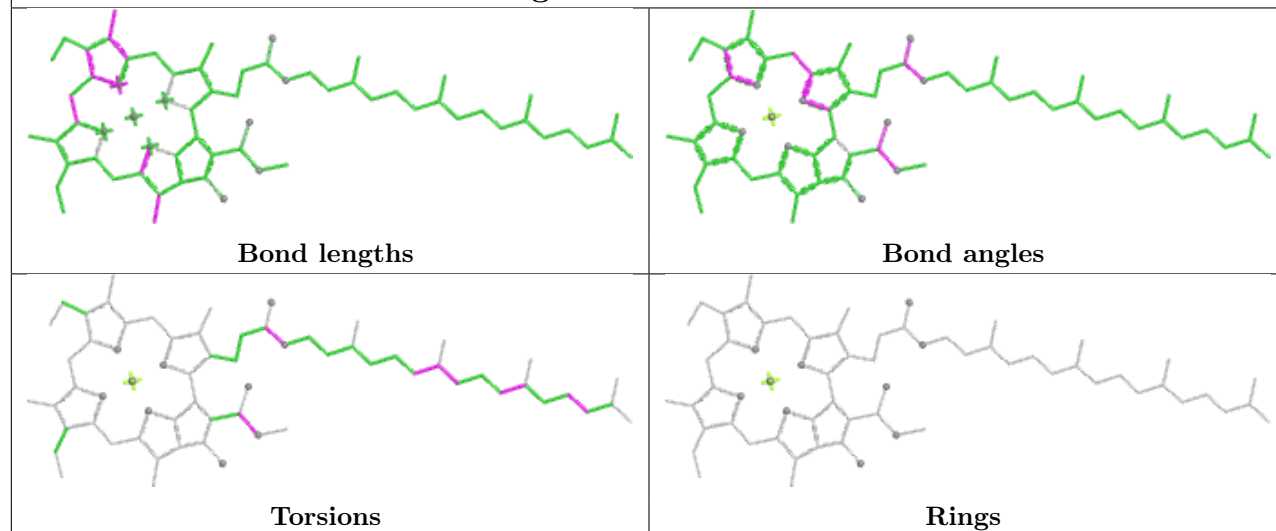


| Ligand CL0 G 851  |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

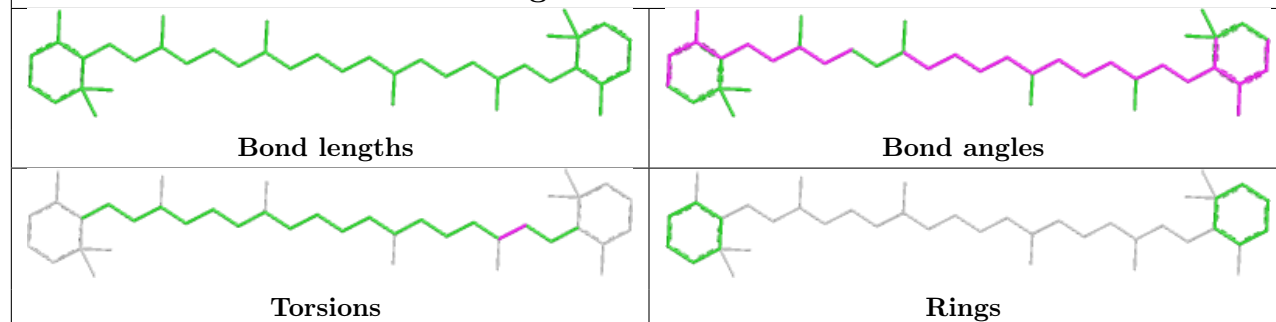
| Ligand CLA A 838  |  |
|---|--|
|    |    |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

| Ligand BCR a 845  |  |
|---|--|
|  |  |
| Bond lengths  | Bond angles  |
|  |  |
| Torsions  | Rings  |

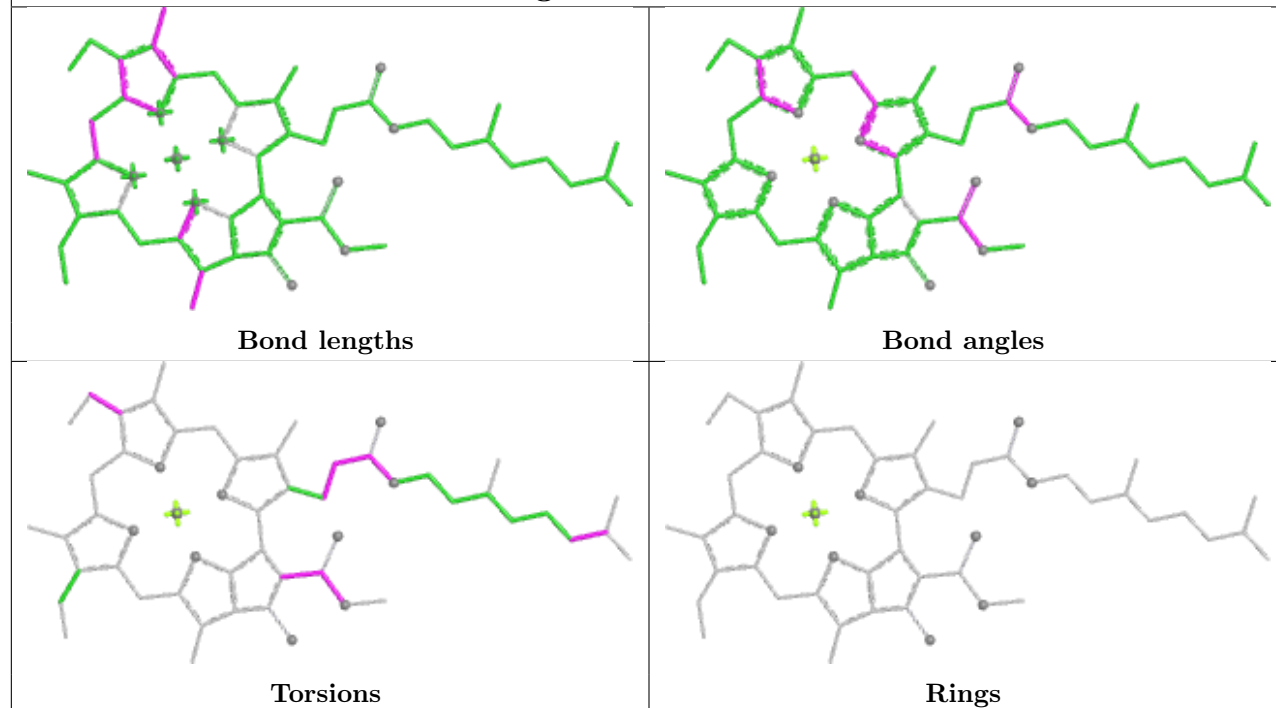
## Ligand CLA A 810

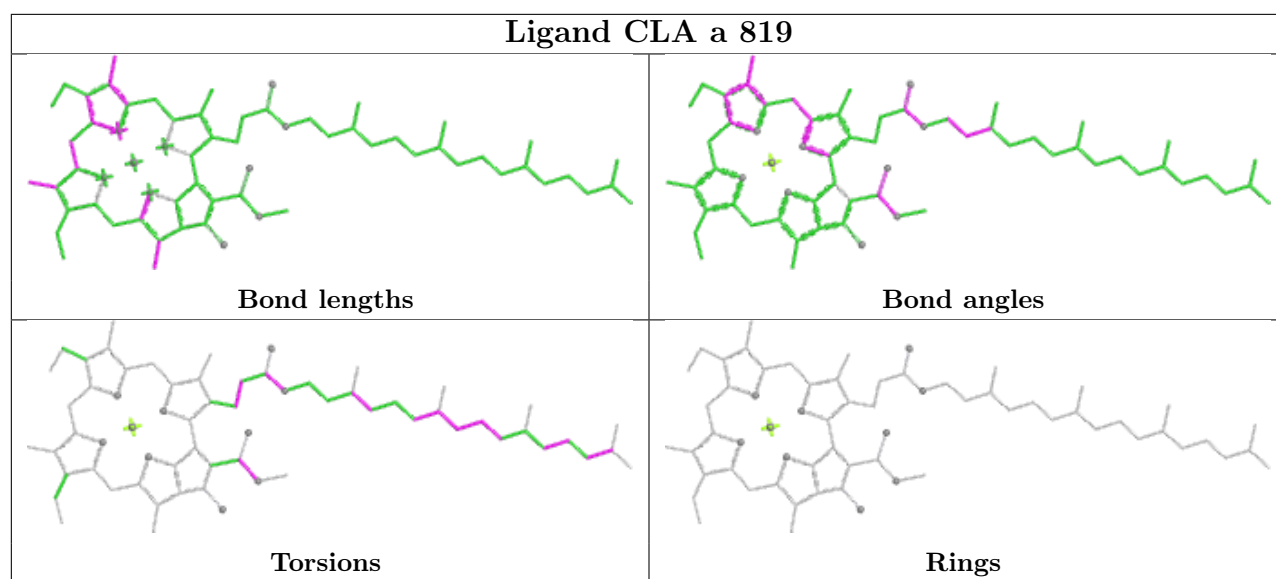


## Ligand BCR G 844

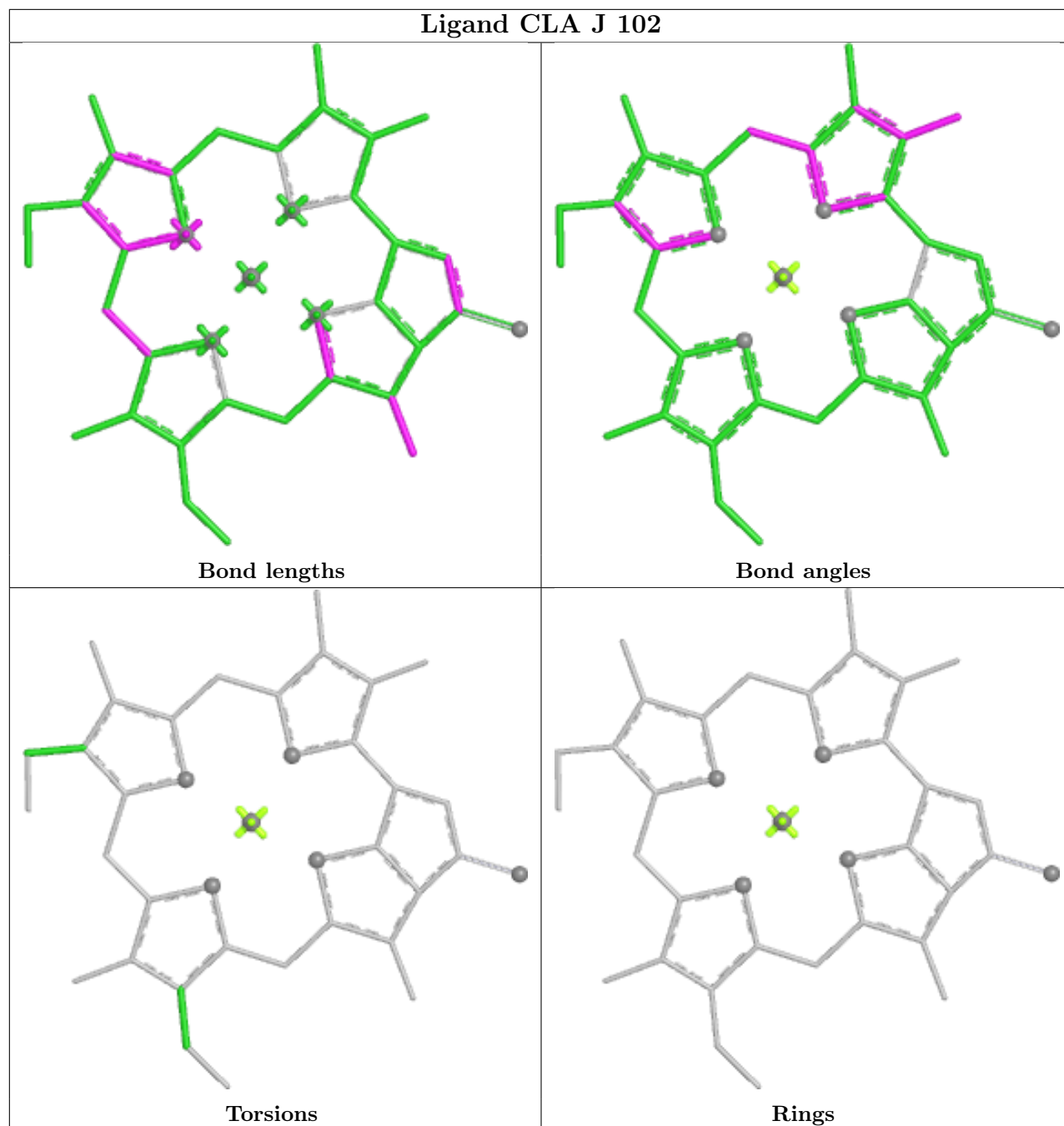


## Ligand CLA b 823

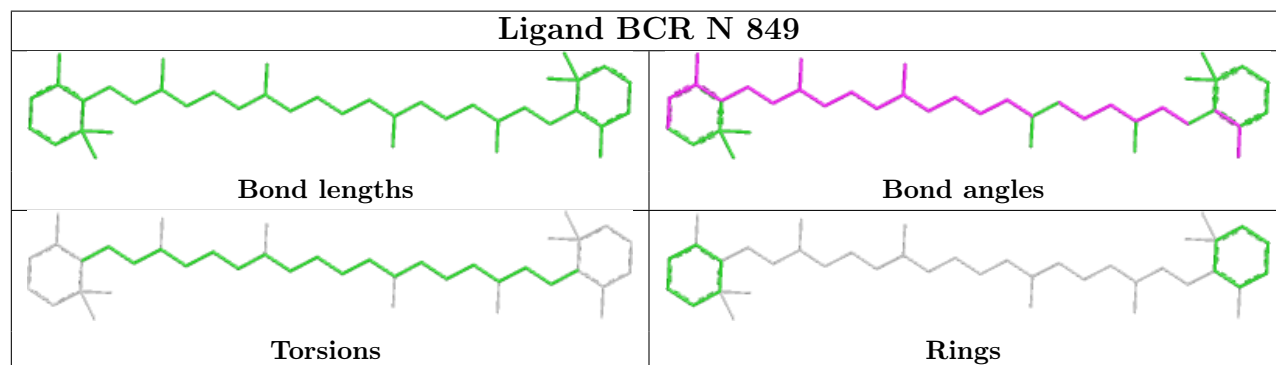


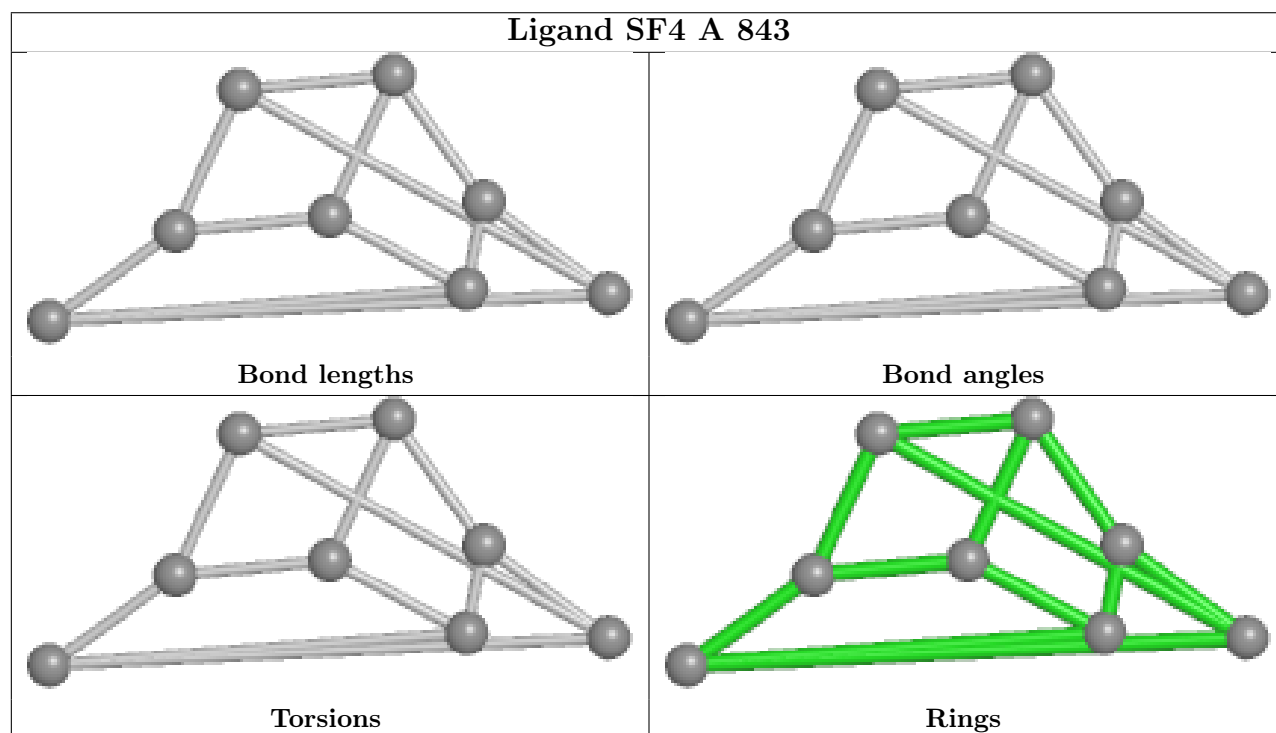
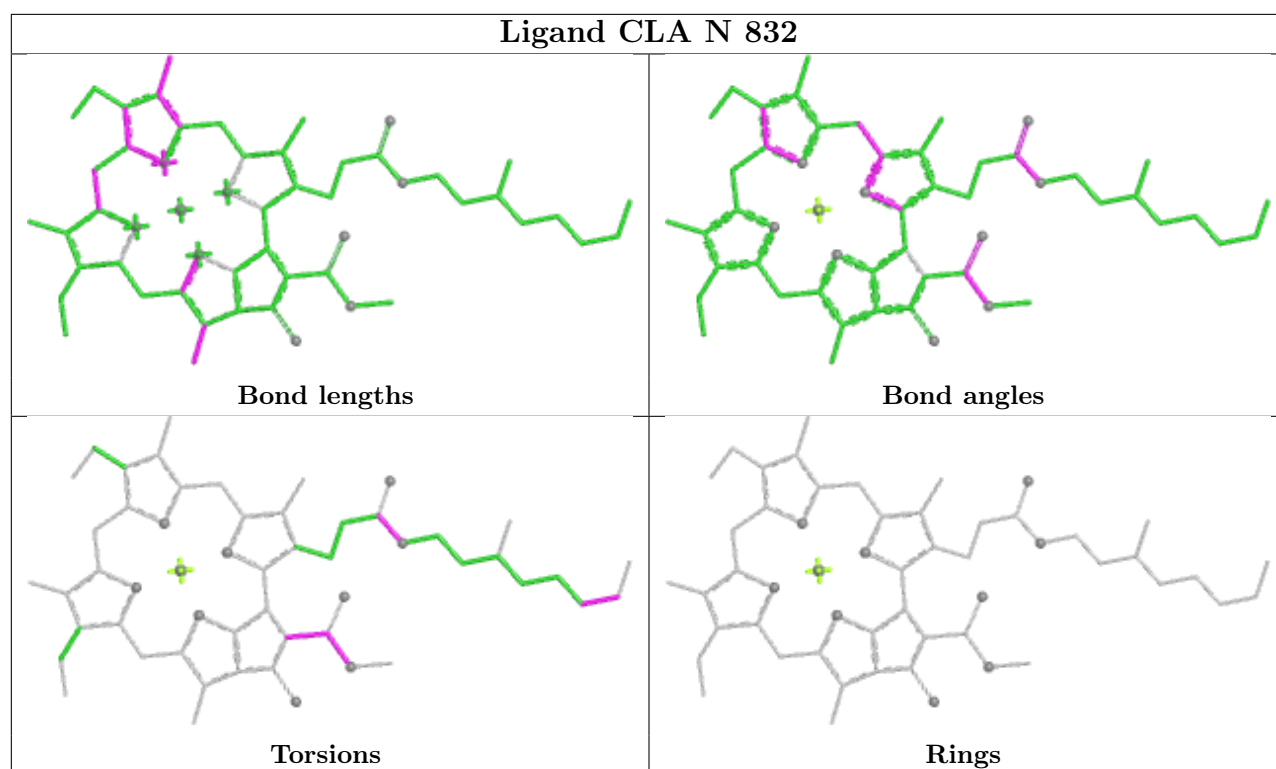


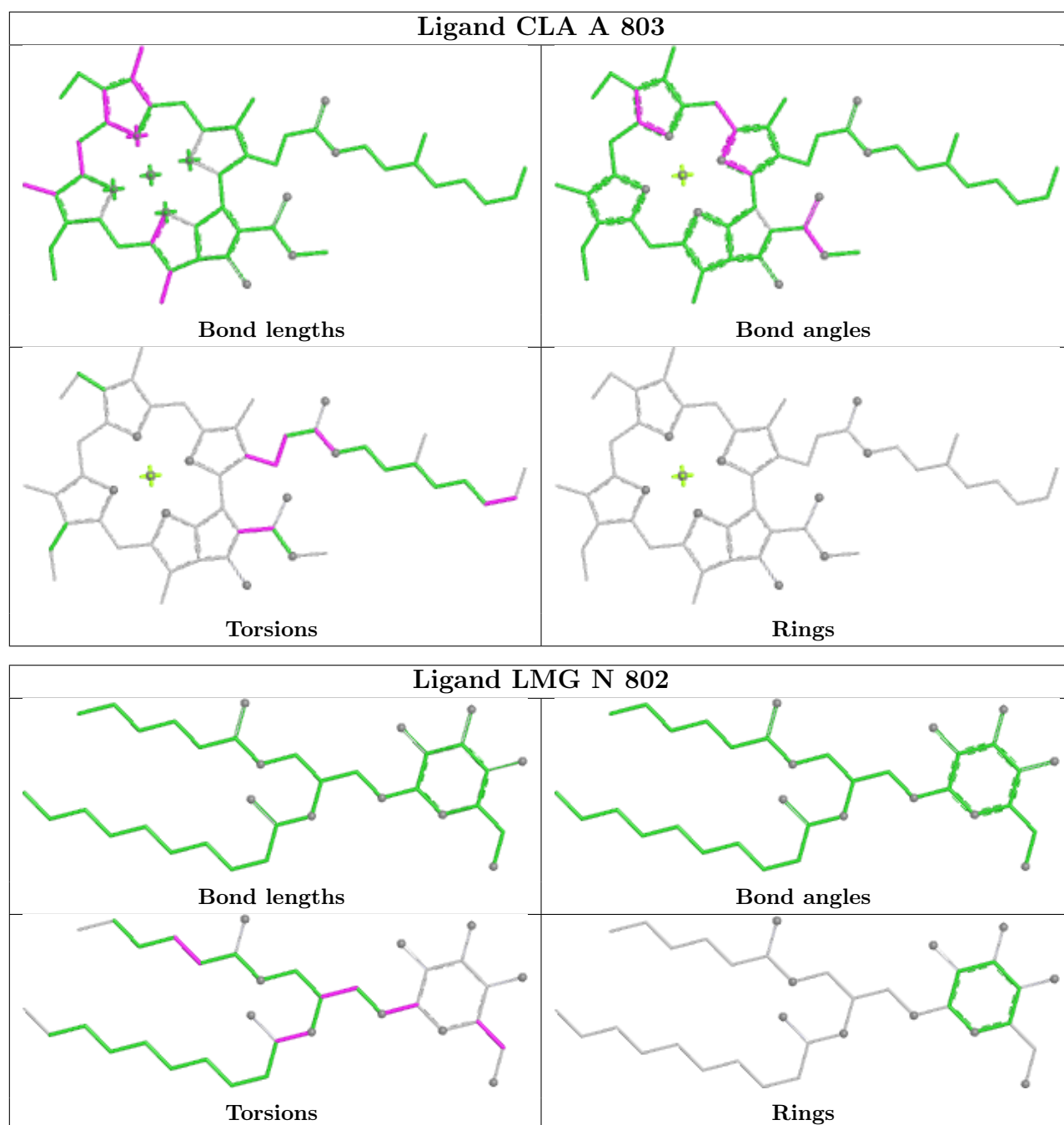
## Ligand CLA J 102

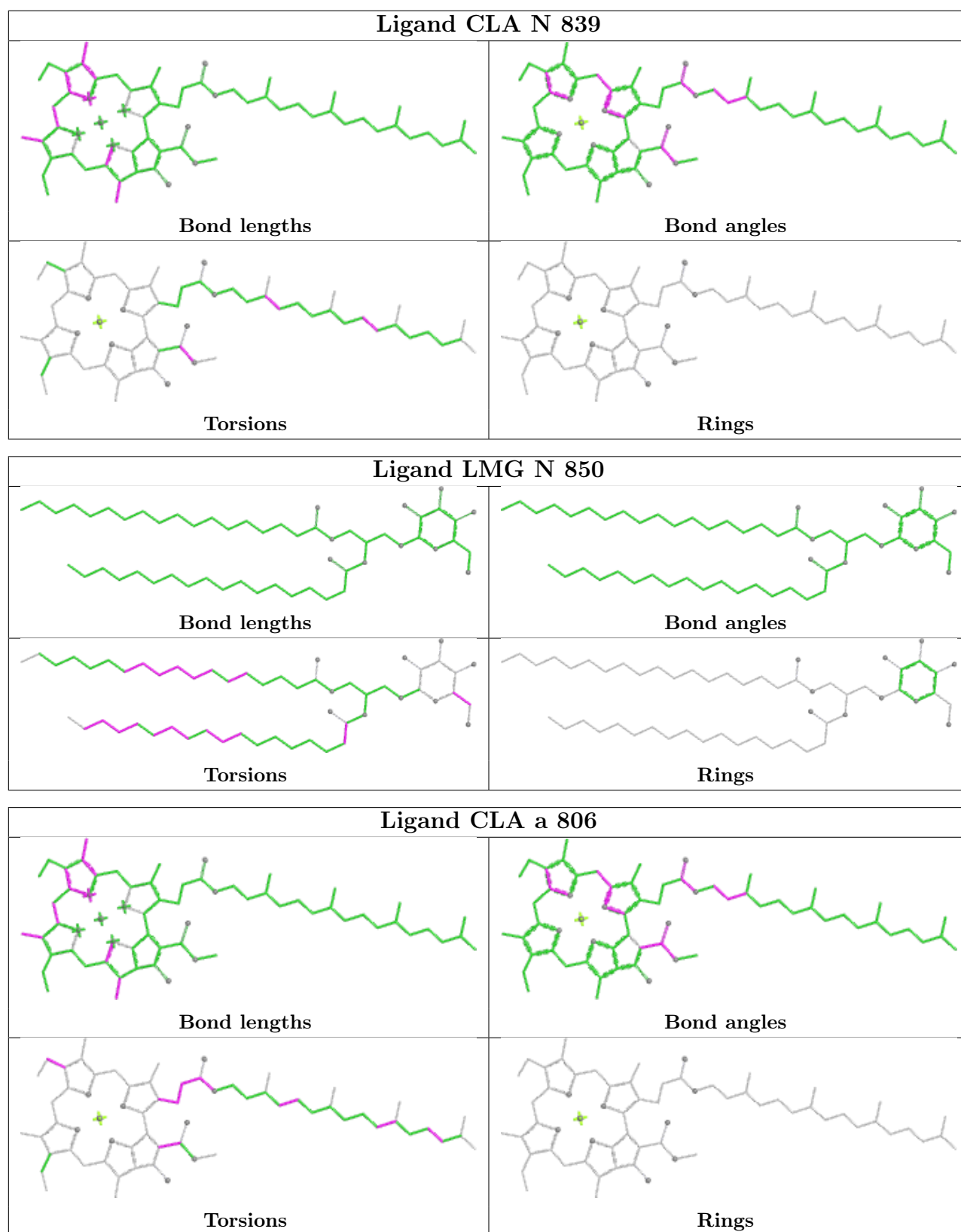


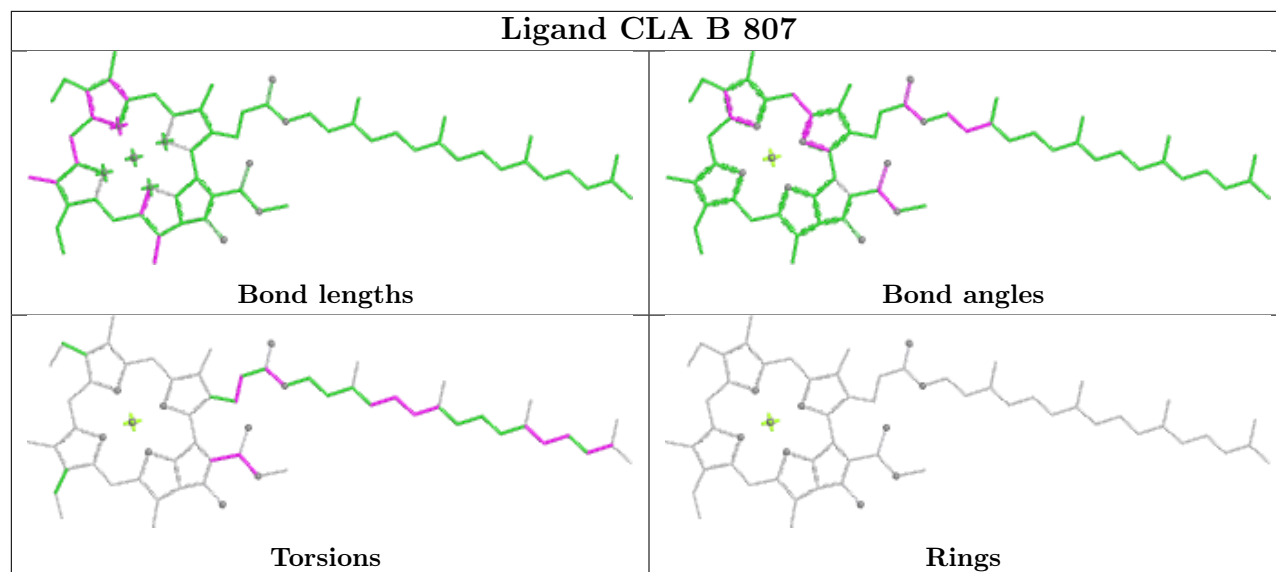
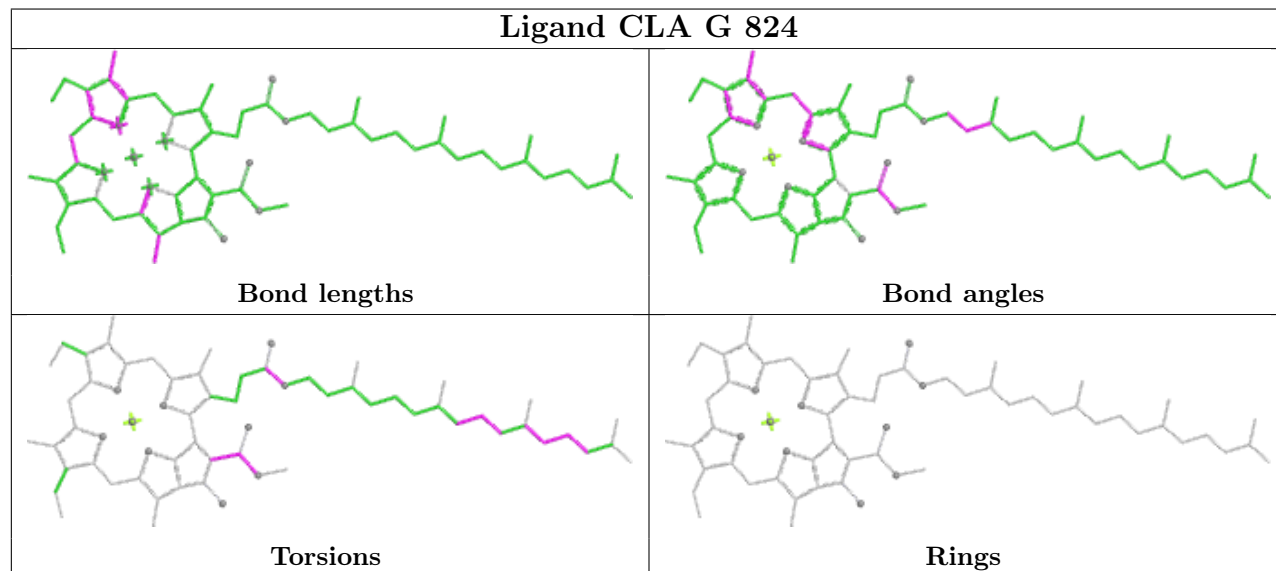
## Ligand BCR N 849



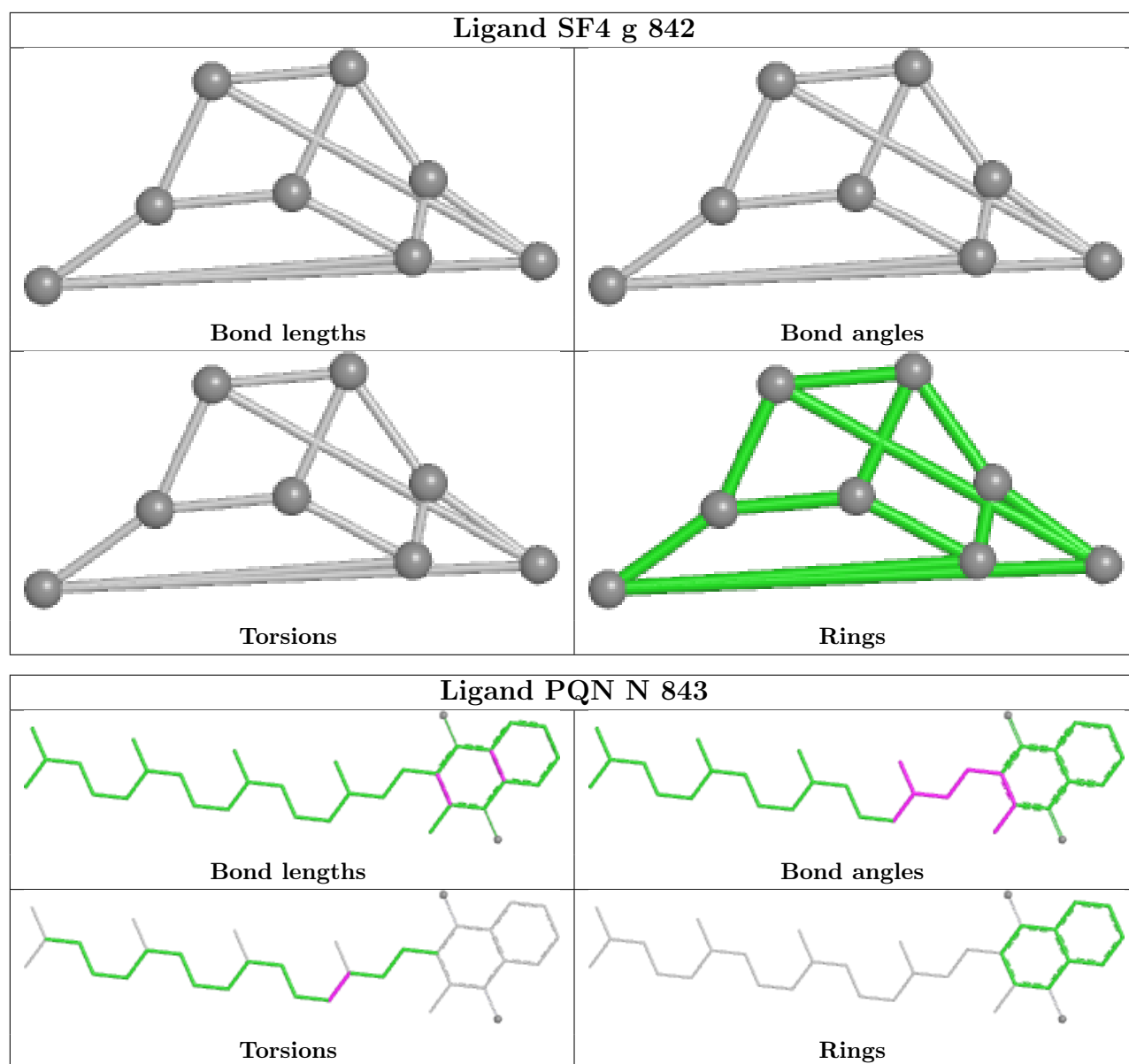




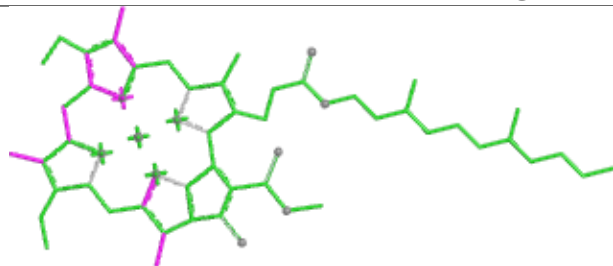


**Ligand CLA B 807****Ligand CLA G 824**

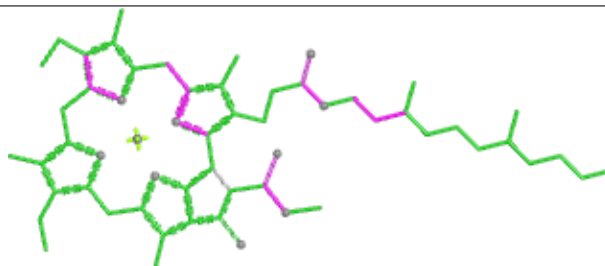




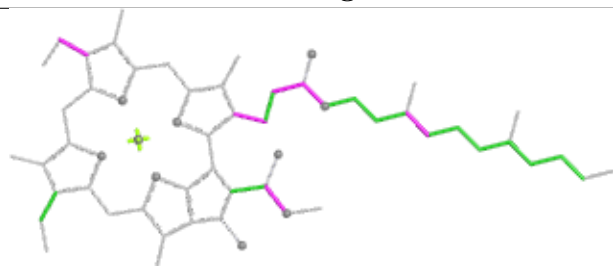
## Ligand CLA N 834



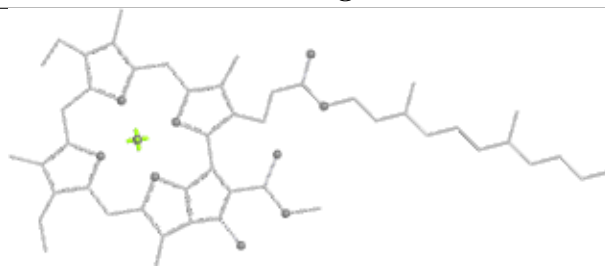
Bond lengths



Bond angles

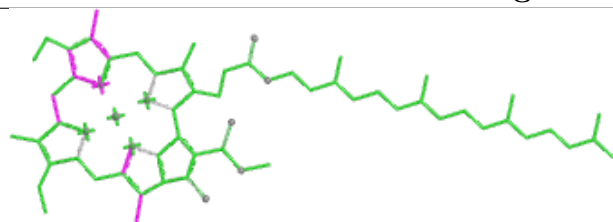


Torsions

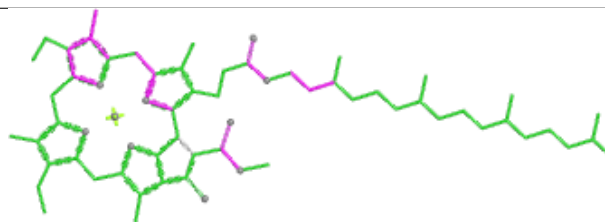


Rings

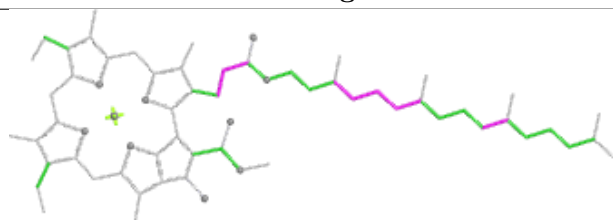
## Ligand CLA A 808



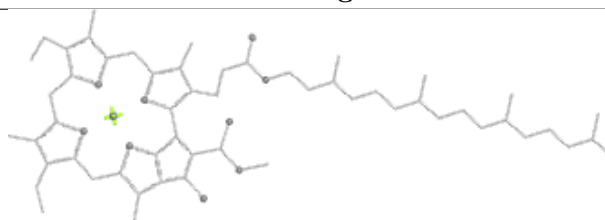
Bond lengths



Bond angles

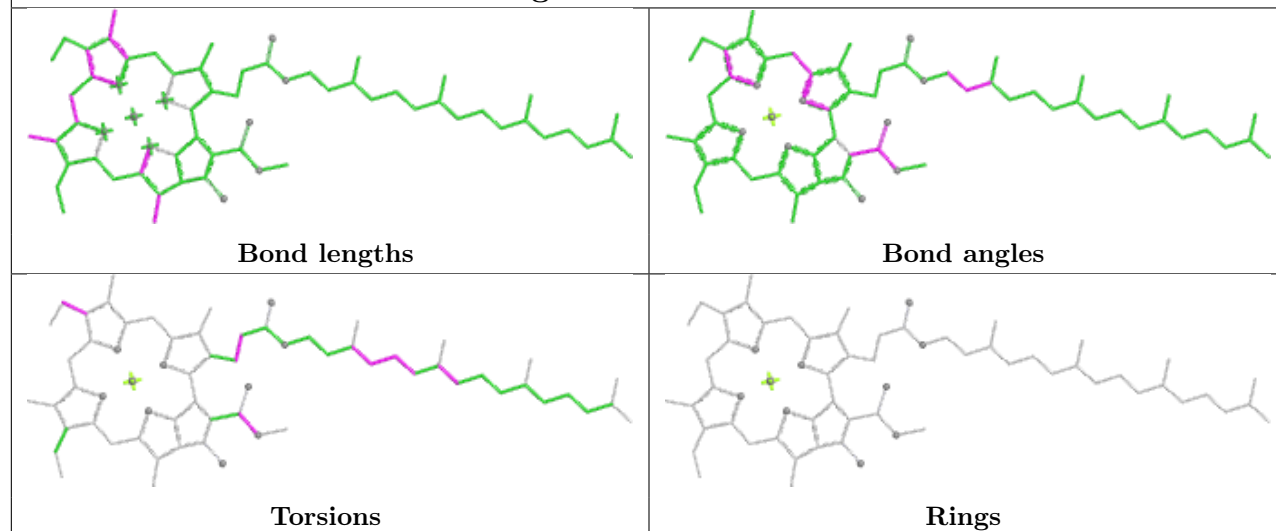


Torsions

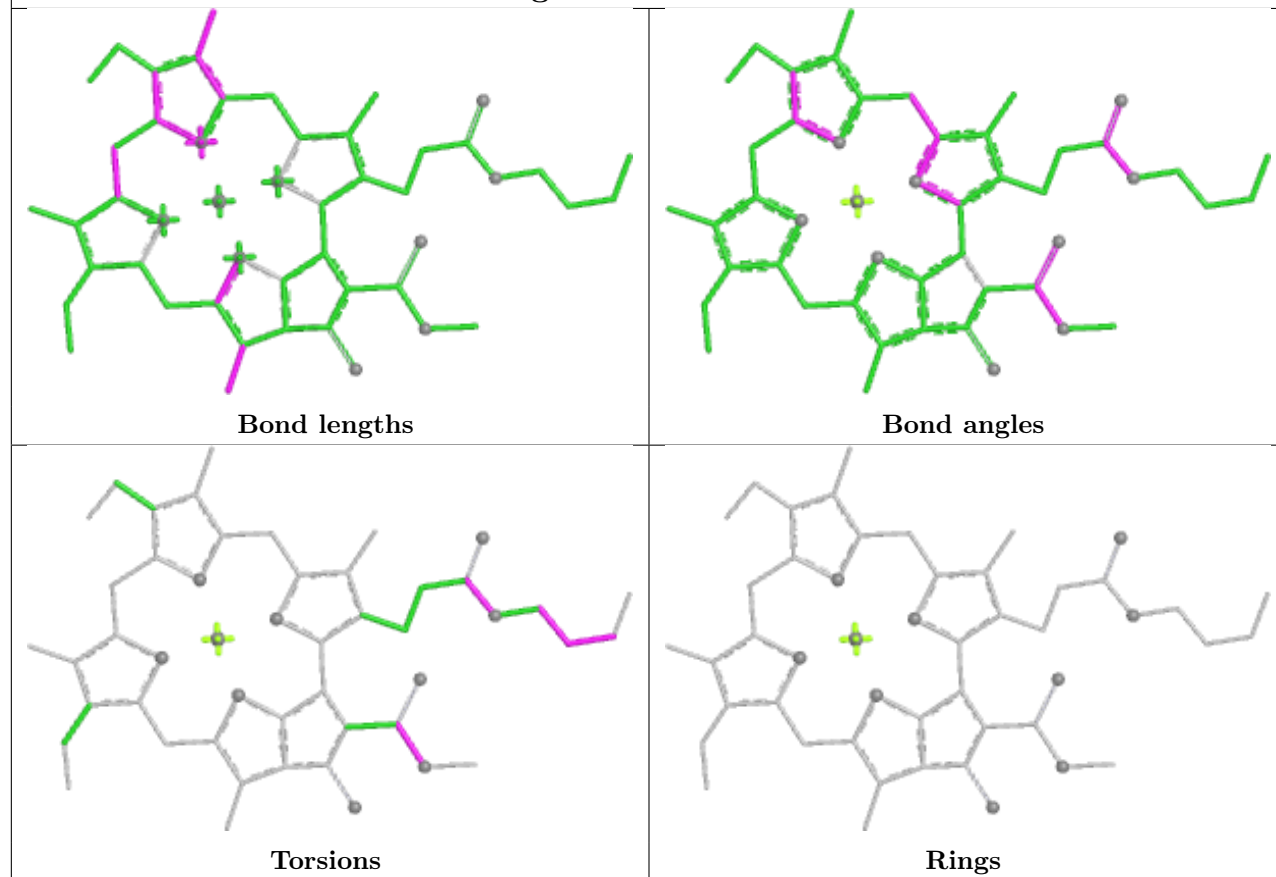


Rings

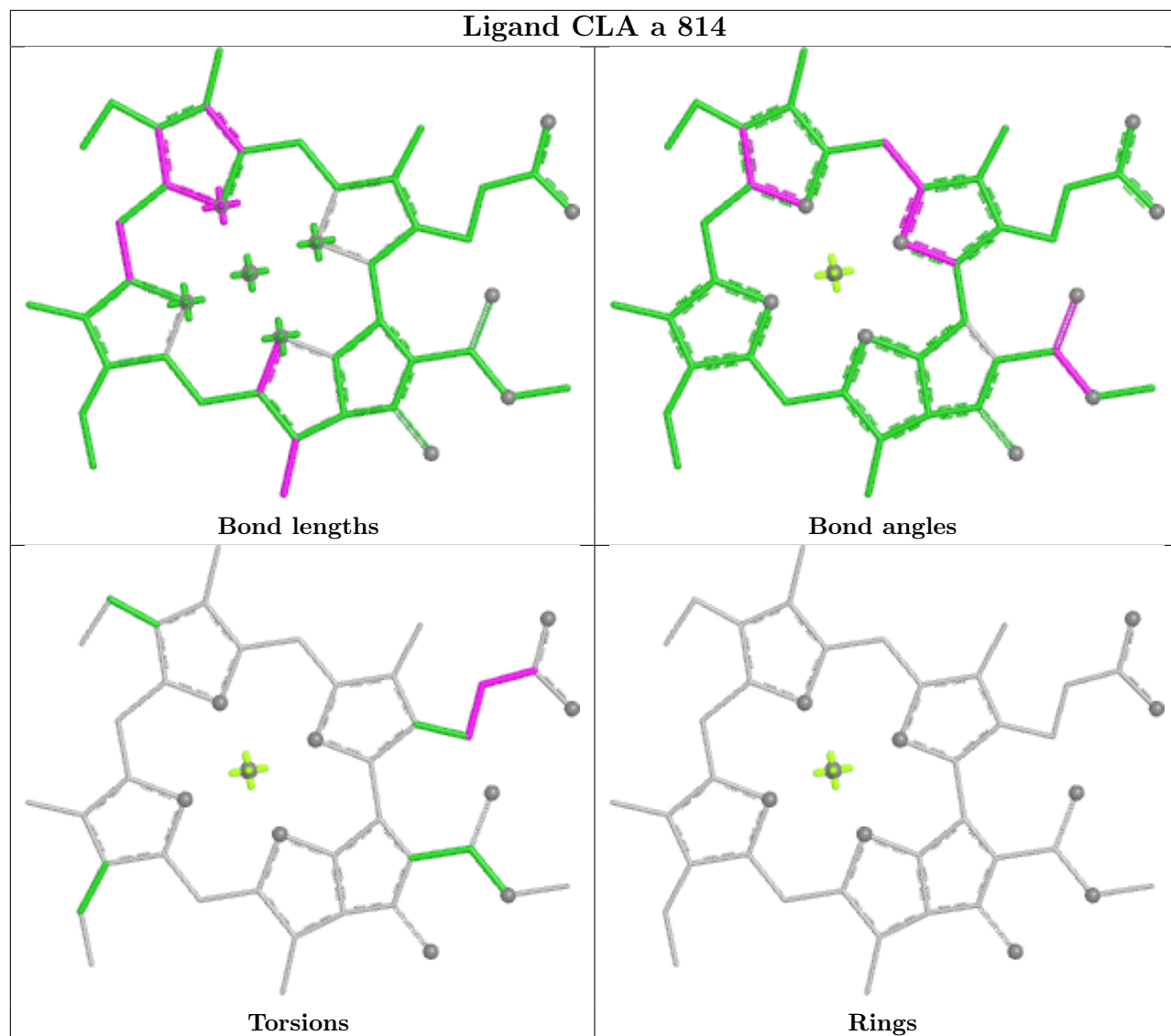
## Ligand CLA A 853



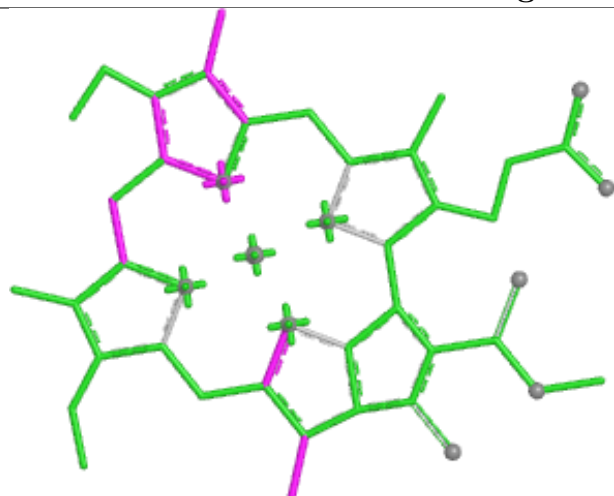
## Ligand CLA N 817



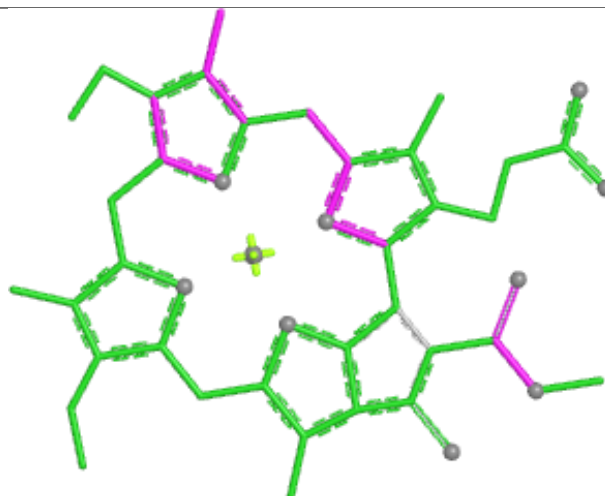
## Ligand CLA a 814



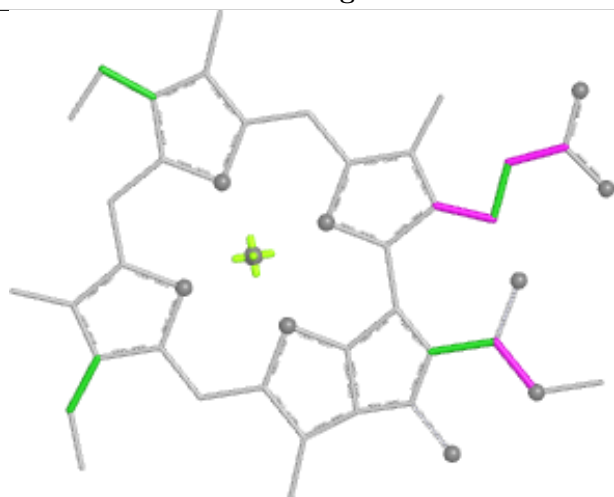
## Ligand CLA n 834



Bond lengths



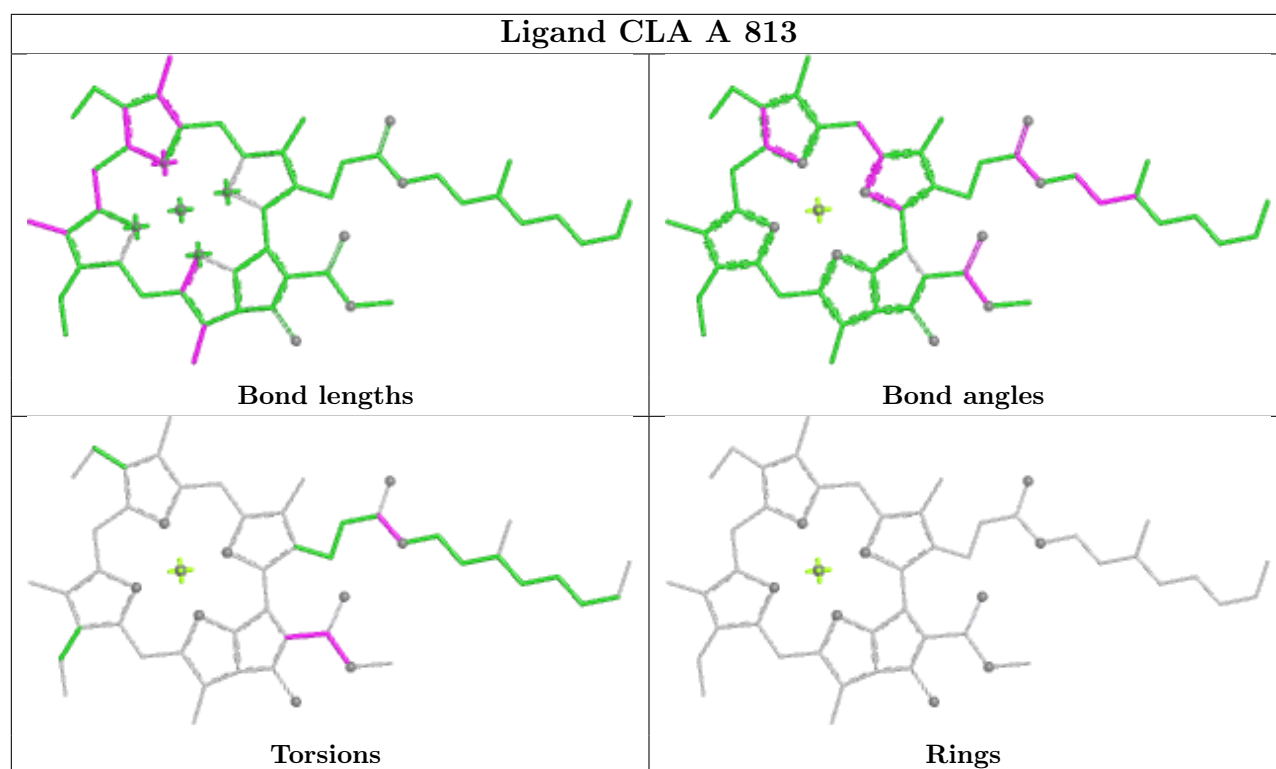
Bond angles



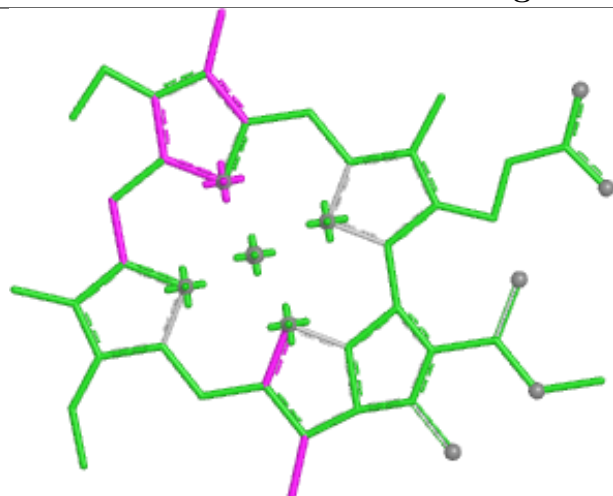
Torsions



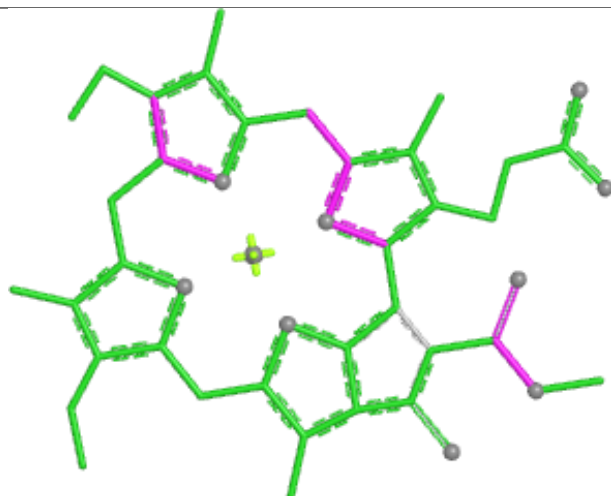
Rings



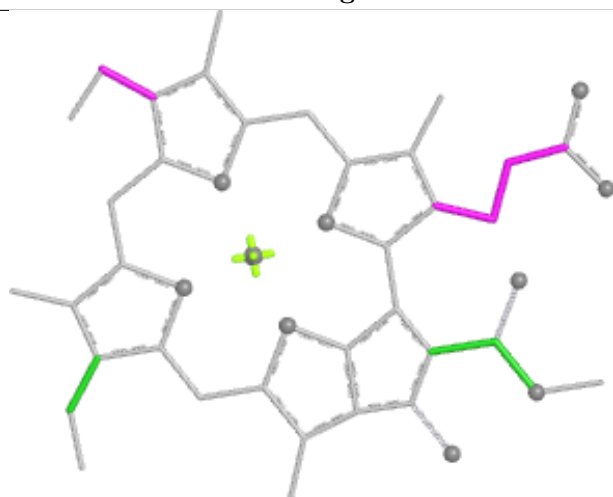
## Ligand CLA N 822



Bond lengths



Bond angles

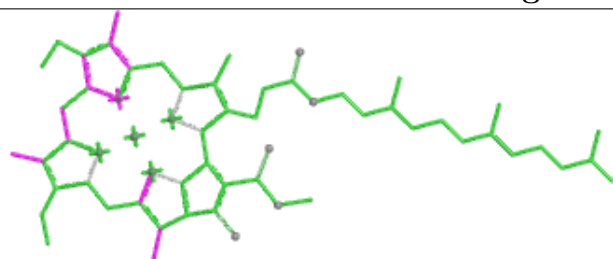


Torsions

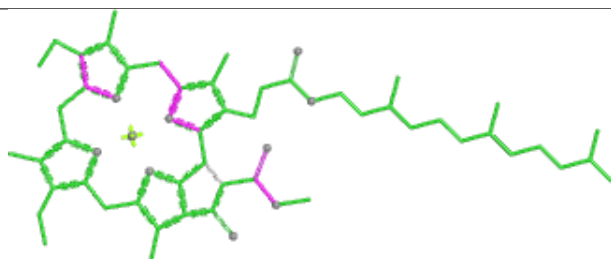


Rings

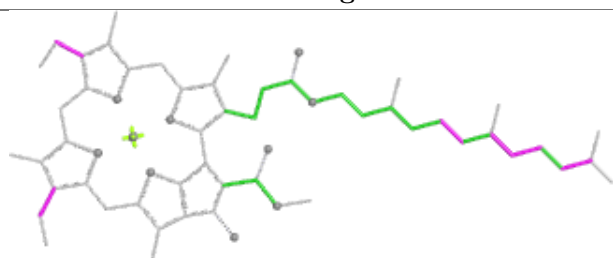
## Ligand CLA I 203



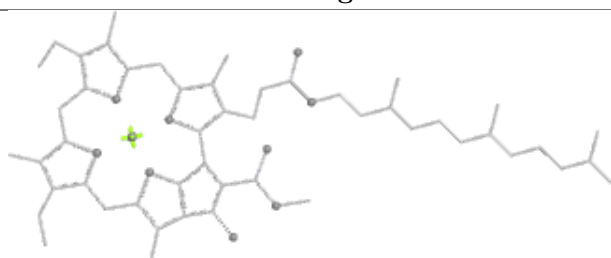
Bond lengths



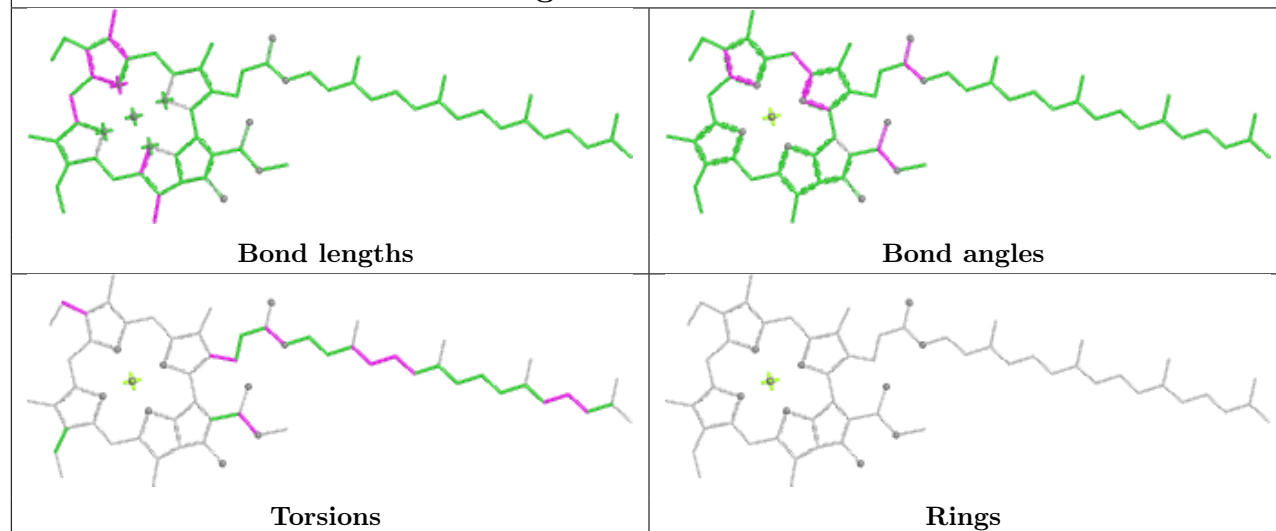
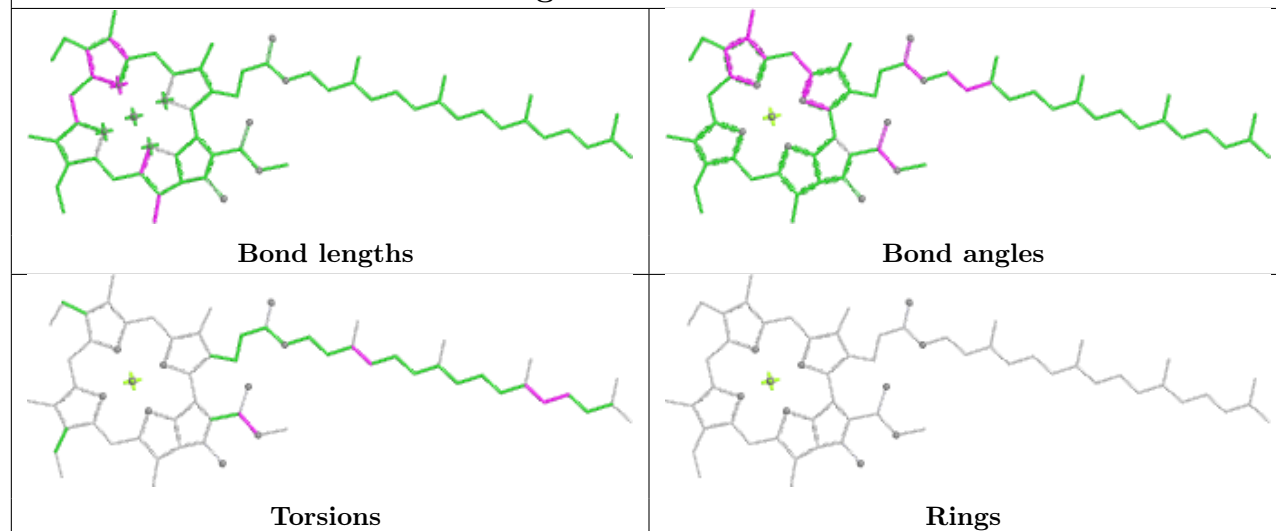
Bond angles



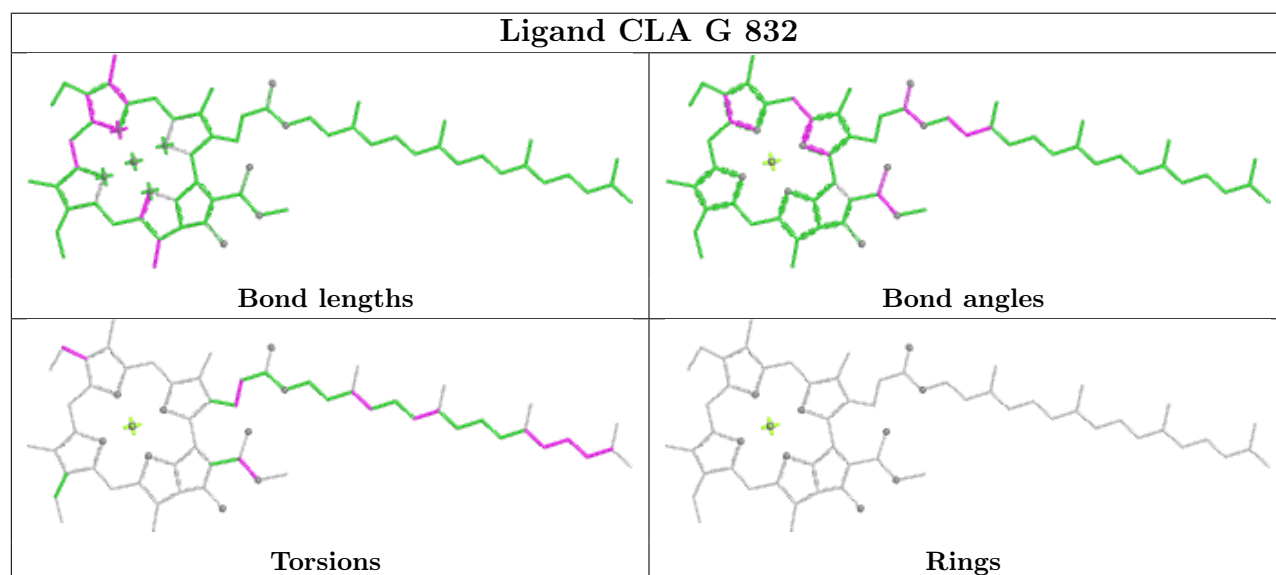
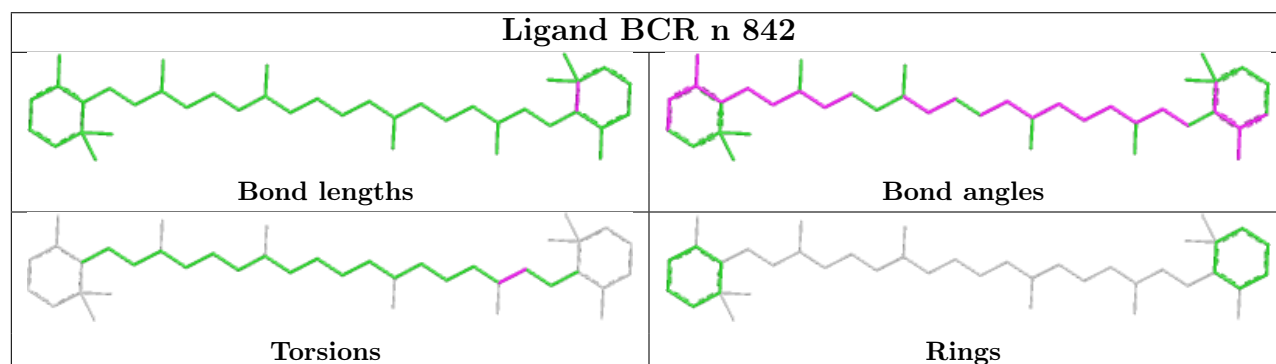
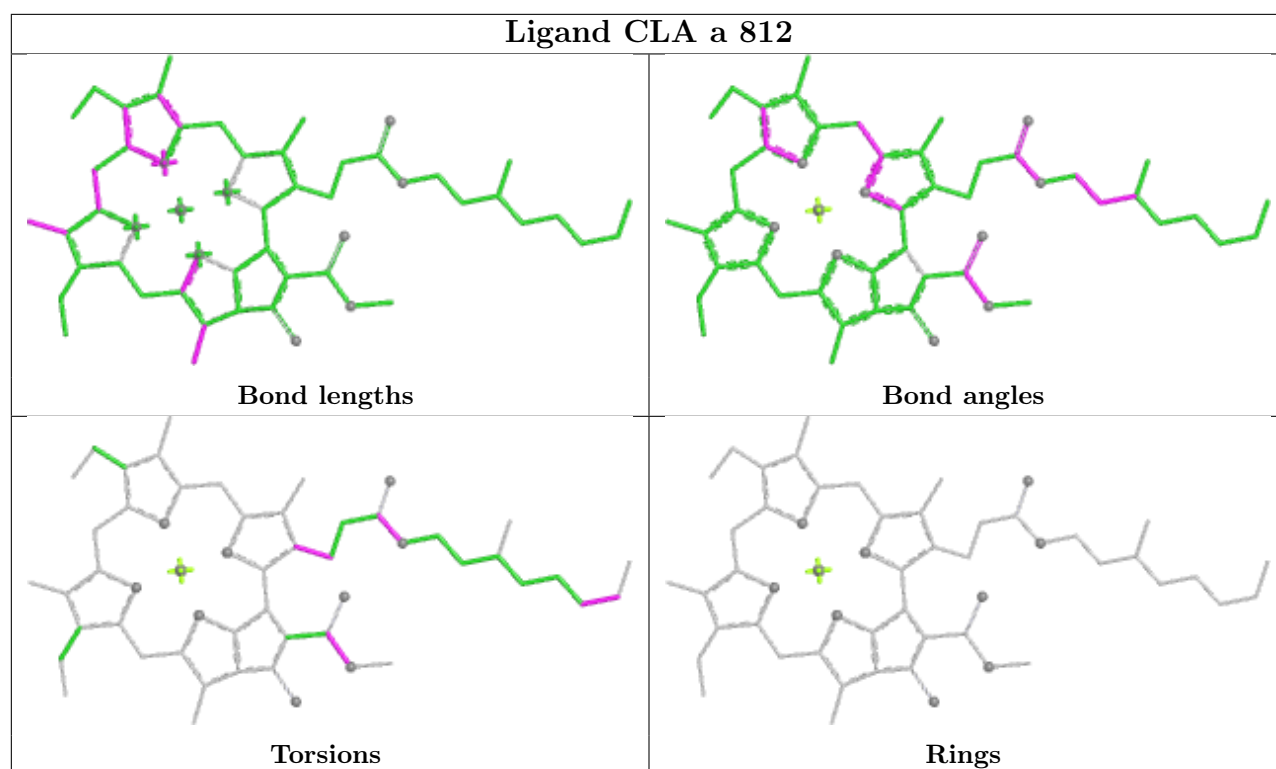
Torsions



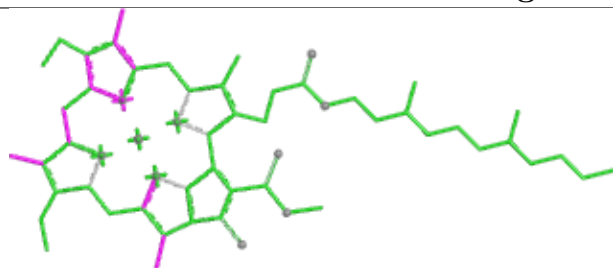
Rings

**Ligand CLA a 837****Ligand CLA a 831**

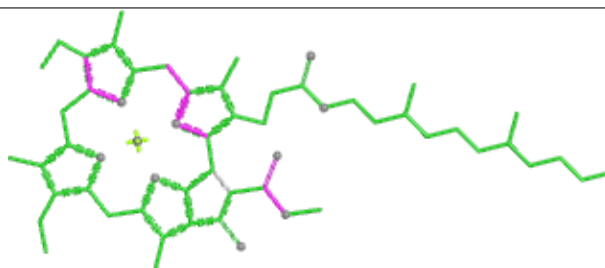




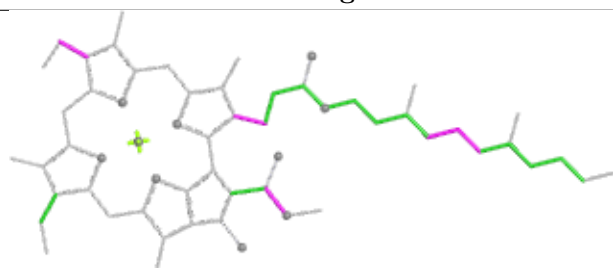
## Ligand CLA b 851



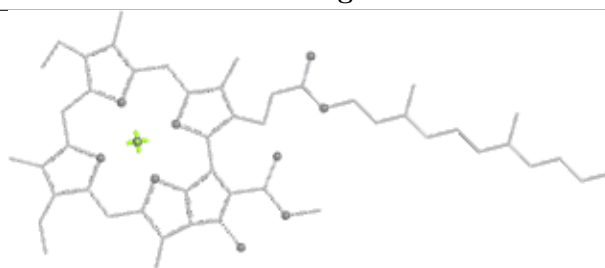
Bond lengths



Bond angles

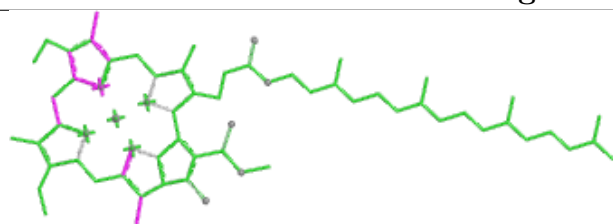


Torsions

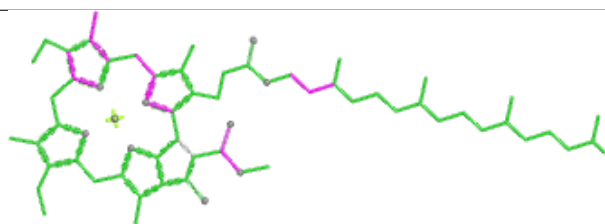


Rings

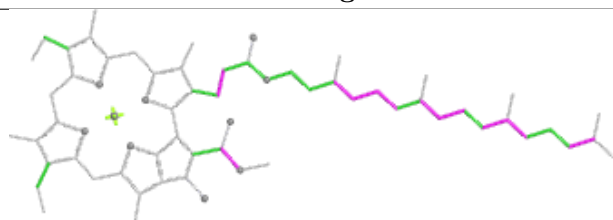
## Ligand CLA a 826



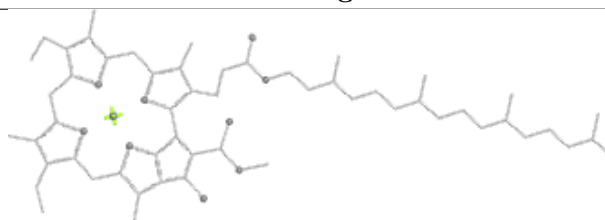
Bond lengths



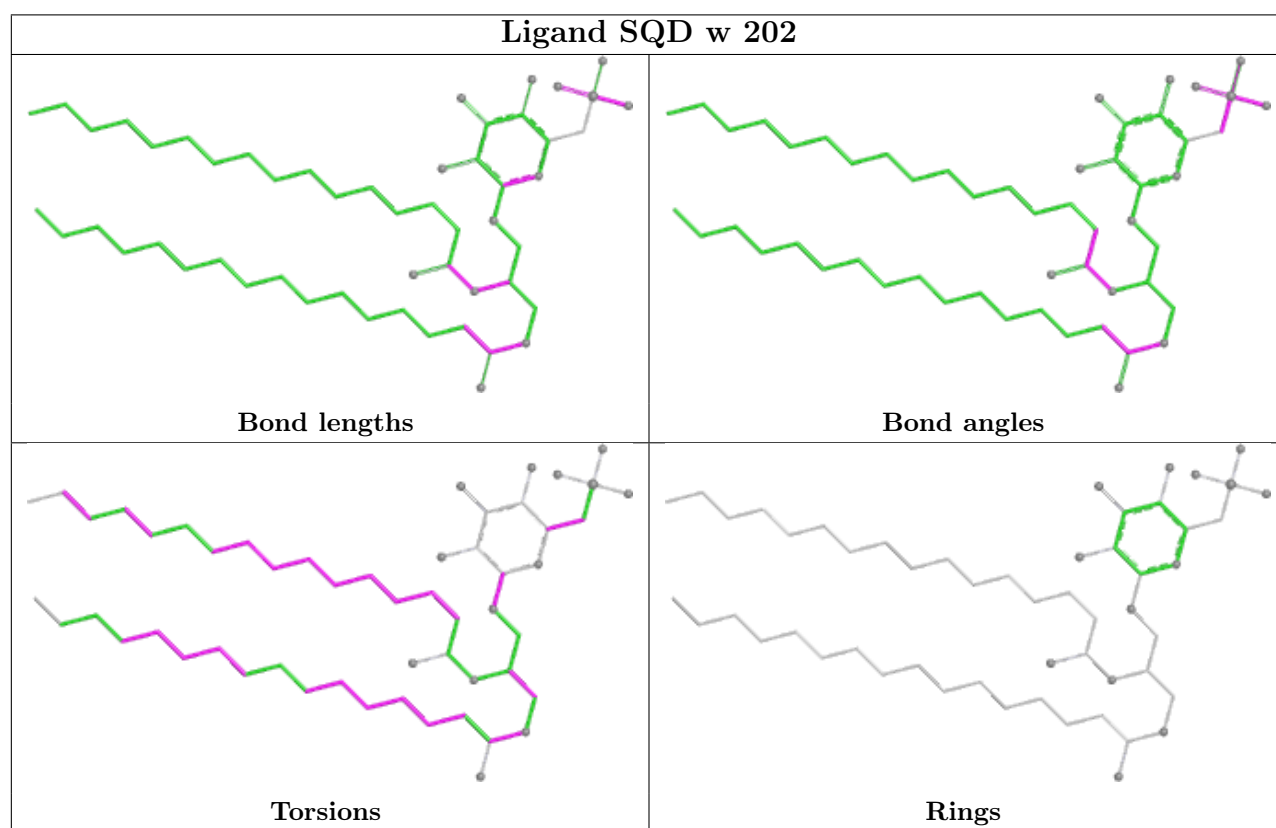
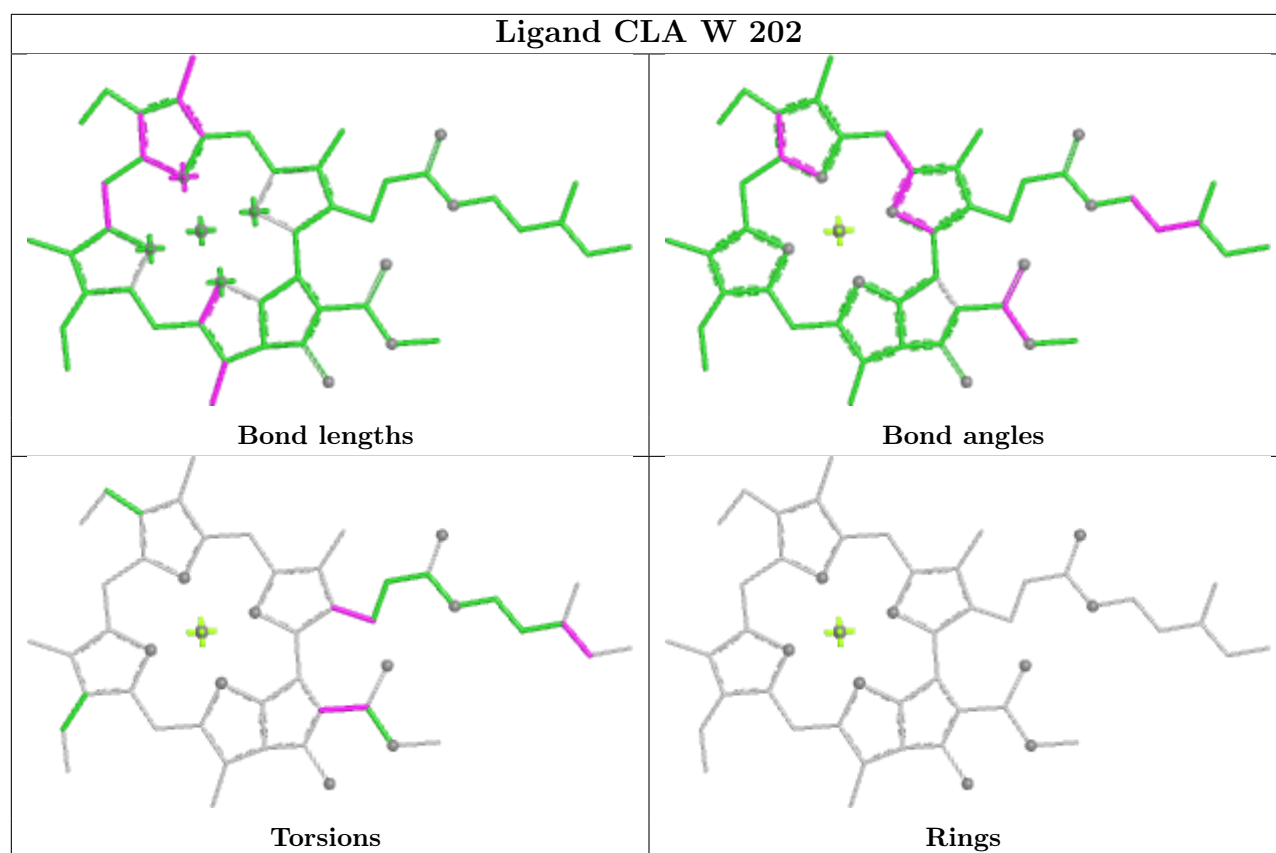
Bond angles

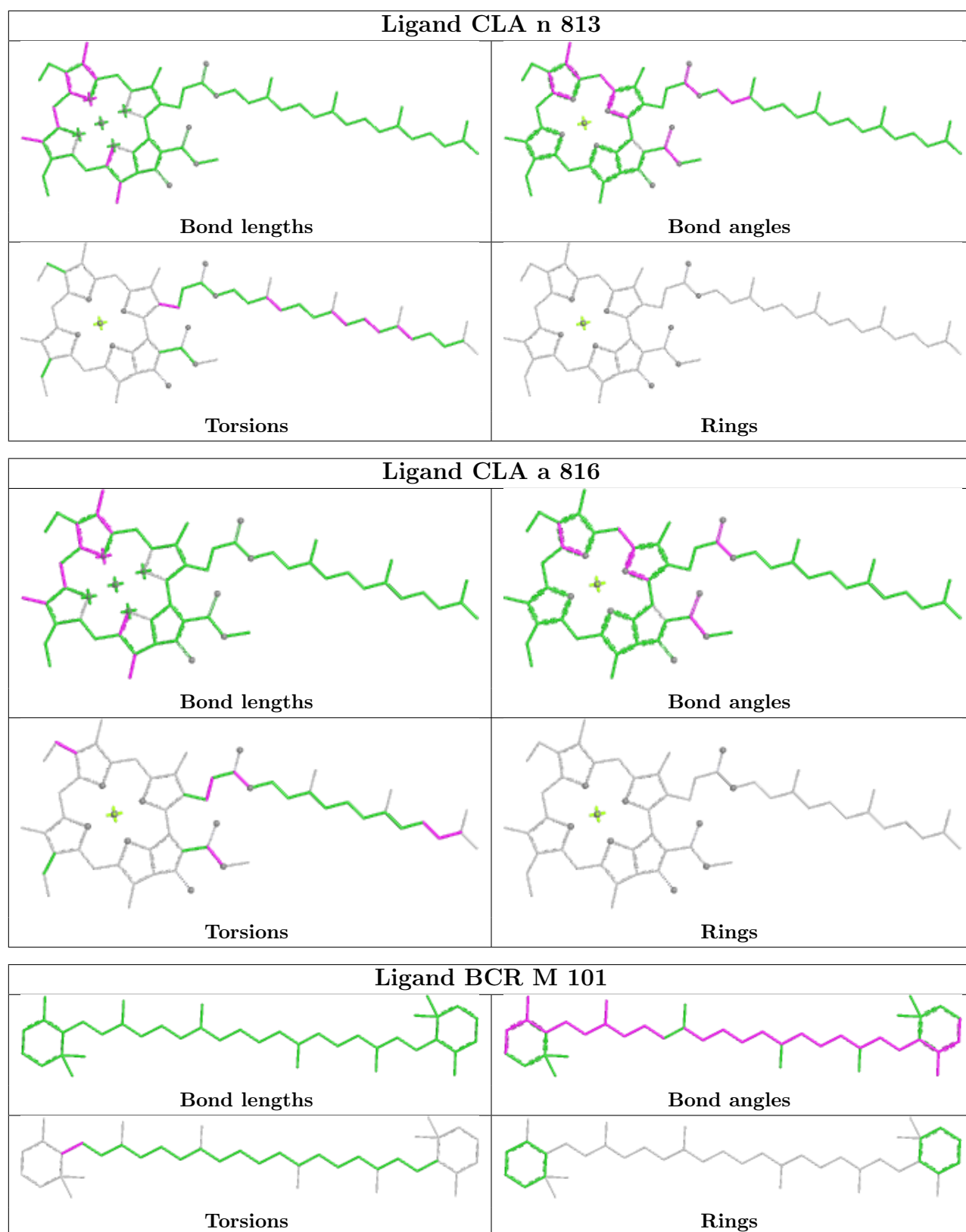


Torsions

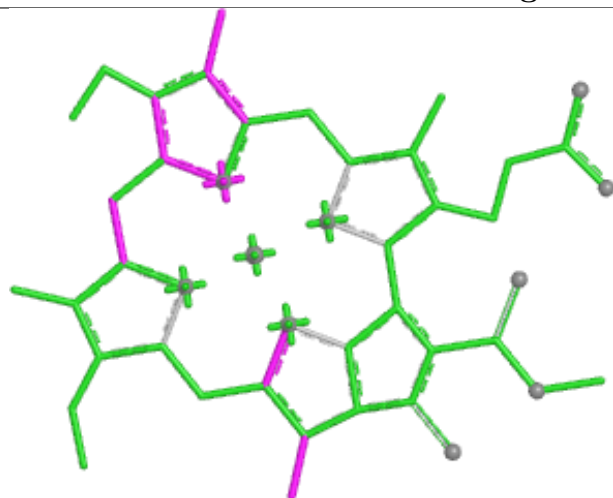


Rings

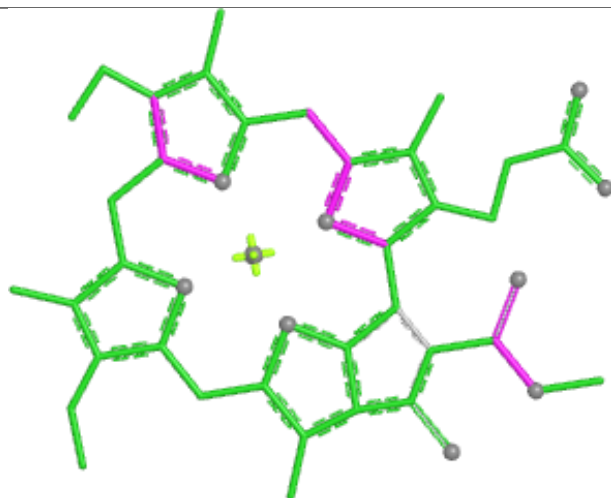




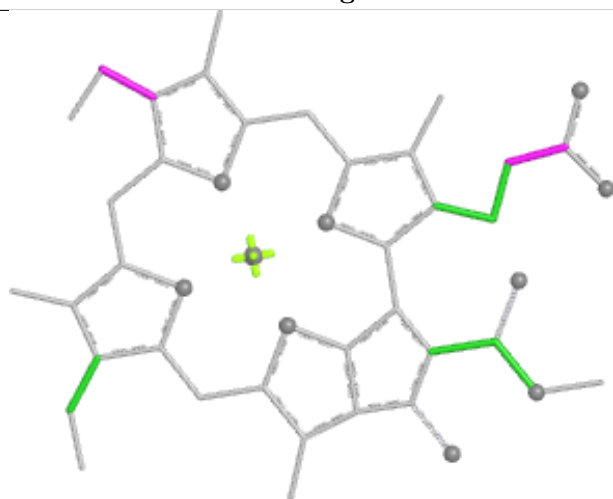
## Ligand CLA s 202



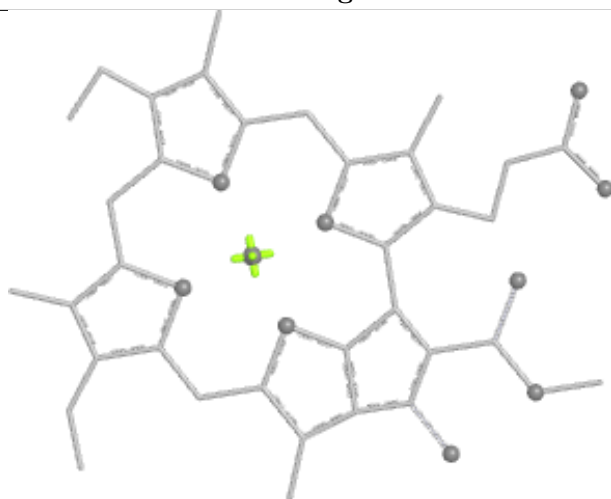
Bond lengths



Bond angles

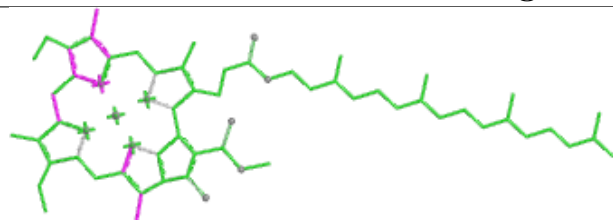


Torsions

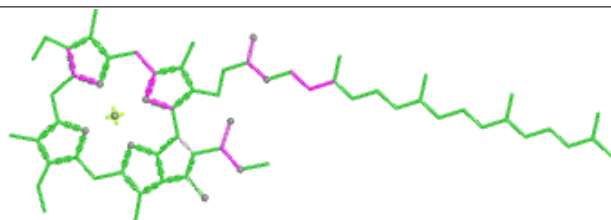


Rings

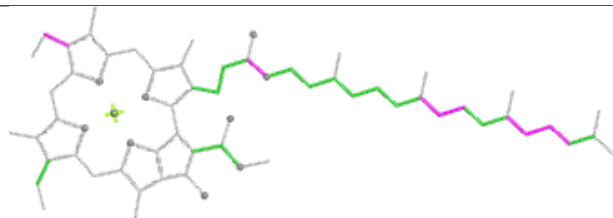
## Ligand CLA a 823



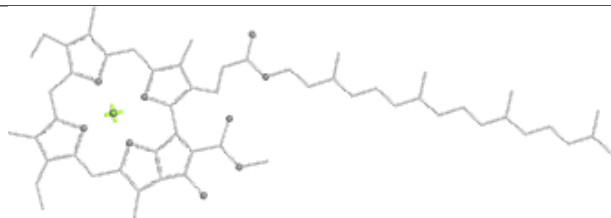
Bond lengths



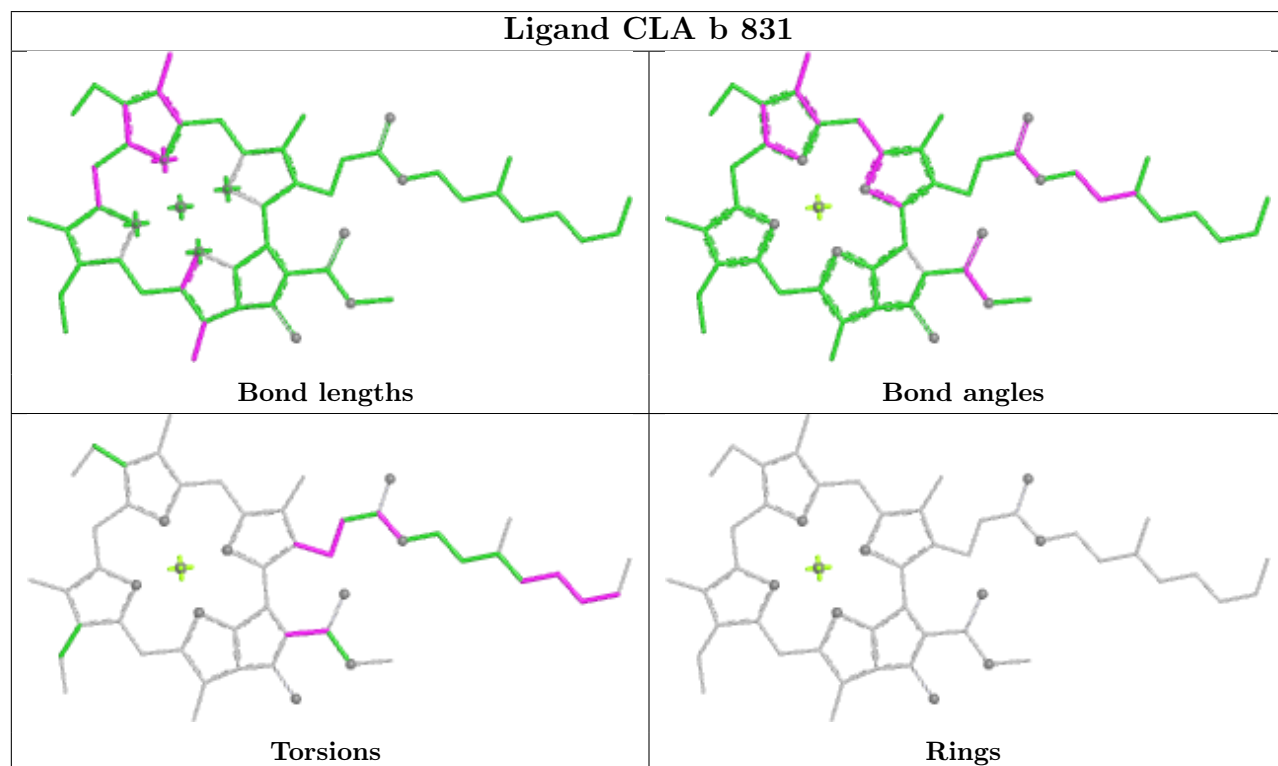
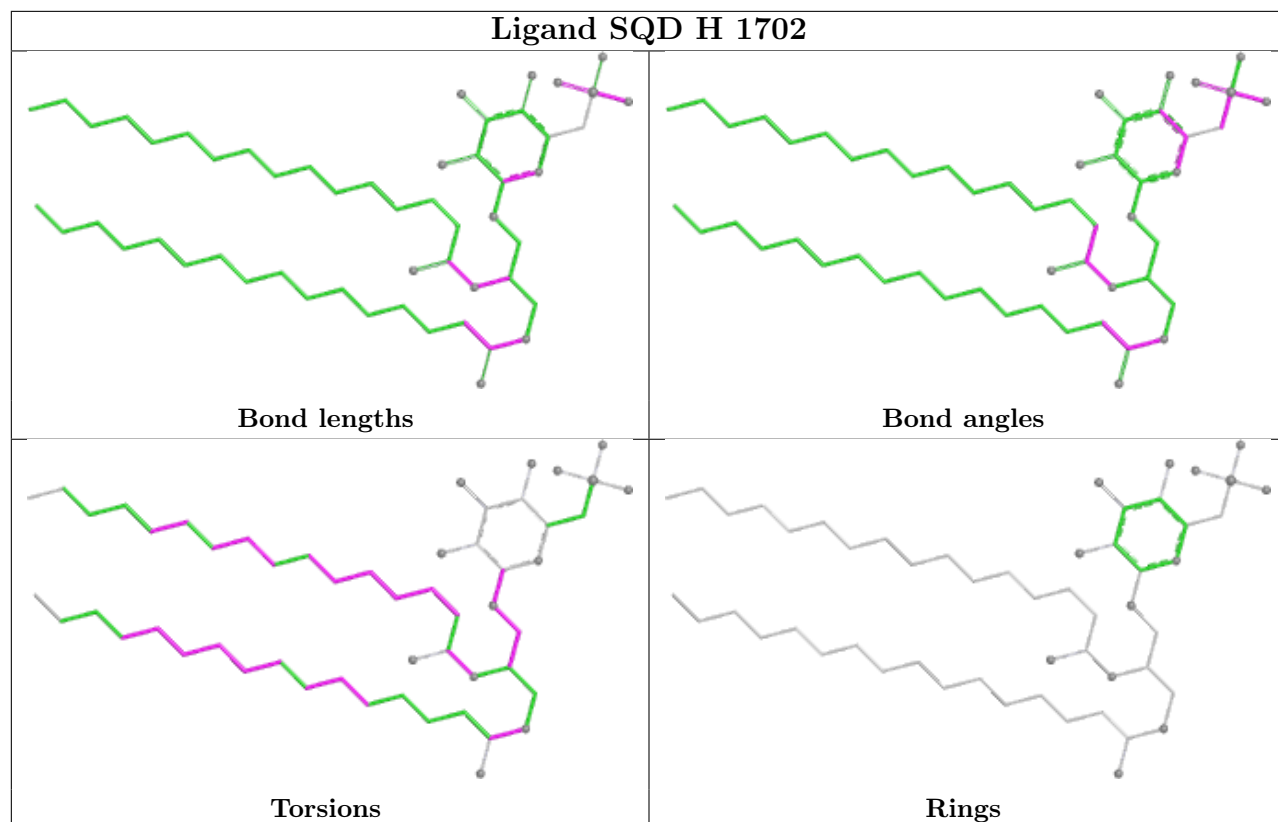
Bond angles

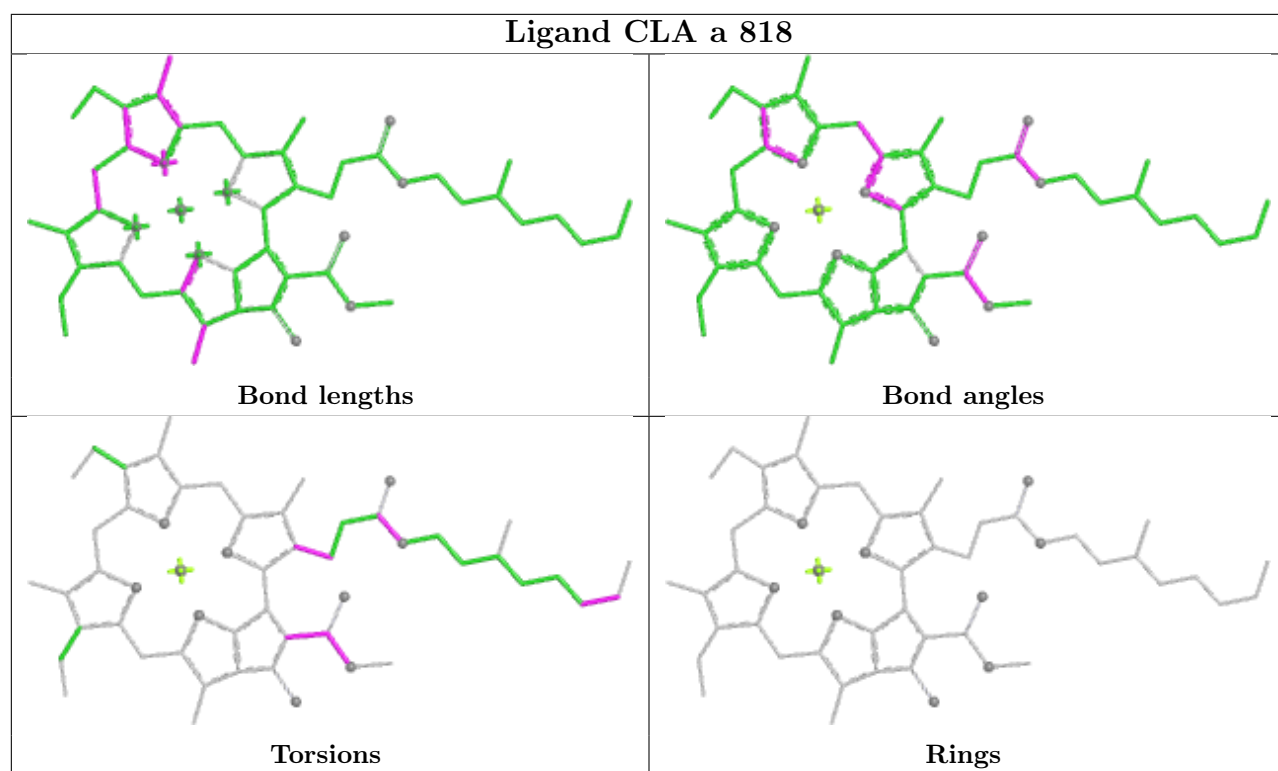


Torsions

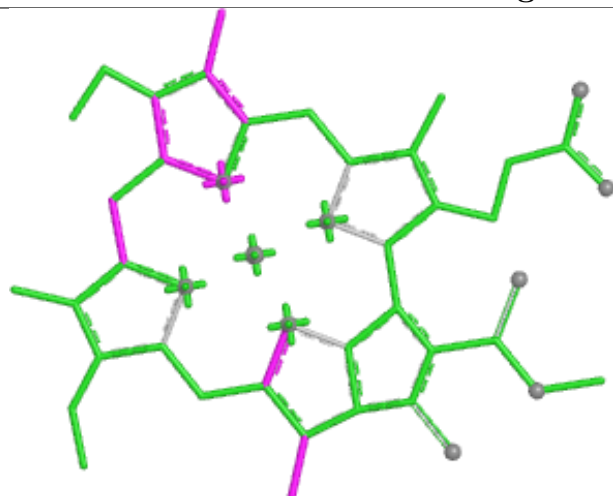


Rings

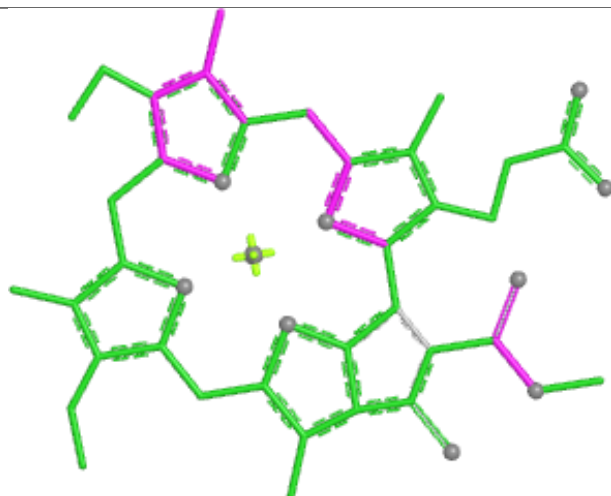




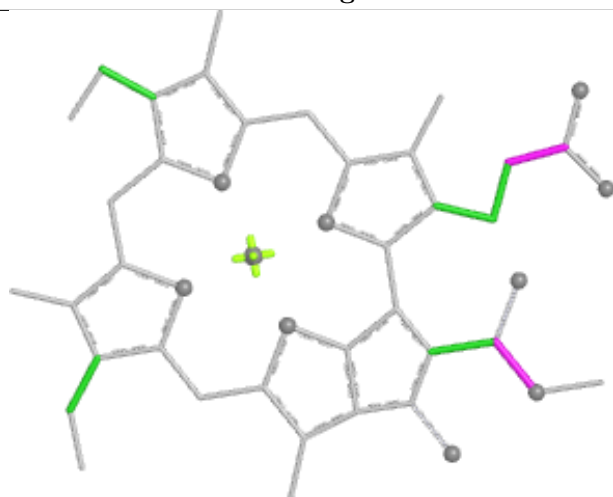
## Ligand CLA b 835



Bond lengths



Bond angles



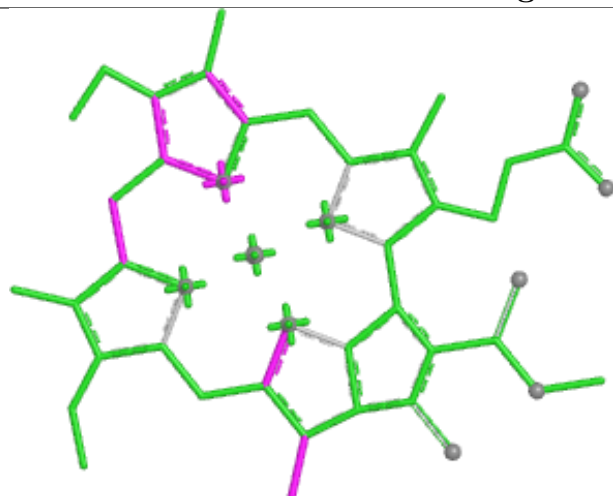
Torsions



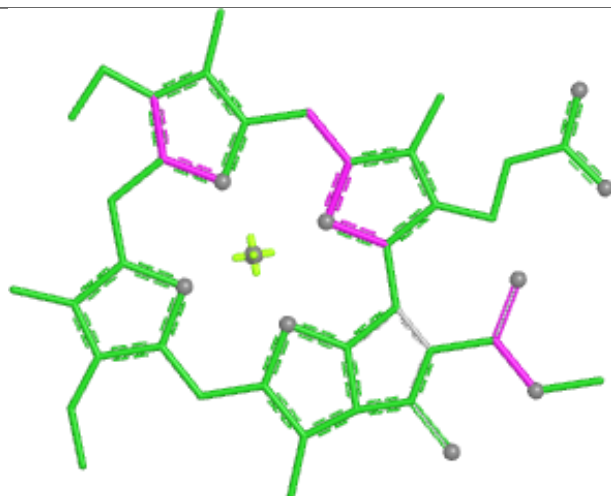
Rings



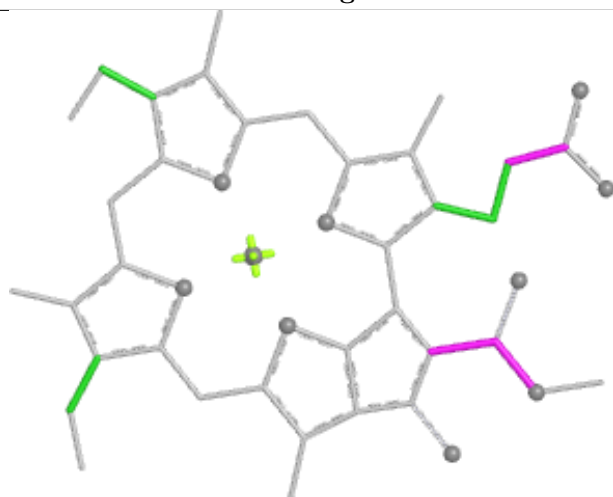
## Ligand CLA b 836



Bond lengths



Bond angles

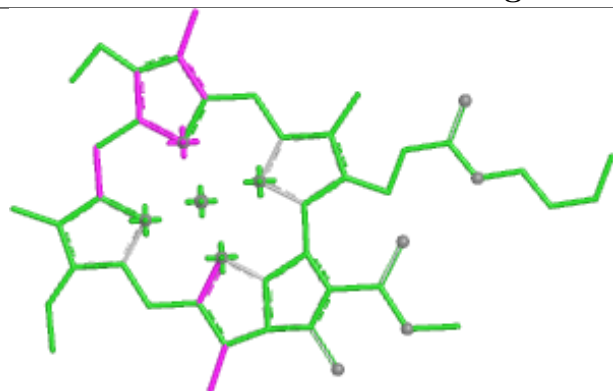


Torsions

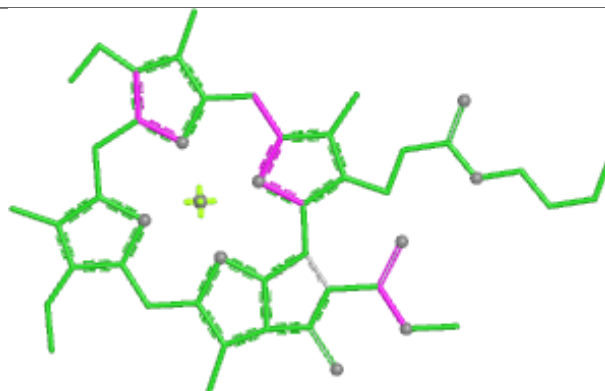


Rings

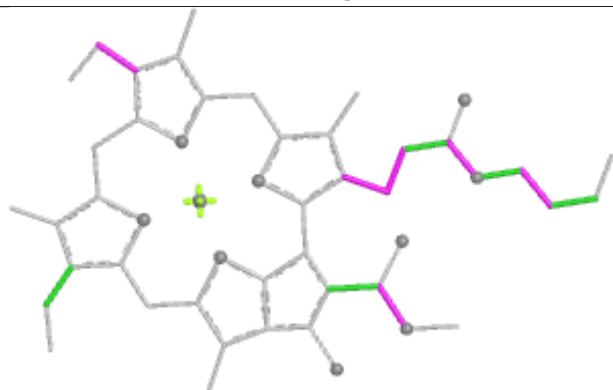
## Ligand CLA H 1701



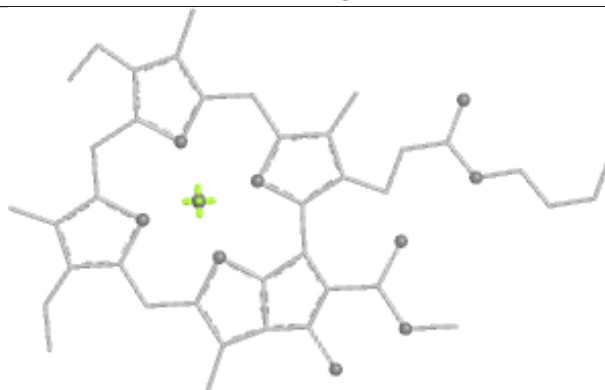
Bond lengths



Bond angles

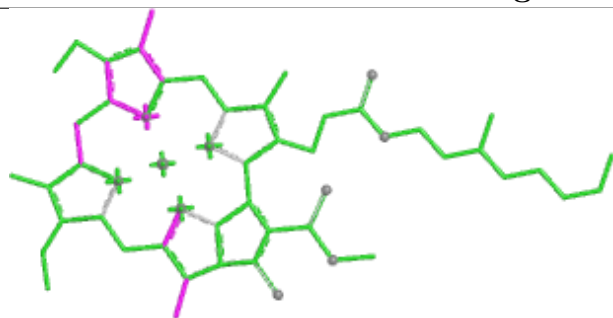


Torsions

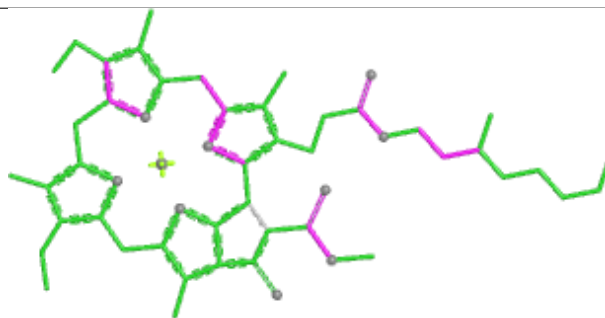


Rings

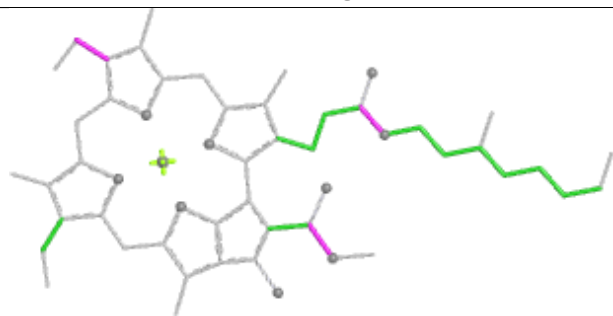
## Ligand CLA A 834



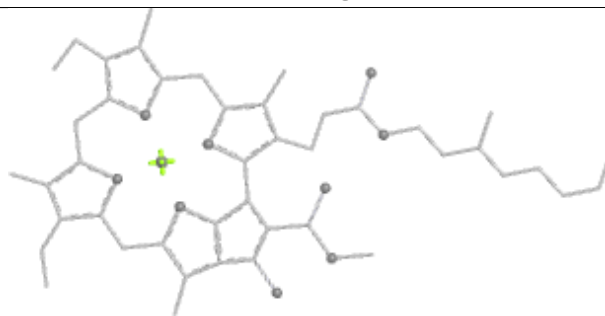
Bond lengths



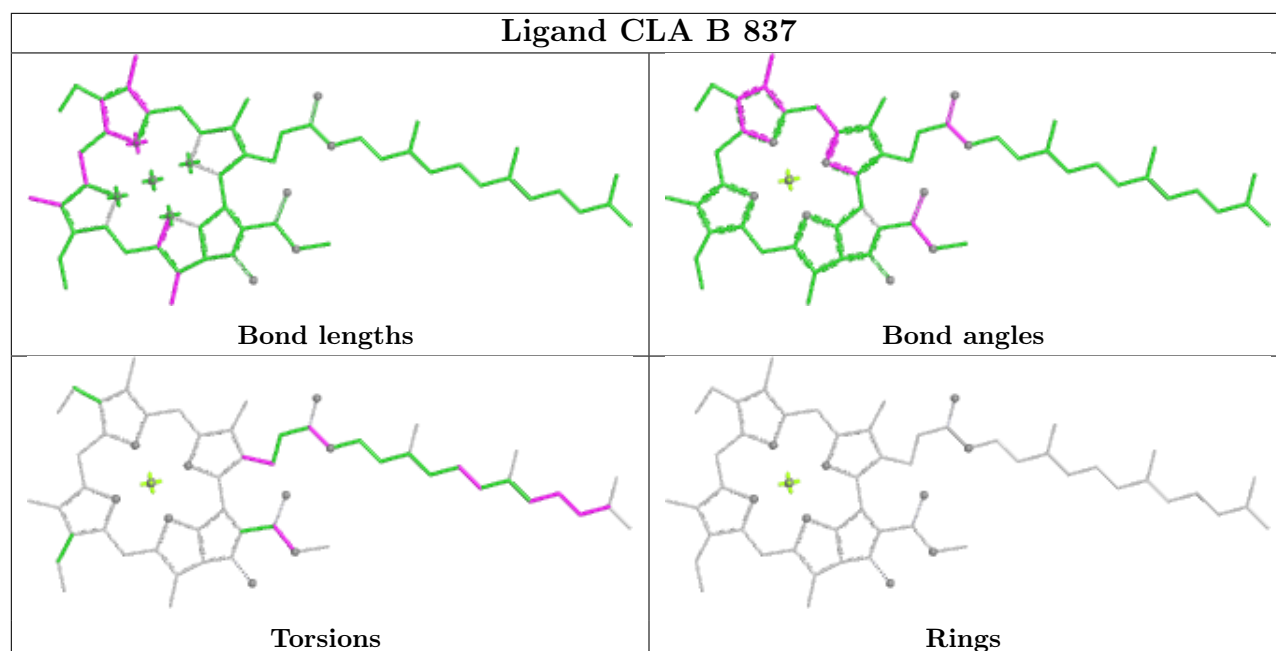
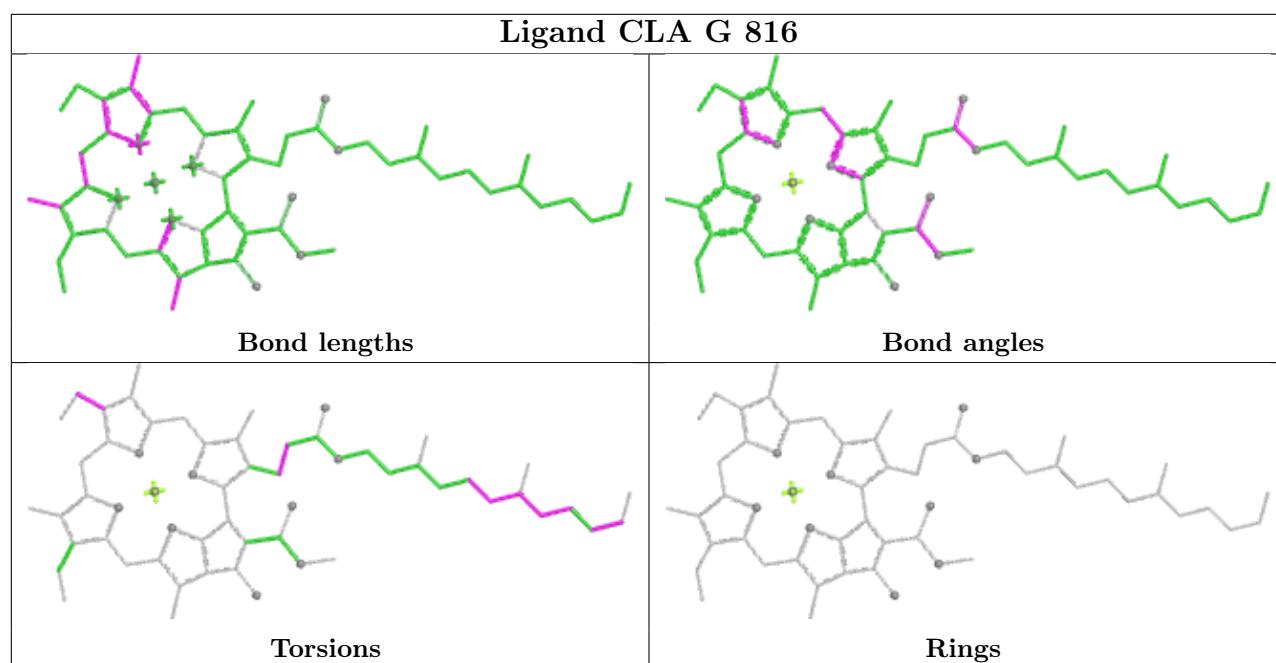
Bond angles

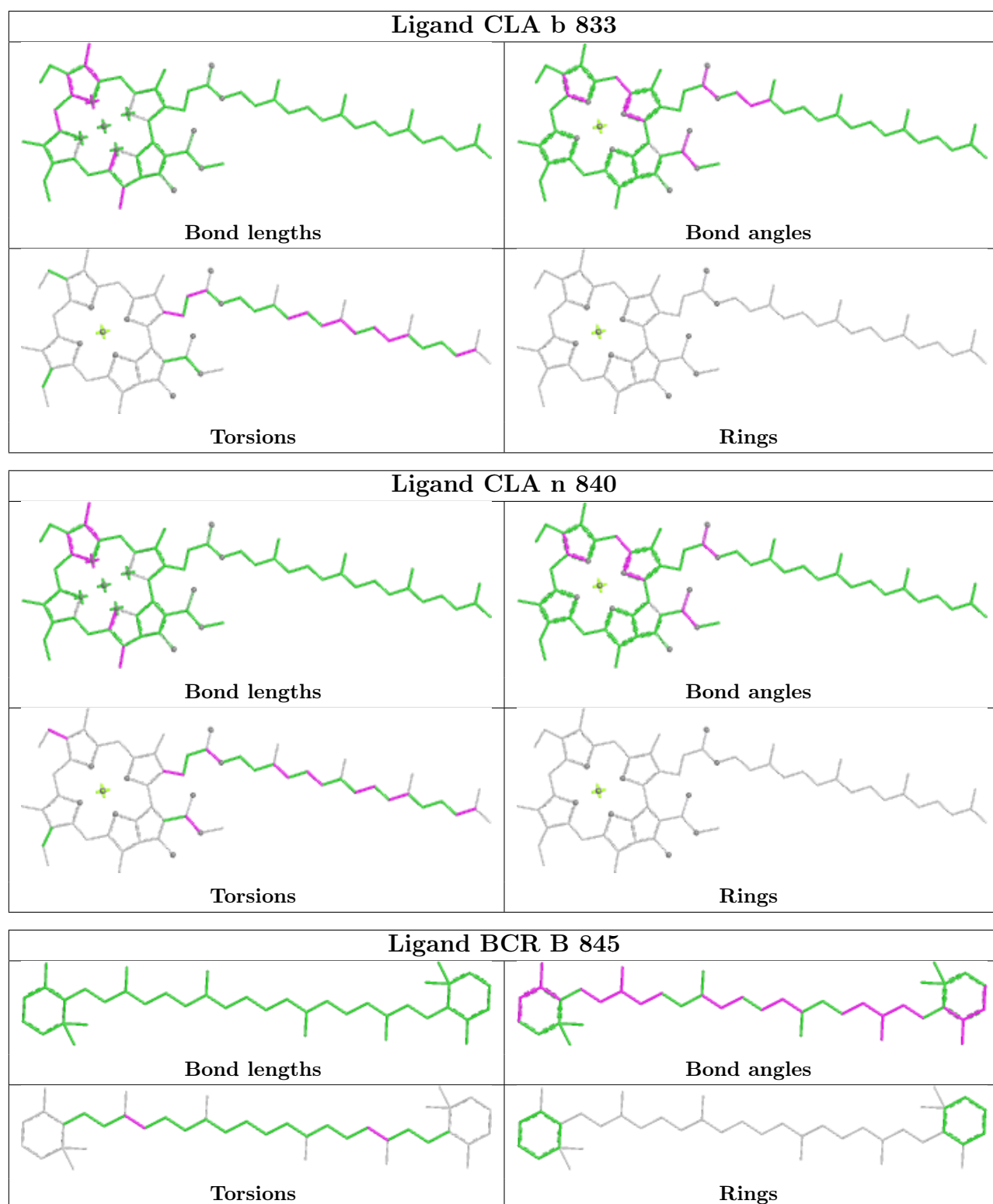


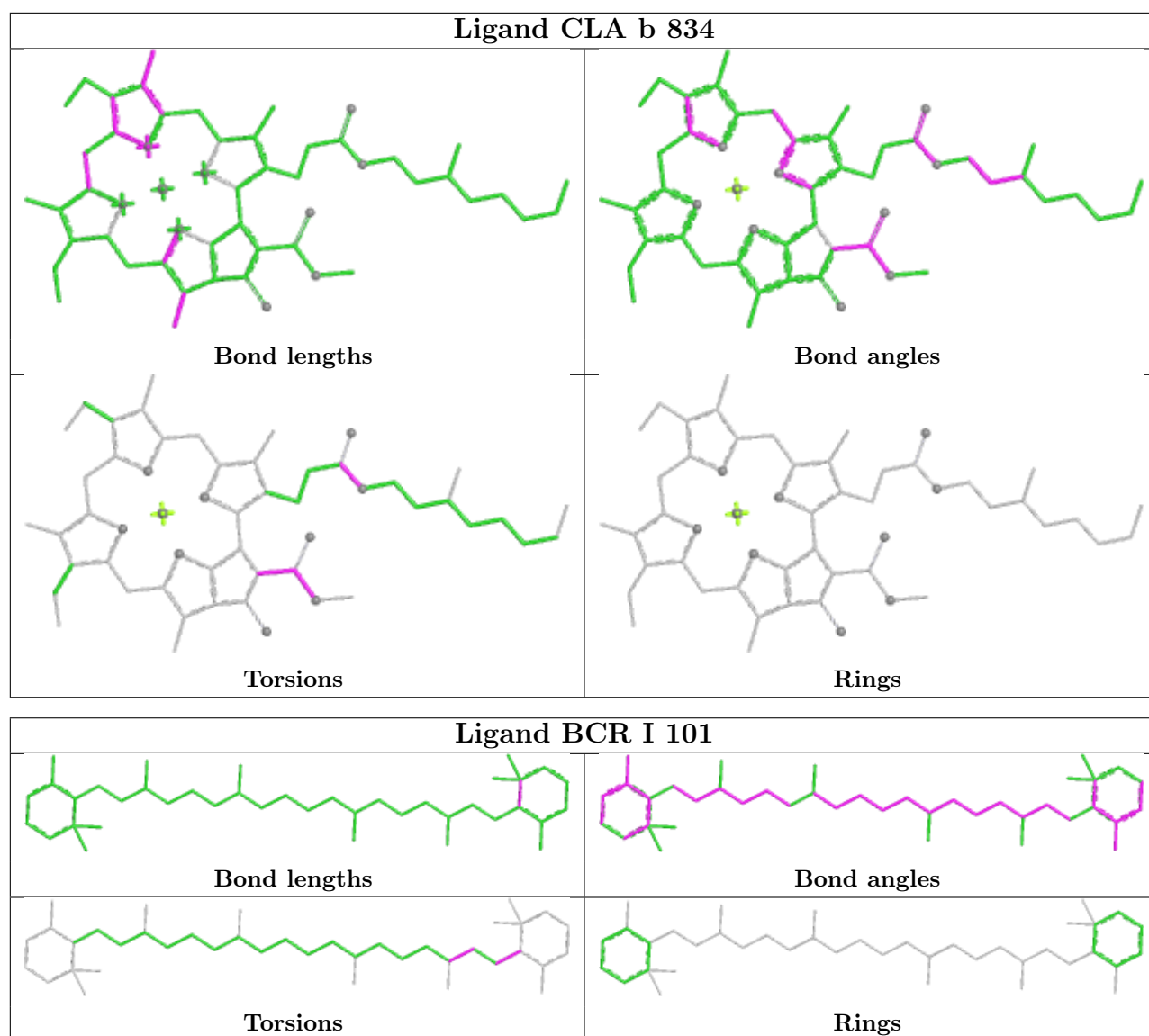
Torsions



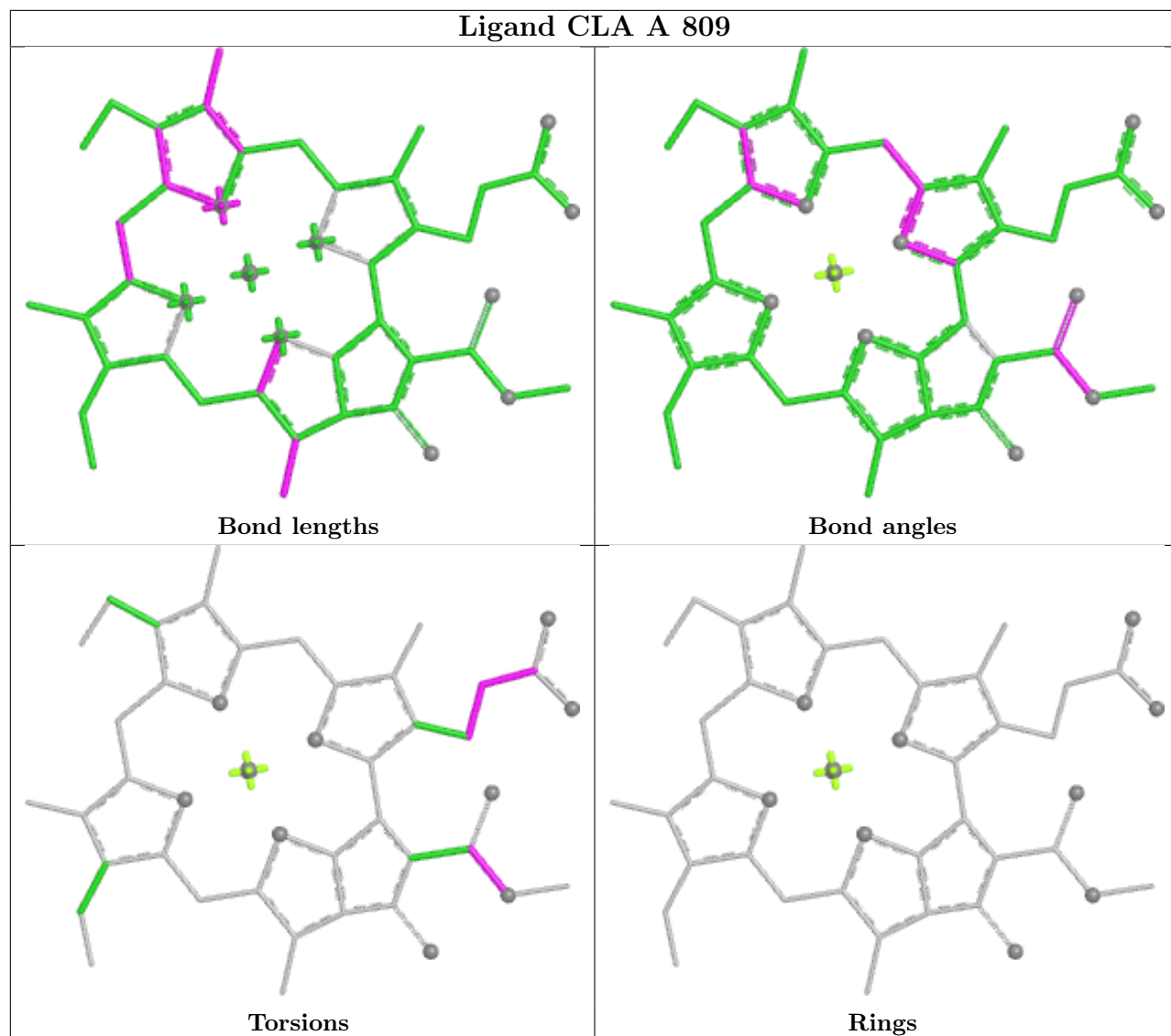
Rings



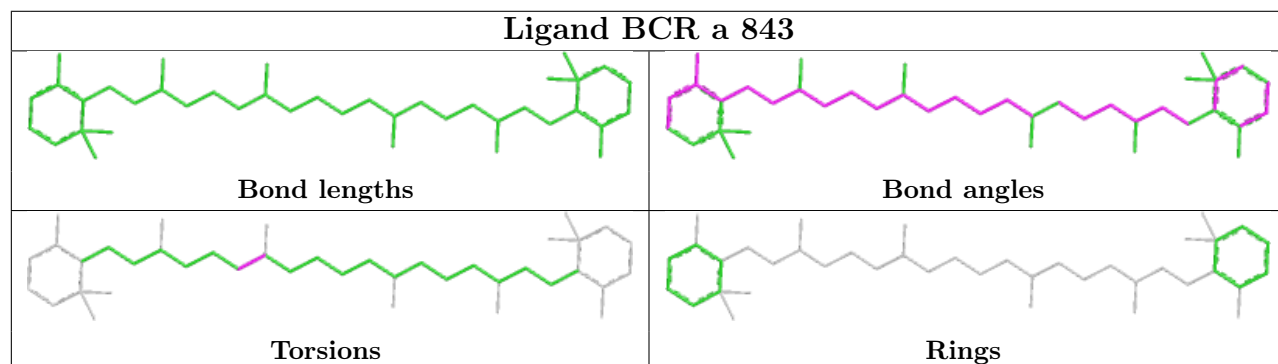


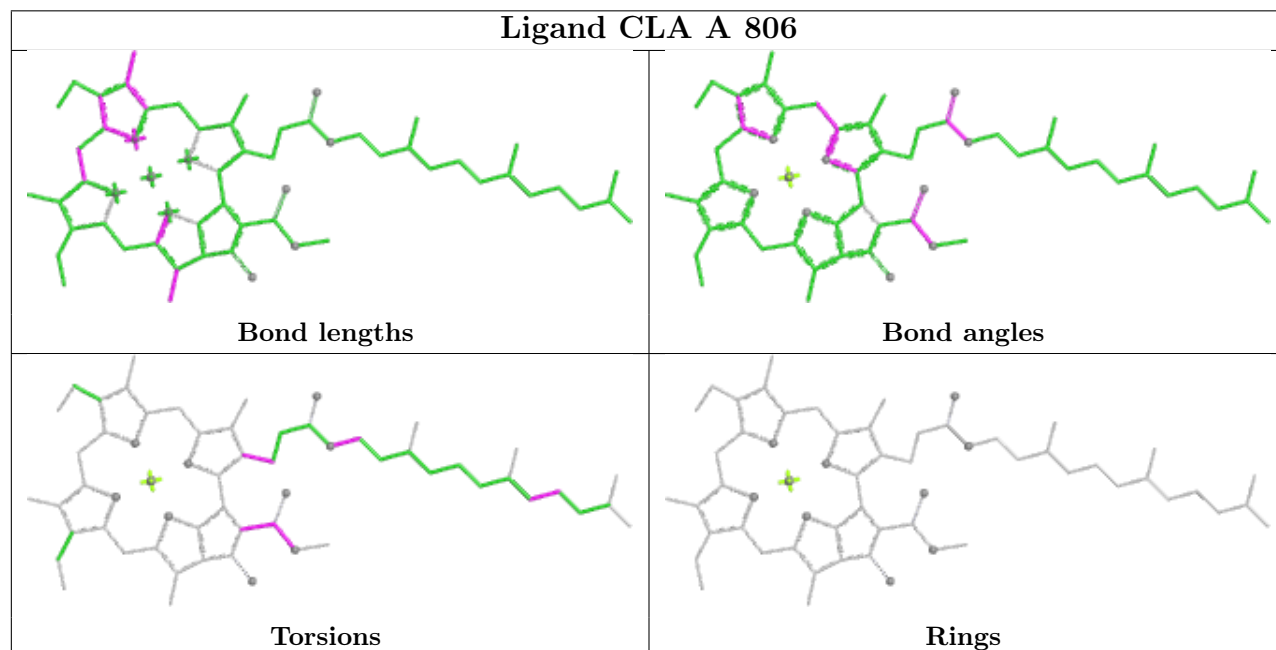
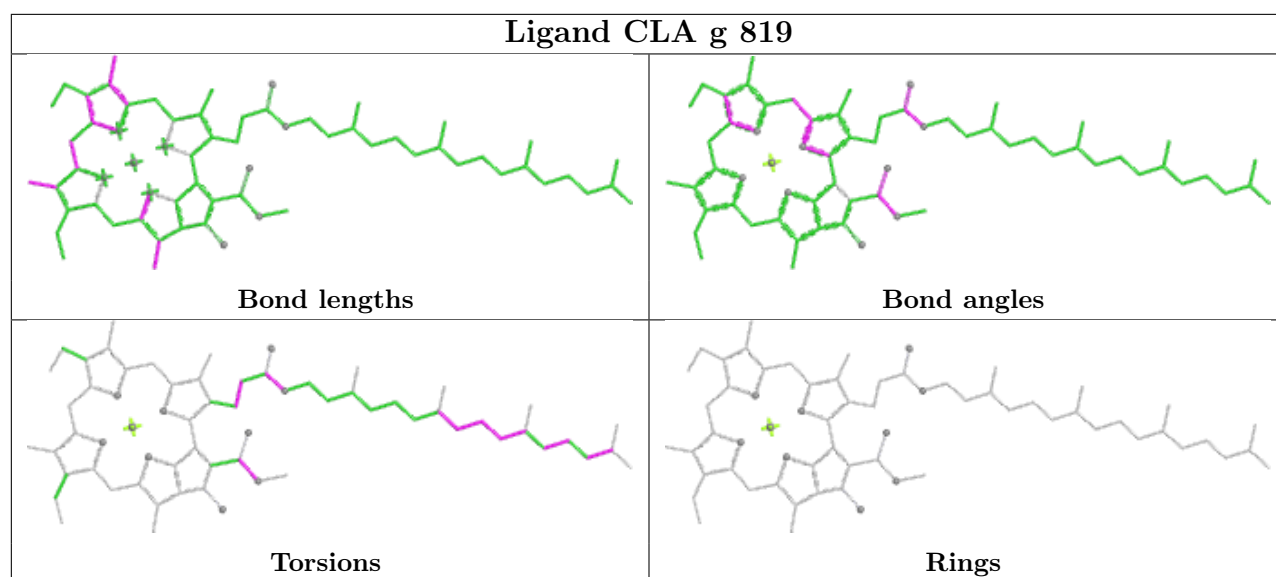


## Ligand CLA A 809

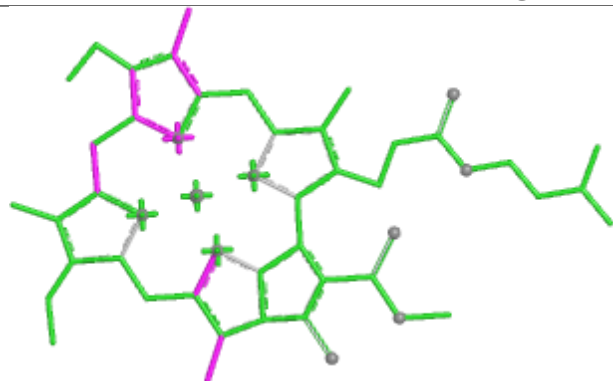


## Ligand BCR a 843

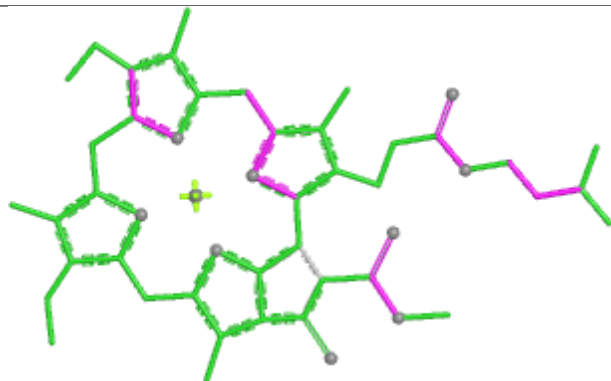




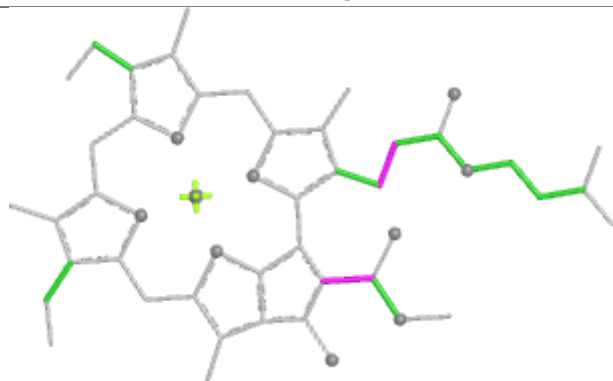
## Ligand CLA N 816



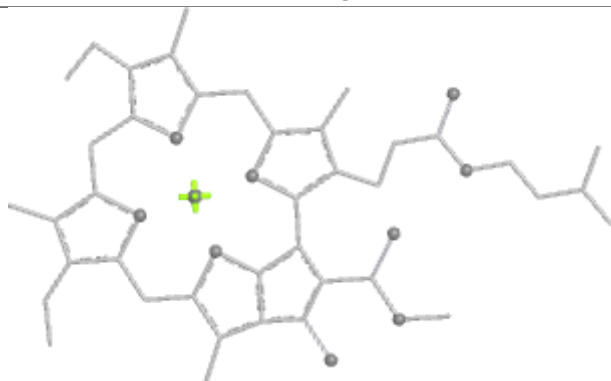
Bond lengths



Bond angles

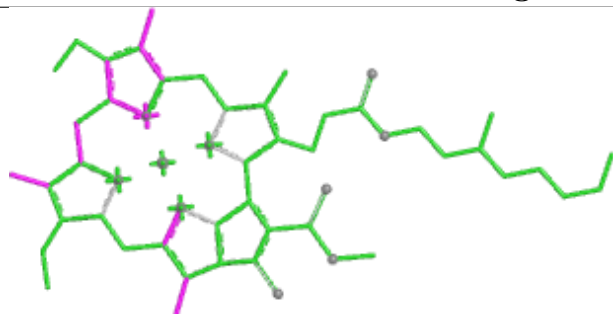


Torsions

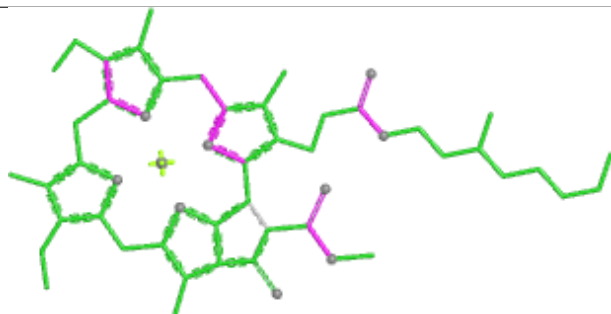


Rings

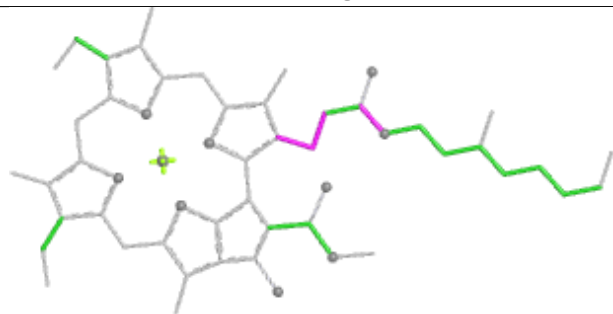
## Ligand CLA G 819



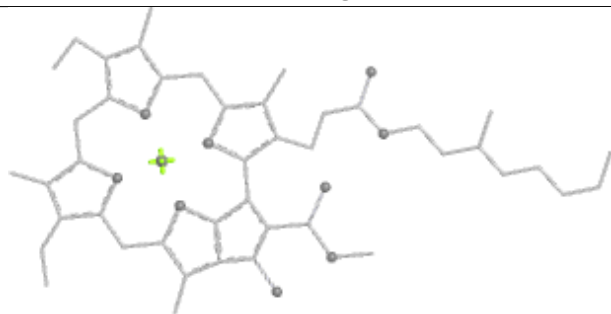
Bond lengths



Bond angles

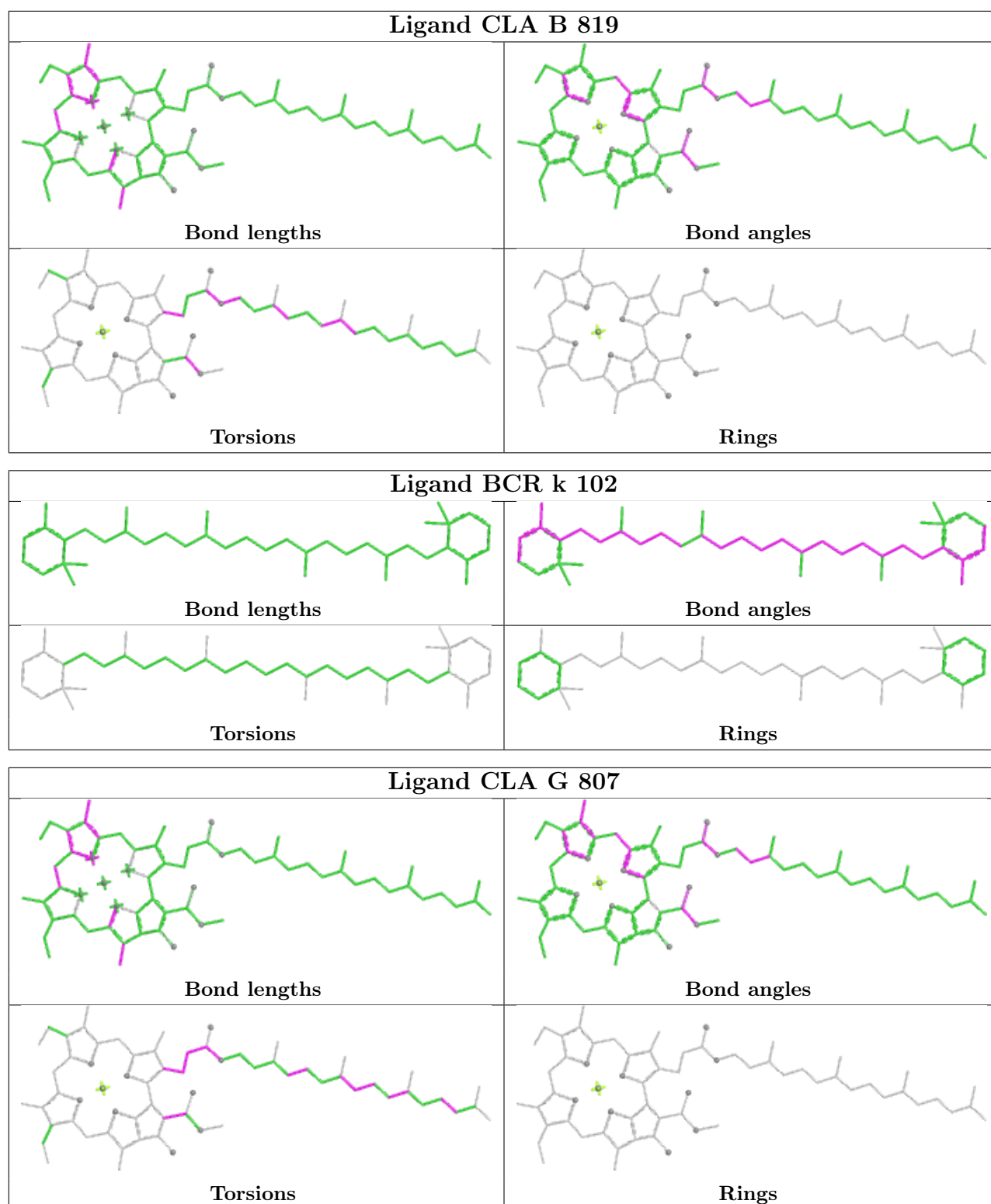


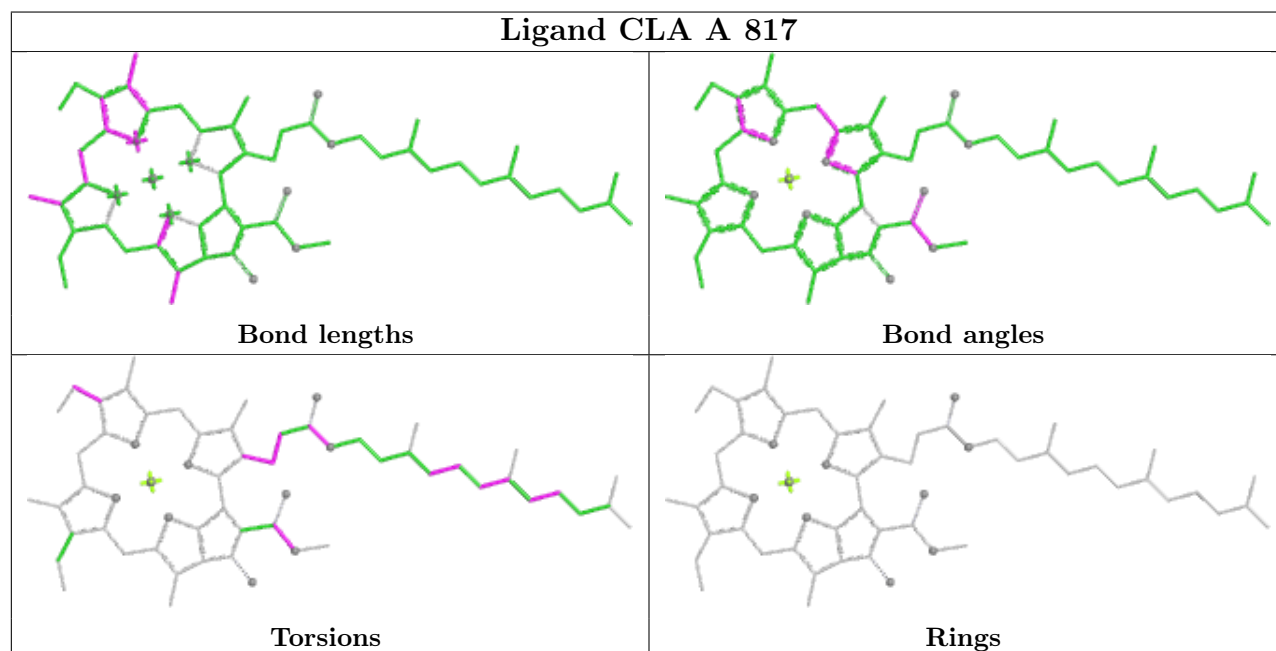
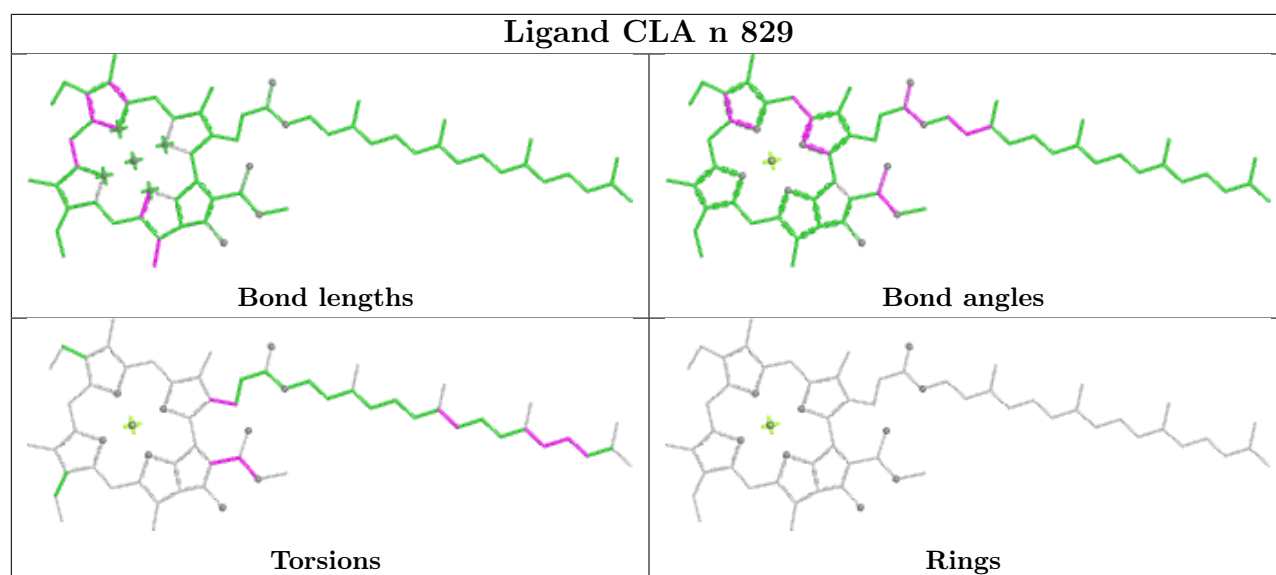
Torsions

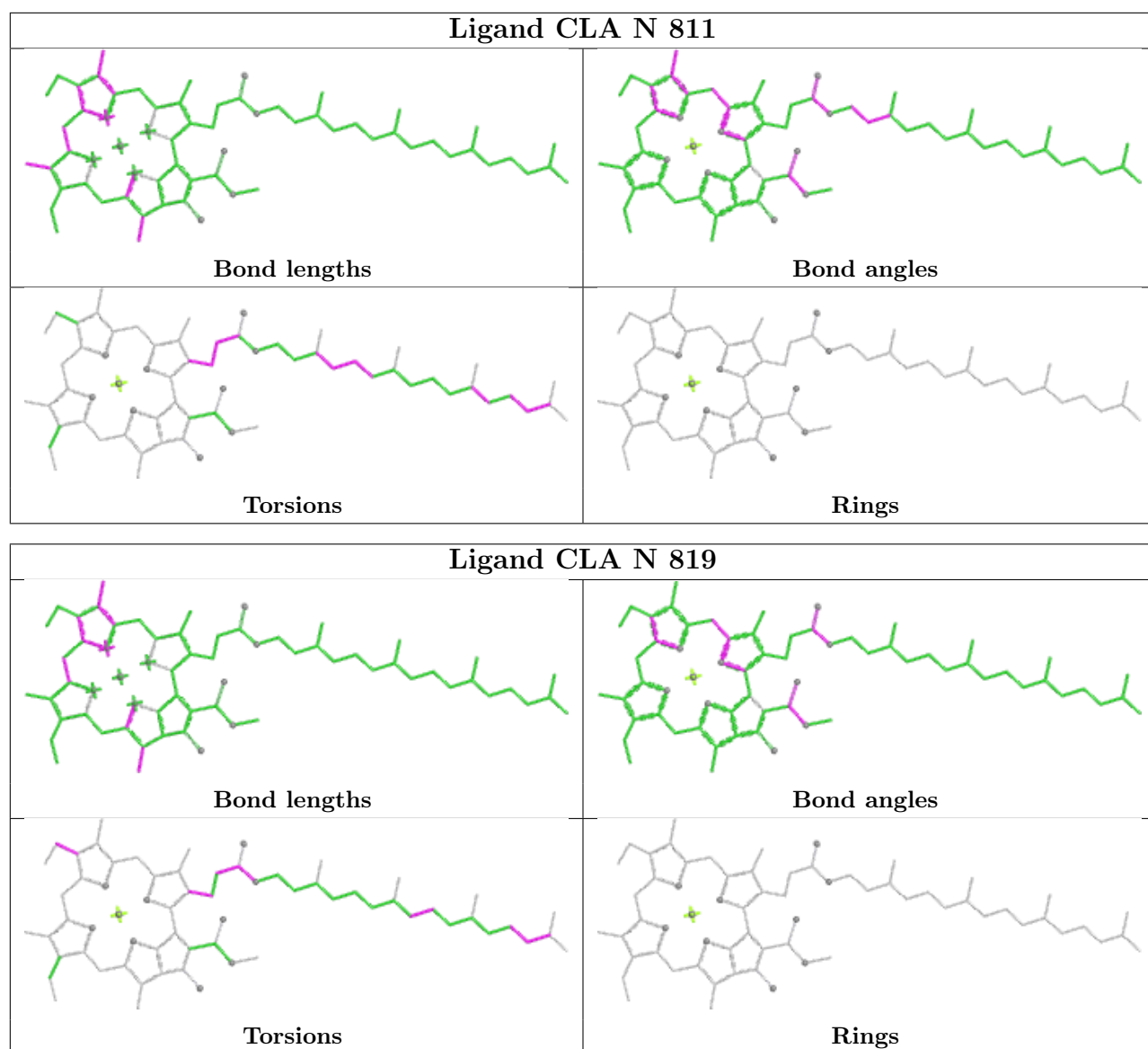


Rings

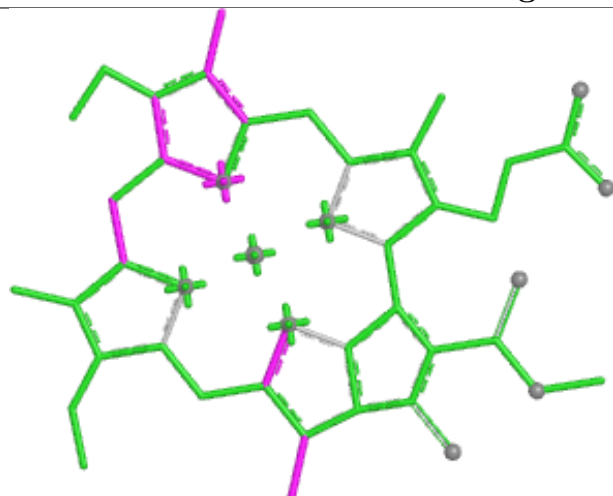




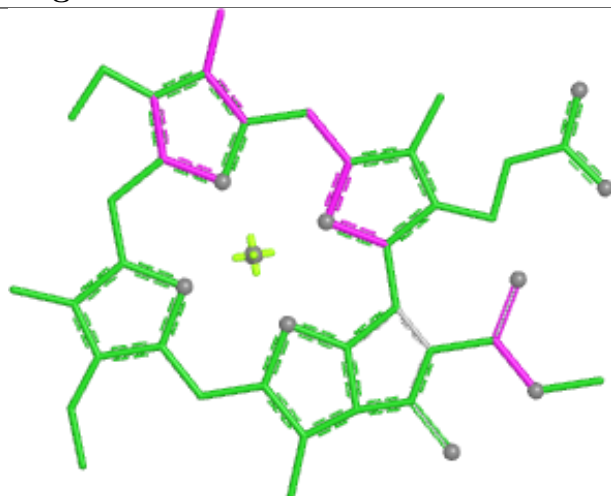




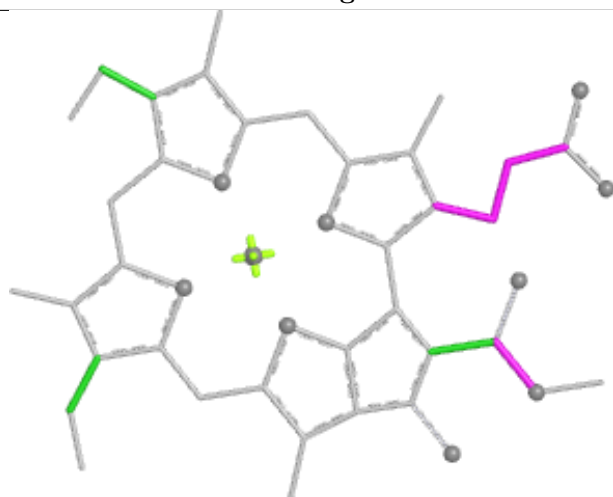
## Ligand CLA g 820



Bond lengths



Bond angles

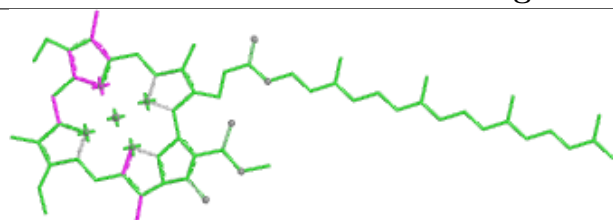


Torsions

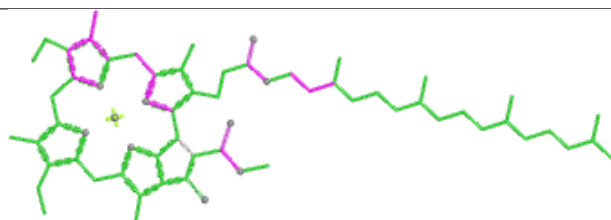


Rings

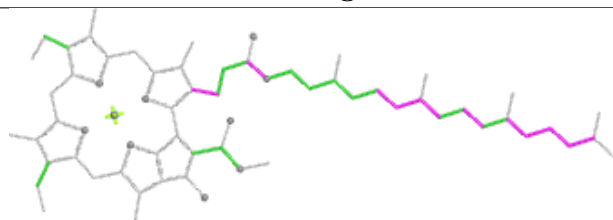
## Ligand CLA A 818



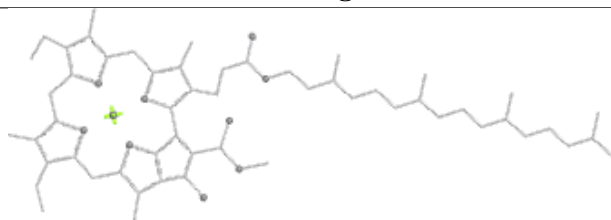
Bond lengths



Bond angles

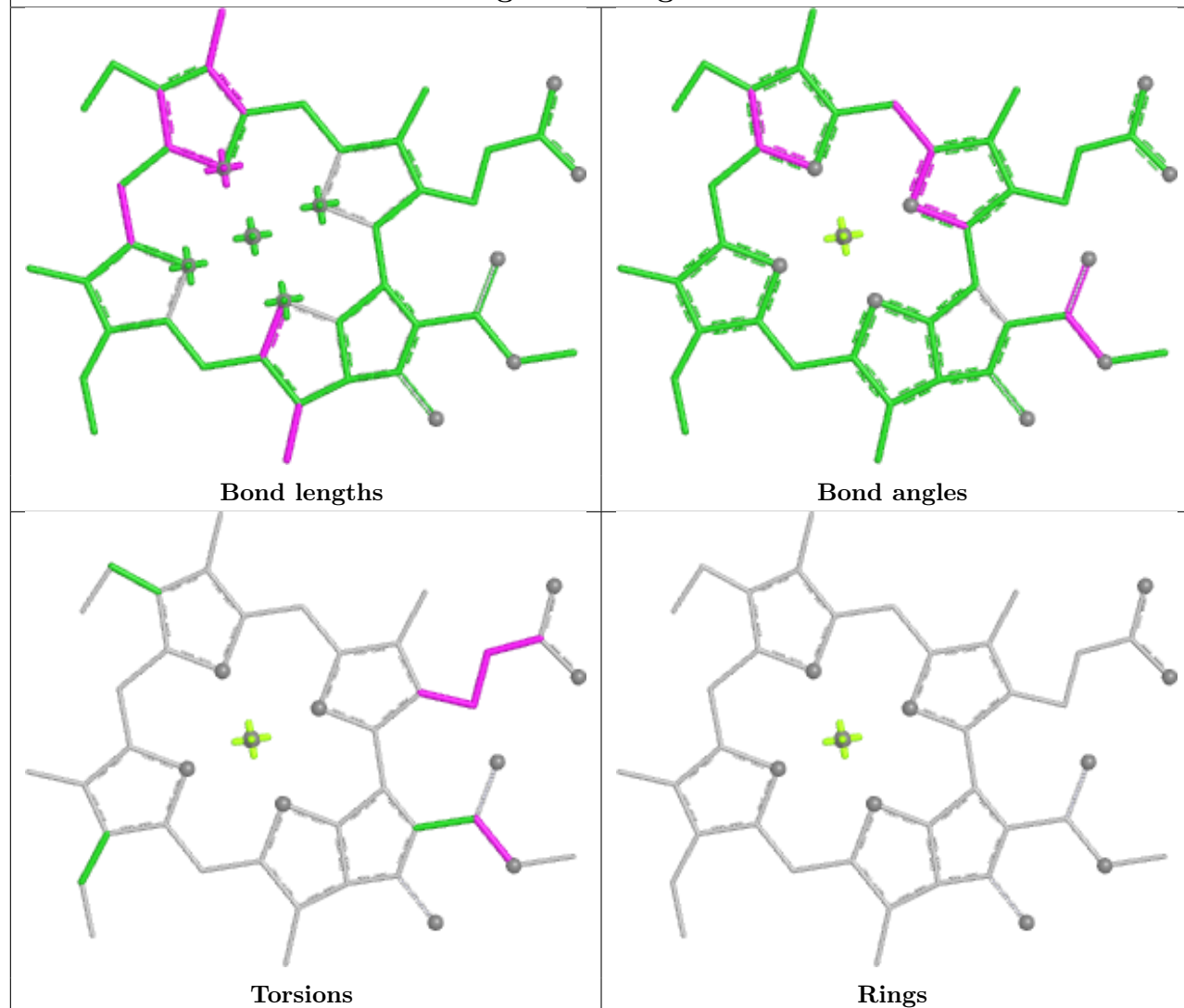


Torsions

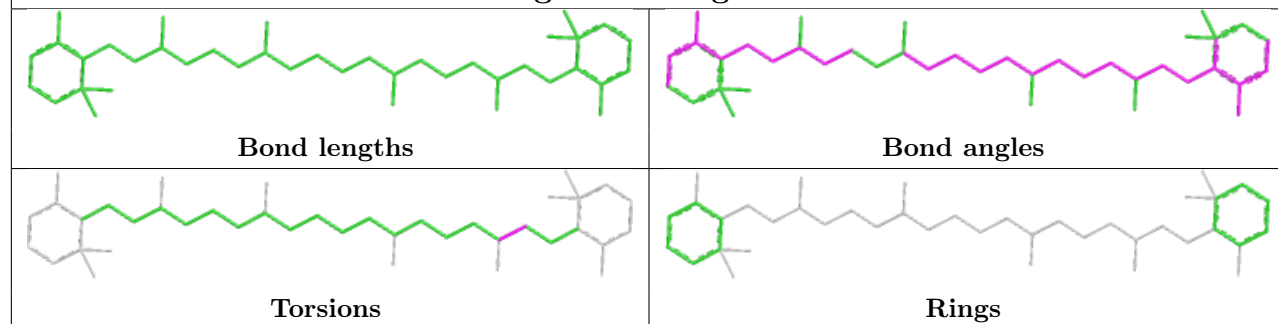


Rings

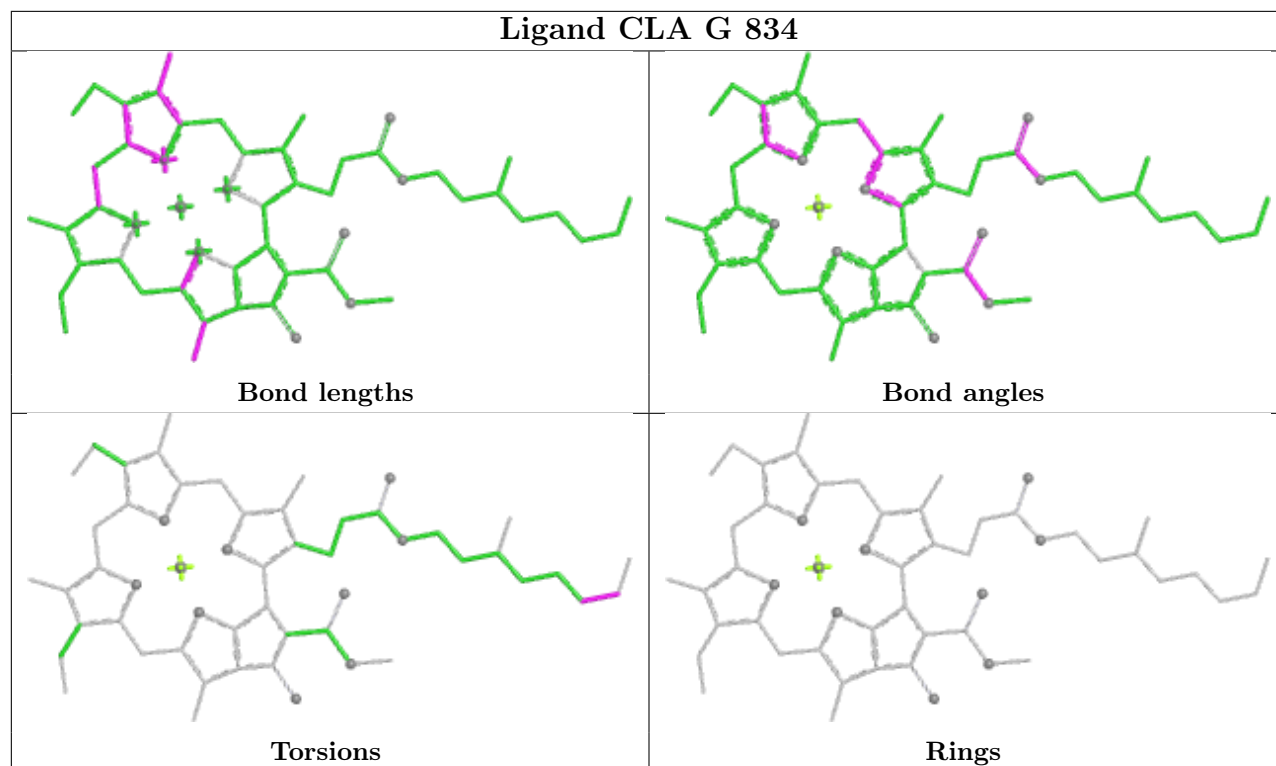
## Ligand CLA g 808



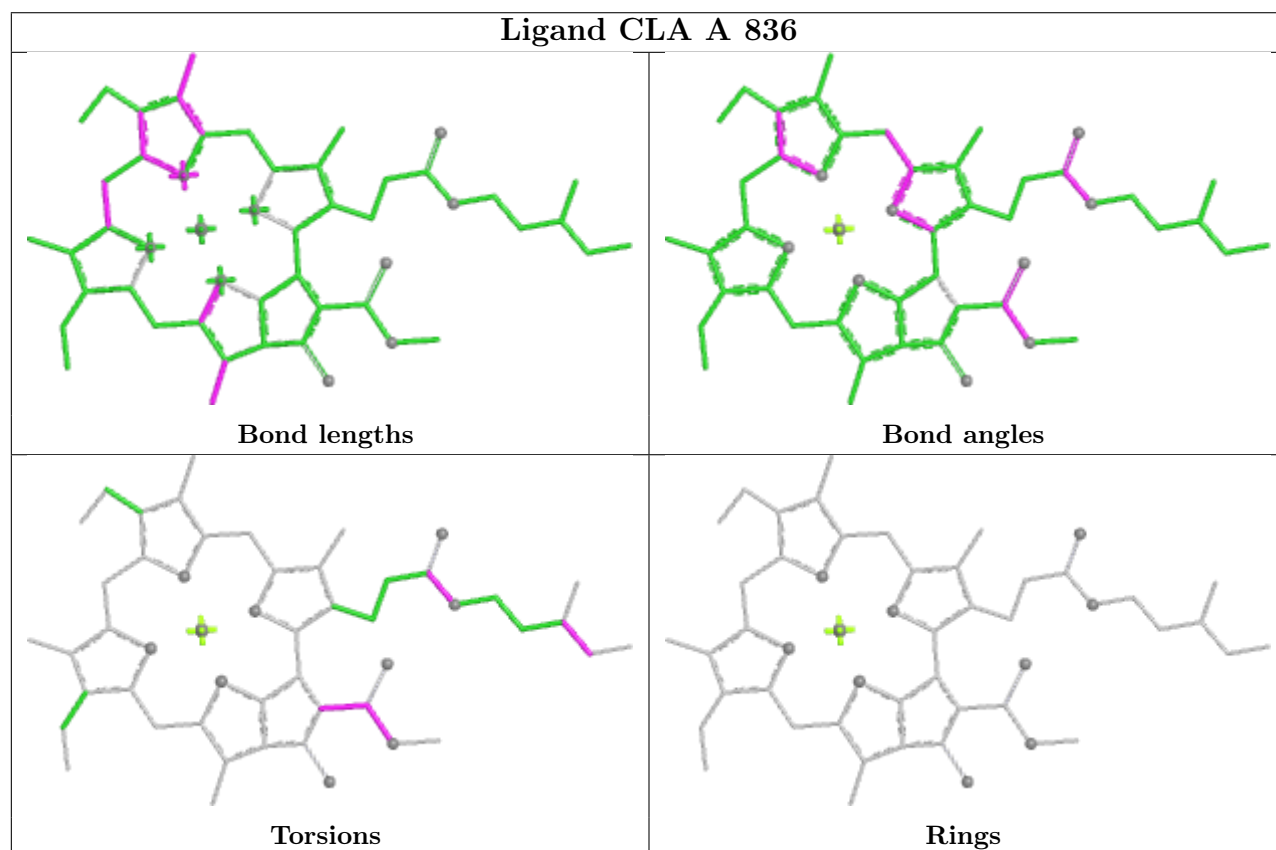
## Ligand BCR g 844

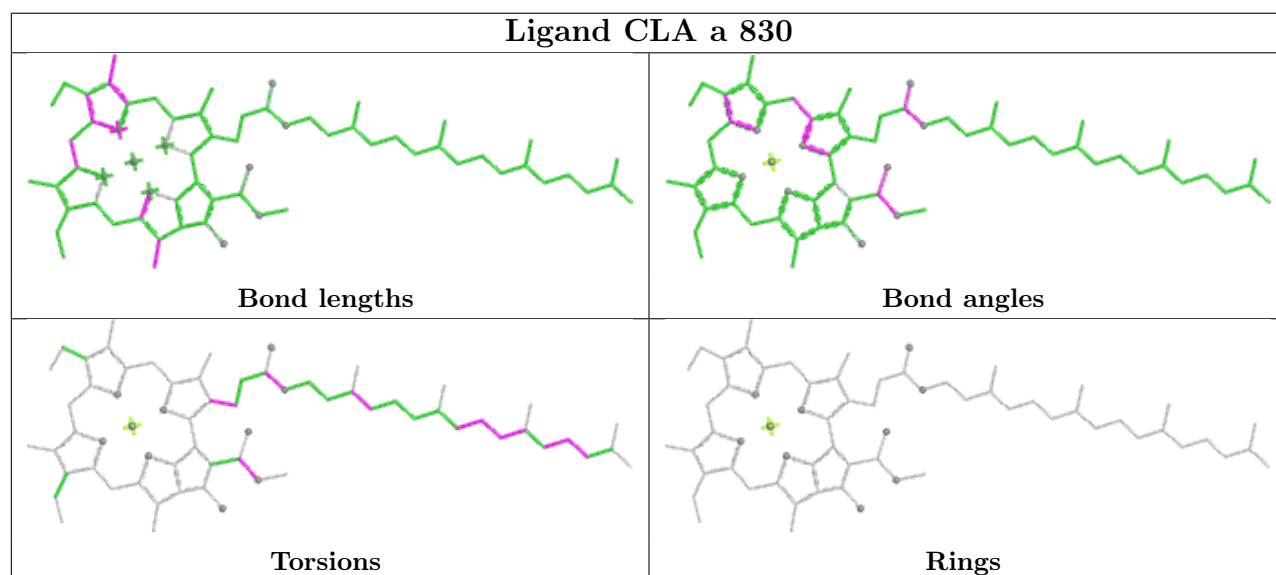
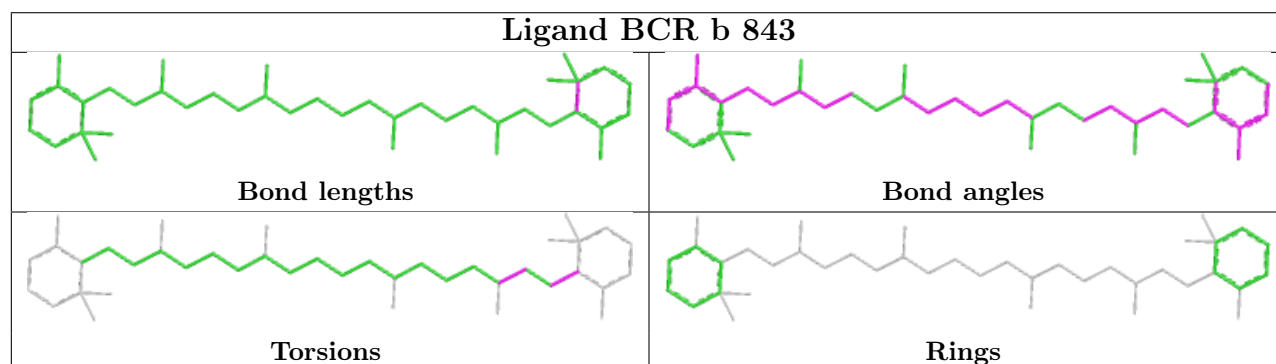
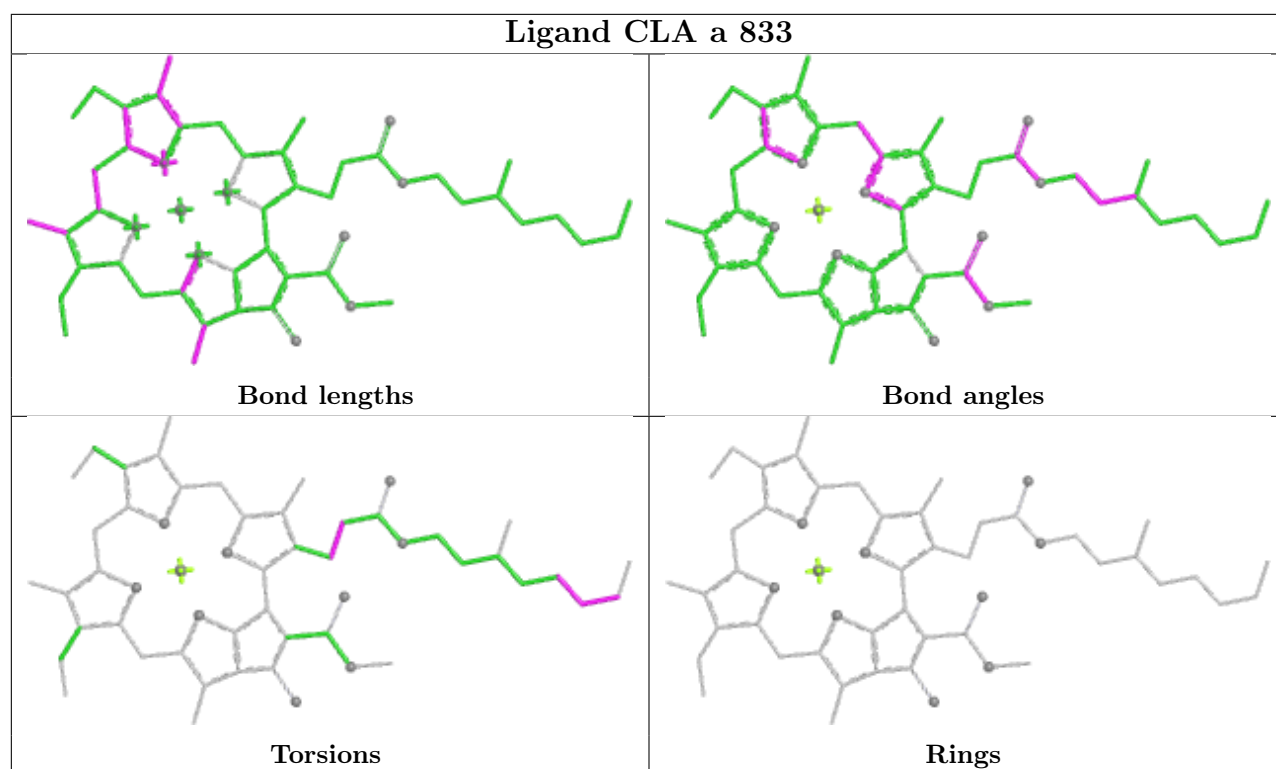


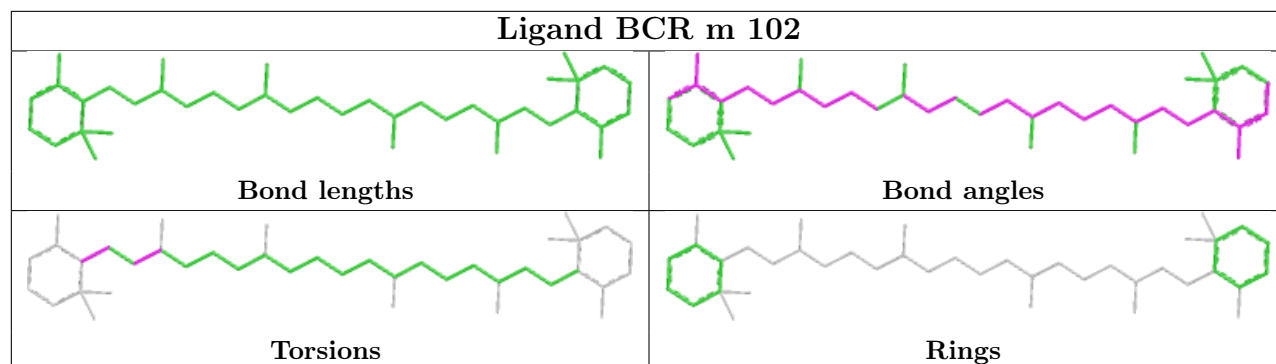
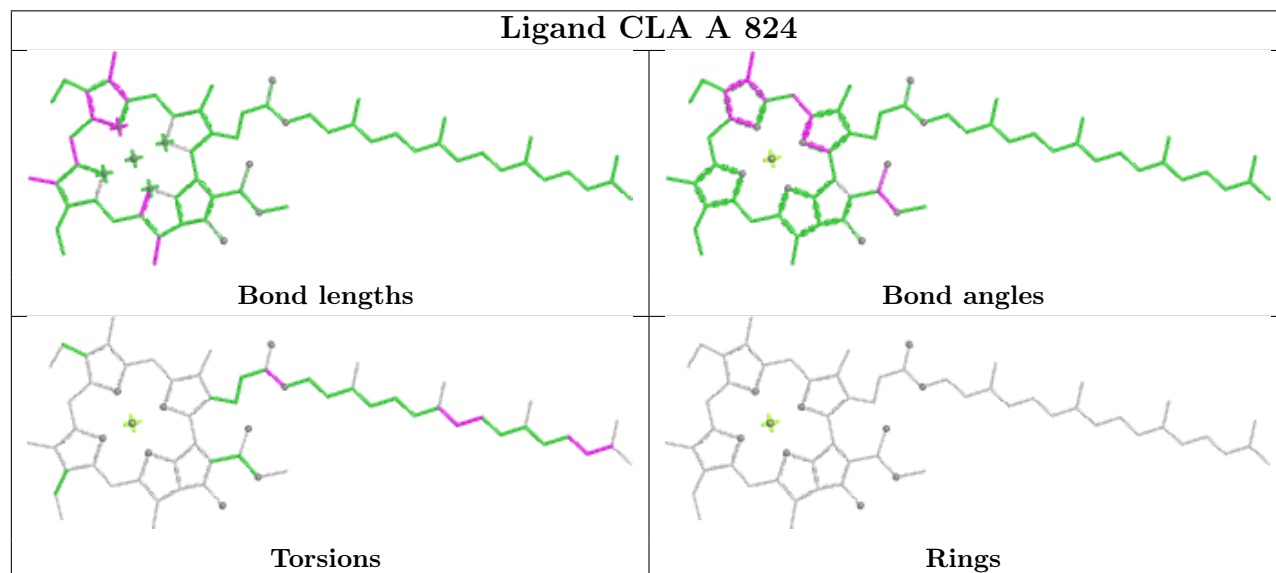
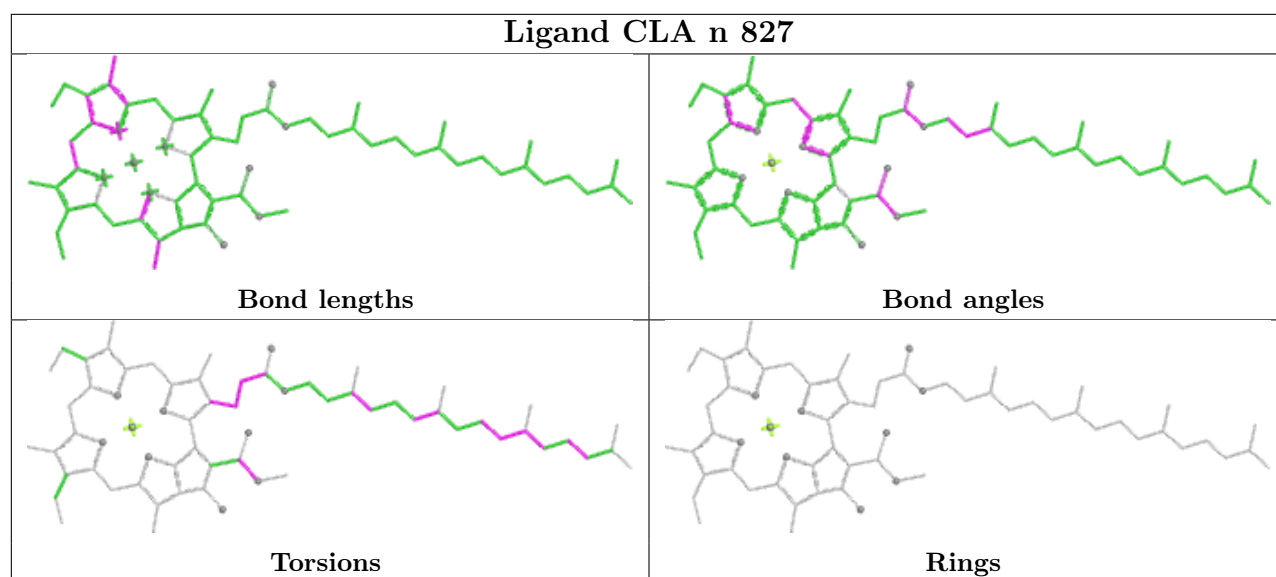
## Ligand CLA G 834



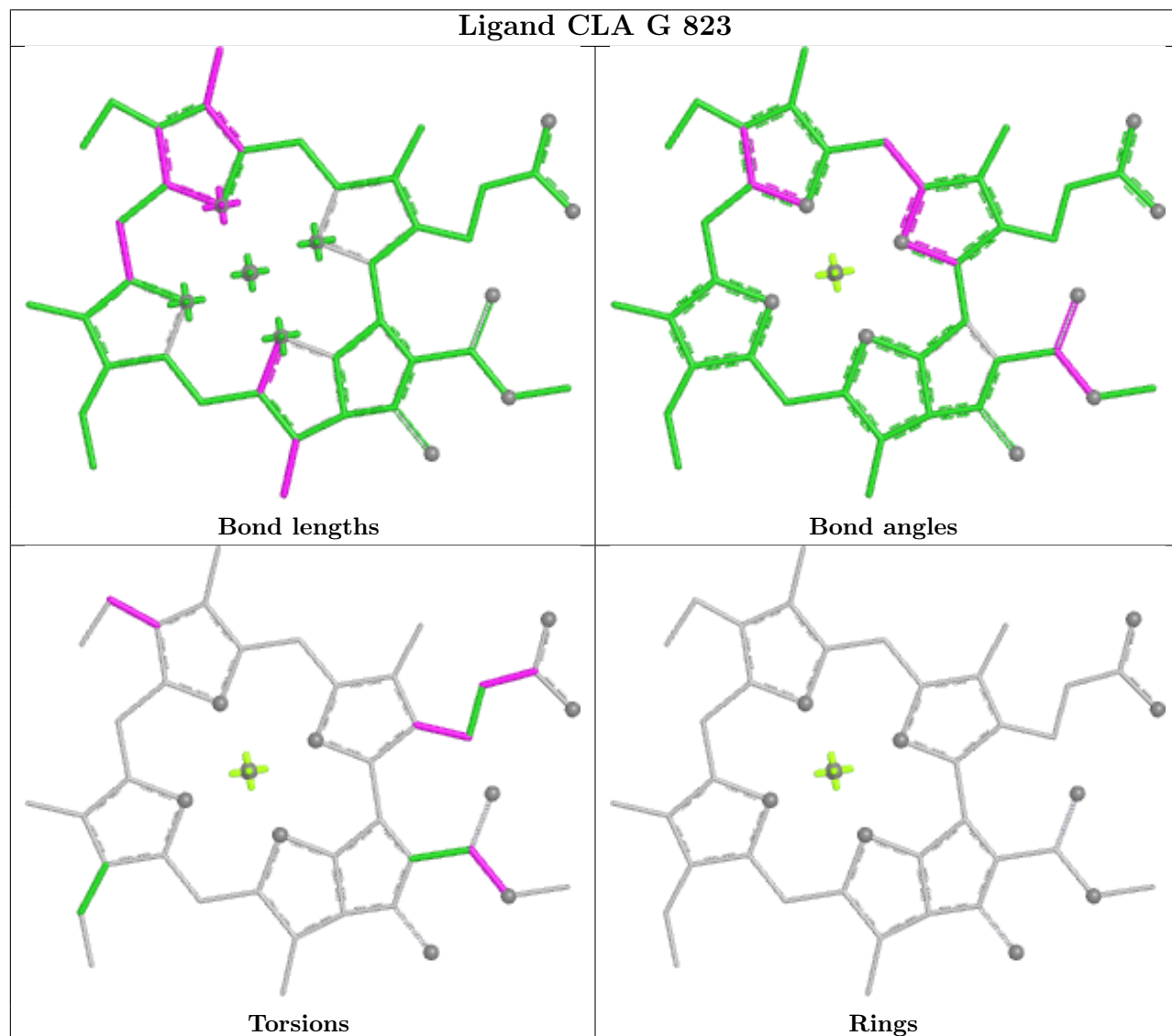
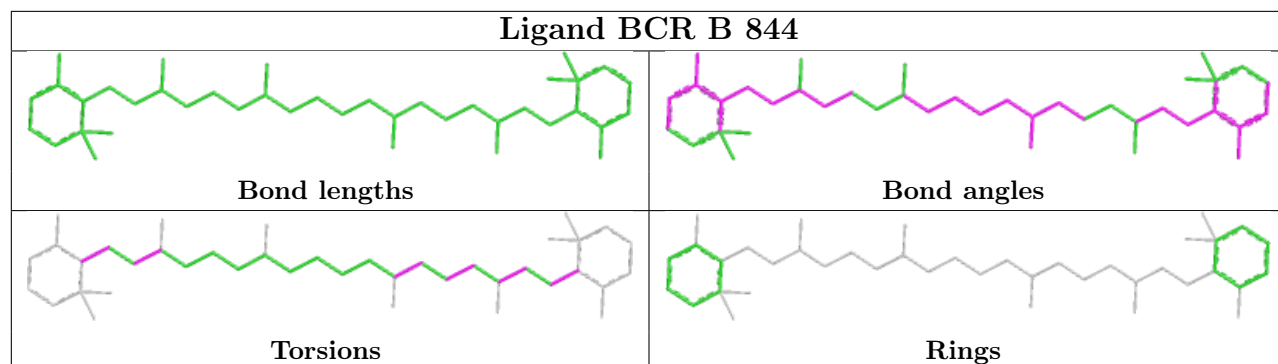
## Ligand CLA A 836



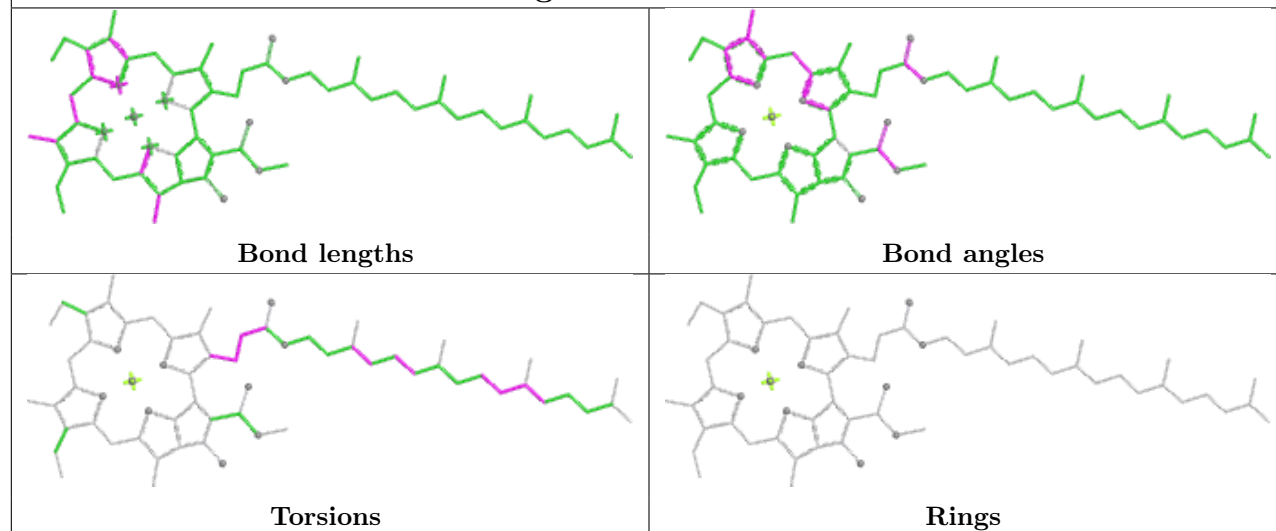




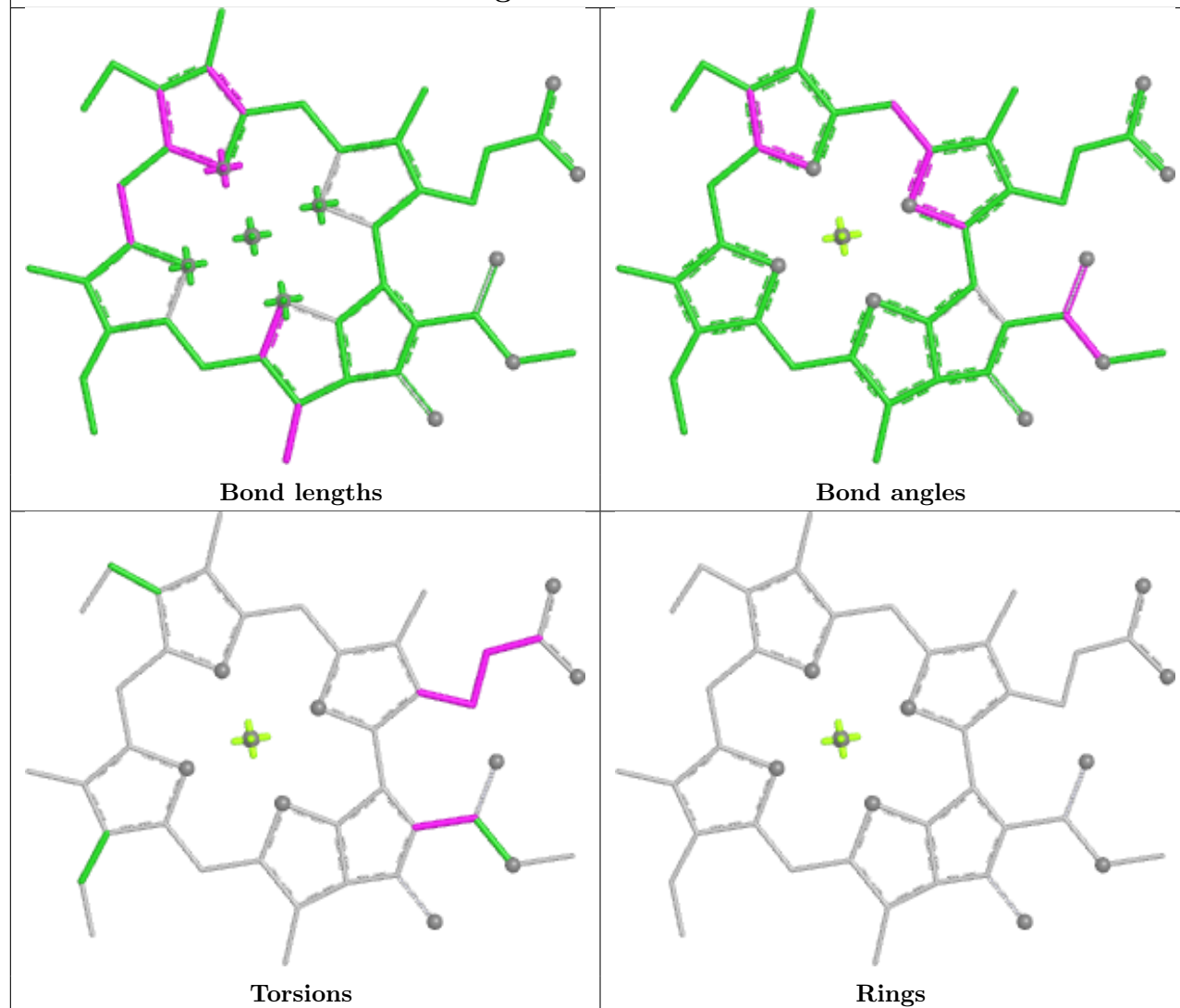




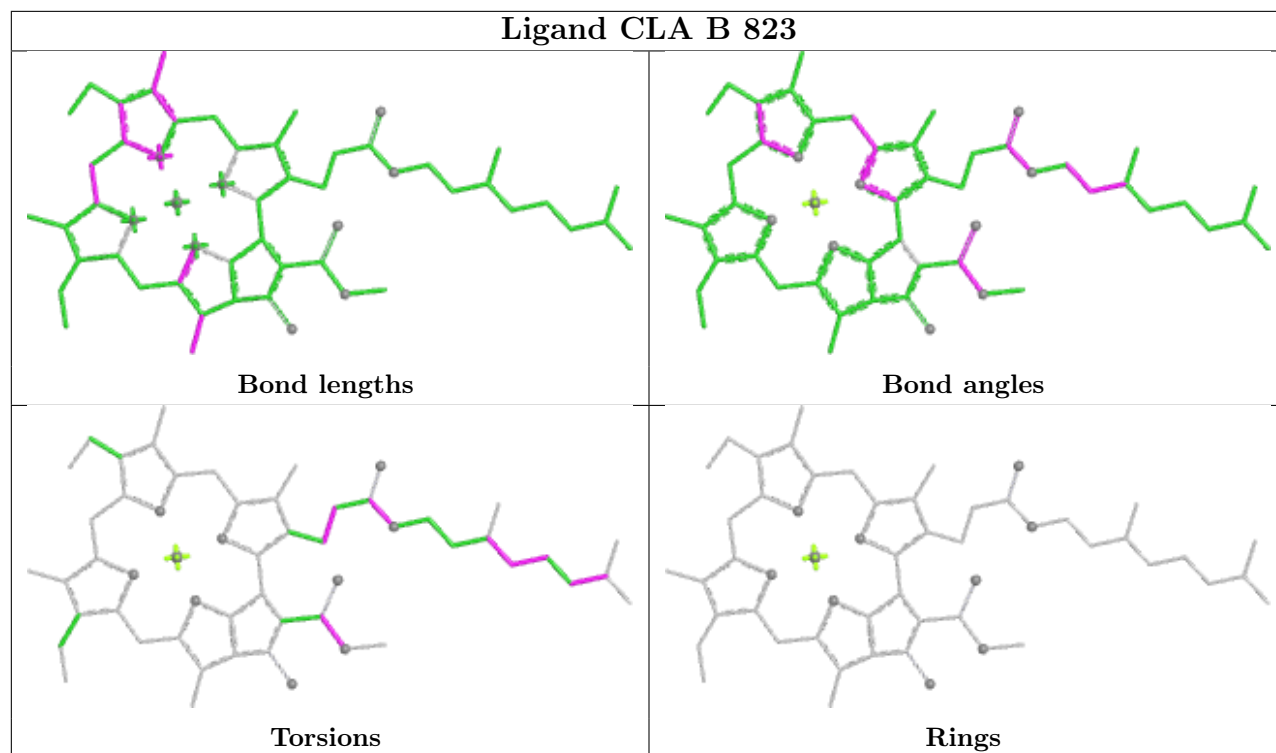
## Ligand CLA b 814



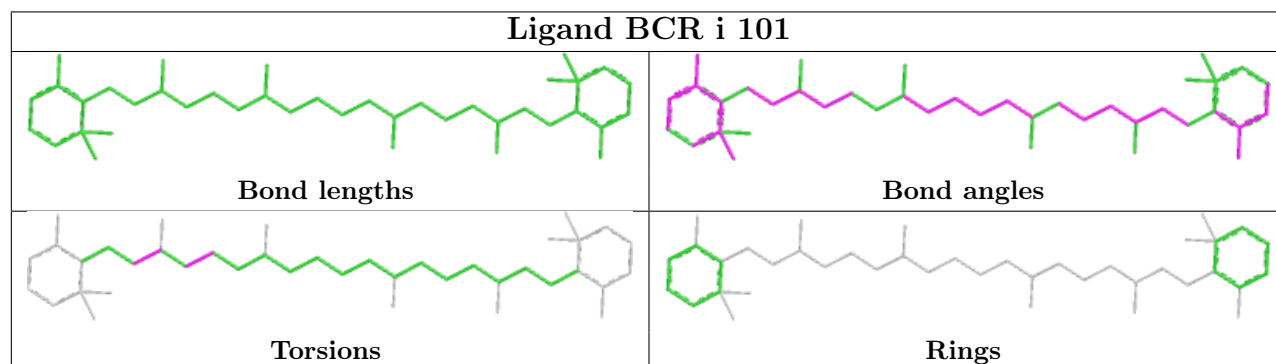
## Ligand CLA b 822



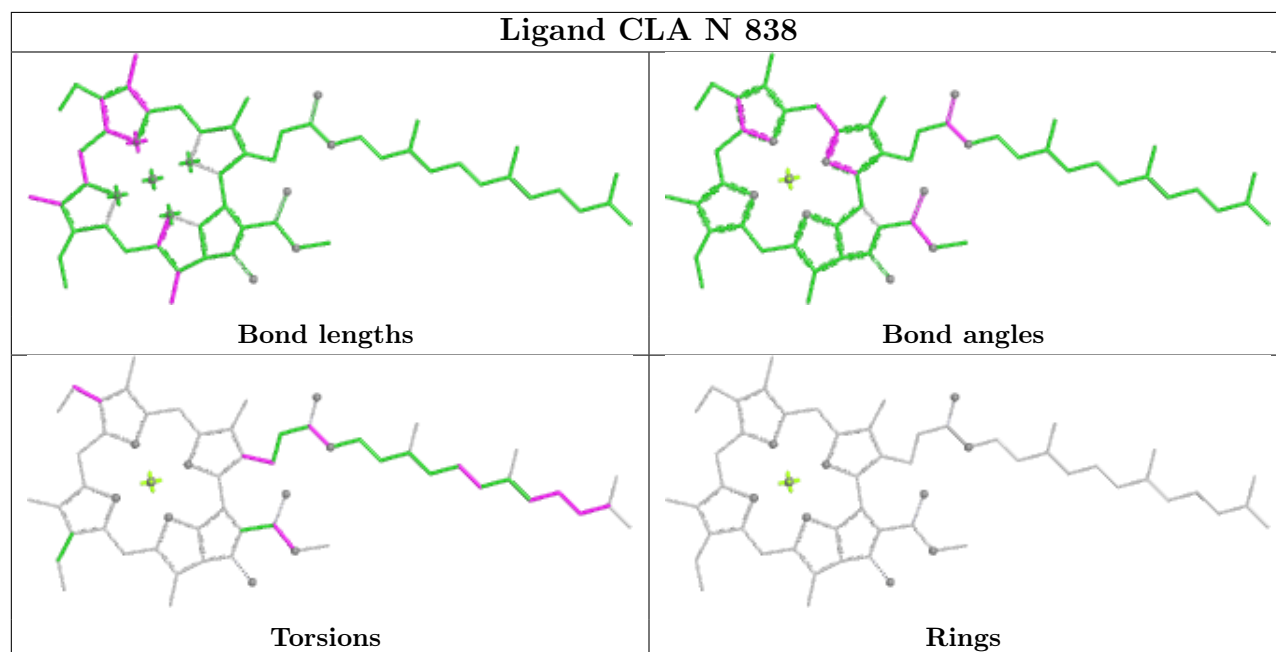
## Ligand CLA B 823

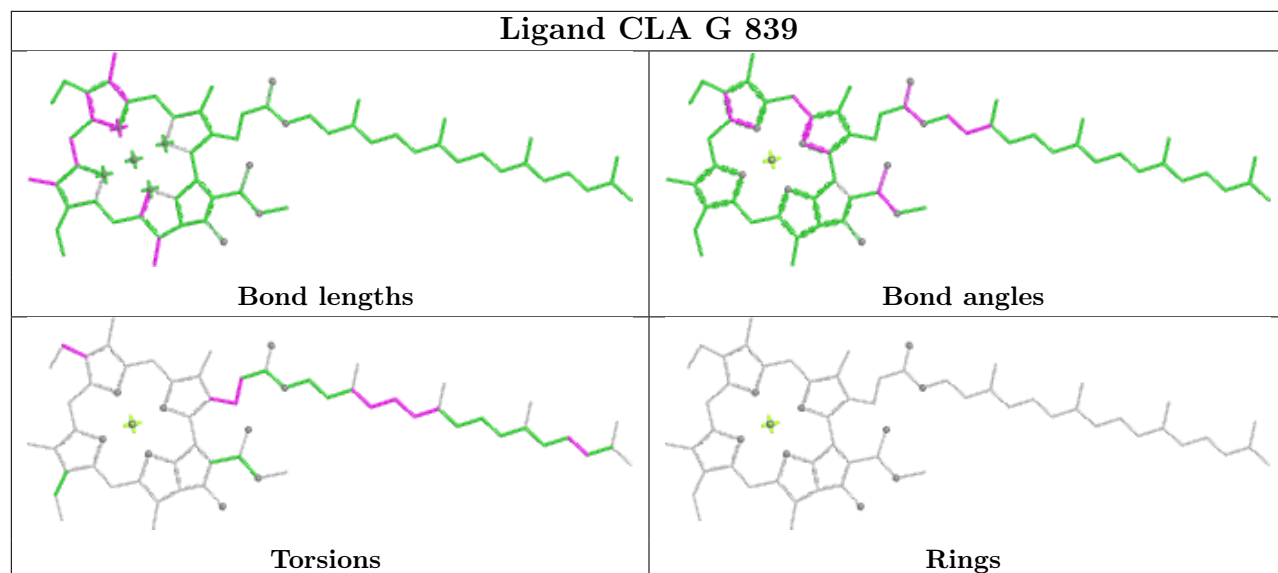
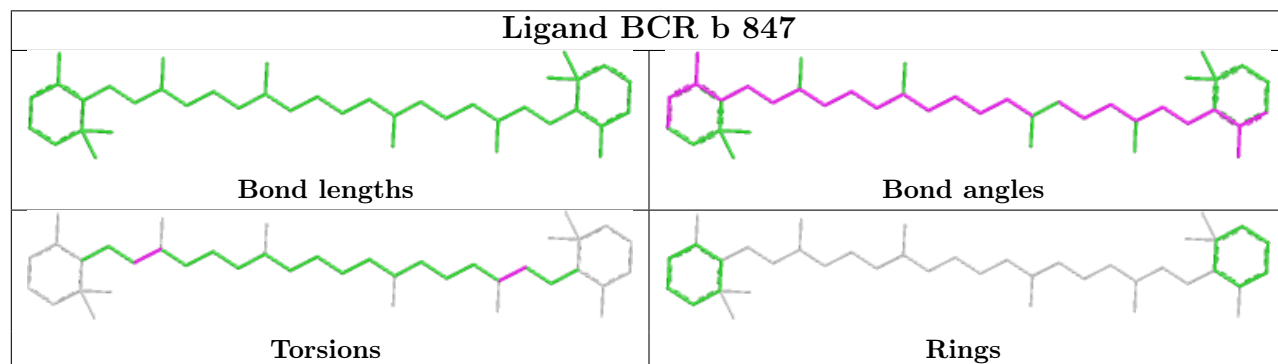
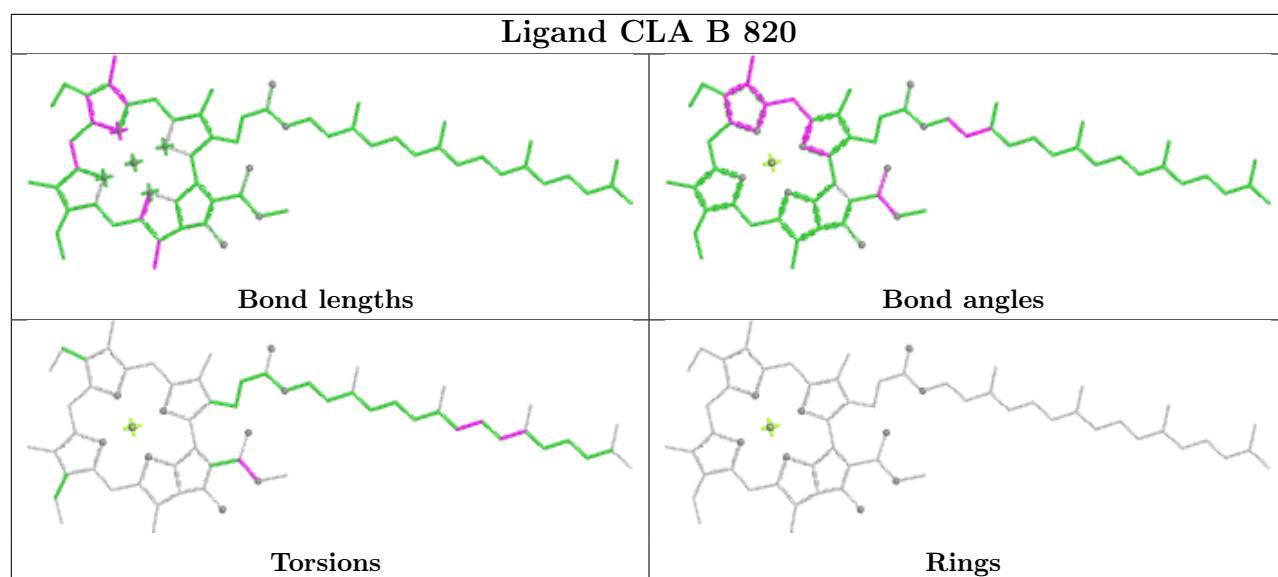


## Ligand BCR i 101

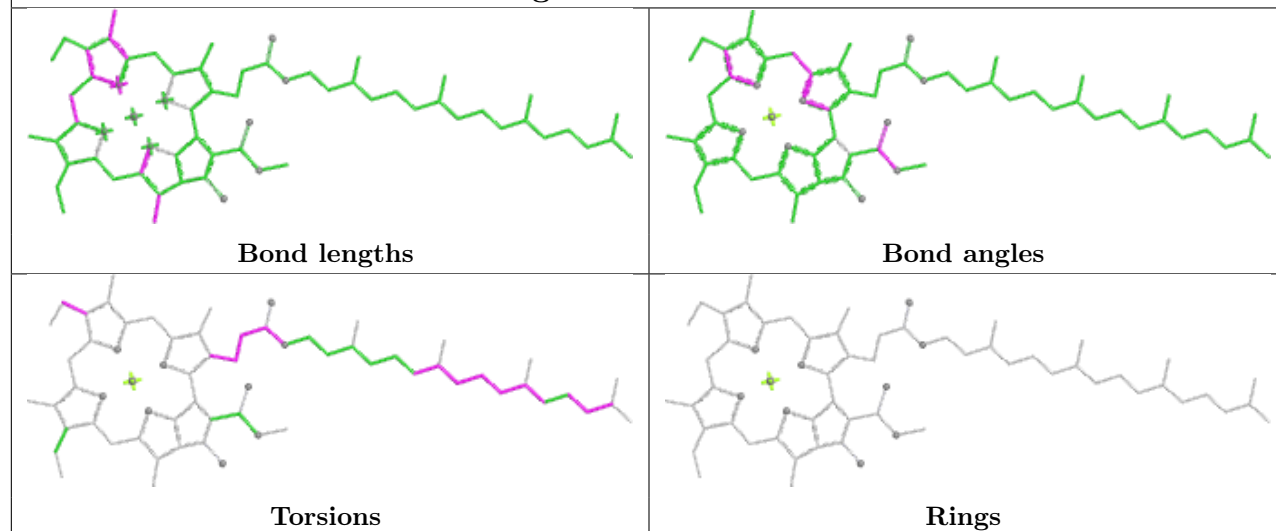


## Ligand CLA N 838

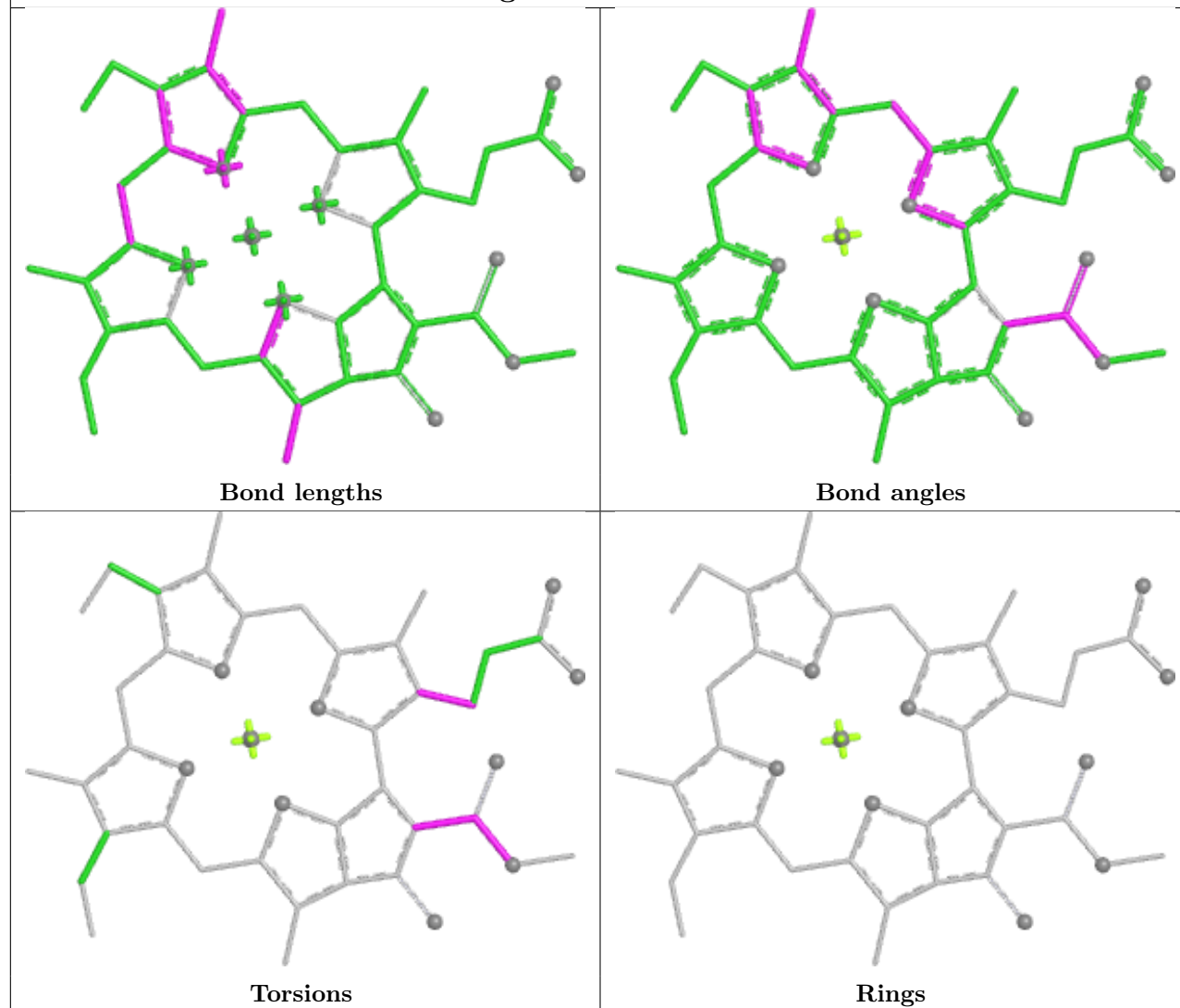


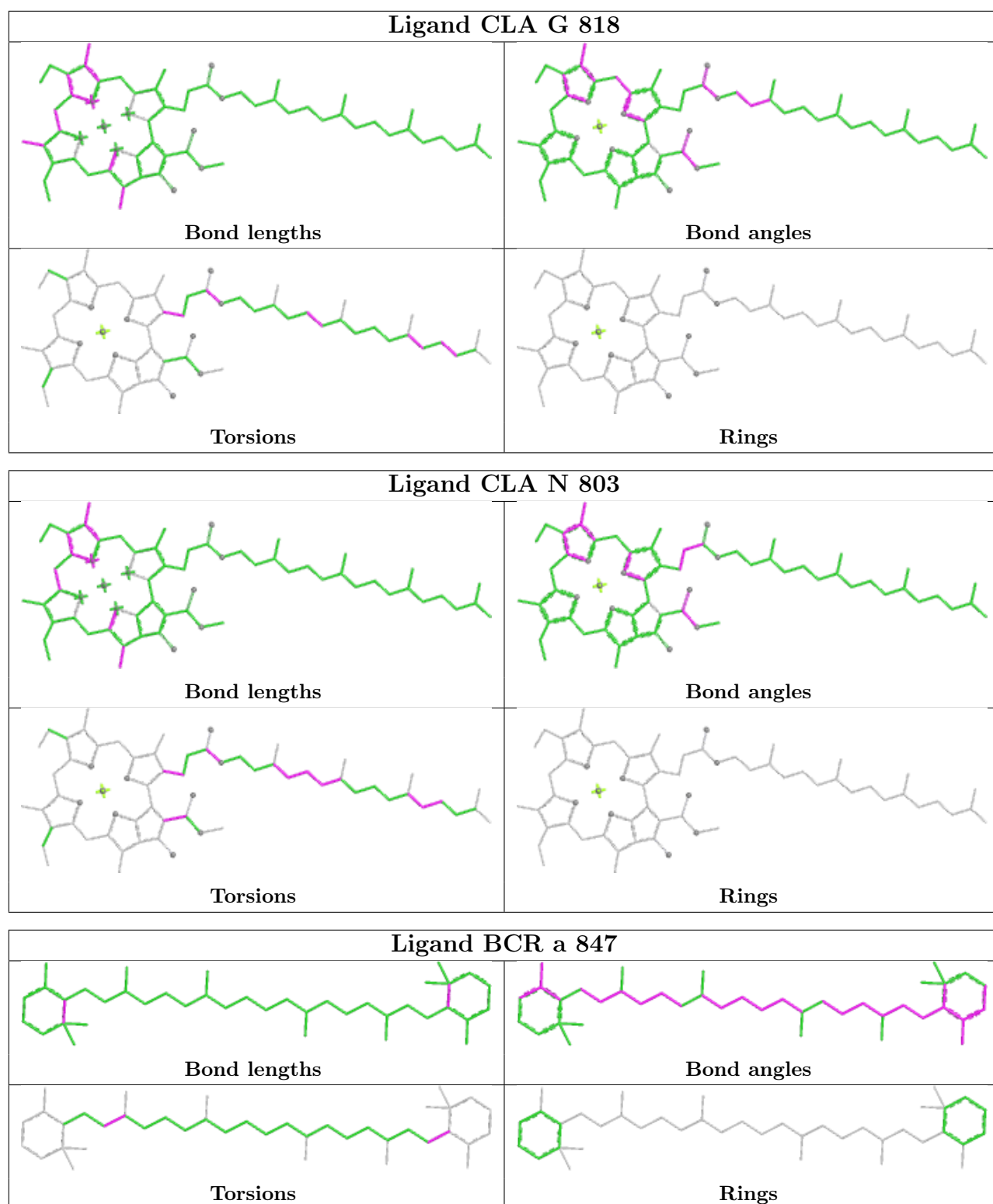


## Ligand CLA B 818

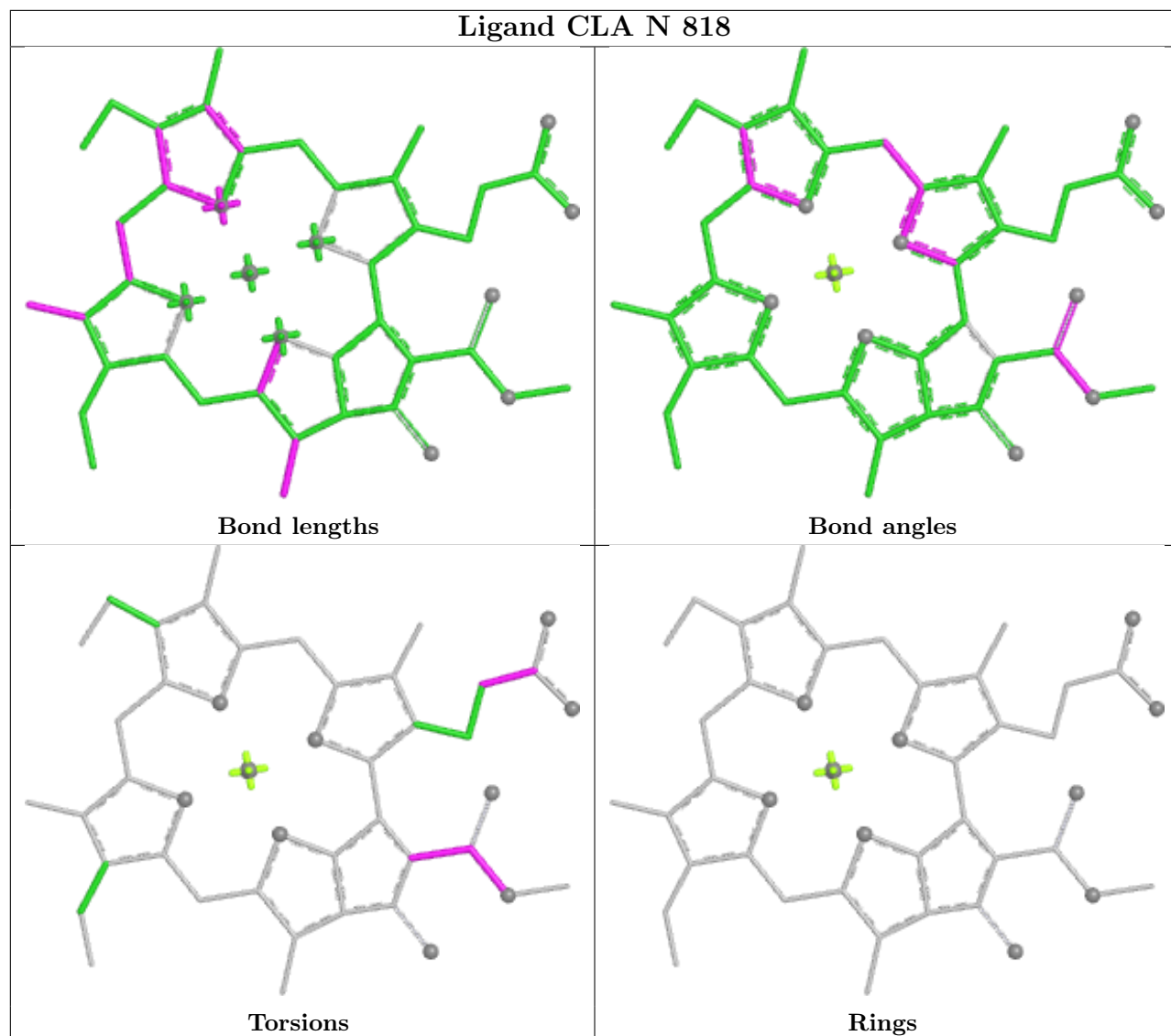


## Ligand CLA I 202

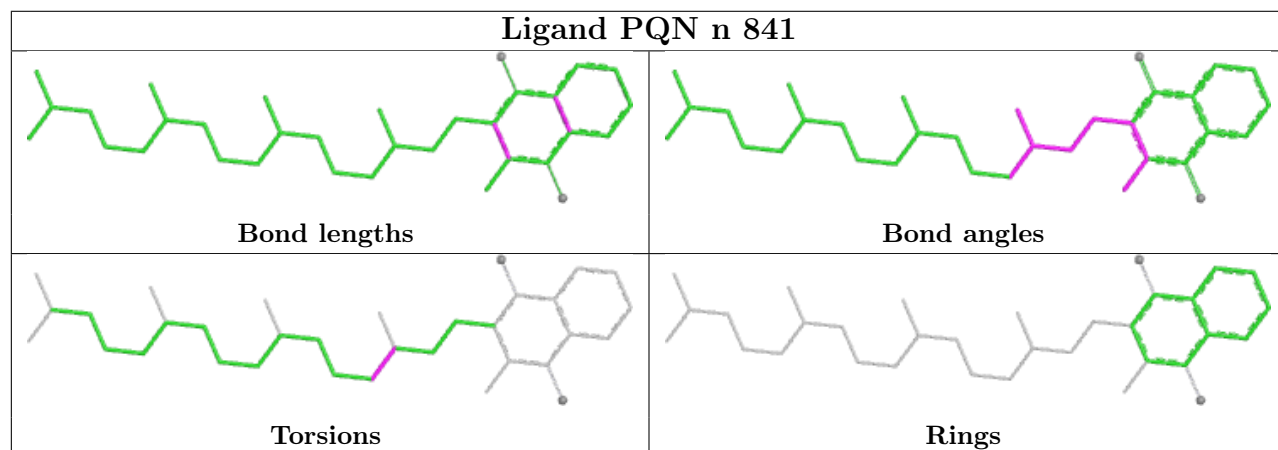


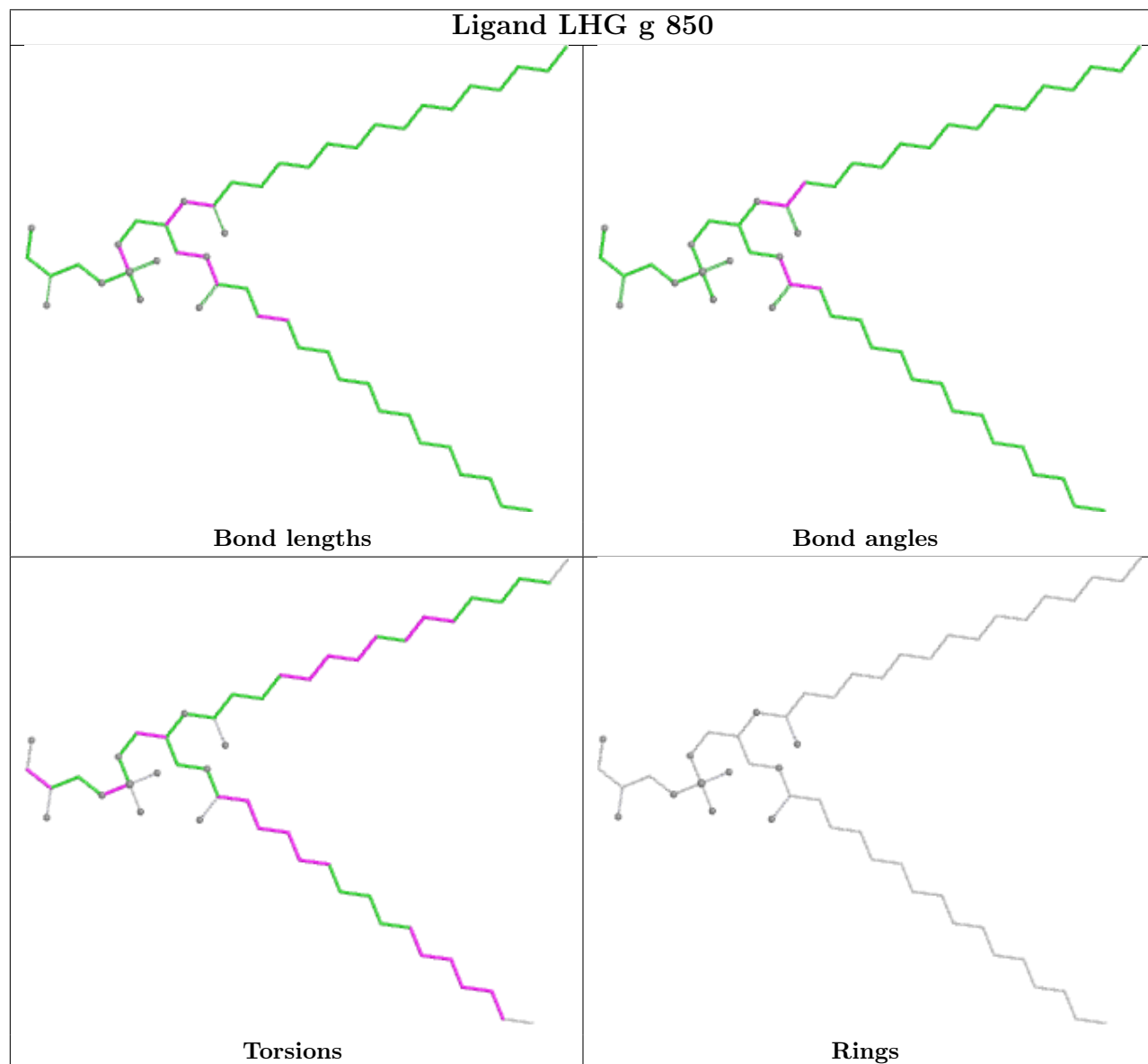
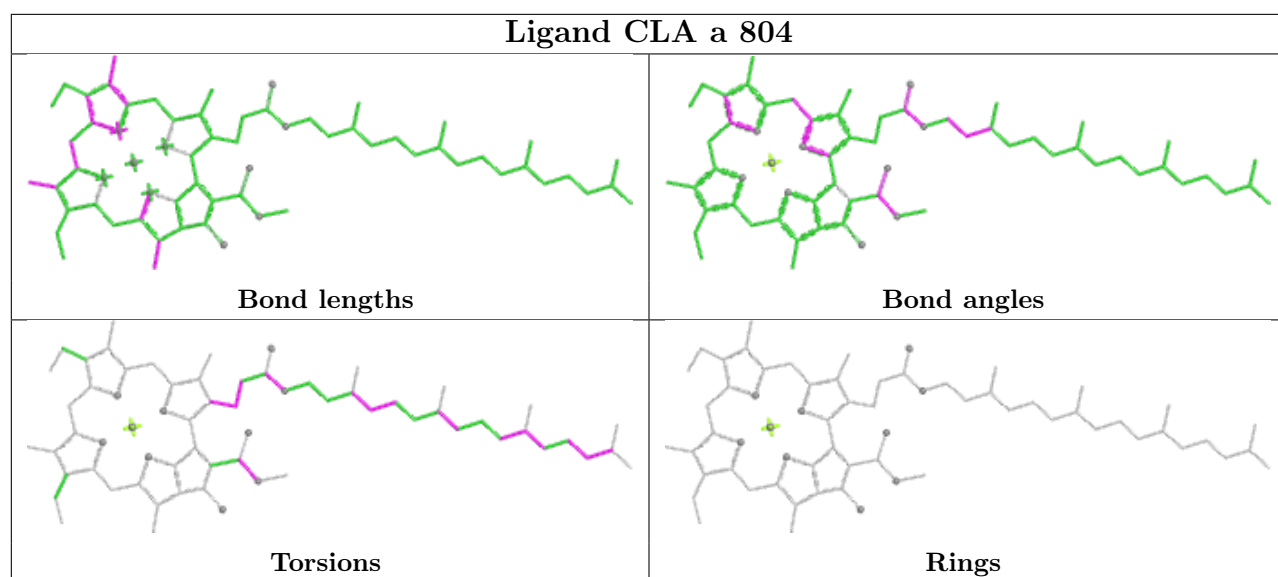


## Ligand CLA N 818

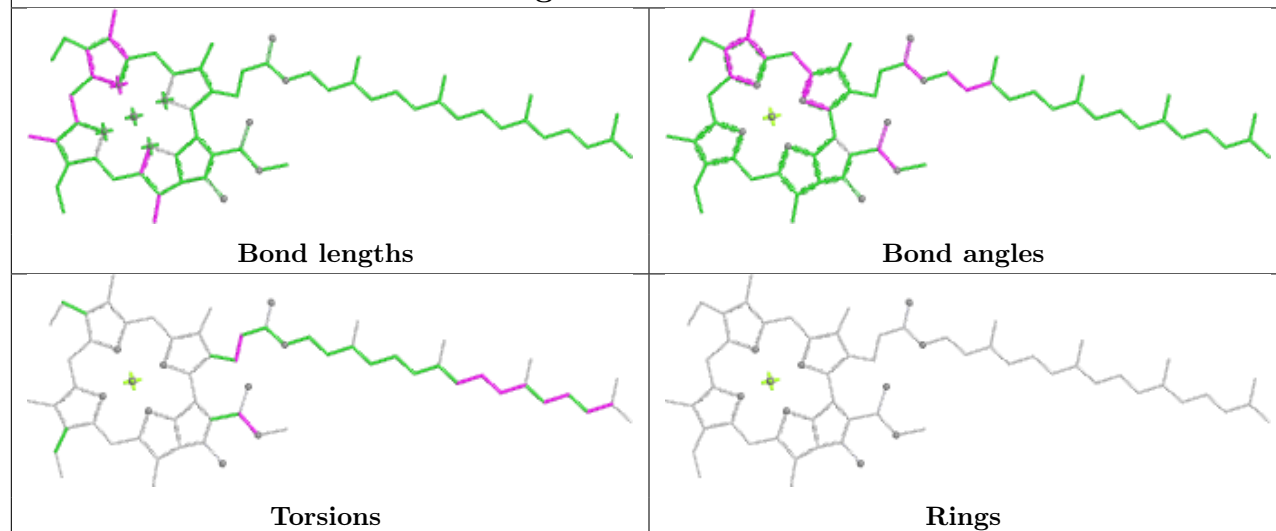
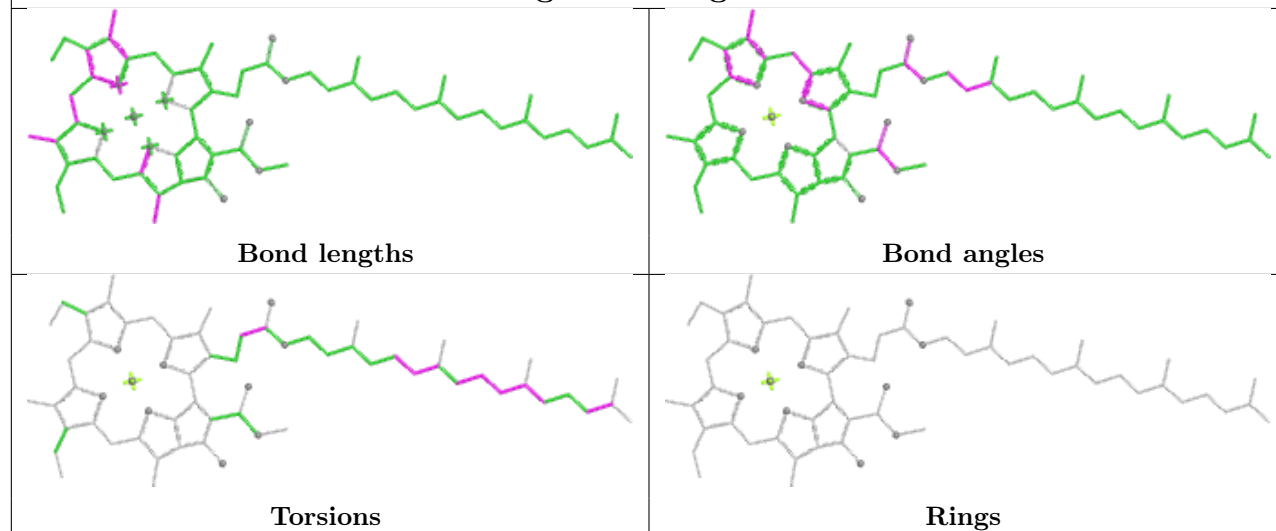


## Ligand PQN n 841

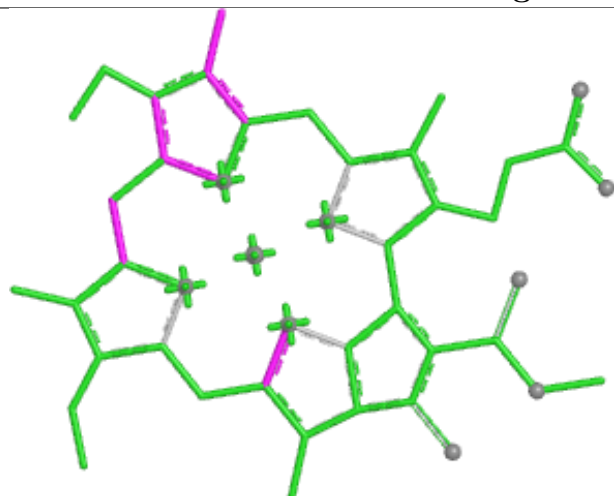




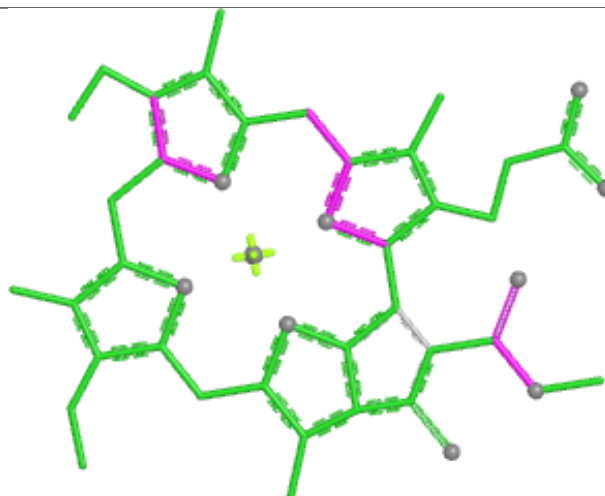


**Ligand CLA b 830****Ligand CLA g 825**

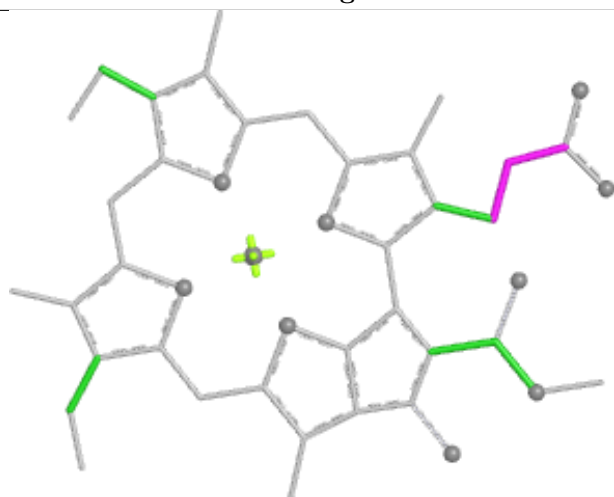
## Ligand CLA G 815



Bond lengths



Bond angles

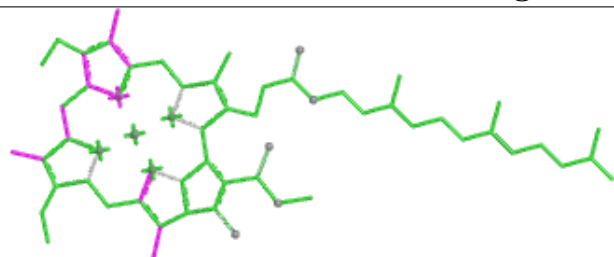


Torsions

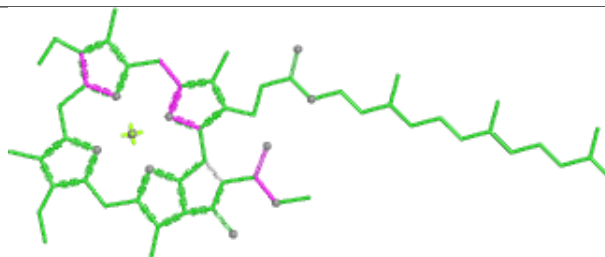


Rings

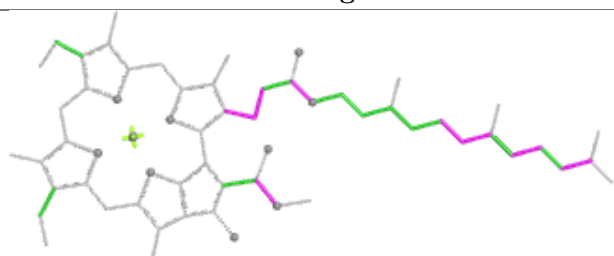
## Ligand CLA N 833



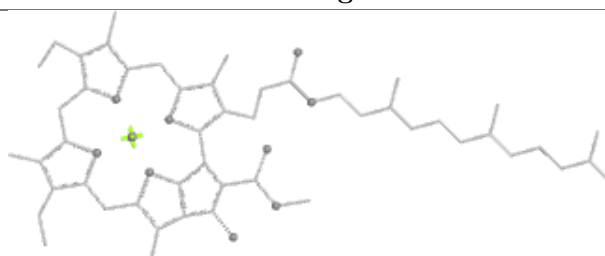
Bond lengths



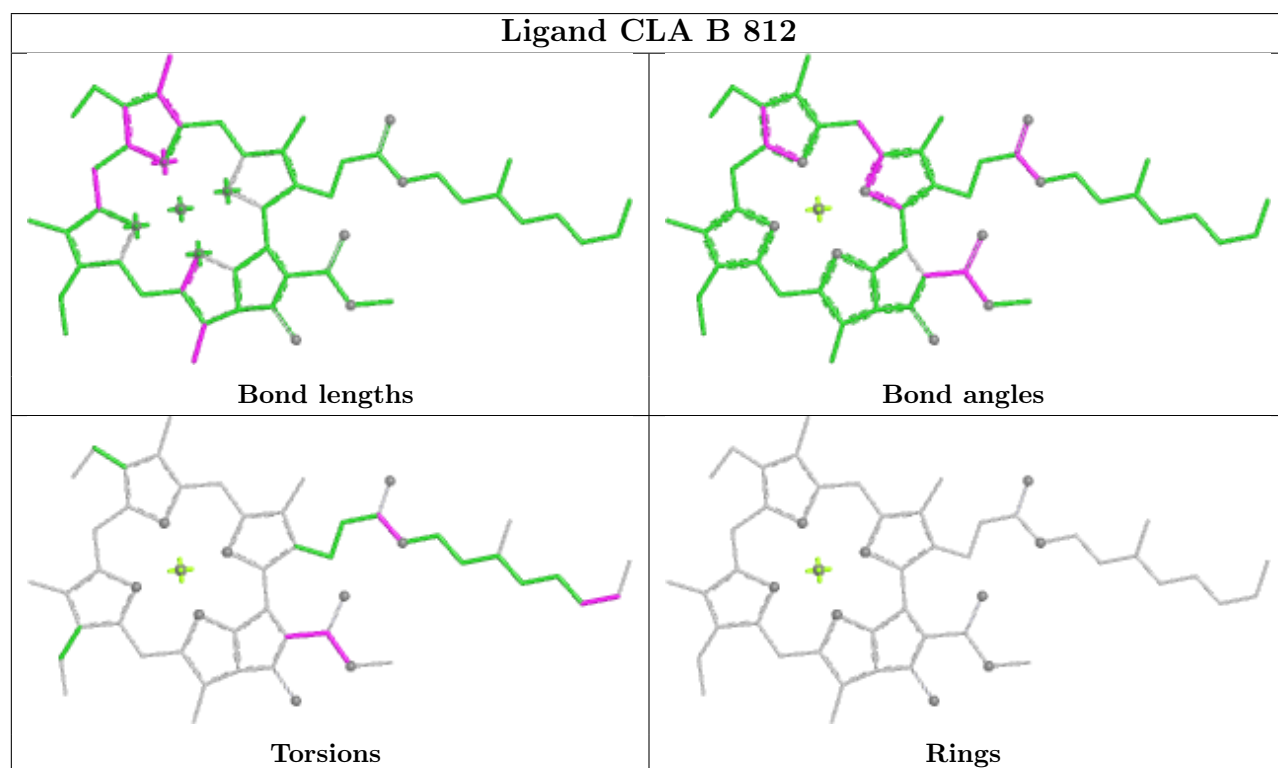
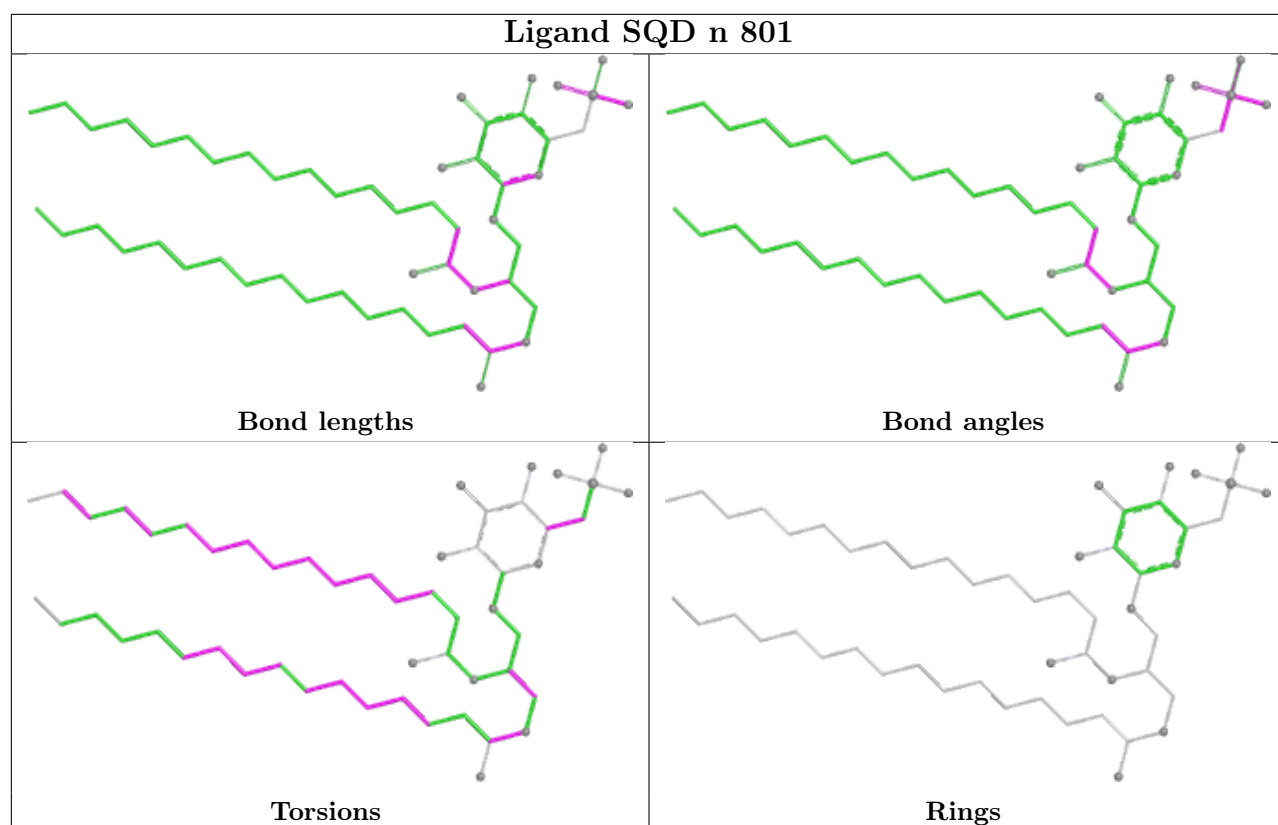
Bond angles

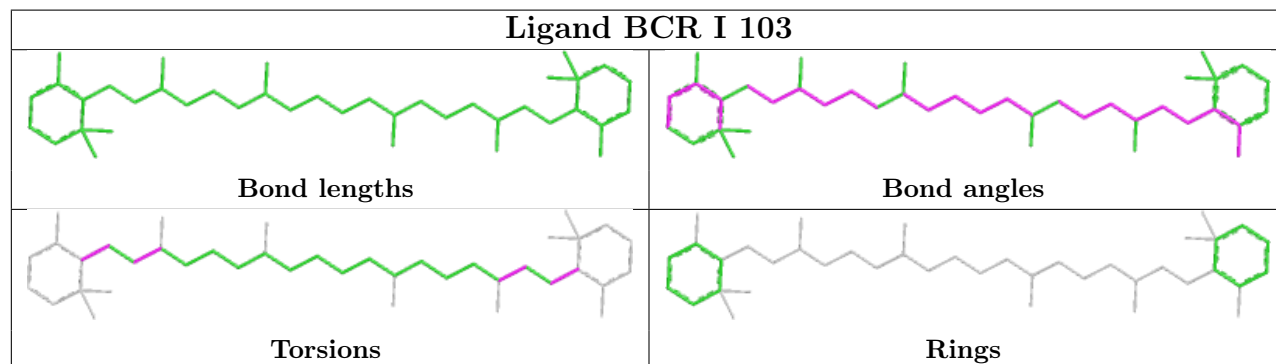
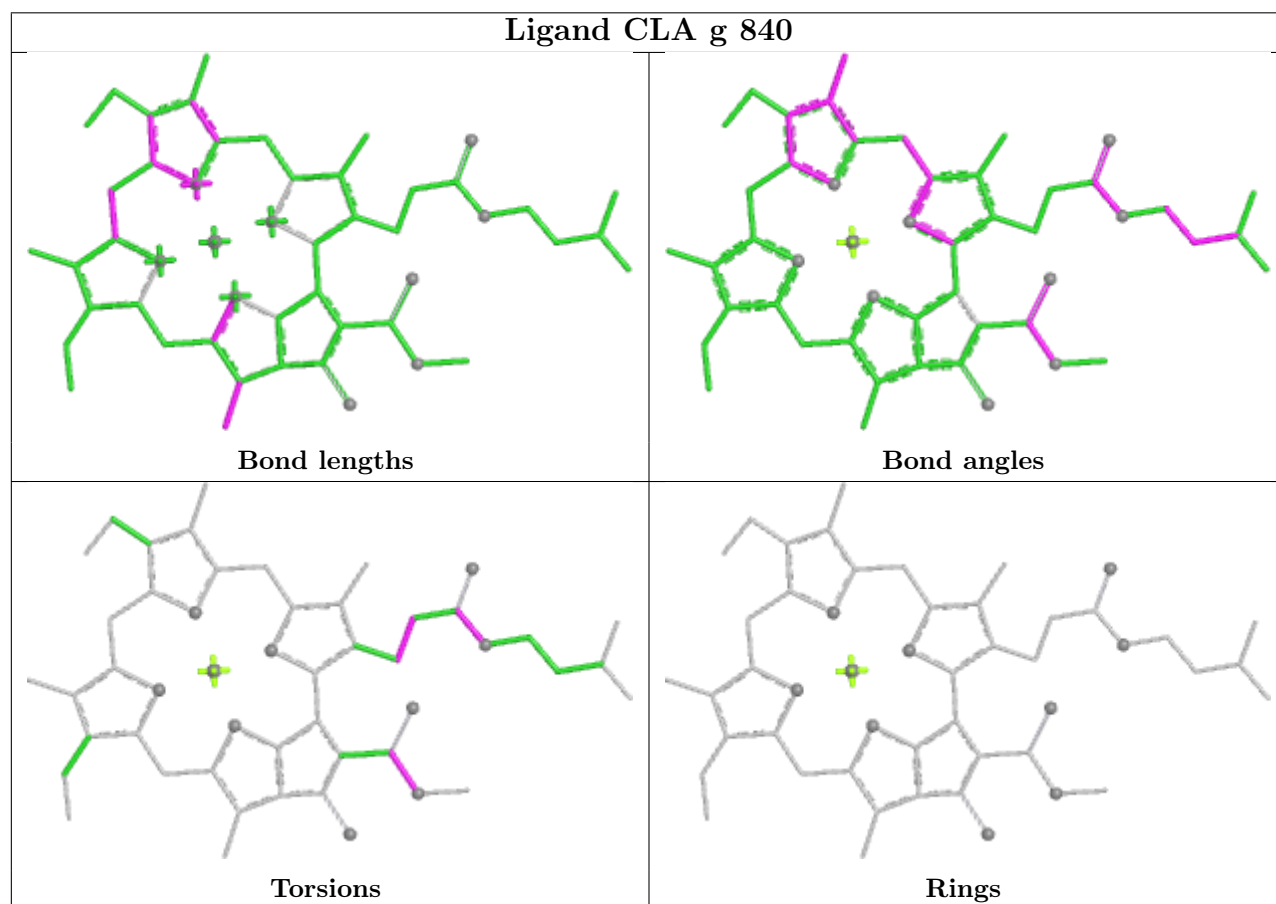
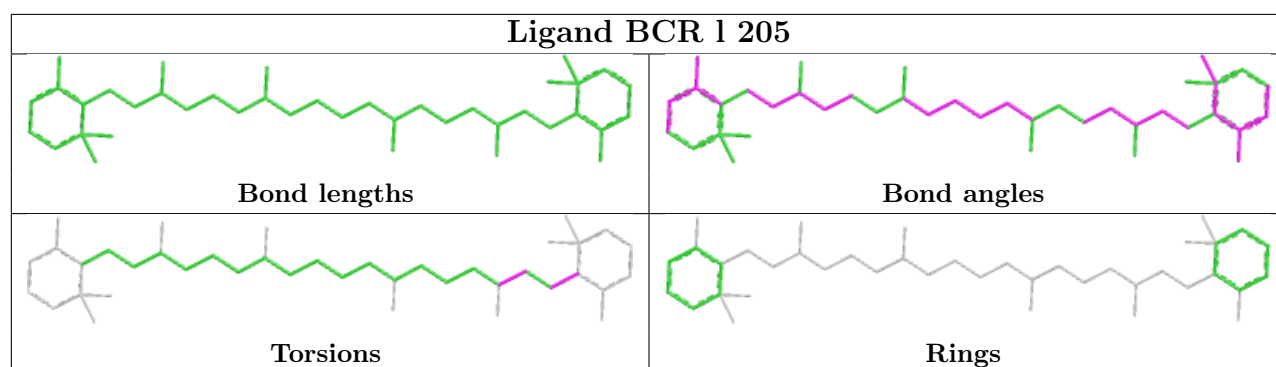


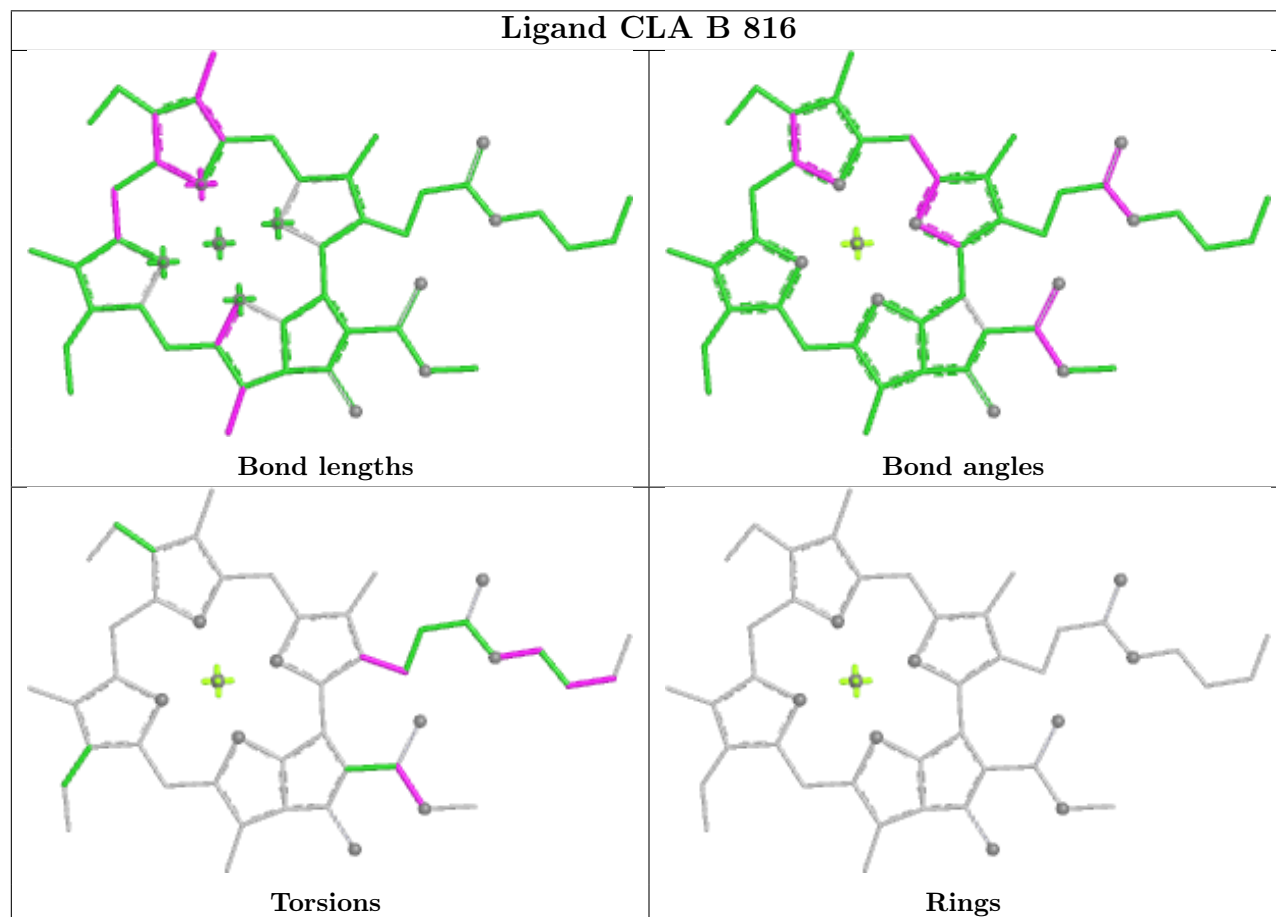
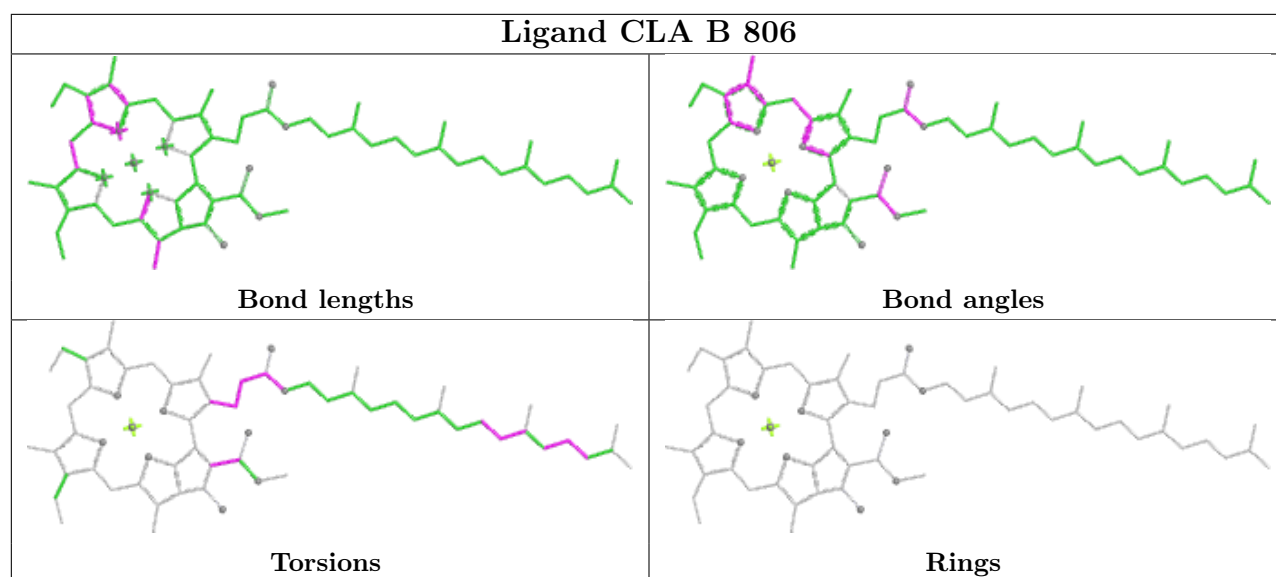
Torsions

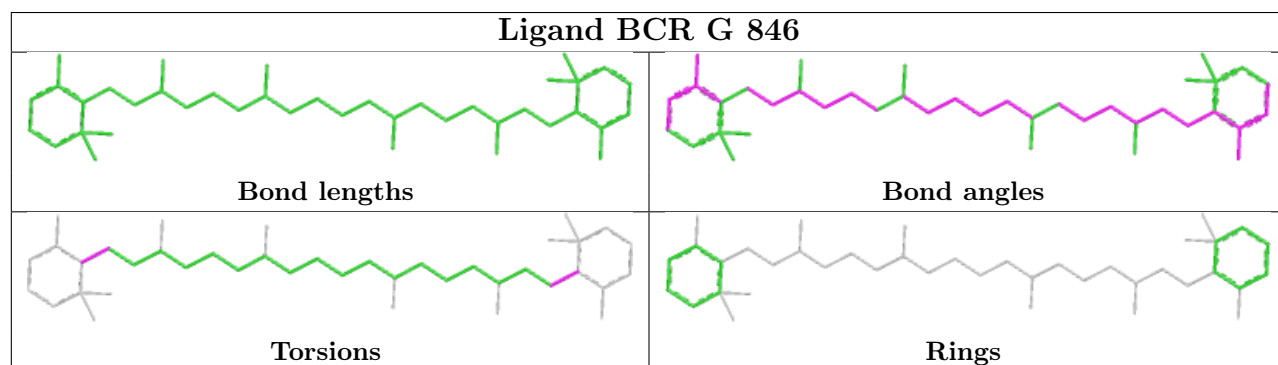
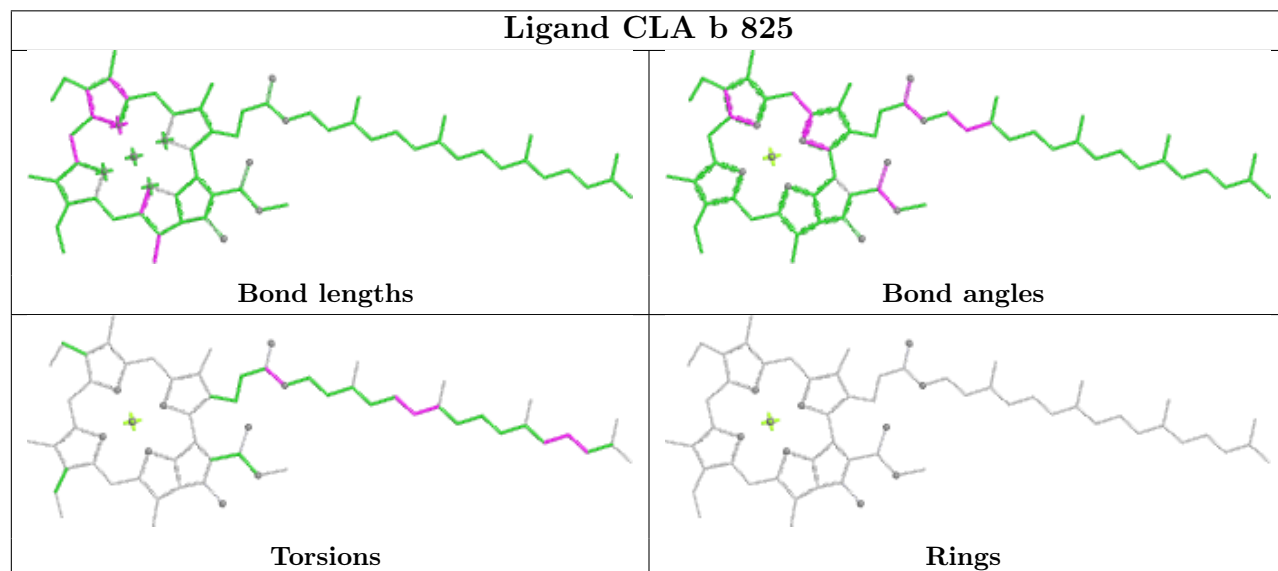
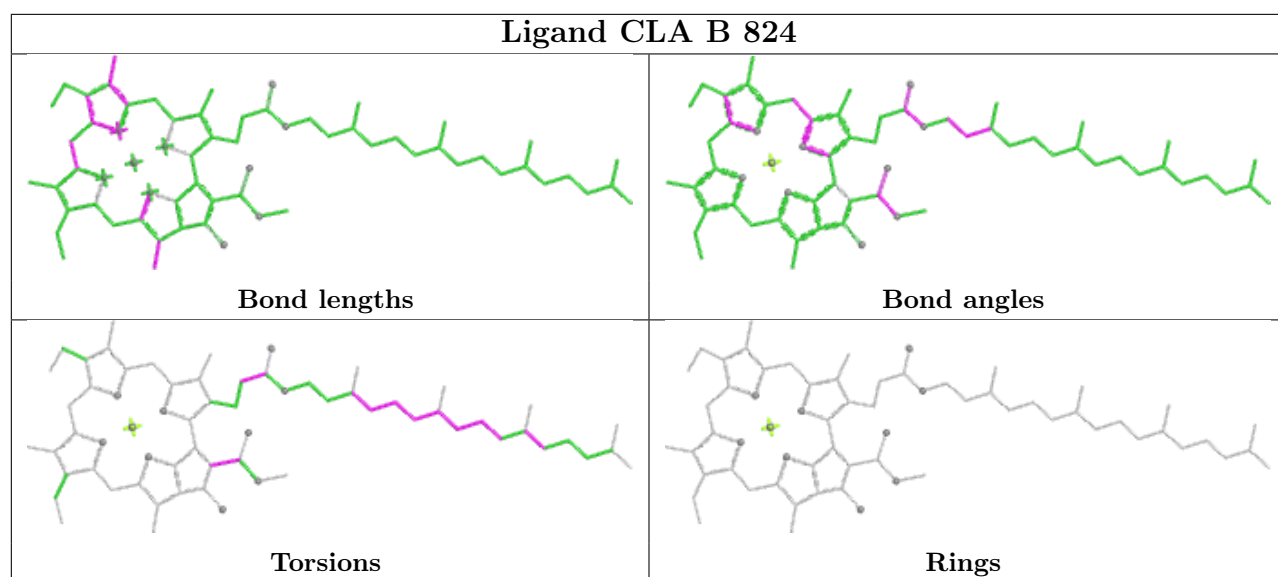


Rings

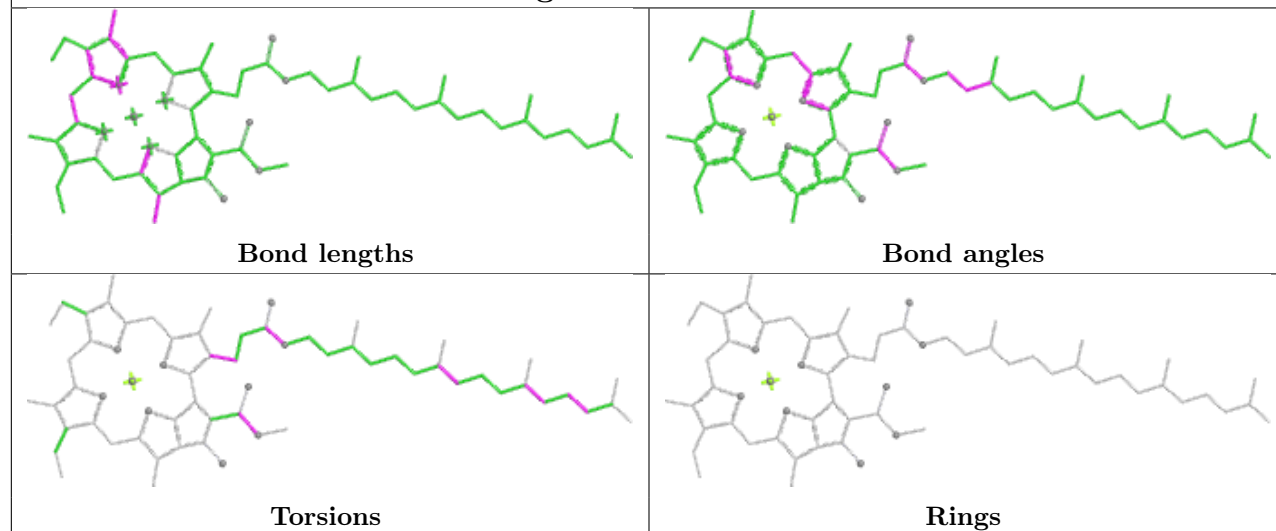




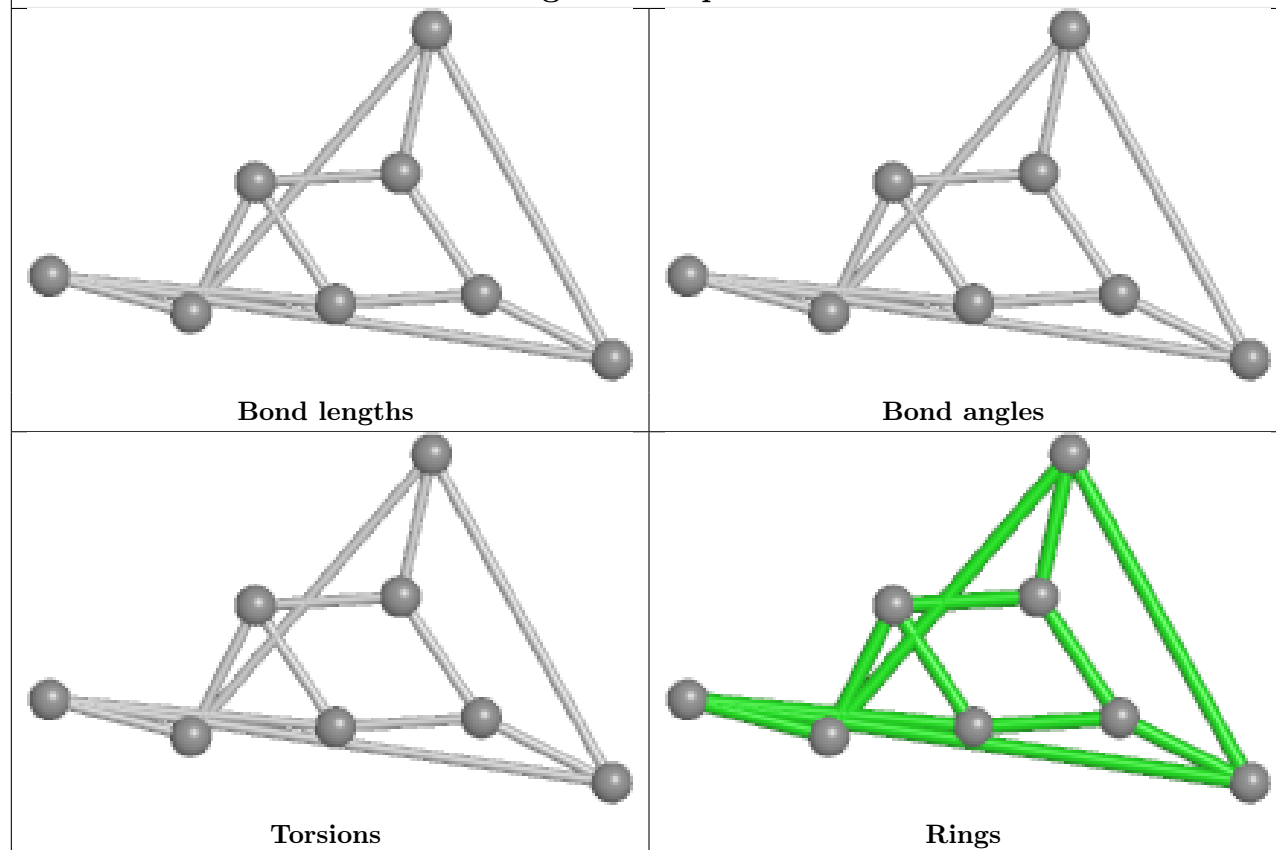




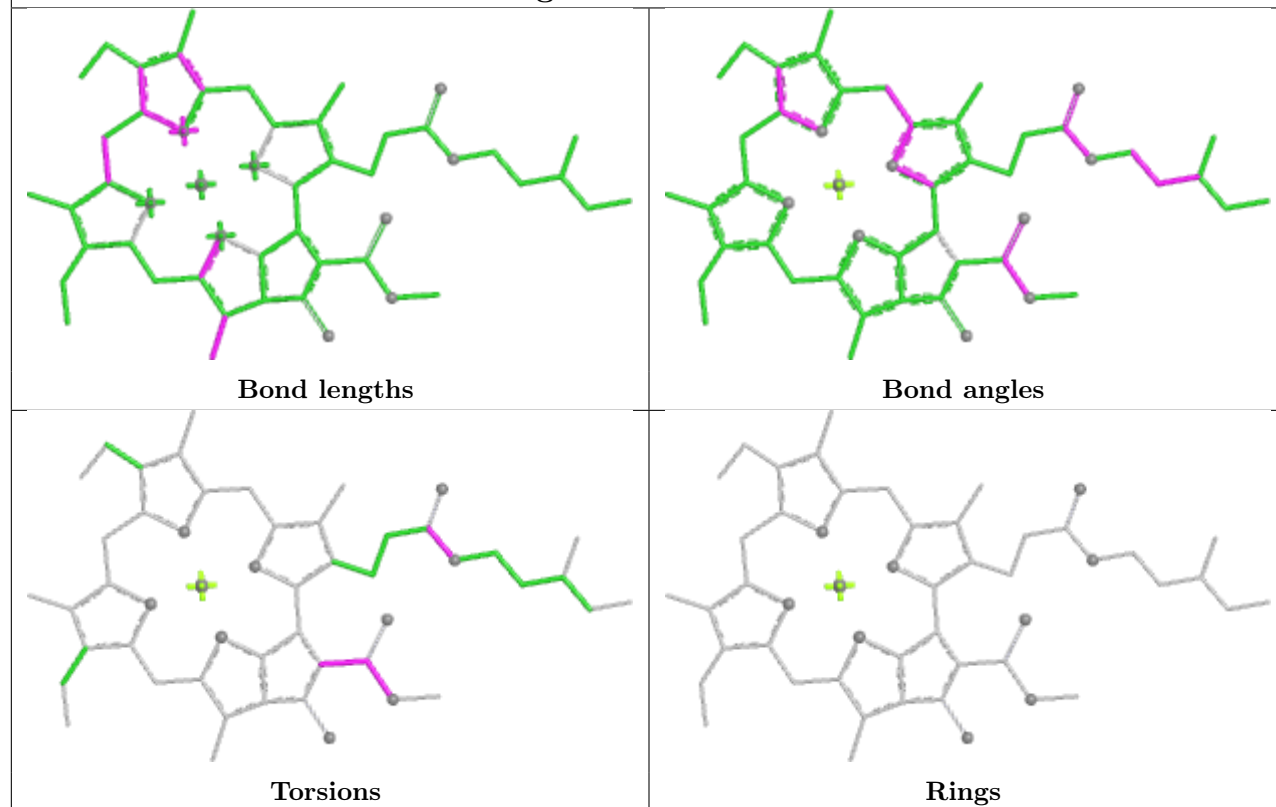
## Ligand CLA a 817



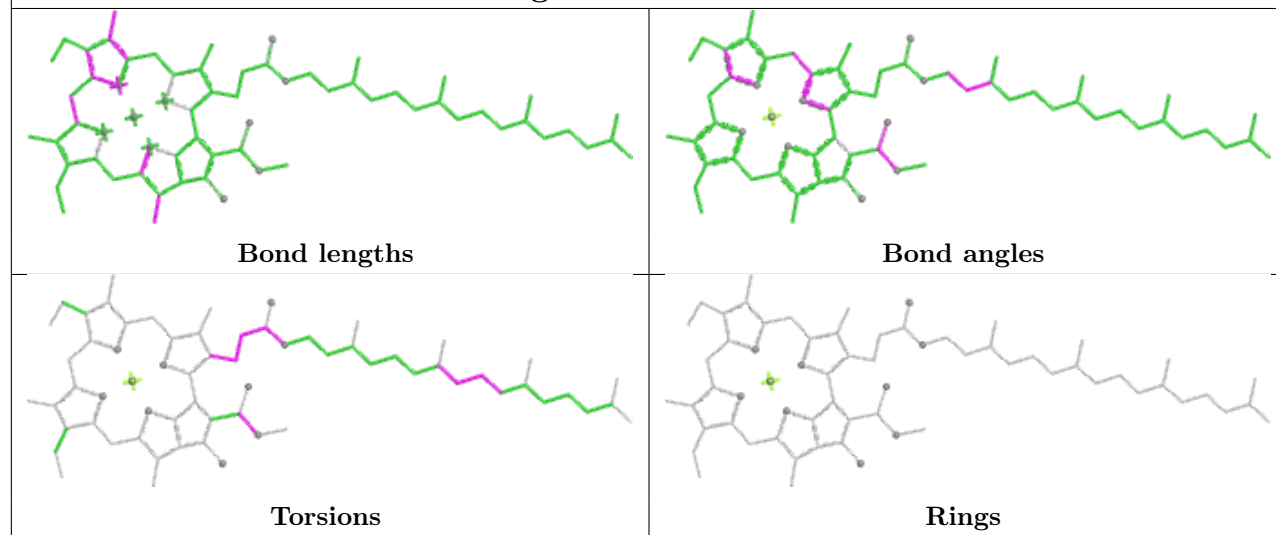
## Ligand SF4 p 102



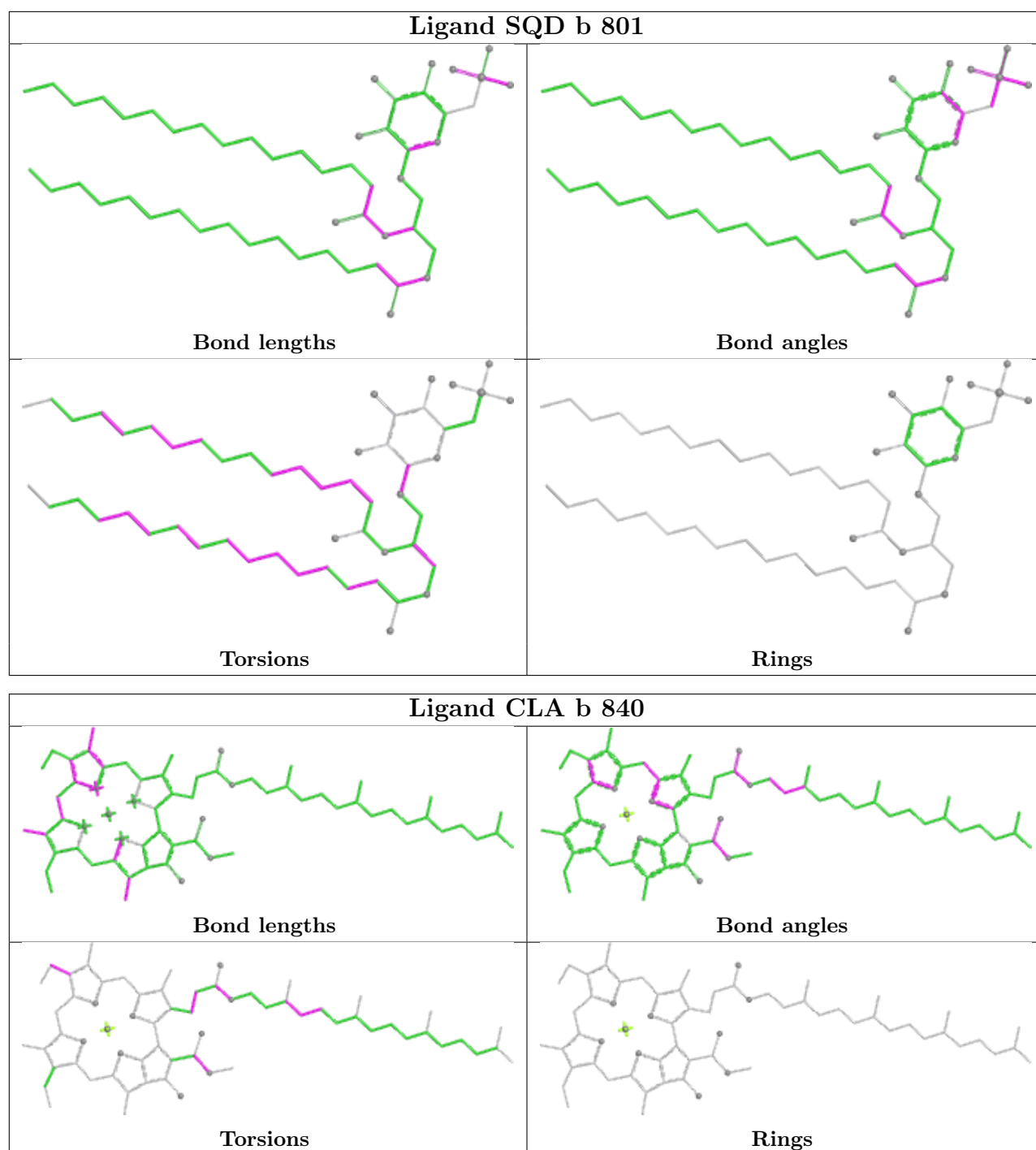
## Ligand CLA a 835



## Ligand CLA G 827







## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

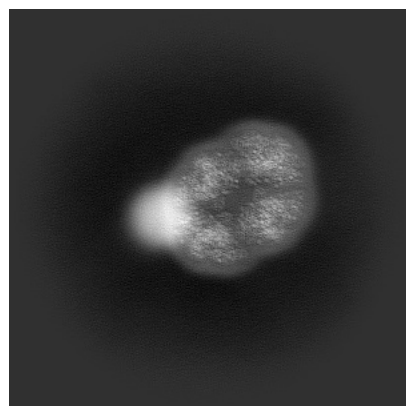
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65883. These allow visual inspection of the internal detail of the map and identification of artifacts.

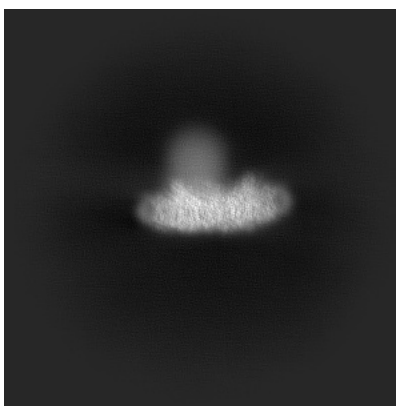
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

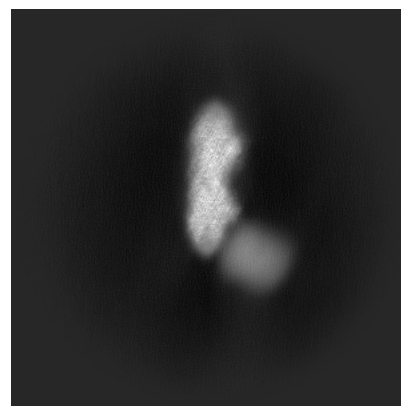
#### 6.1.1 Primary map



X

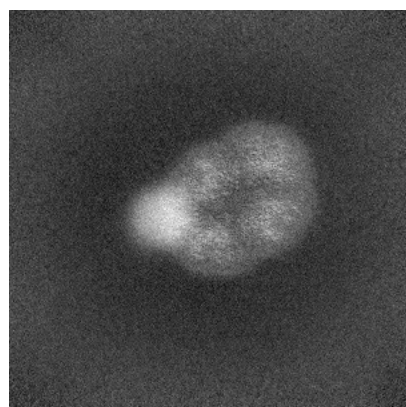


Y

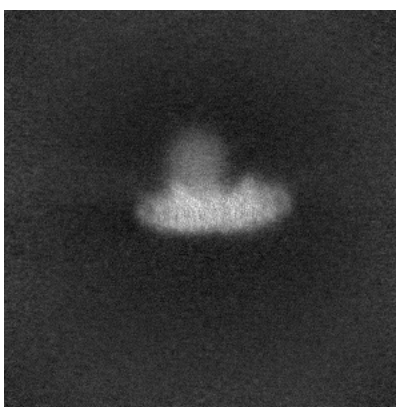


Z

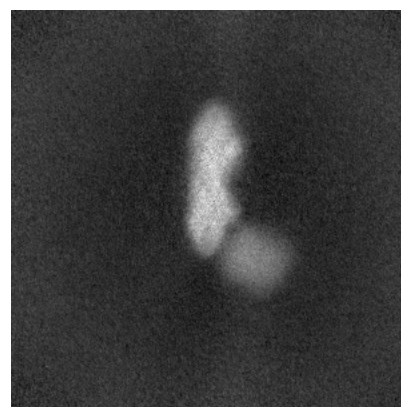
#### 6.1.2 Raw map



X



Y

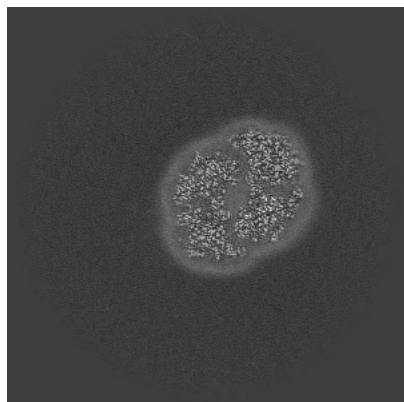


Z

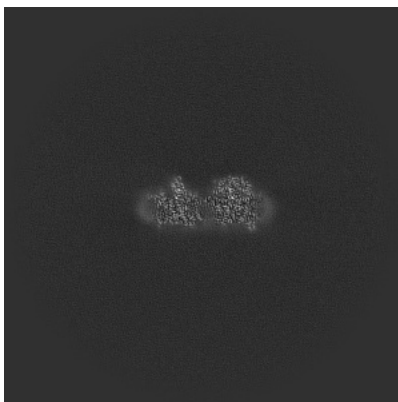
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

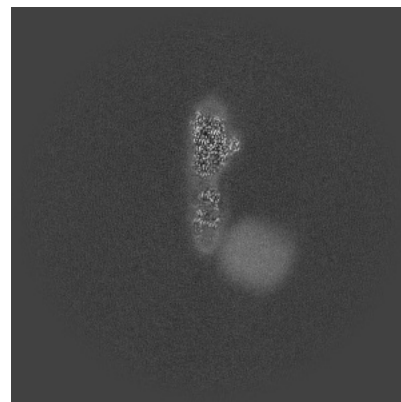
### 6.2.1 Primary map



X Index: 330

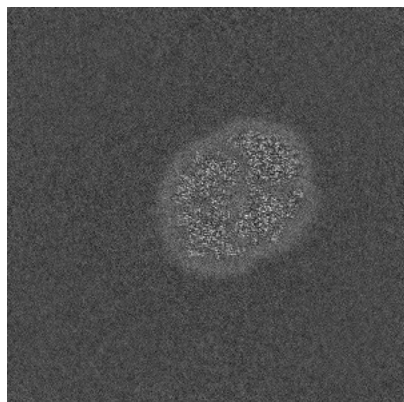


Y Index: 330

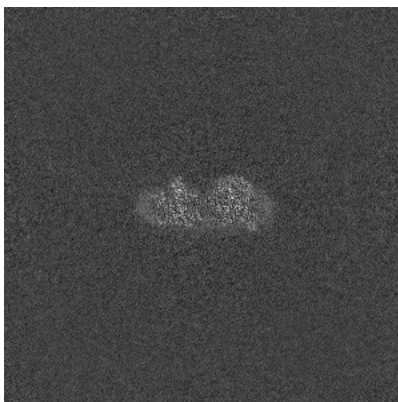


Z Index: 330

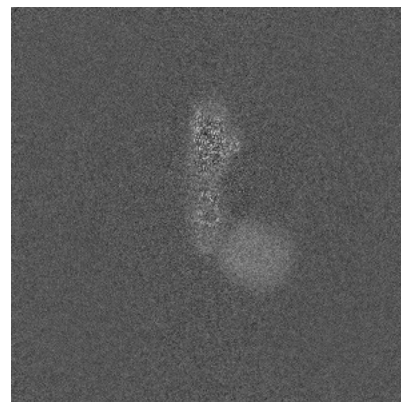
### 6.2.2 Raw map



X Index: 330



Y Index: 330

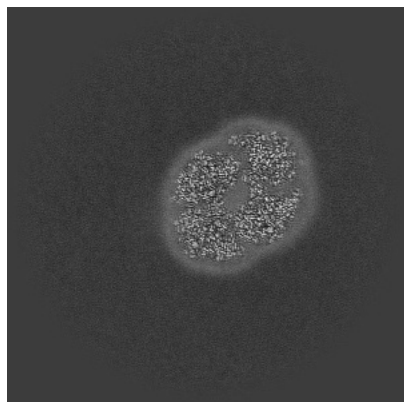


Z Index: 330

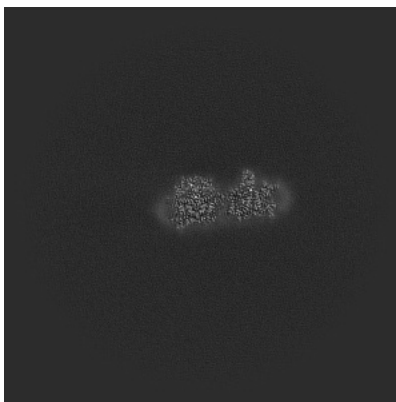
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

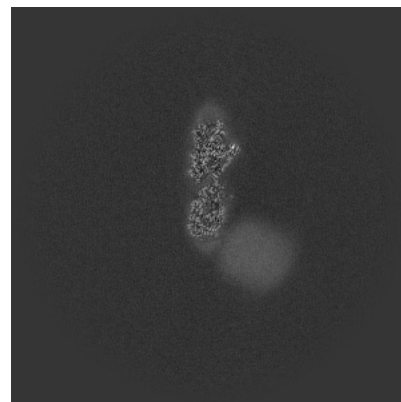
### 6.3.1 Primary map



X Index: 335

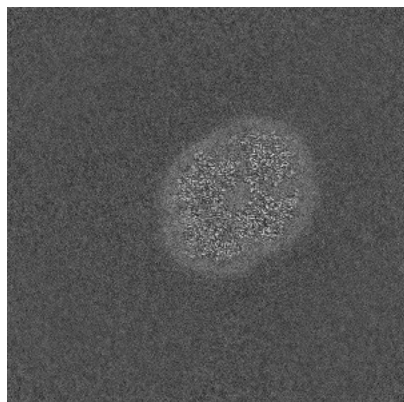


Y Index: 427

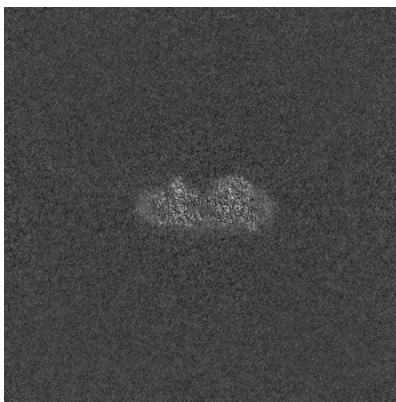


Z Index: 309

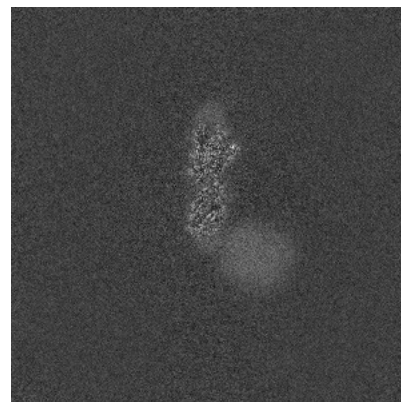
### 6.3.2 Raw map



X Index: 334



Y Index: 330



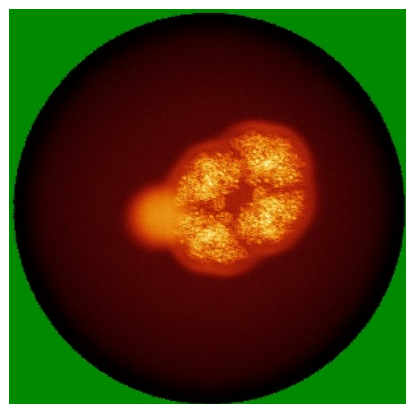
Z Index: 308

The images above show the largest variance slices of the map in three orthogonal directions.

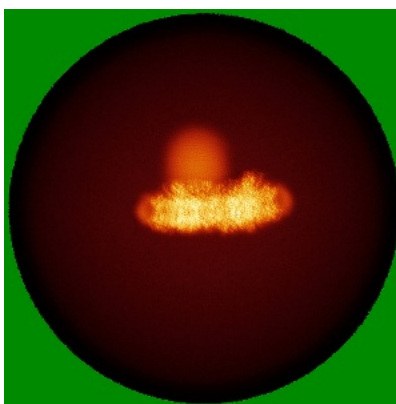


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

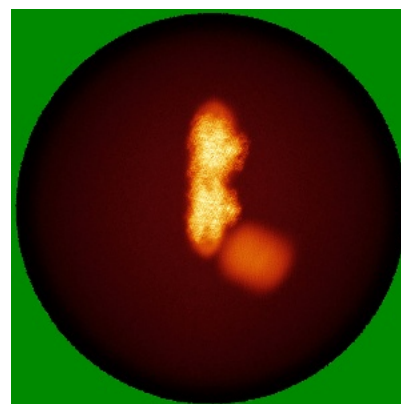
### 6.4.1 Primary map



X

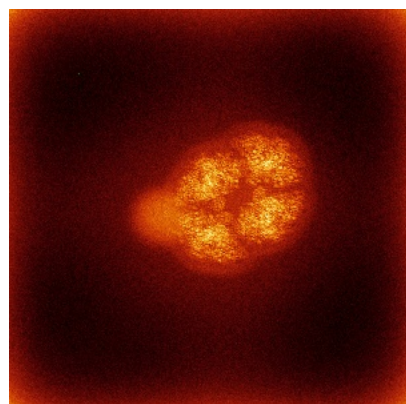


Y

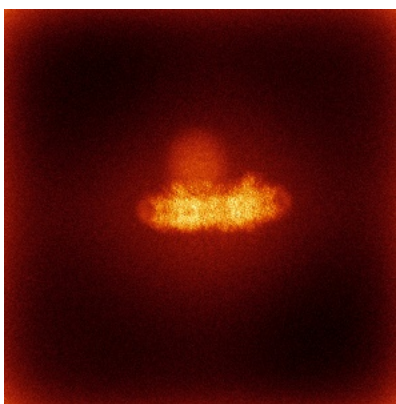


Z

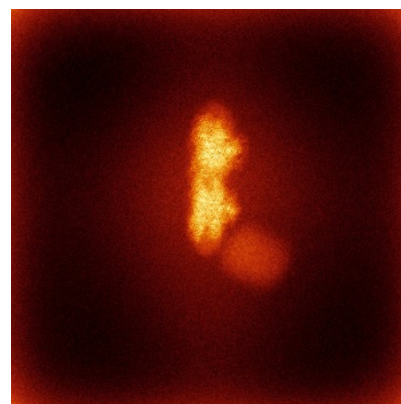
### 6.4.2 Raw map



X



Y

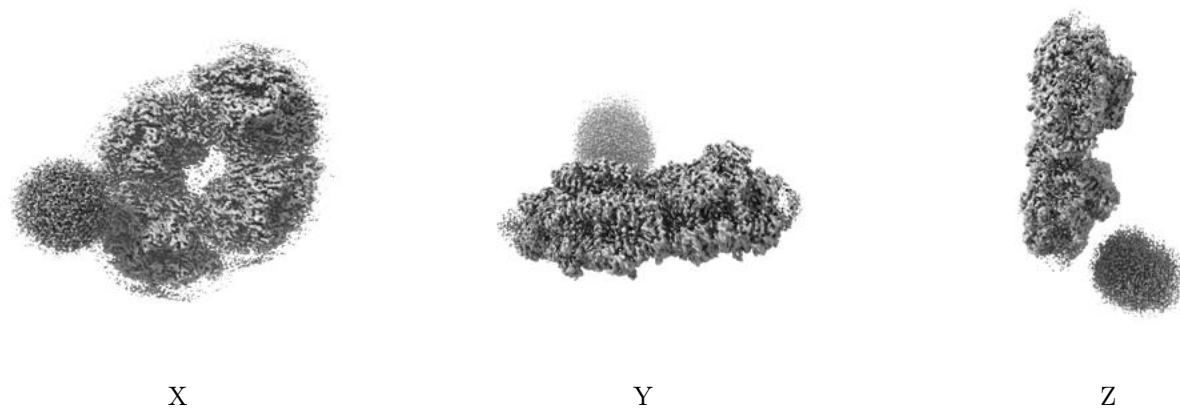


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.185. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

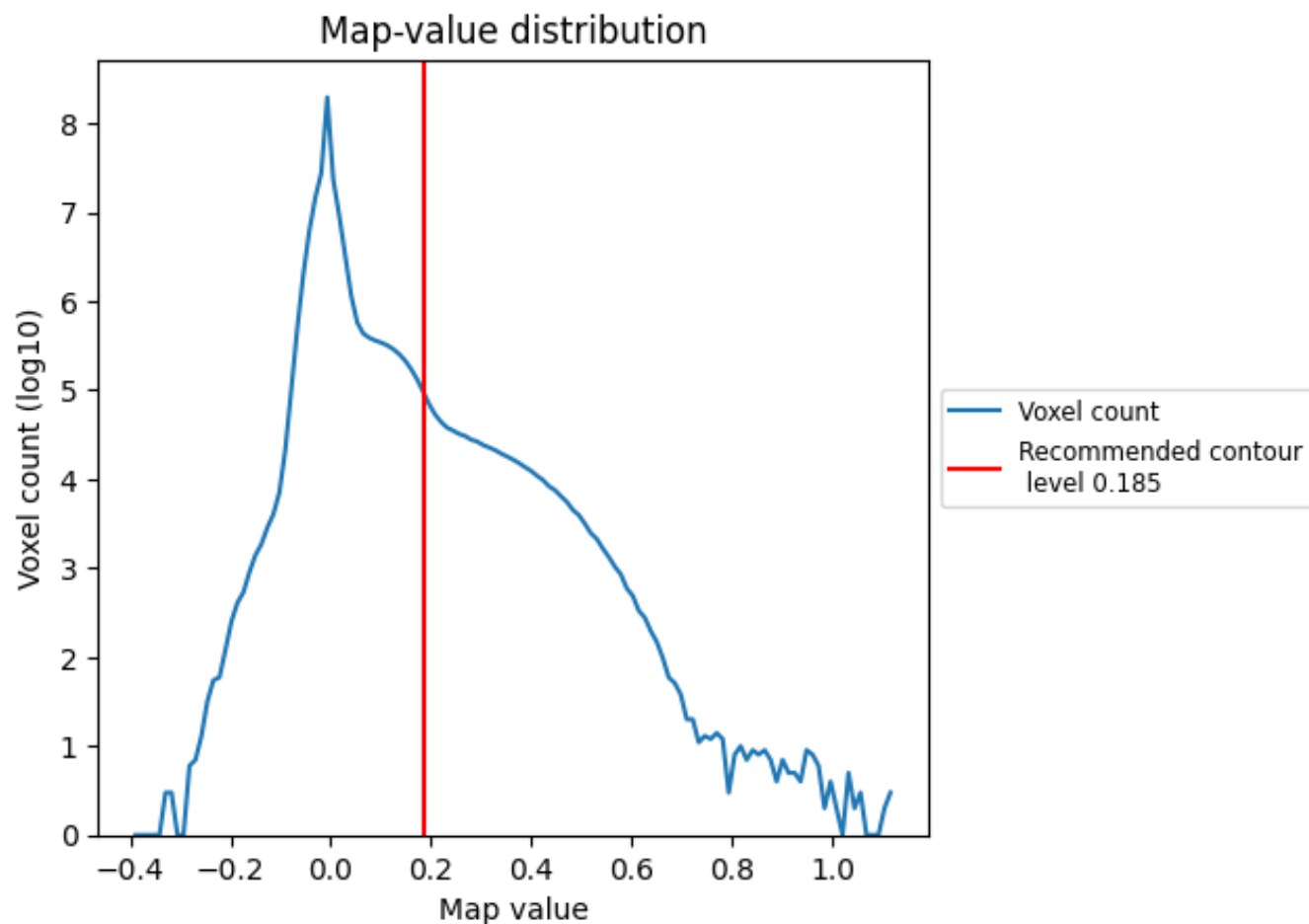
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

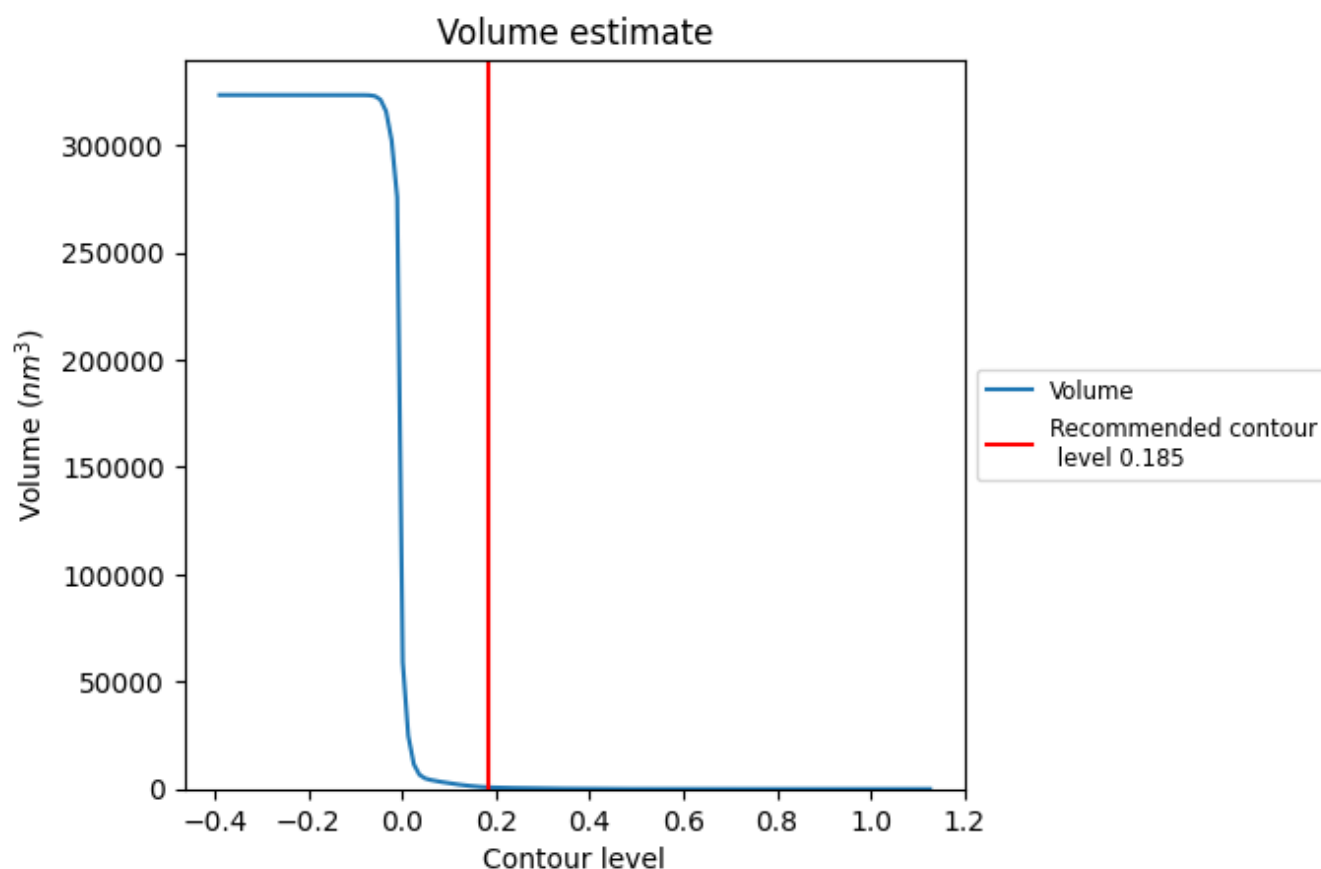
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)

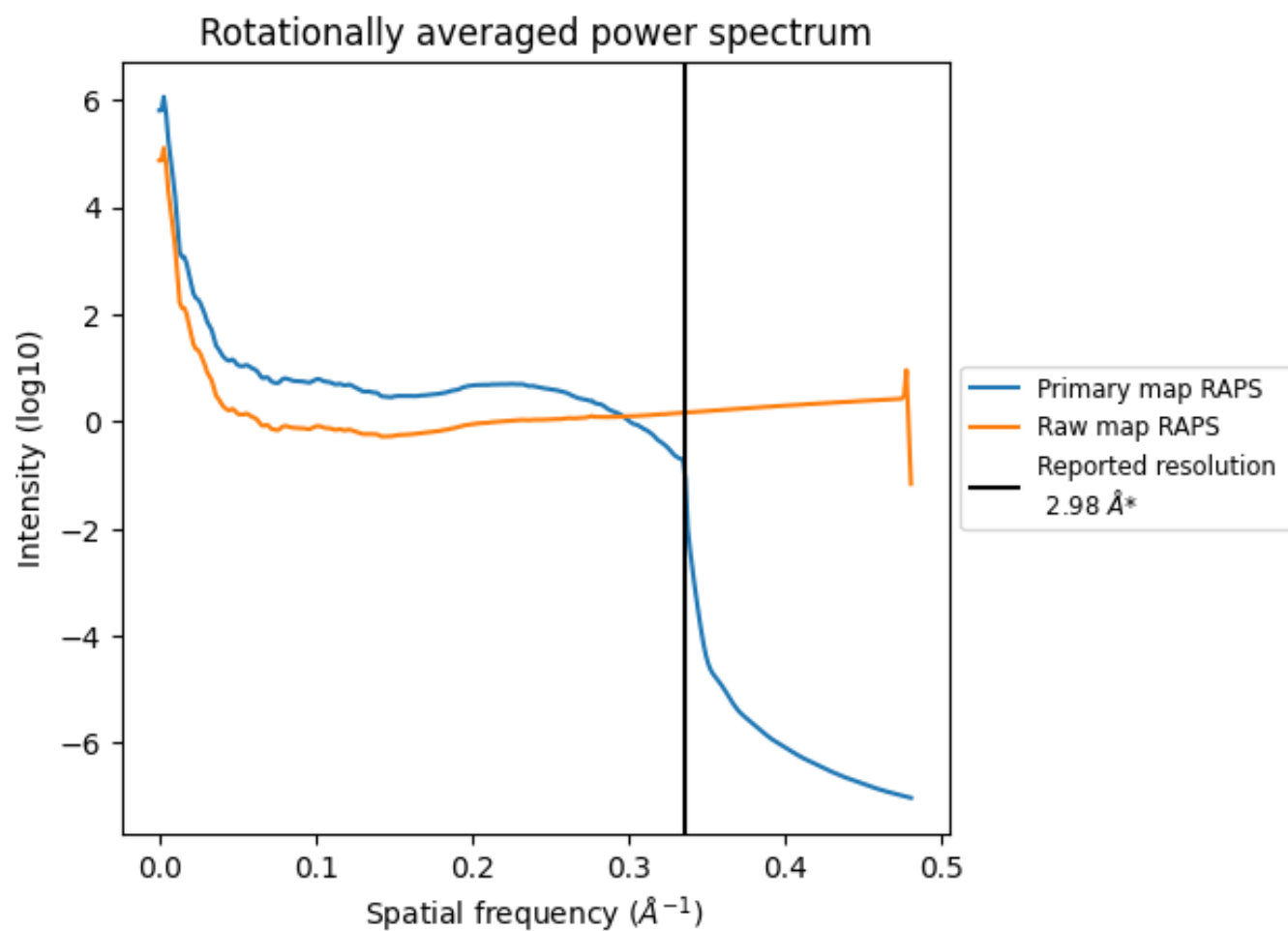


The volume at the recommended contour level is 767  $\text{nm}^3$ ; this corresponds to an approximate mass of 693 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum ⓘ

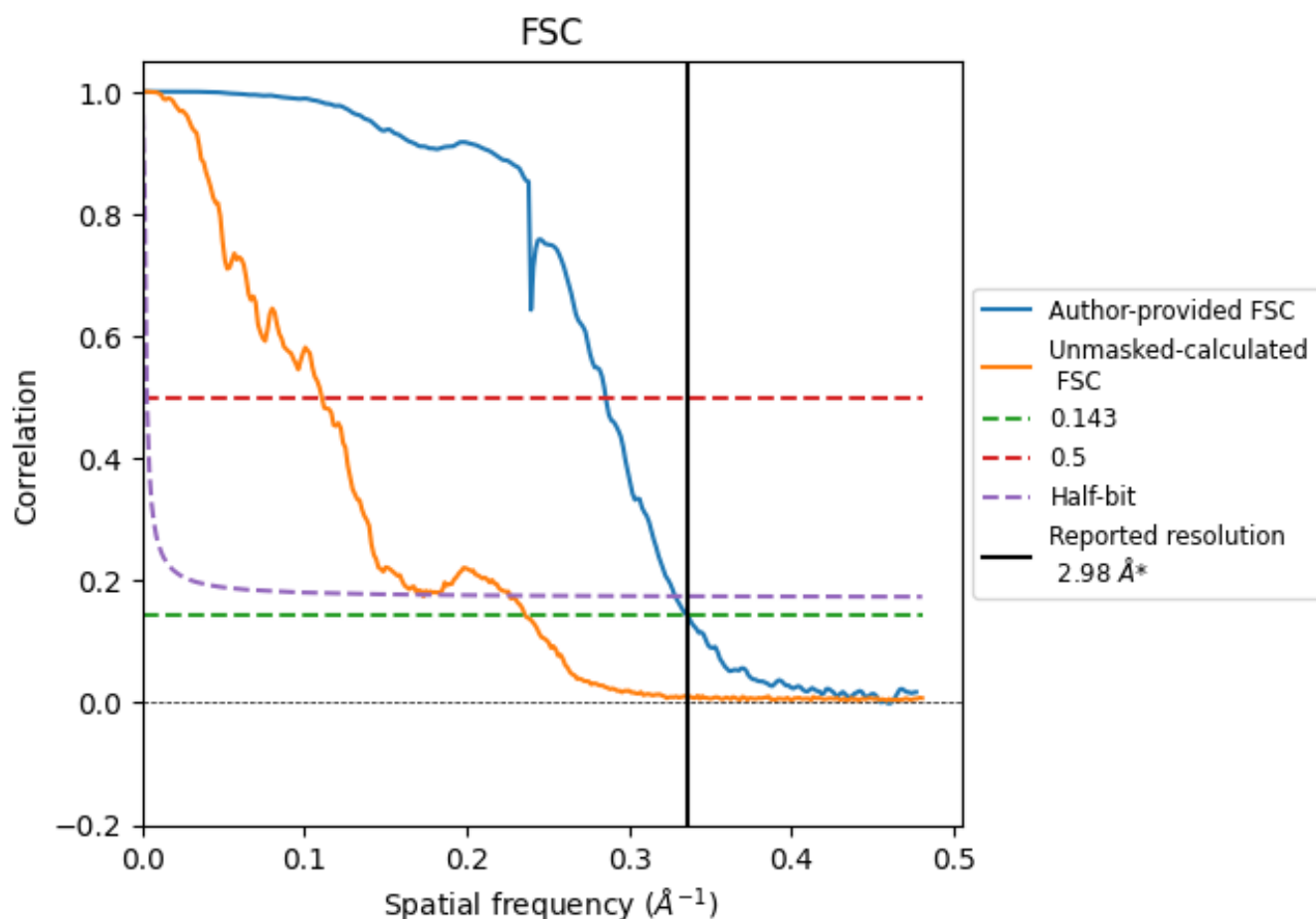


\*Reported resolution corresponds to spatial frequency of 0.336 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.336 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

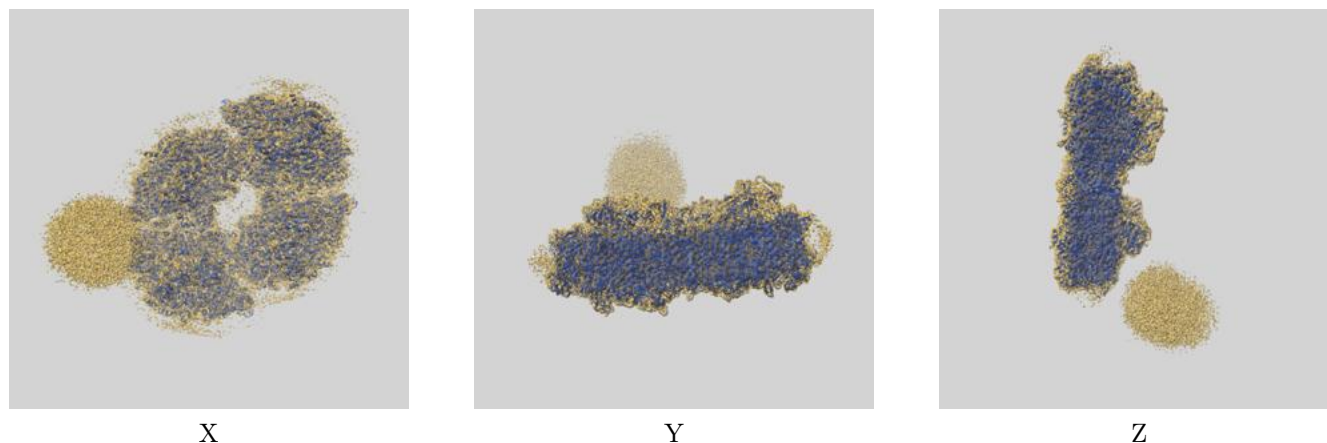
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.98                               | -    | -        |
| Author-provided FSC curve | 2.98                               | 3.50 | 3.04     |
| Unmasked-calculated*      | 4.24                               | 9.04 | 5.78     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 2.98 by more than 10 %

## 9 Map-model fit [i](#)

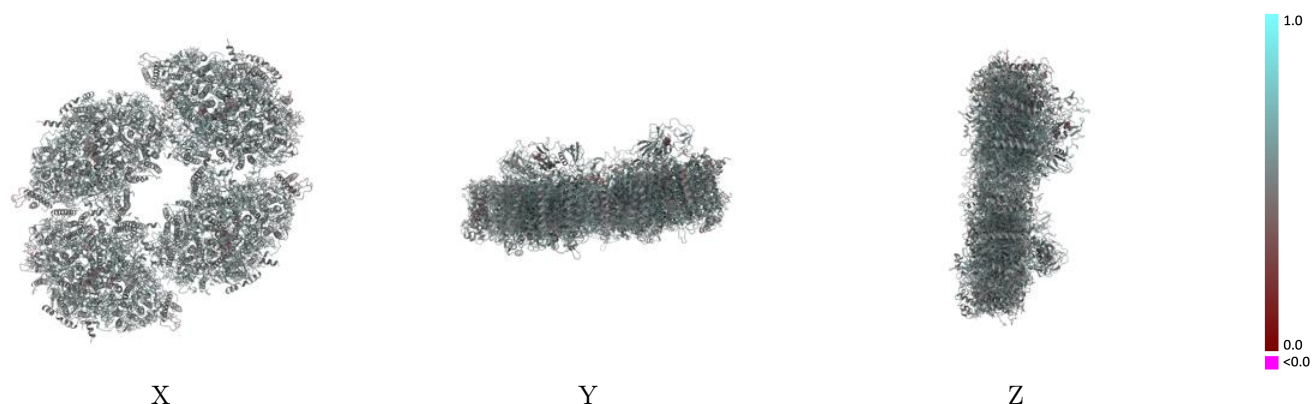
This section contains information regarding the fit between EMDB map EMD-65883 and PDB model 9WD5. Per-residue inclusion information can be found in section [3](#) on page [47](#).

### 9.1 Map-model overlay [i](#)



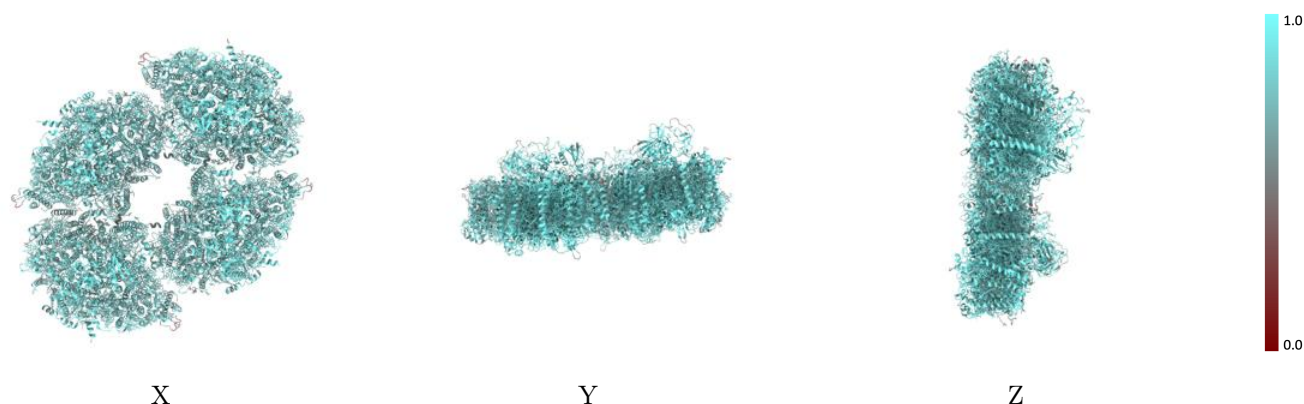
The images above show the 3D surface view of the map at the recommended contour level 0.185 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



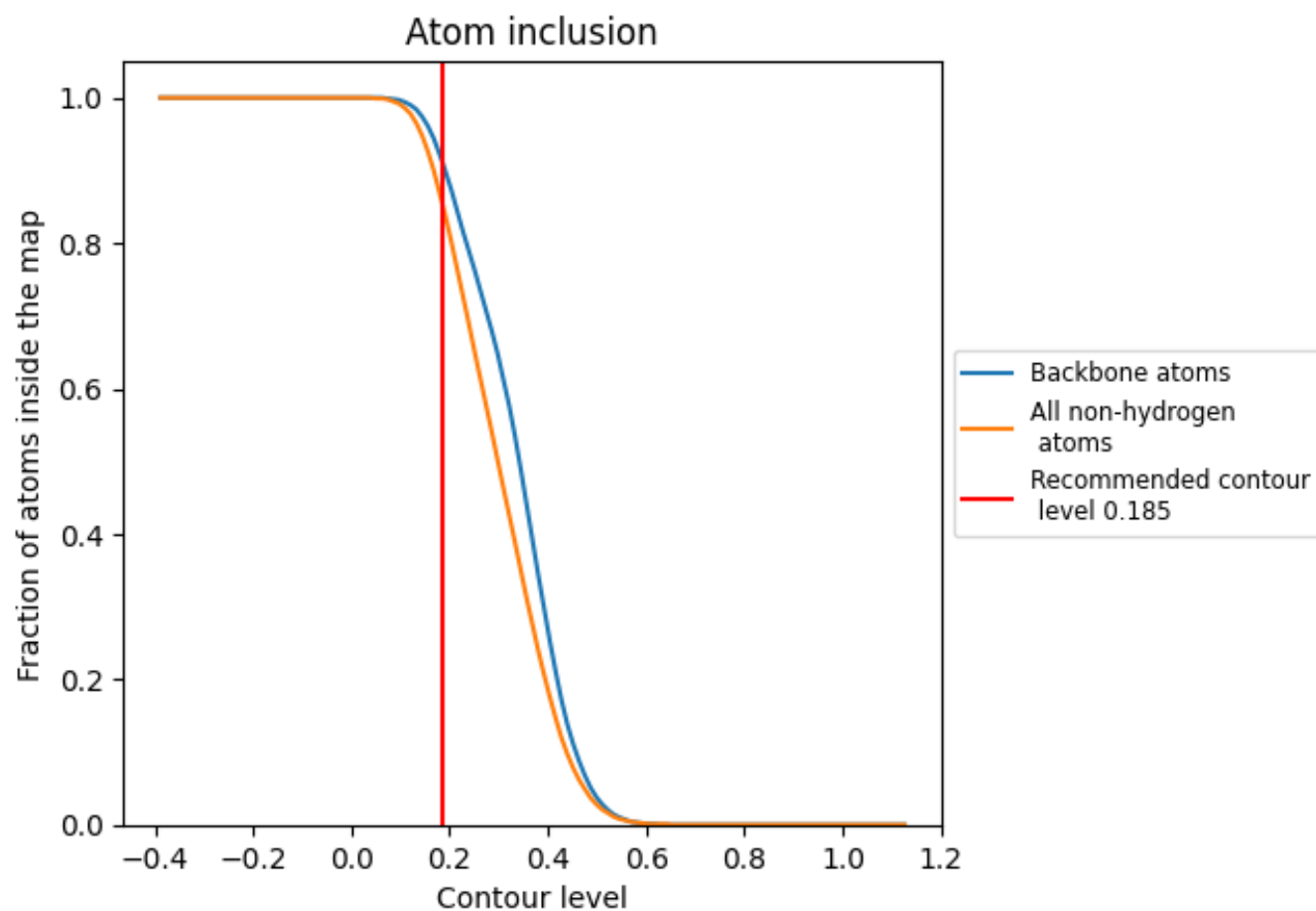
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.185).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ































The table lists the average atom inclusion at the recommended contour level (0.185) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.8550   |  0.5300   |
| 1     |  0.7220   |  0.4730   |
| A     |  0.8720   |  0.5330   |
| B     |  0.8600   |  0.5380   |
| C     |  0.9270   |  0.5160   |
| D     |  0.8760   |  0.5210   |
| E     |  0.8260   |  0.5260   |
| F     |  0.8440   |  0.5160   |
| G     |  0.8790   |  0.5400   |
| H     |  0.7940   |  0.5160   |
| I     |  0.7620   |  0.5260   |
| J     |  0.8230   |  0.5080   |
| K     |  0.7070   |  0.4420   |
| L     |  0.7900   |  0.5260   |
| M     |  0.7830  |  0.5170  |
| N     |  0.8720 |  0.5430 |
| P     |  0.9270 |  0.5110 |
| Q     |  0.8720 |  0.5280 |
| R     |  0.8540 |  0.5240 |
| S     |  0.8300 |  0.5190 |
| T     |  0.8530 |  0.5110 |
| U     |  0.7150 |  0.4570 |
| V     |  0.8490 |  0.5360 |
| W     |  0.8430 |  0.5280 |
| X     |  0.7990 |  0.5050 |
| Y     |  0.7640 |  0.5170 |
| a     |  0.8590 |  0.5340 |
| b     |  0.8620 |  0.5290 |
| c     |  0.9420 |  0.5120 |
| d     |  0.8680 |  0.5170 |
| e     |  0.8430 |  0.5180 |
| f     |  0.8060 |  0.4940 |
| g     |  0.8720 |  0.5430 |
| h     |  0.7300 |  0.4690 |
| i     |  0.7920 |  0.5160 |



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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| j     |  0.8350 |  0.4920 |
| k     |  0.6840 |  0.4650 |
| l     |  0.8230 |  0.5290 |
| m     |  0.7300 |  0.5130 |
| n     |  0.8690 |  0.5390 |
| p     |  0.9400 |  0.5290 |
| q     |  0.8910 |  0.5330 |
| r     |  0.8190 |  0.5270 |
| s     |  0.8040 |  0.4900 |
| t     |  0.8170 |  0.4980 |
| u     |  0.6530 |  0.4800 |
| v     |  0.7910 |  0.5220 |
| w     |  0.8350 |  0.5360 |
| x     |  0.7630 |  0.4950 |
| y     |  0.7970 |  0.5220 |