# wwPDB EM Validation Summary Report (i)

May 26, 2024 – 04:36 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 7RX2 |
| EMDB ID | : | EMD-24722 |
| Title | : | afTMEM16 in C22 lipid nanodiscs with MSP1E3 scaffold protein in the presnece of Ca2+ |
| Authors | : | Falzone, M.E.; Accardi, A. |
| Deposited on | : | 2021-08-21 |
| Resolution | : | 2.70 Å(reported) |

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

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

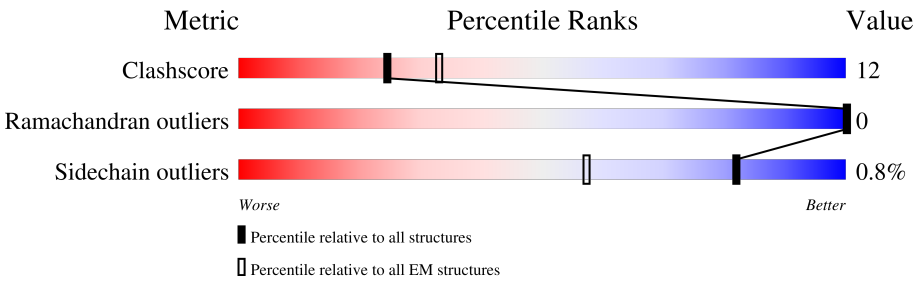
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev92 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

# 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 2.70 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 (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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 >=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 <=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 | A | 735 | 61% 22% 16% |
| 1 | B | 735 | 61% 22% 16% |

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10390 atoms, of which 12 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.

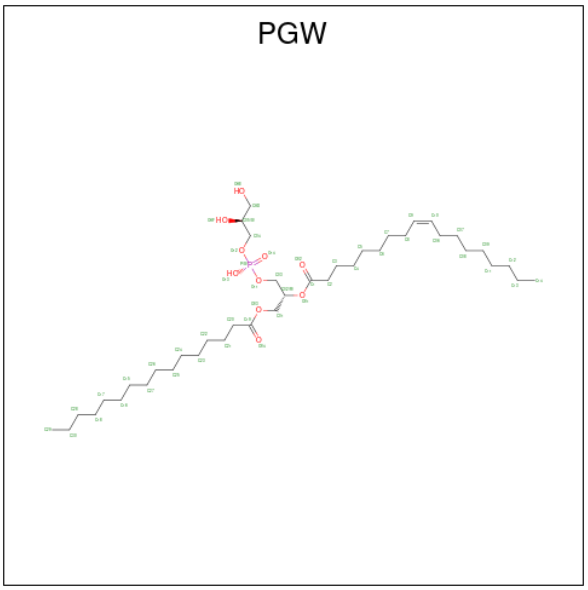
- Molecule 1 is a protein called afTMEM16 lipid scramblase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | B | 615 | 4969 | 3251 | 832 | 867 | 19 | 0 | 0 |
| 1 | A | 615 | 4969 | 3251 | 832 | 867 | 19 | 0 | 0 |

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Ca | |
| 2 | B | 2 | 2 | 2 | 0 |
| 2 | A | 2 | 2 | 2 | 0 |

- Molecule 3 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: $C_{40}H_{77}O_{10}P$).



| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 3 | B | 1 | Total C O<br>26 21 5 | 0 |
| 3 | B | 1 | Total C O P<br>41 30 10 1 | 0 |
| 3 | B | 1 | Total C O P<br>26 17 8 1 | 0 |
| 3 | B | 1 | Total C O P<br>38 29 8 1 | 0 |
| 3 | B | 1 | Total C O P<br>30 21 8 1 | 0 |
| 3 | B | 1 | Total C O P<br>30 21 8 1 | 0 |
| 3 | B | 1 | Total C O P<br>24 15 8 1 | 0 |
| 3 | A | 1 | Total C O P<br>24 15 8 1 | 0 |
| 3 | A | 1 | Total C O<br>26 21 5 | 0 |
| 3 | A | 1 | Total C O P<br>41 30 10 1 | 0 |
| 3 | A | 1 | Total C O P<br>26 17 8 1 | 0 |
| 3 | A | 1 | Total C O P<br>38 29 8 1 | 0 |
| 3 | A | 1 | Total C O P<br>30 21 8 1 | 0 |
| 3 | A | 1 | Total C O P<br>30 21 8 1 | 0 |

- Molecule 4 is water.

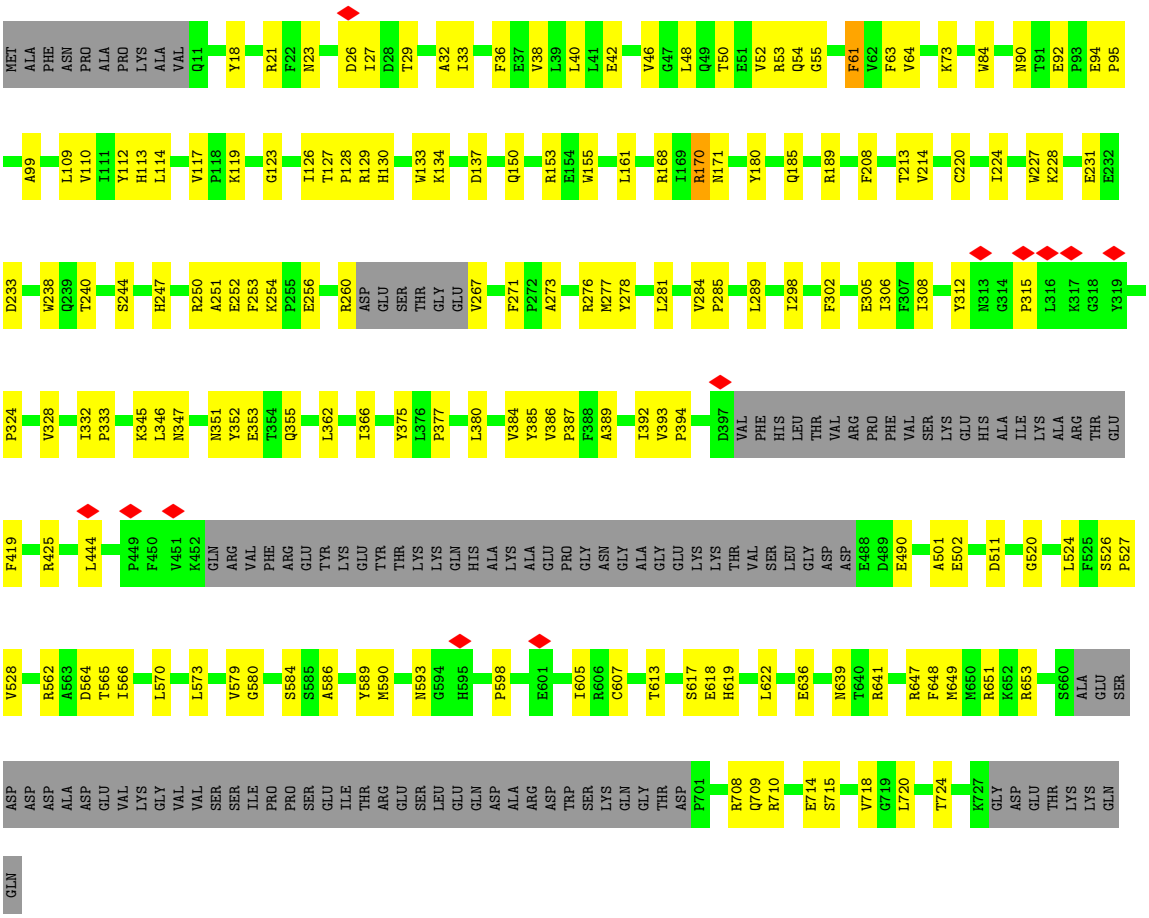
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 4 | B | 3 | Total H O<br>9 6 3 | 0 |
| 4 | A | 3 | Total H O<br>9 6 3 | 0 |

# 3 Residue-property plots (i)

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.

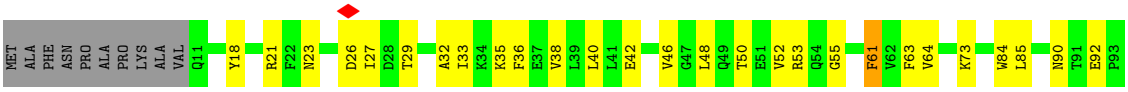
• Molecule 1: afTMEM16 lipid scramblase

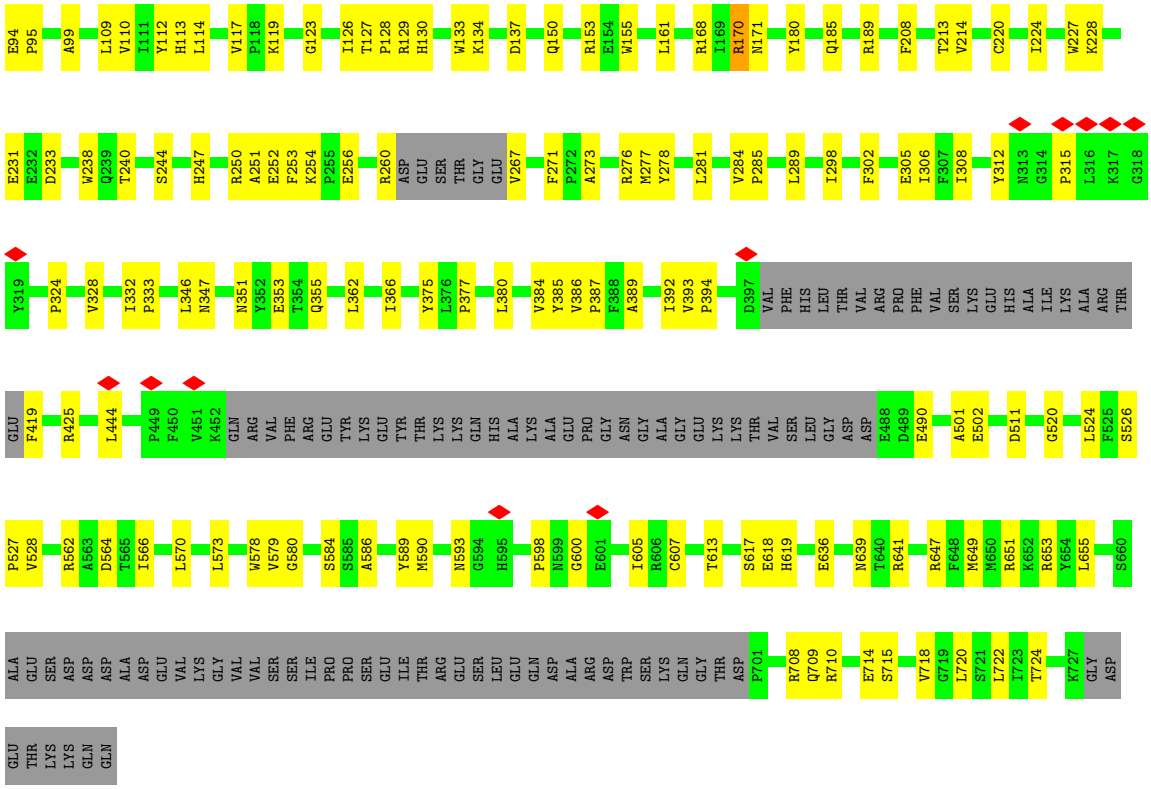
Chain B:




• Molecule 1: afTMEM16 lipid scramblase

Chain A:




E94 P95 A99 L109 V110 I111 Y112 H113 L114 V117 P118 K119 G123 I126 T127 P128 R129 H130 W133 K134 D137 Q150 R153 E154 W155 L161 R168 I169 R170 N171 Y180 Q185 R189 F208 T213 V214 C220 I224 W227 K228
E231 E232 D233 W238 Q239 T240 S244 H247 R250 A251 E252 F253 K254 P255 E256 R260 ASP GLU SER THR GLY GLU V267 F271 P272 A273 R276 M277 Y278 L281 V284 P285 L289 I298 F302 E305 I306 F307 I308 Y312 N313 G314 P315 L316 K317 G318
Y319 P324 V328 I332 P333 L346 N347 N351 Y352 E353 T354 Q355 L362 I366 Y375 L376 P377 L380 V384 Y385 V386 P387 F388 A389 I392 V393 P394 D397 VAL PHE HIS LEU THR VAL ARG PRO PHE VAL SER LYS GLU HIS ALA ILE LYS ALA ARG THR
GLU F419 R425 L444 P449 F450 V451 K452 GLN ARG VAL PHE ARG GLU TYR LYS GLU TYR THR LYS LYS GLN HIS ALA LYS ALA GLU PRO GLY ASN GLY ALA GLY GLU LYS LYS THR VAL SER LEU GLY ASP ASP E488 D489 E490 A501 E502 D511 G520 L524 F525 S526
P527 V528 R562 A563 D564 T565 I566 L570 L573 W578 V579 G580 S584 S585 A586 Y589 M590 N593 G594 H595 P598 N599 G600 E601 I605 R606 C607 T613 S617 E618 H619 E636 N639 T640 R641 R647 F648 M649 M650 R651 K652 R653 Y654 L655 S660
ALA GLU SER ASP ASP ASP ALA ASP GLU VAL LYS GLY VAL VAL SER SER ILE PRO PRO SER GLU ILE THR ARG GLU SER LEU GLU GLN ASP ALA ARG ASP TRP SER LYS GLN GLY THR ASP P701 R708 Q709 R710 E714 S715 V718 G719 L720 S721 L722 I723 T724 K727 GLY ASP
GLU THR LYS LYS GLN GLN

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 132332 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 42.7884 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 0.087 | Depositor |
| Minimum map value | -0.046 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.003 | Depositor |
| Recommended contour level | 0.013 | Depositor |
| Map size (Å) | 271.3728, 271.3728, 271.3728 | wwPDB |
| Map dimensions | 384, 384, 384 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.7067, 0.7067, 0.7067 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PGW, CA

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 | A | 0.44 | 0/5101 | 0.47 | 0/6933 |
| 1 | B | 0.44 | 0/5101 | 0.47 | 0/6933 |
| All | All | 0.44 | 0/10202 | 0.47 | 0/13866 |

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 (i)

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 | A | 4969 | 0 | 4947 | 122 | 0 |
| 1 | B | 4969 | 0 | 4947 | 125 | 0 |
| 2 | A | 2 | 0 | 0 | 0 | 0 |
| 2 | B | 2 | 0 | 0 | 0 | 0 |
| 3 | A | 215 | 0 | 239 | 17 | 0 |
| 3 | B | 215 | 0 | 239 | 15 | 0 |
| 4 | A | 3 | 6 | 0 | 0 | 0 |
| 4 | B | 3 | 6 | 0 | 0 | 0 |
| All | All | 10378 | 12 | 10372 | 244 | 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 12.

The worst 5 of 244 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) |
|---|---|---|---|
| 1:A:129:ARG:HA | 1:A:134:LYS:HA | 1.40 | 1.03 |
| 1:B:129:ARG:HA | 1:B:134:LYS:HA | 1.40 | 0.98 |
| 1:B:189:ARG:HD3 | 3:B:805:PGW:H03A | 1.47 | 0.96 |
| 1:A:189:ARG:HD3 | 3:A:1506:PGW:H03A | 1.47 | 0.94 |
| 1:A:524:LEU:HD23 | 1:A:580:GLY:HA2 | 1.62 | 0.82 |

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 | A | 605/735 (82%) | 571 (94%) | 34 (6%) | 0 | 100 | 100 |
| 1 | B | 605/735 (82%) | 571 (94%) | 34 (6%) | 0 | 100 | 100 |
| All | All | 1210/1470 (82%) | 1142 (94%) | 68 (6%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains (i)

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 | A | 529/646 (82%) | 525 (99%) | 4 (1%) | 81 | 93 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | B | 529/646 (82%) | 525 (99%) | 4 (1%) | 81 93 |
| All | All | 1058/1292 (82%) | 1050 (99%) | 8 (1%) | 82 93 |

5 of 8 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 593 | ASN |
| 1 | A | 444 | LEU |
| 1 | A | 61 | PHE |
| 1 | B | 593 | ASN |
| 1 | A | 170 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 150 | GLN |
| 1 | A | 283 | GLN |
| 1 | A | 499 | ASN |
| 1 | A | 370 | ASN |
| 1 | B | 370 | ASN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 for Mogul analysis.

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 | $\#\|Z\| > 2$ |
| 3 | PGW | B | 806 | - | 37,37,50 | 1.09 | 5 (13%) | 41,42,56 | 1.23 | 3 (7%) |
| 3 | PGW | B | 803 | - | 25,25,50 | 1.18 | 3 (12%) | 27,27,56 | 1.38 | 2 (7%) |
| 3 | PGW | A | 1504 | - | 25,25,50 | 1.18 | 3 (12%) | 27,27,56 | 1.38 | 2 (7%) |
| 3 | PGW | B | 804 | - | 40,40,50 | 0.29 | 0 | 43,46,56 | 0.34 | 0 |
| 3 | PGW | A | 1508 | - | 29,29,50 | 1.21 | 4 (13%) | 33,34,56 | 1.07 | 2 (6%) |
| 3 | PGW | A | 1506 | - | 25,25,50 | 1.30 | 4 (16%) | 29,30,56 | 1.44 | 3 (10%) |
| 3 | PGW | A | 1501 | - | 23,23,50 | 0.49 | 0 | 27,28,56 | 0.64 | 1 (3%) |
| 3 | PGW | B | 805 | - | 25,25,50 | 1.30 | 4 (16%) | 29,30,56 | 1.44 | 3 (10%) |
| 3 | PGW | B | 807 | - | 29,29,50 | 1.21 | 4 (13%) | 33,34,56 | 1.07 | 2 (6%) |
| 3 | PGW | A | 1507 | - | 37,37,50 | 1.09 | 5 (13%) | 41,42,56 | 1.23 | 3 (7%) |
| 3 | PGW | A | 1509 | - | 28,28,50 | 1.24 | 5 (17%) | 30,32,56 | 1.28 | 2 (6%) |
| 3 | PGW | A | 1505 | - | 40,40,50 | 0.29 | 0 | 43,46,56 | 0.34 | 0 |
| 3 | PGW | B | 808 | - | 28,28,50 | 1.24 | 5 (17%) | 30,32,56 | 1.28 | 2 (6%) |
| 3 | PGW | B | 809 | - | 23,23,50 | 0.48 | 0 | 27,28,56 | 0.64 | 1 (3%) |

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 |
|---|---|---|---|---|---|---|---|
| 3 | PGW | B | 806 | - | - | 18/39/39/55 | - |
| 3 | PGW | B | 803 | - | - | 9/27/27/55 | - |
| 3 | PGW | A | 1504 | - | - | 9/27/27/55 | - |
| 3 | PGW | B | 804 | - | - | 22/45/45/55 | - |
| 3 | PGW | A | 1508 | - | - | 8/31/31/55 | - |
| 3 | PGW | A | 1506 | - | - | 8/27/27/55 | - |
| 3 | PGW | A | 1501 | - | - | 8/25/25/55 | - |
| 3 | PGW | B | 805 | - | - | 8/27/27/55 | - |
| 3 | PGW | B | 807 | - | - | 8/31/31/55 | - |
| 3 | PGW | A | 1507 | - | - | 18/39/39/55 | - |
| 3 | PGW | A | 1509 | - | - | 15/28/28/55 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | PGW | A | 1505 | - | - | 22/45/45/55 | - |
| 3 | PGW | B | 808 | - | - | 15/28/28/55 | - |
| 3 | PGW | B | 809 | - | - | 8/25/25/55 | - |

The worst 5 of 42 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | A | 1508 | PGW | O01-C1 | 2.95 | 1.42 | 1.34 |
| 3 | B | 807 | PGW | O01-C1 | 2.94 | 1.42 | 1.34 |
| 3 | A | 1504 | PGW | O01-C1 | 2.89 | 1.42 | 1.34 |
| 3 | B | 803 | PGW | O01-C1 | 2.87 | 1.42 | 1.34 |
| 3 | B | 805 | PGW | O01-C1 | 2.86 | 1.42 | 1.34 |

The worst 5 of 26 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | B | 805 | PGW | O01-C1-C2 | 4.93 | 122.12 | 111.50 |
| 3 | A | 1506 | PGW | O01-C1-C2 | 4.93 | 122.12 | 111.50 |
| 3 | A | 1504 | PGW | O01-C1-C2 | 4.27 | 120.70 | 111.50 |
| 3 | B | 803 | PGW | O01-C1-C2 | 4.27 | 120.70 | 111.50 |
| 3 | B | 806 | PGW | O01-C1-C2 | 3.88 | 119.87 | 111.50 |

There are no chirality outliers.

5 of 176 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | B | 803 | PGW | C01-C02-C03-O11 |
| 3 | B | 803 | PGW | O01-C02-C03-O11 |
| 3 | B | 804 | PGW | C03-O11-P-O13 |
| 3 | B | 804 | PGW | C03-O11-P-O14 |
| 3 | B | 805 | PGW | C03-O11-P-O12 |

There are no ring outliers.

14 monomers are involved in 30 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | B | 806 | PGW | 2 | 0 |
| 3 | B | 803 | PGW | 1 | 0 |
| 3 | A | 1504 | PGW | 1 | 0 |
| 3 | B | 804 | PGW | 6 | 0 |

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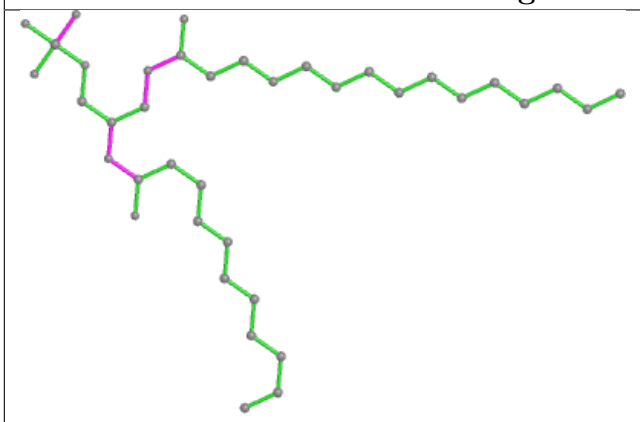
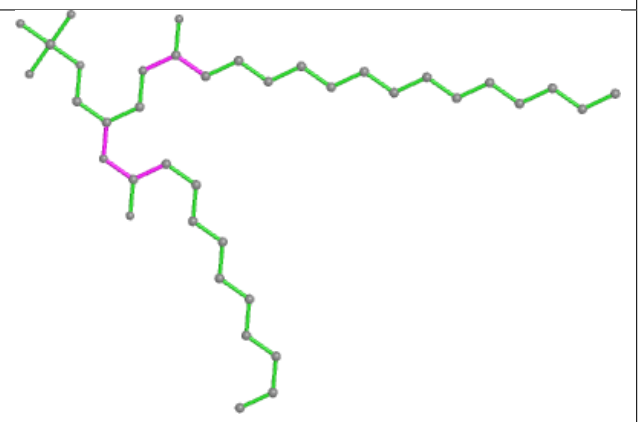
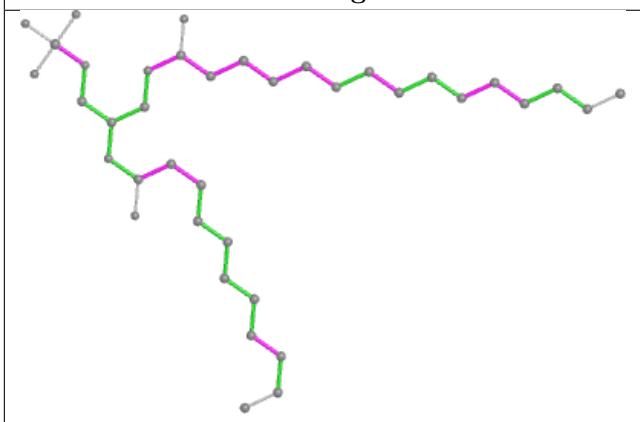
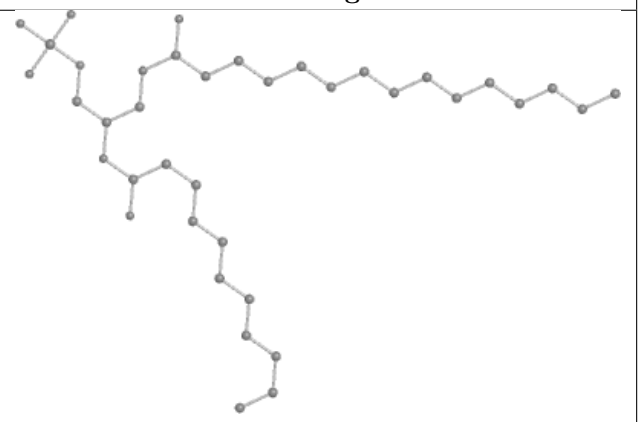
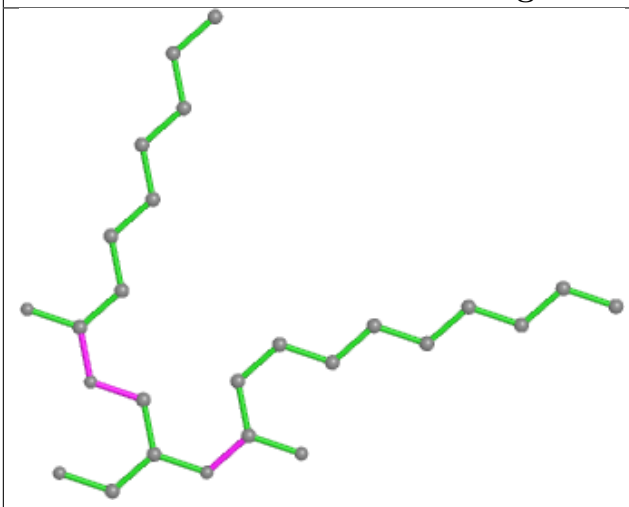
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | A | 1508 | PGW | 1 | 0 |
| 3 | A | 1506 | PGW | 2 | 0 |
| 3 | A | 1501 | PGW | 2 | 0 |
| 3 | B | 805 | PGW | 2 | 0 |
| 3 | B | 807 | PGW | 1 | 0 |
| 3 | A | 1507 | PGW | 3 | 0 |
| 3 | A | 1509 | PGW | 2 | 0 |
| 3 | A | 1505 | PGW | 6 | 0 |
| 3 | B | 808 | PGW | 2 | 0 |
| 3 | B | 809 | PGW | 1 | 0 |

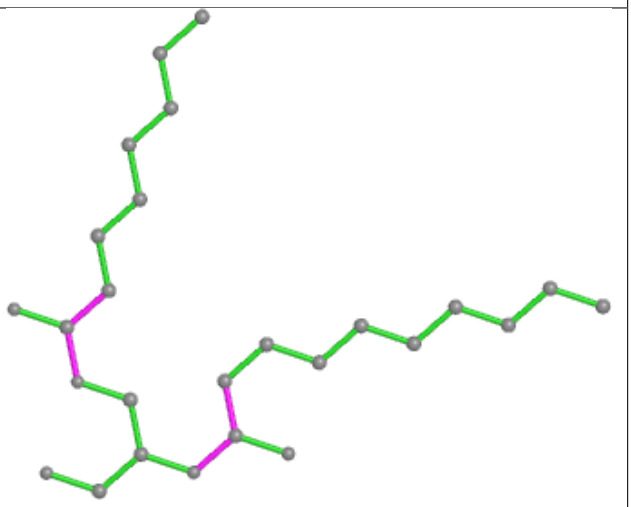
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 PGW B 806 | |
|---|---|
|  |  |
| **Bond lengths** | **Bond angles** |
|  |  |
| **Torsions** | **Rings** |

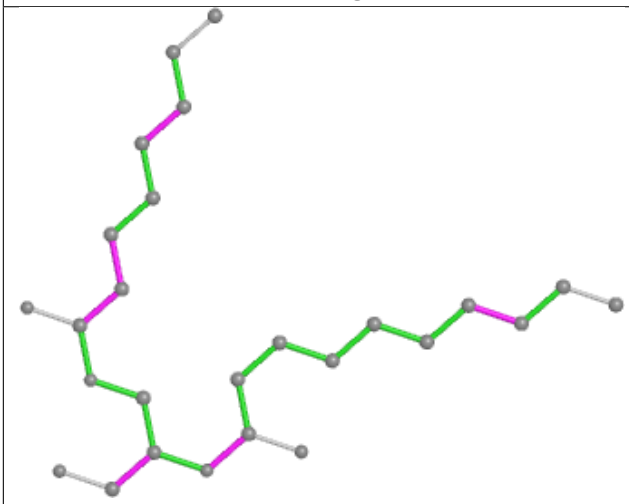
**Ligand PGW B 803**



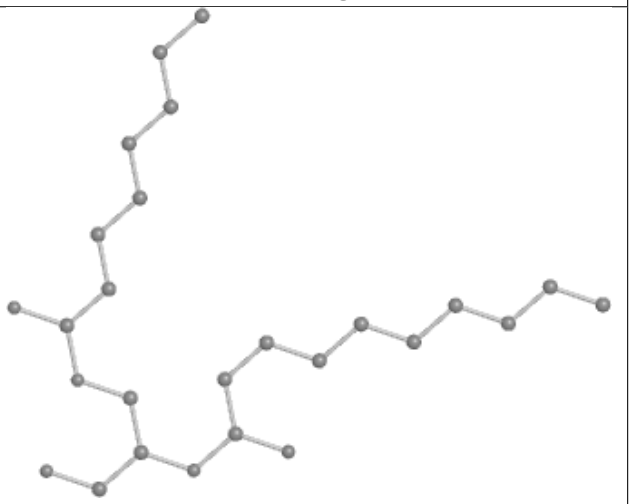
**Bond lengths**



**Bond angles**

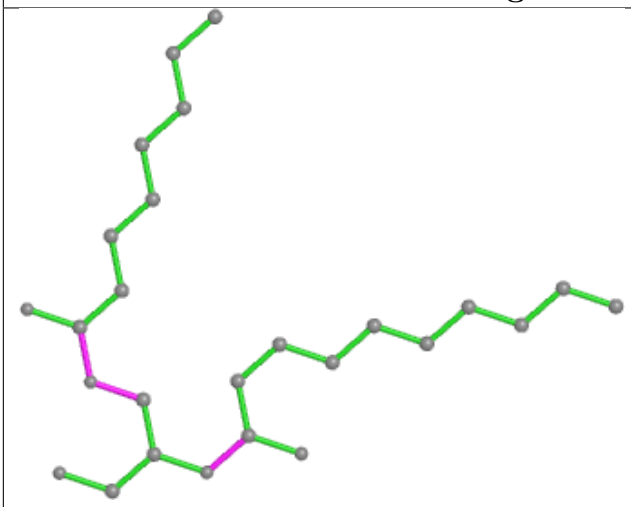


**Torsions**

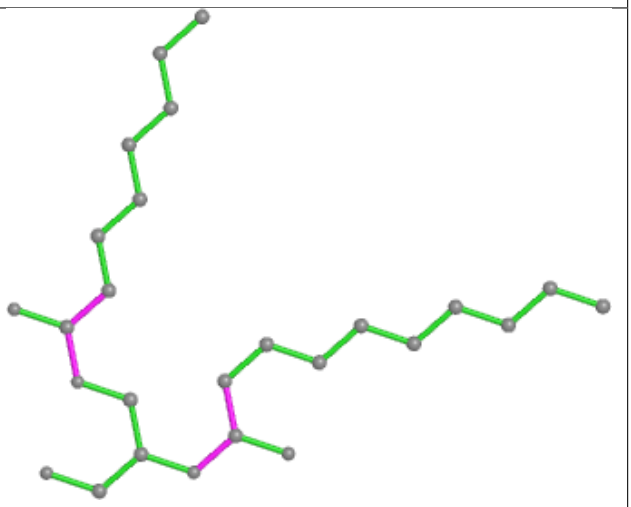


**Rings**

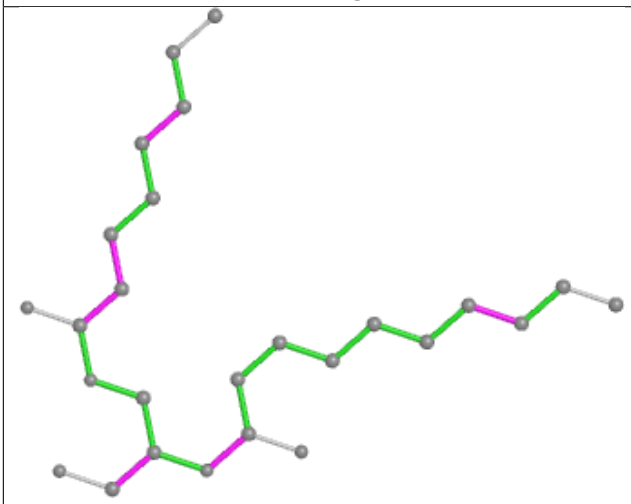
**Ligand PGW A 1504**



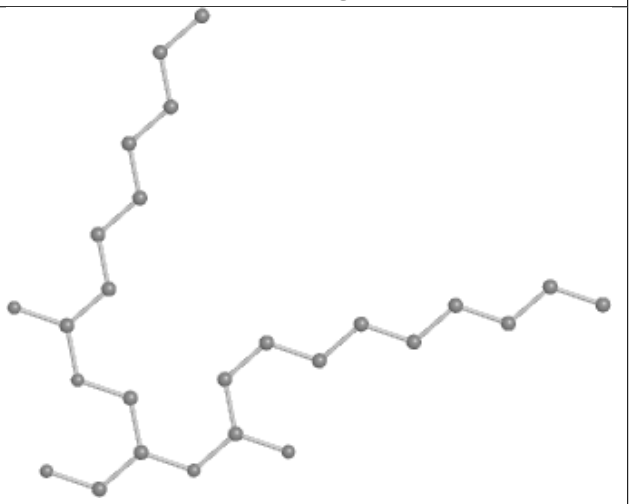
**Bond lengths**



**Bond angles**

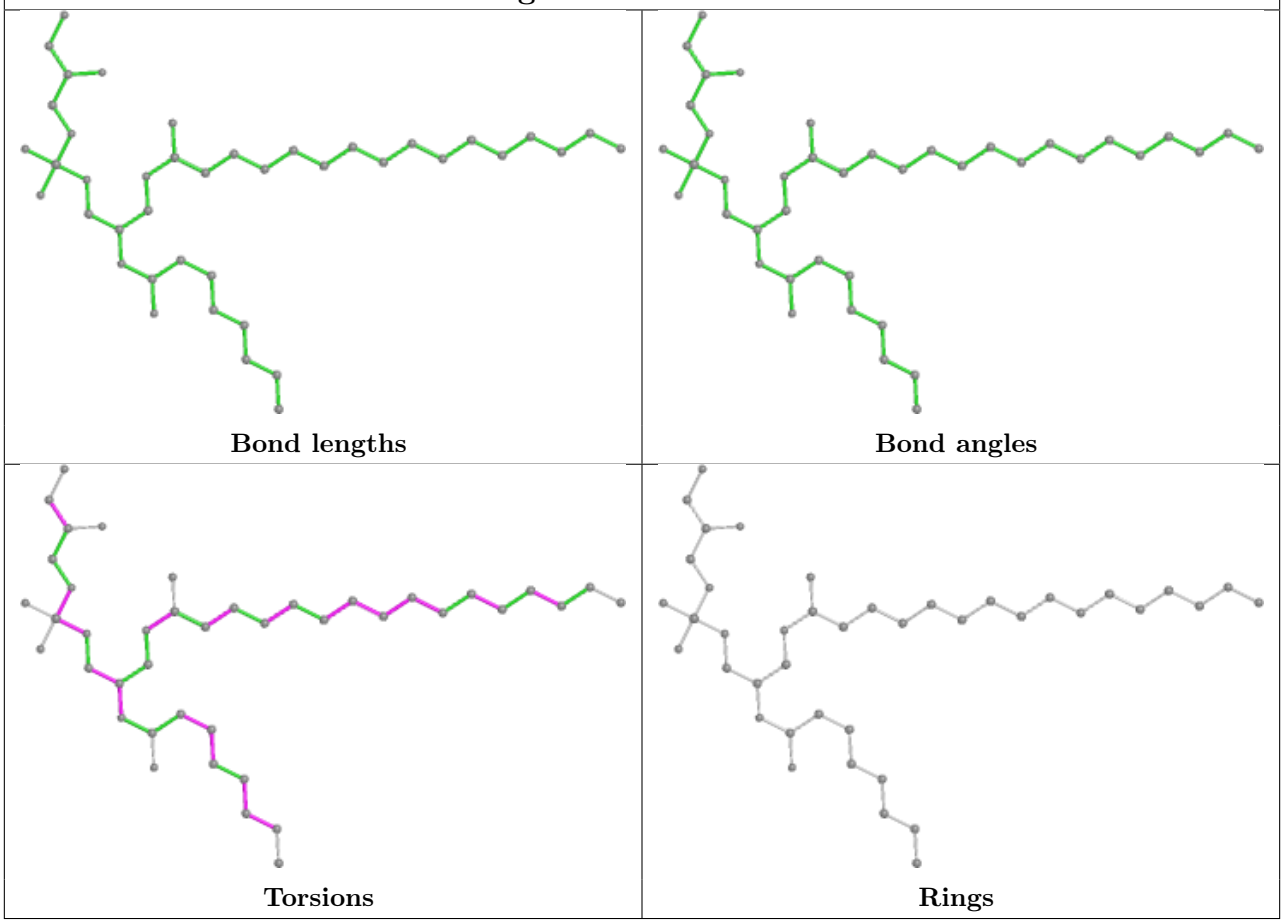


**Torsions**

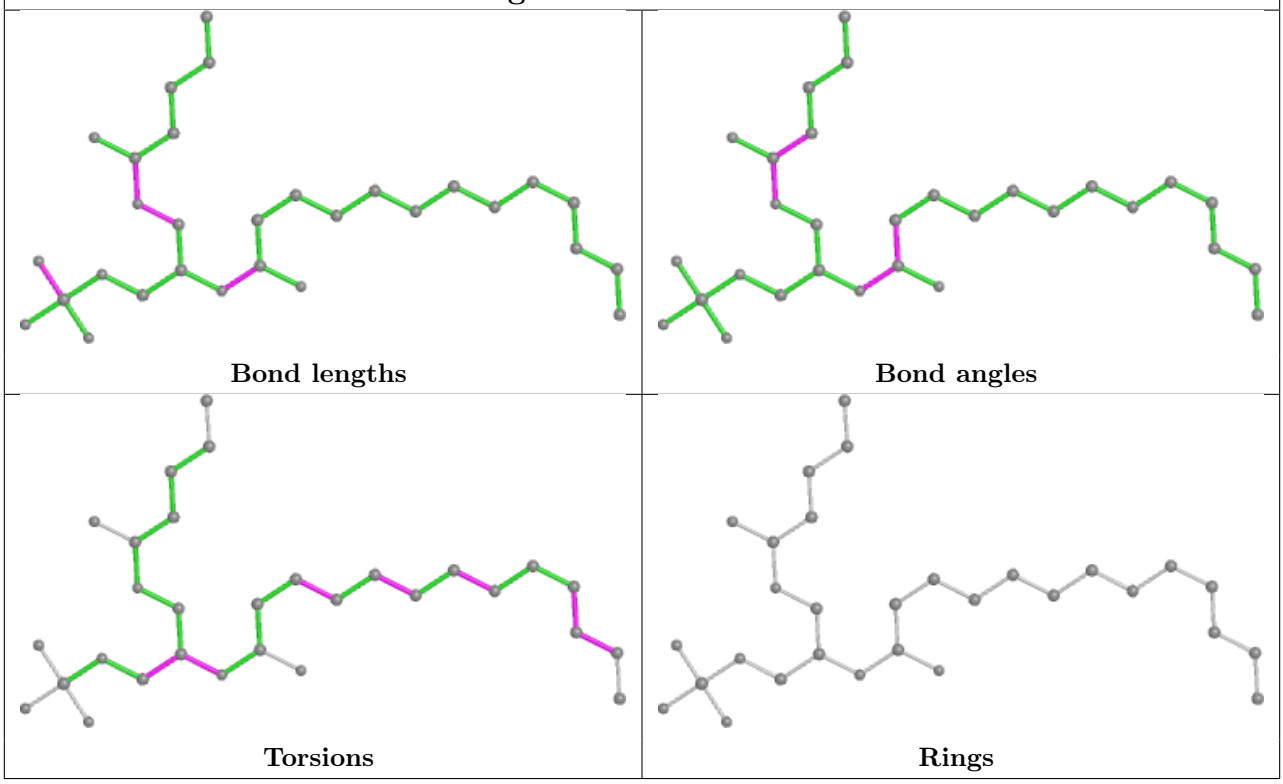


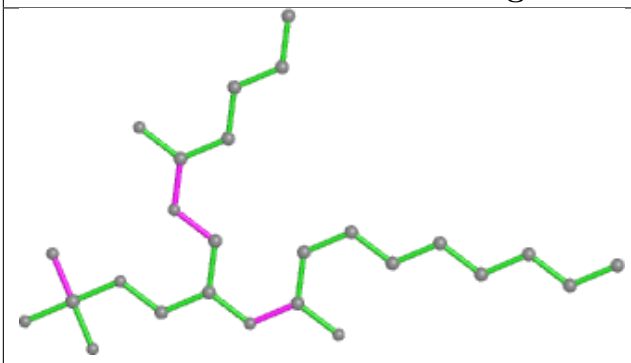
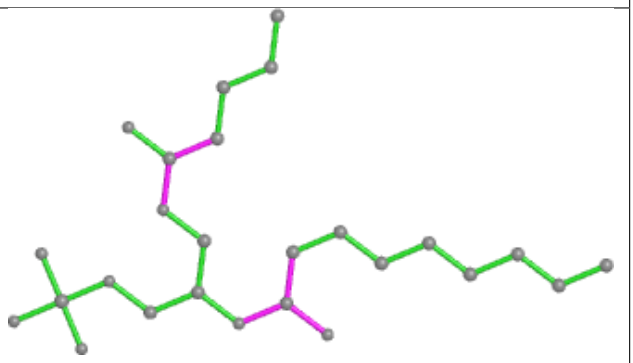
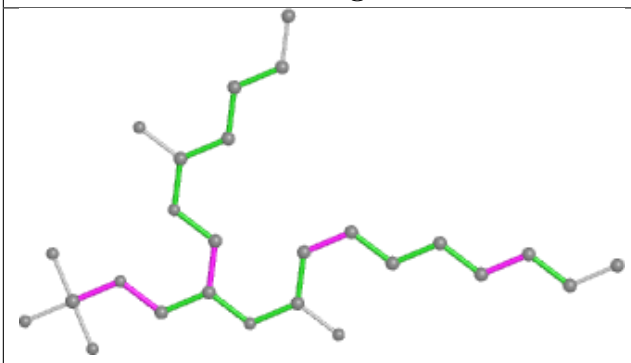
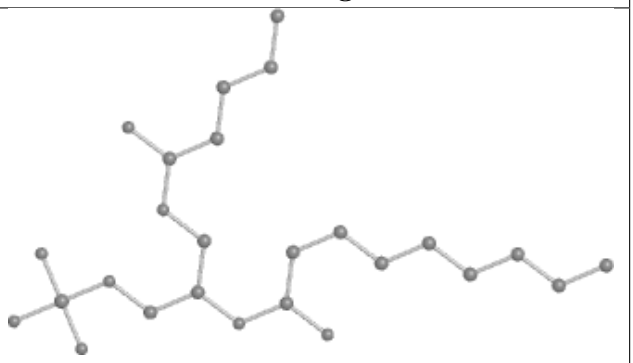
**Rings**

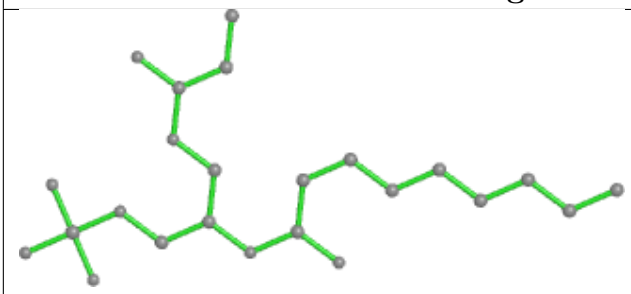
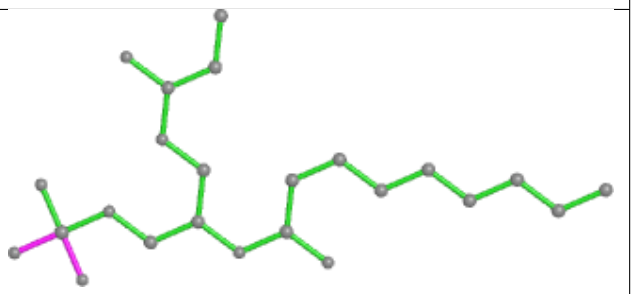
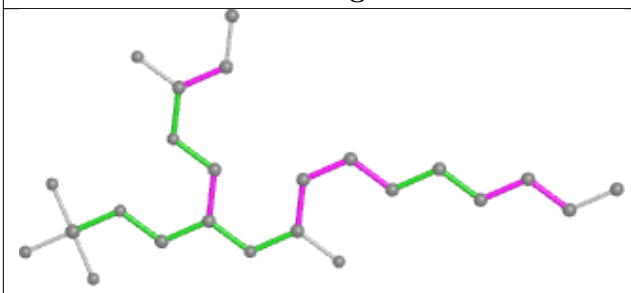
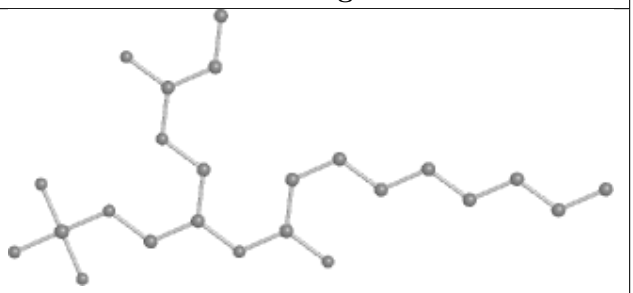
## Ligand PGW B 804



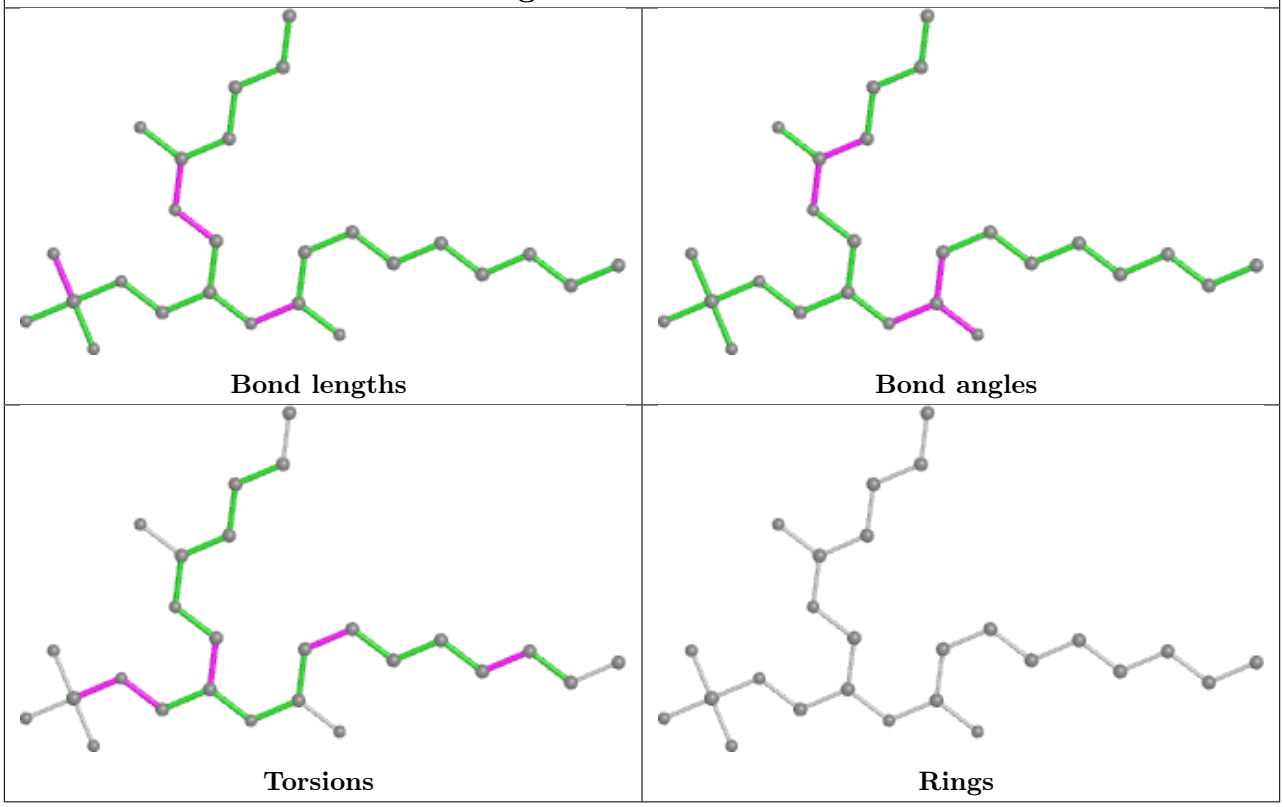

## Ligand PGW A 1508



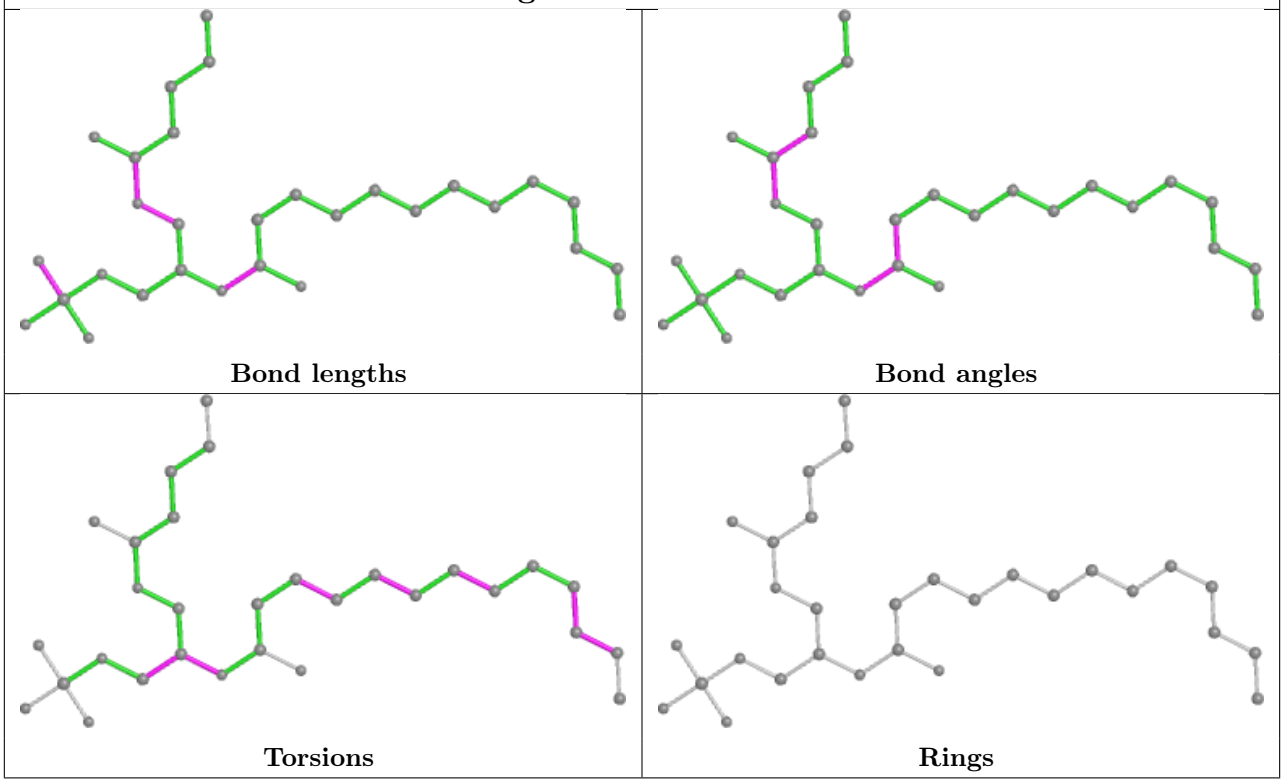
| Ligand PGW A 1506 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand PGW A 1501 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

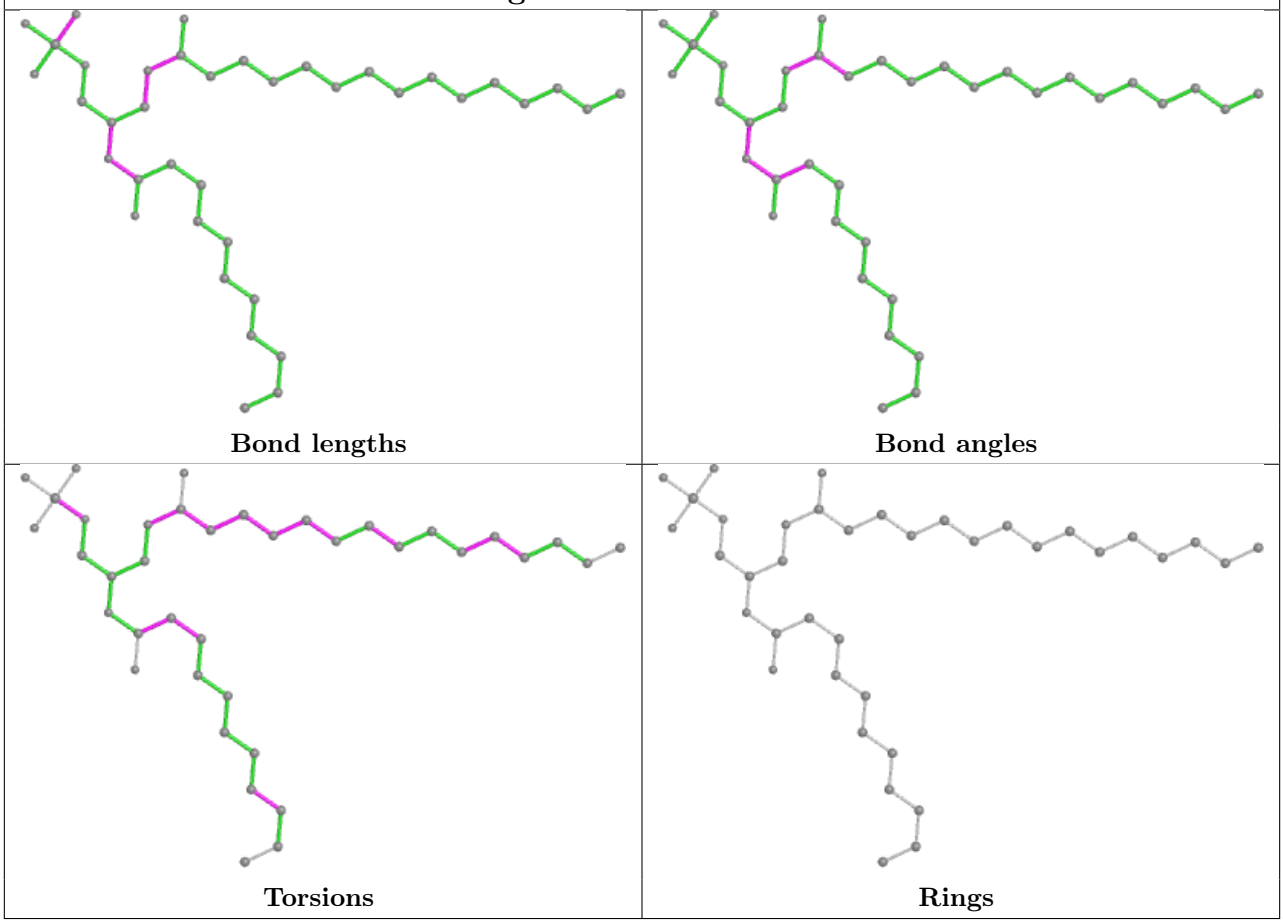
## Ligand PGW B 805



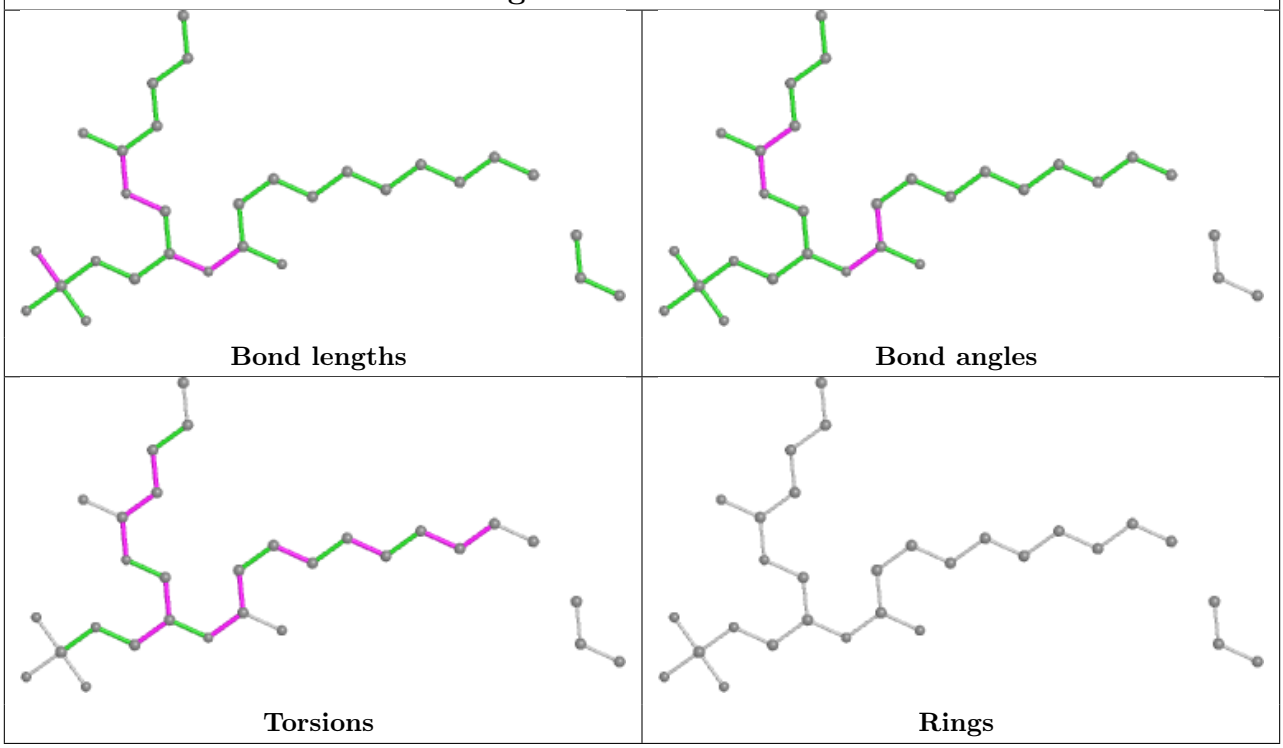

## Ligand PGW B 807



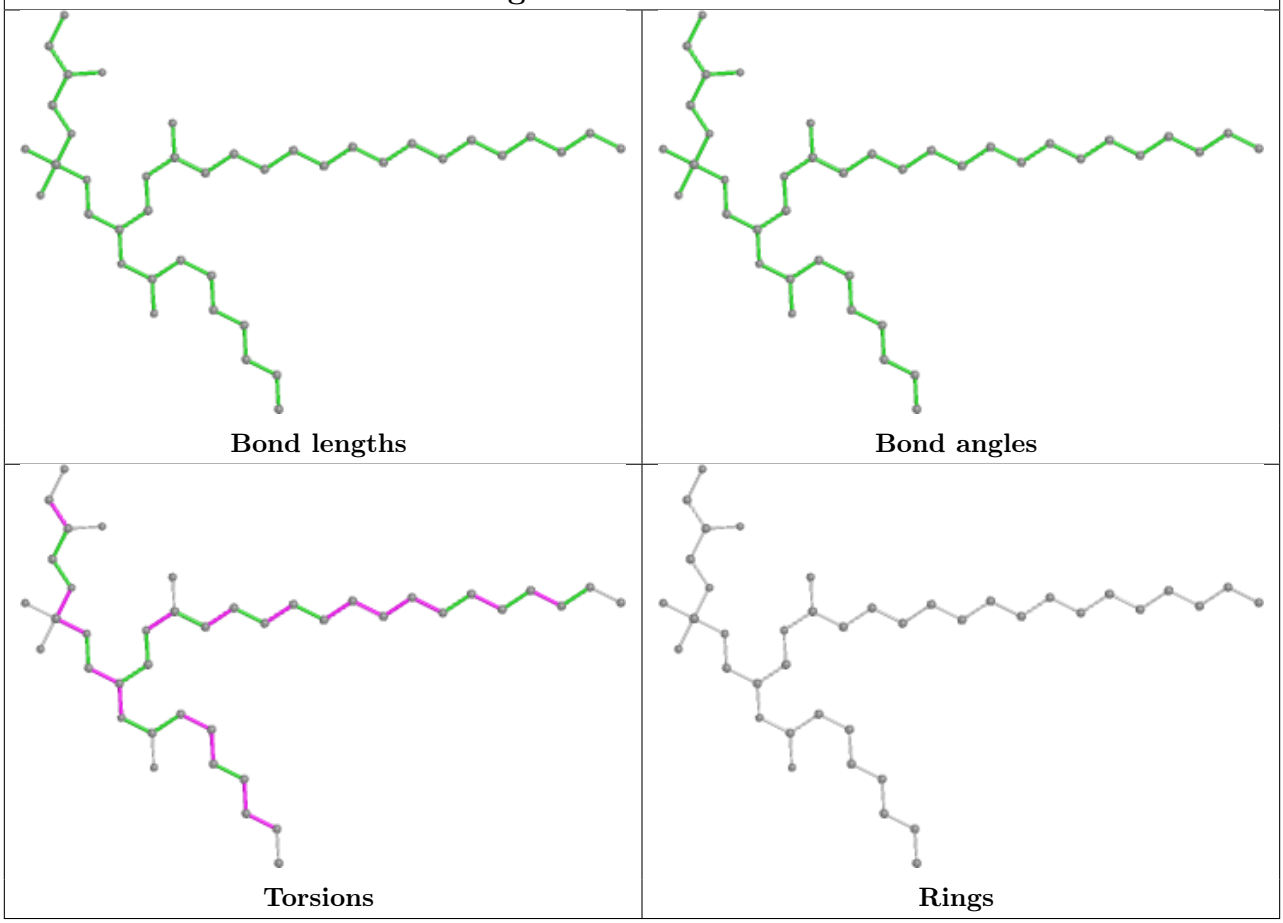
## Ligand PGW A 1507



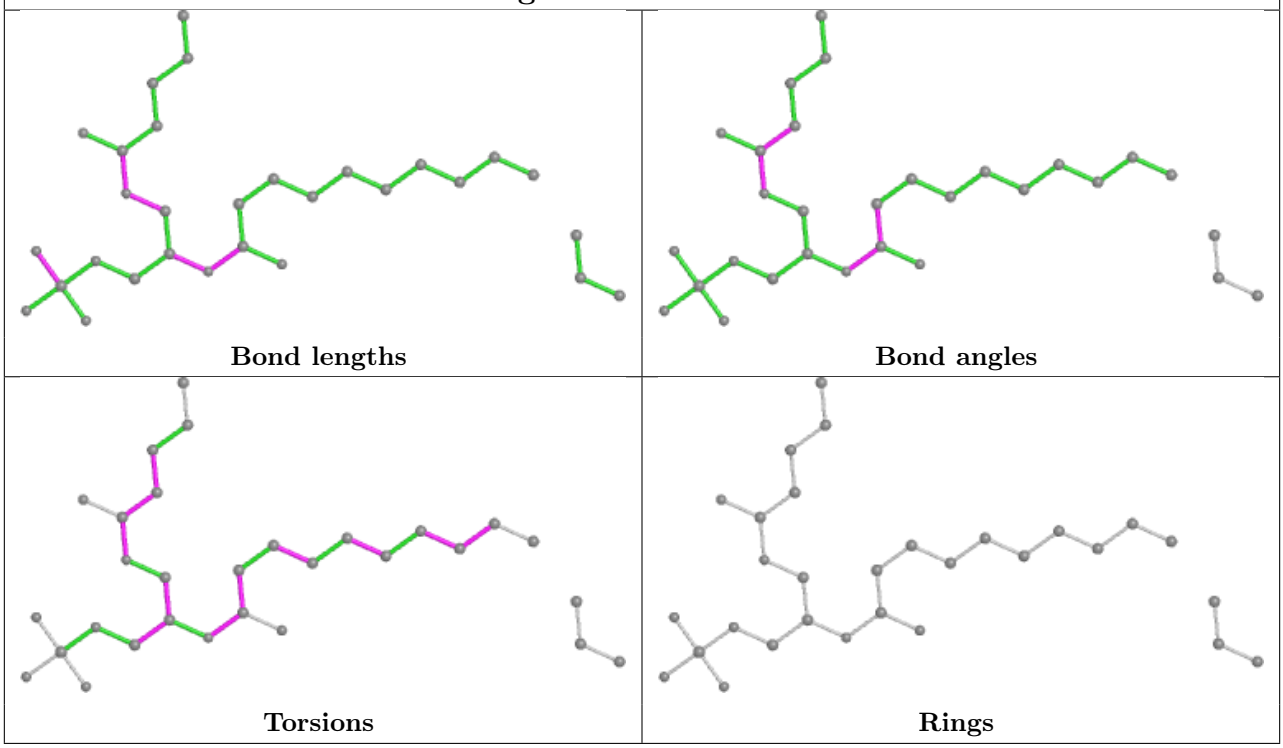

## Ligand PGW A 1509

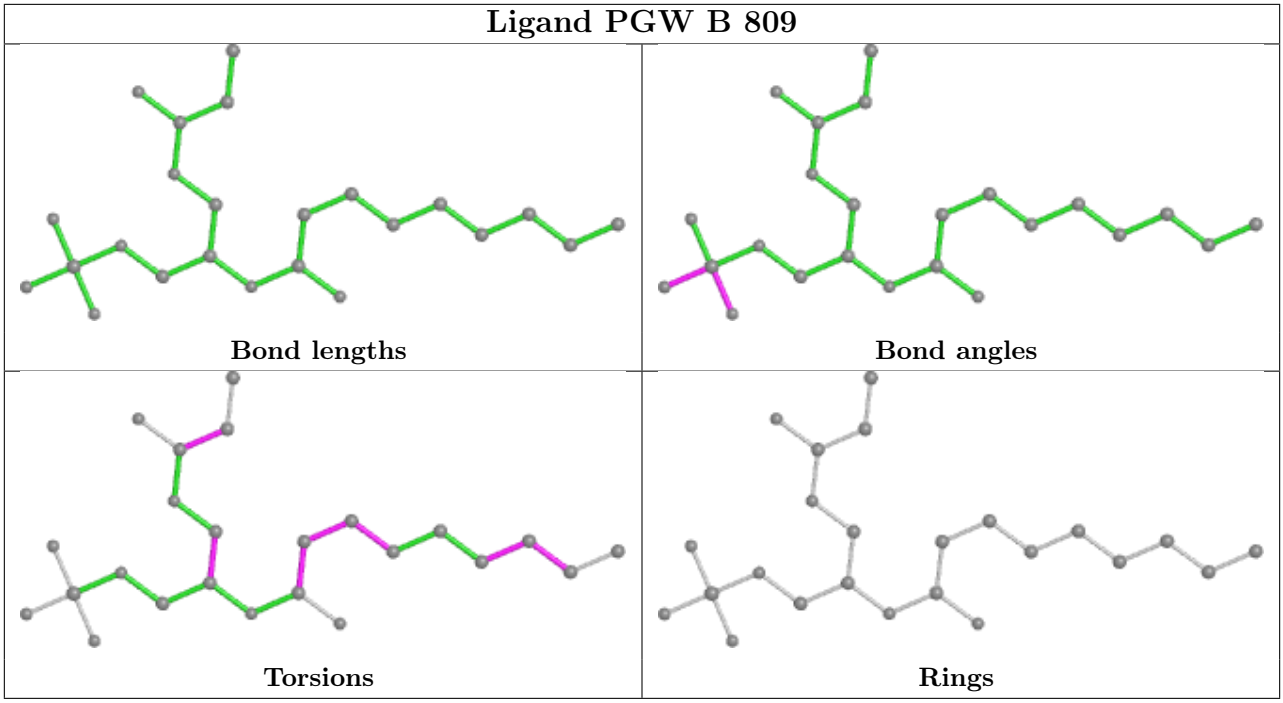


**Ligand PGW A 1505**




**Ligand PGW B 808**






## 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.

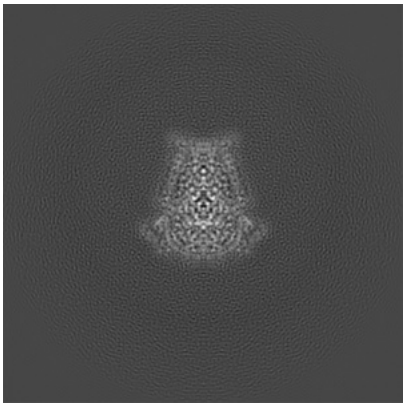
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24722. These allow visual inspection of the internal detail of the map and identification of artifacts.

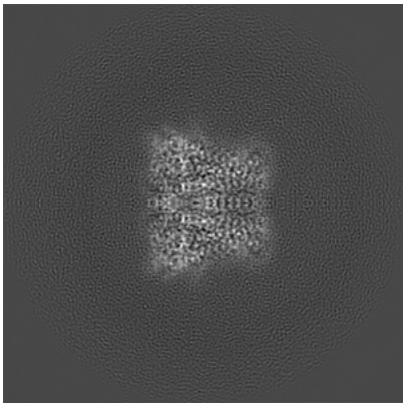
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

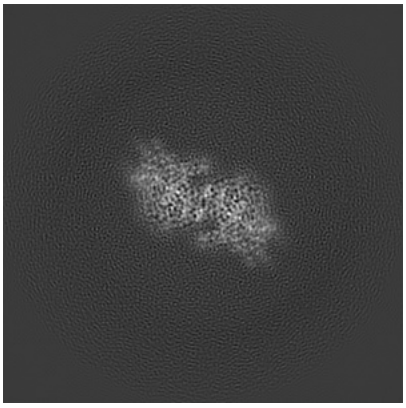
### 6.1.1 Primary map



X



Y

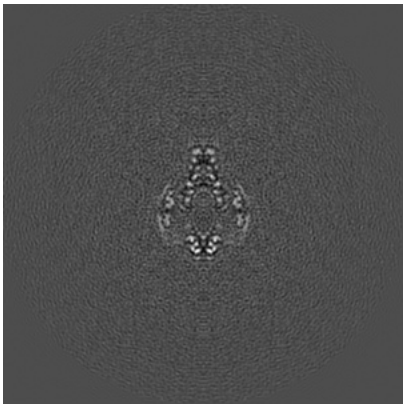


Z

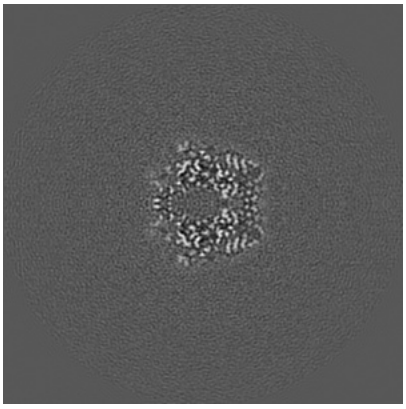
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

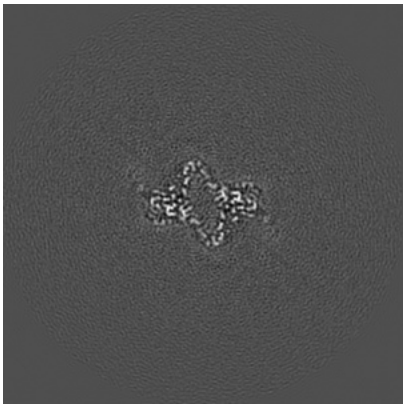
### 6.2.1 Primary map



X Index: 192



Y Index: 192

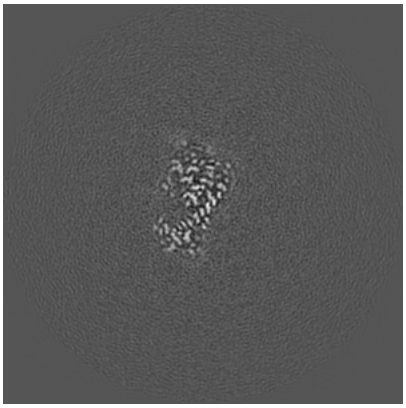


Z Index: 192

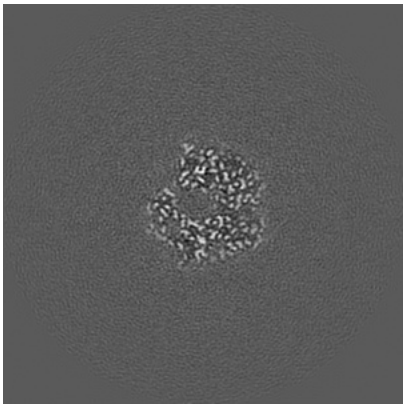
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

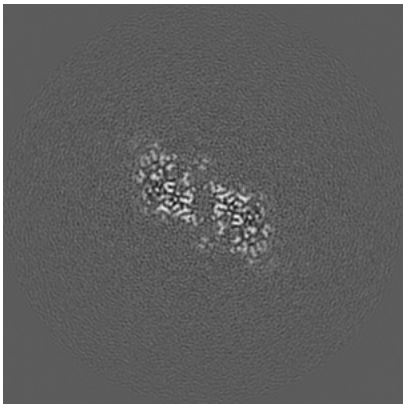
### 6.3.1 Primary map



X Index: 222



Y Index: 196

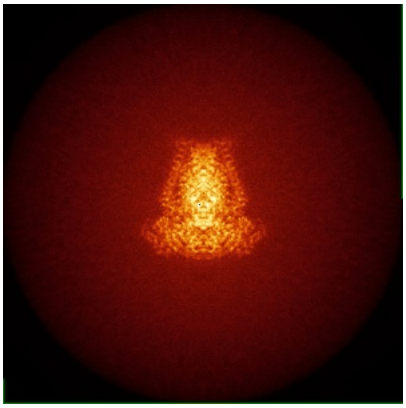


Z Index: 172

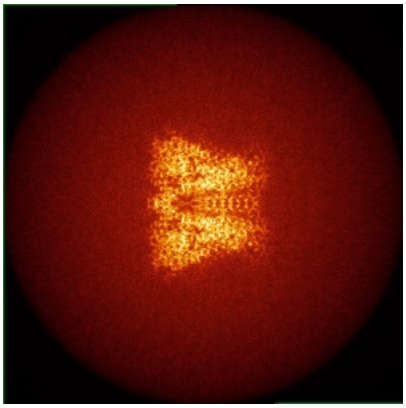
The images above show the largest variance slices of the map in three orthogonal directions.

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

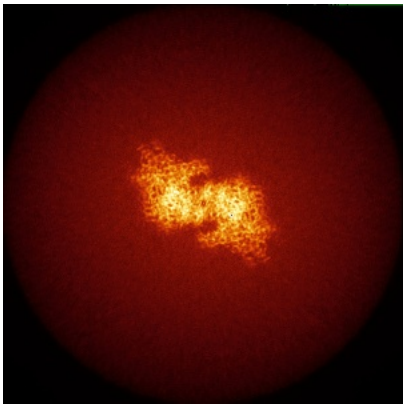
### 6.4.1 Primary map



X



Y



Z

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

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

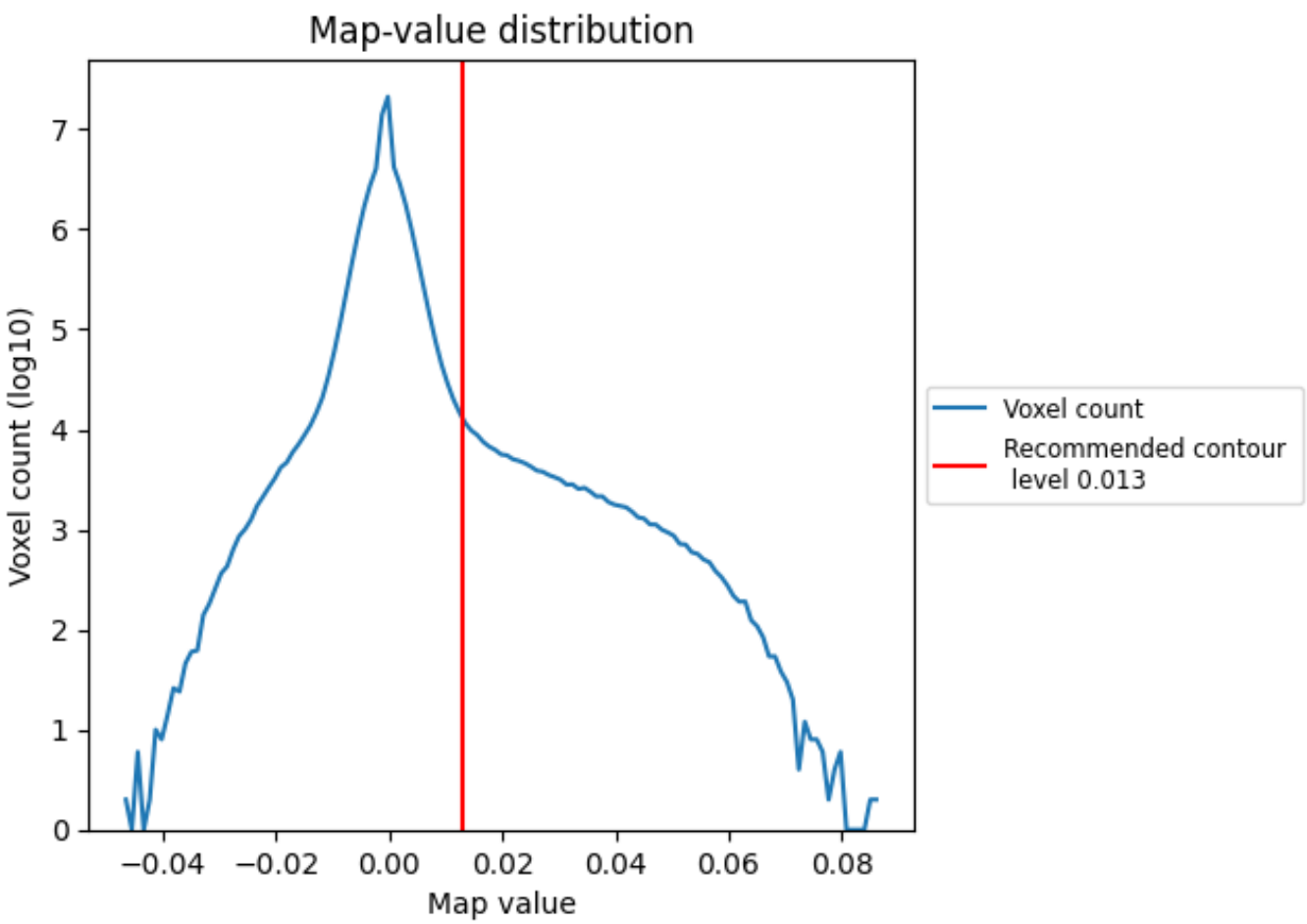
## 6.6 Mask visualisation (i)

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

# 7 Map analysis (i)

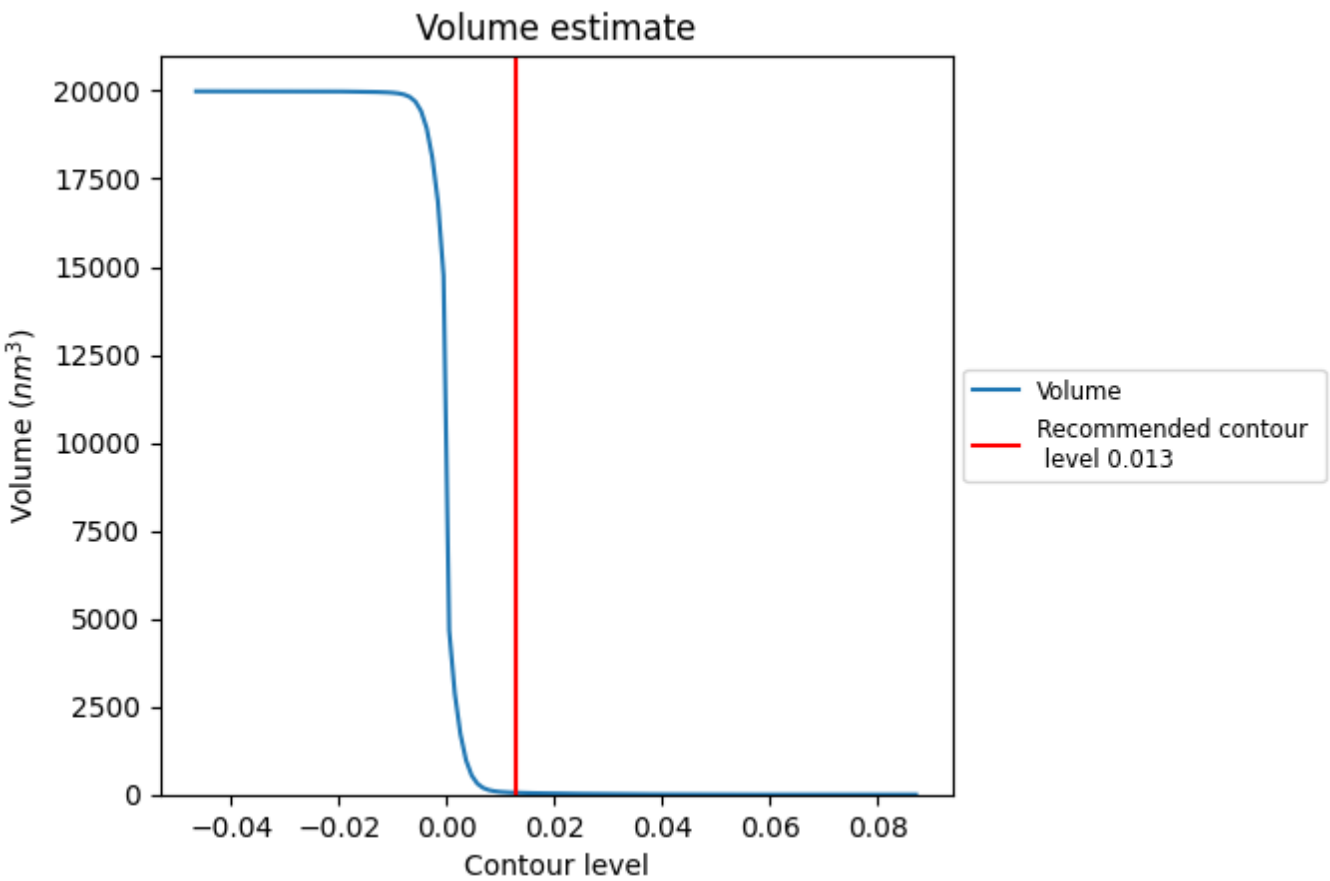
This section contains the results of statistical analysis of the map.

## 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.

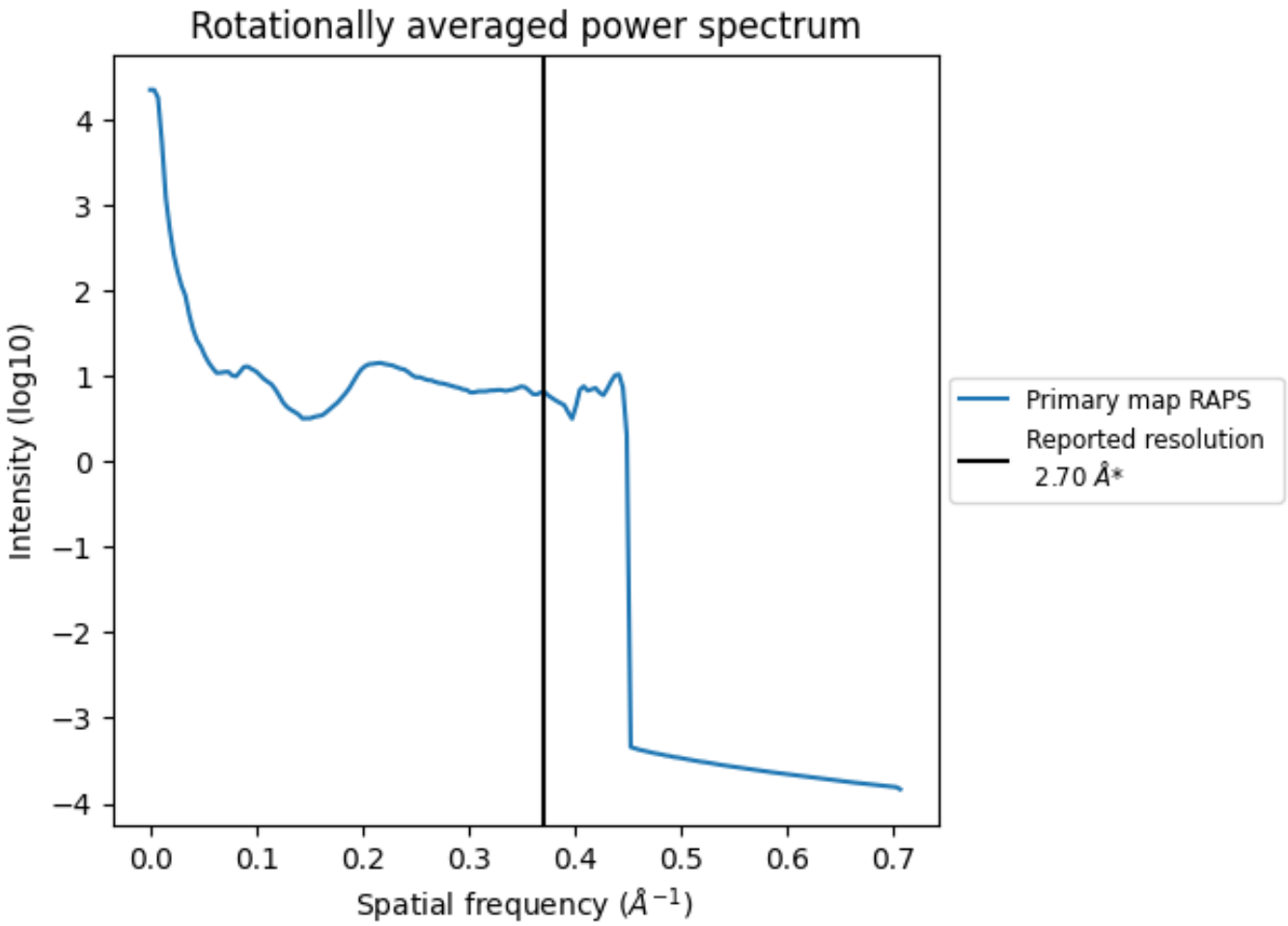
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 51 $nm^3$; this corresponds to an approximate mass of 46 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 (i)

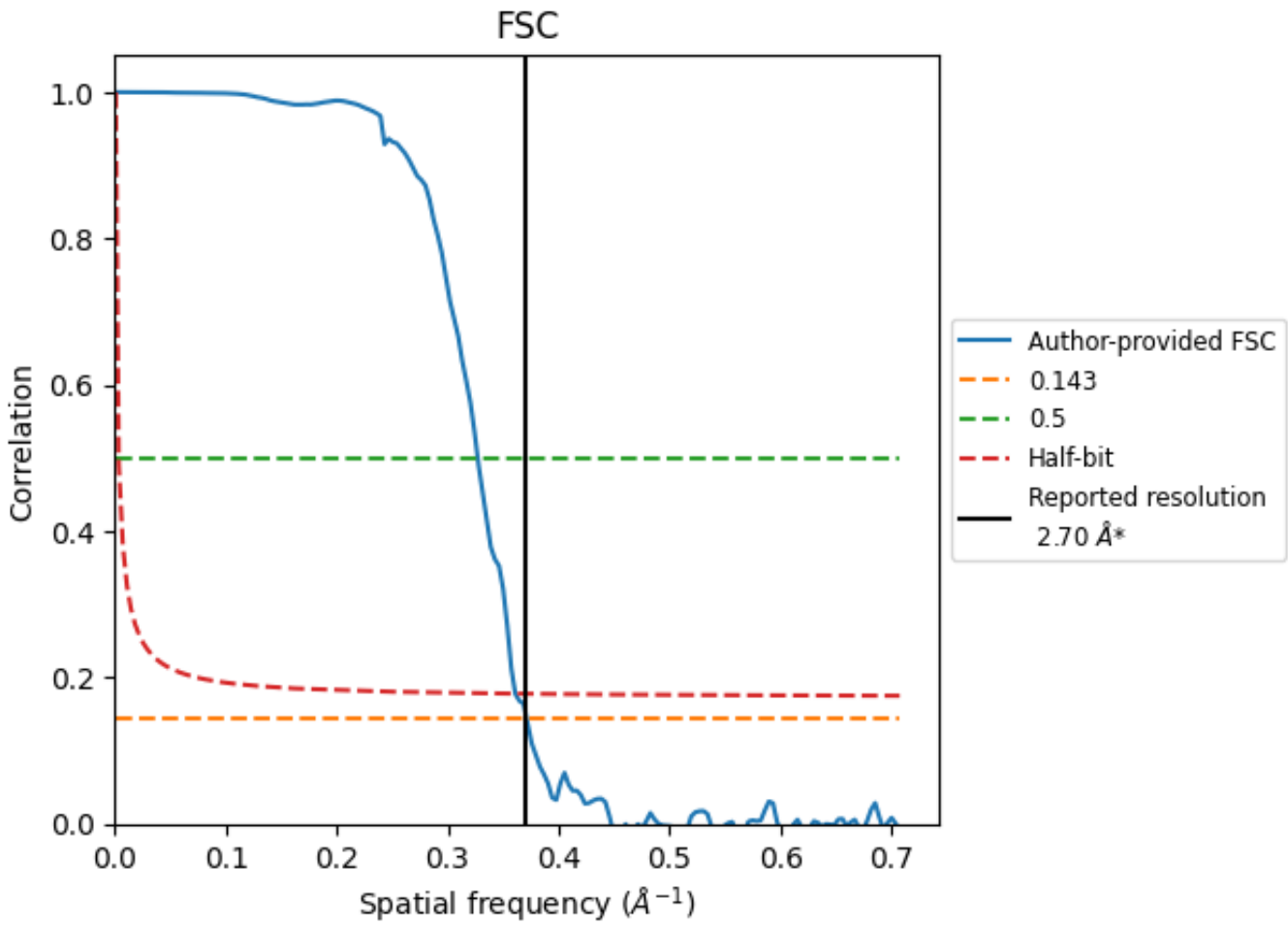



*Reported resolution corresponds to spatial frequency of 0.370 Å$^{-1}$

# 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 0.370 Å$^{-1}$

## 8.2 Resolution estimates (i)

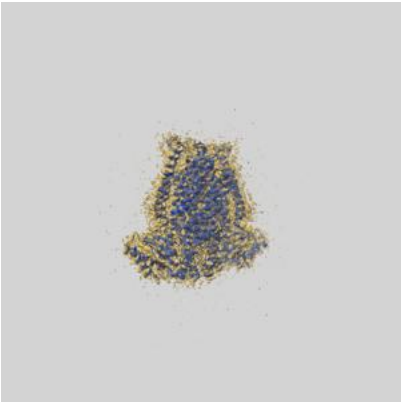
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.70 | - | - |
| Author-provided FSC curve | 2.69 | 3.06 | 2.77 |
| Unmasked-calculated* | - | - | - |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

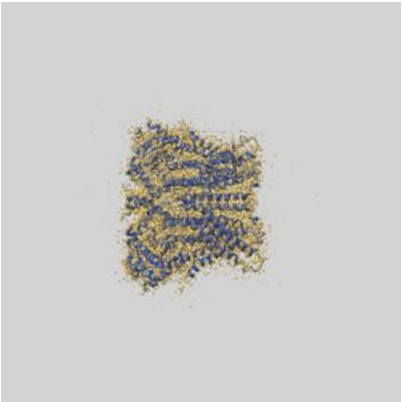
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24722 and PDB model 7RX2. Per-residue inclusion information can be found in section 3 on page 5.

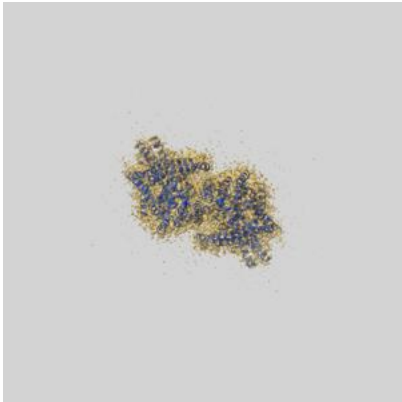
## 9.1 Map-model overlay (i)



X



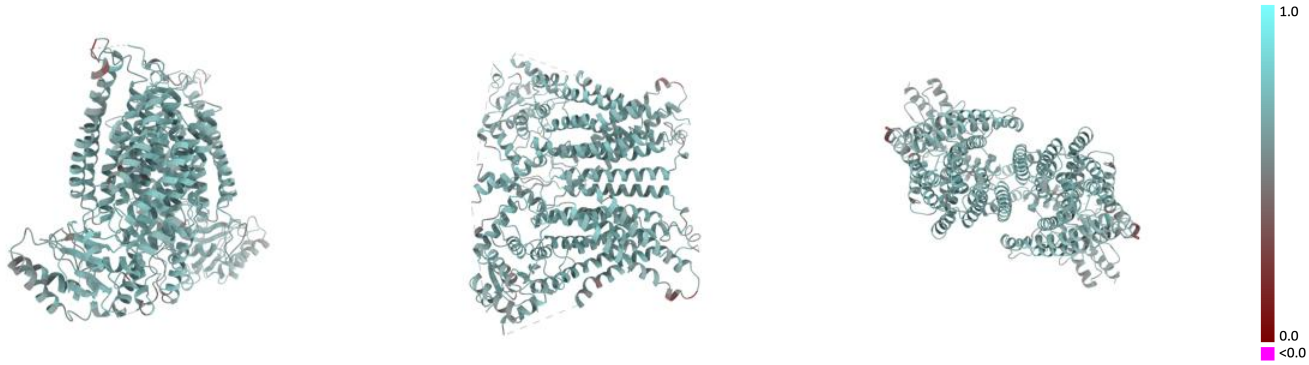
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013 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.

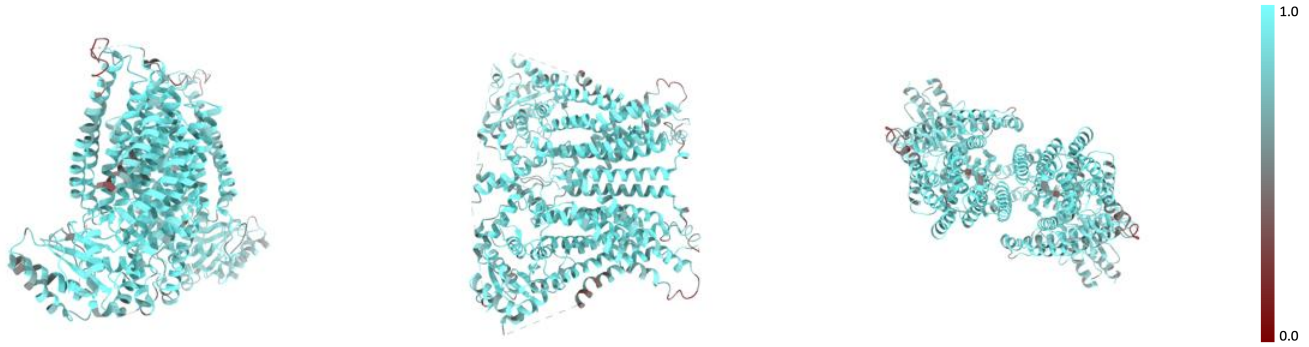
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according 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.

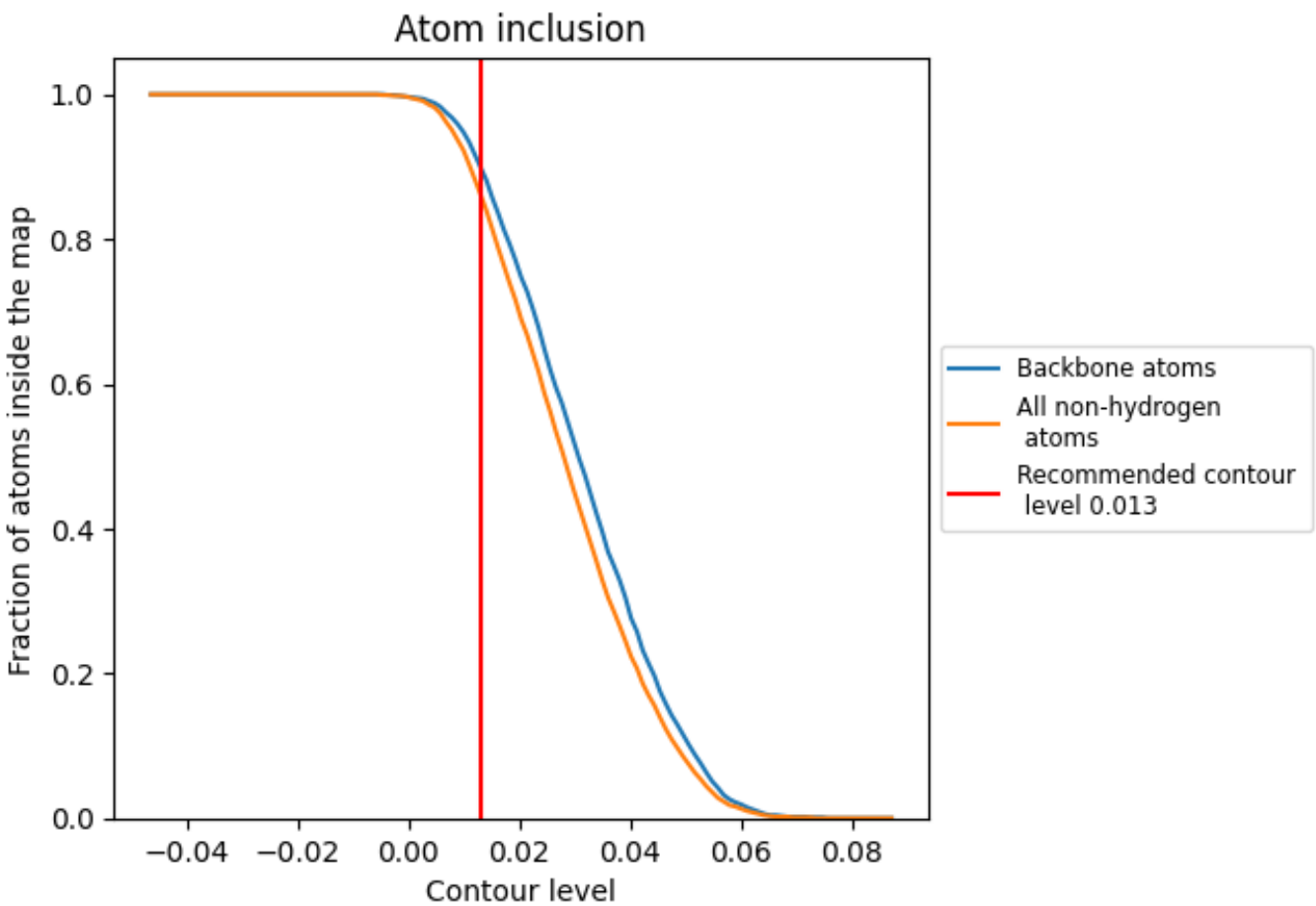
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

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 (0.013).

## 9.4 Atom inclusion (i)




At the recommended contour level, 90% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8620 | 0.6320 |
| A | 0.8630 | 0.6320 |
| B | 0.8620 | 0.6320 |