



# Full wwPDB EM Validation Report ⓘ

Jun 18, 2024 – 12:14 AM JST

PDB ID : 8YR2  
EMDB ID : EMD-39533  
Title : Structure of NET-Nisoxetine in outward-open state  
Authors : Zhang, H.; Xu, E.H.; Jiang, Y.  
Deposited on : 2024-03-20  
Resolution : 2.89 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.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) : 2.37.1

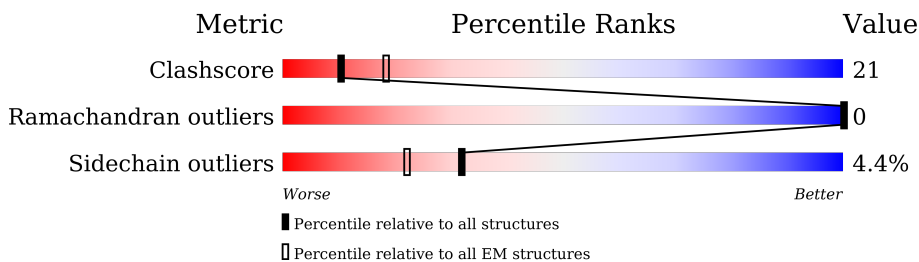
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.89 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  $\geq 3$ , 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	A	617	 66% 23% 8%
1	B	617	 66% 24% 8%

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
6	CLR	A	716	-	-	X	-
6	CLR	B	717	-	-	X	-
6	CLR	B	718	-	-	X	-

## 2 Entry composition [i](#)

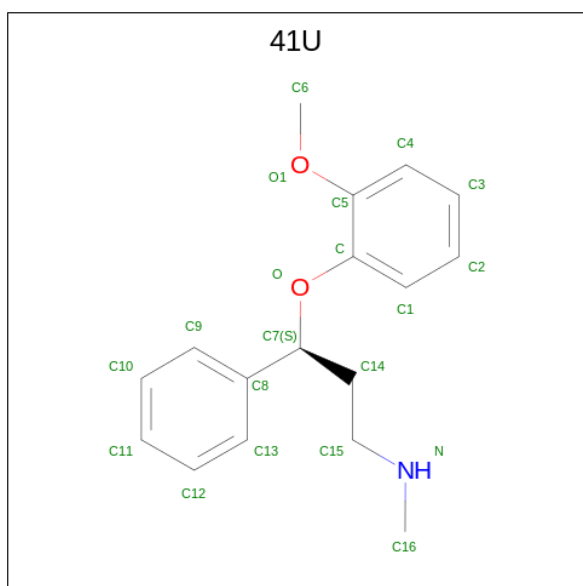
There are 8 unique types of molecules in this entry. The entry contains 9894 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sodium-dependent noradrenaline transporter.

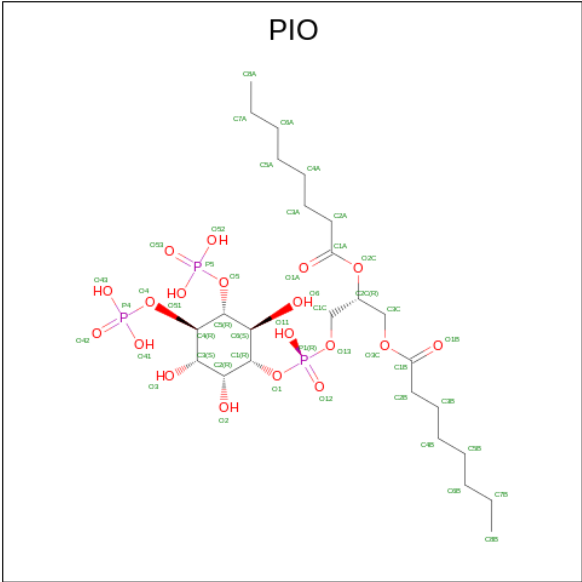
Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	565	Total	C	N	O	S	0	0
			4516	3026	706	764	20		
1	A	565	Total	C	N	O	S	0	0
			4516	3026	706	764	20		

- Molecule 2 is nisoxetine (three-letter code: 41U) (formula: C<sub>17</sub>H<sub>21</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			20	17	1	2	
2	A	1	Total	C	N	O	0
			20	17	1	2	

- Molecule 3 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (three-letter code: PIO) (formula: C<sub>25</sub>H<sub>49</sub>O<sub>19</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	O	P	0
			47	25	19	3	
3	A	1	Total	C	O	P	0
			47	25	19	3	

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
4	B	2	Total	Na	0
			2	2	
4	A	2	Total	Na	0
			2	2	

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Cl	0
			1	1	
5	A	1	Total	Cl	0
			1	1	

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



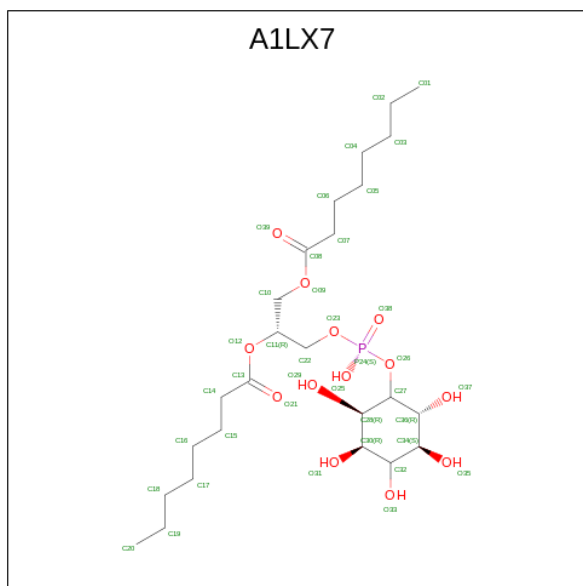
Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	

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Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	

- Molecule 7 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(2R,3R,5S,6R)-2,3,4,5,6-pentakis(oxidanyl)cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (three-letter code: A1LX7) (formula:  $C_{25}H_{47}O_{13}P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	O	P	0
			39	25	13	1	
7	B	1	Total	C	O	P	0
			39	25	13	1	
7	A	1	Total	C	O	P	0
			39	25	13	1	
7	A	1	Total	C	O	P	0
			39	25	13	1	

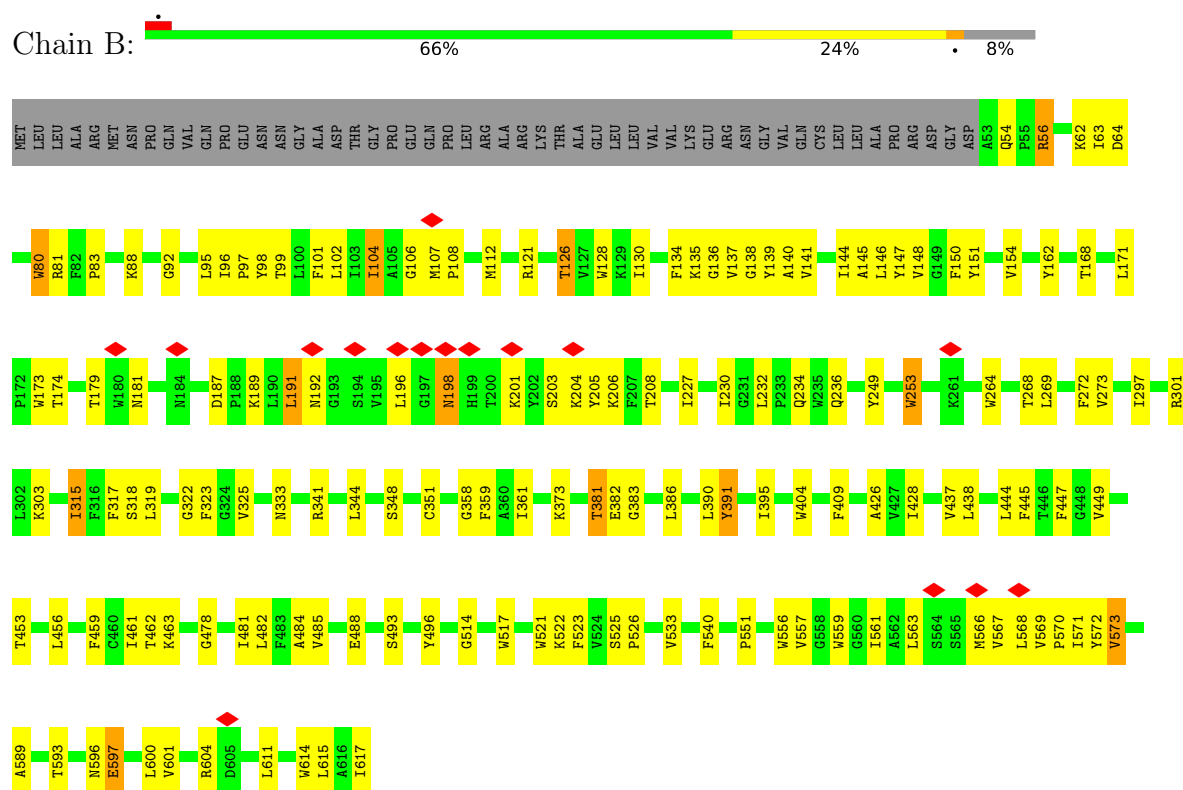
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	B	3	Total 3	O 3	0
8	A	3	Total 3	O 3	0

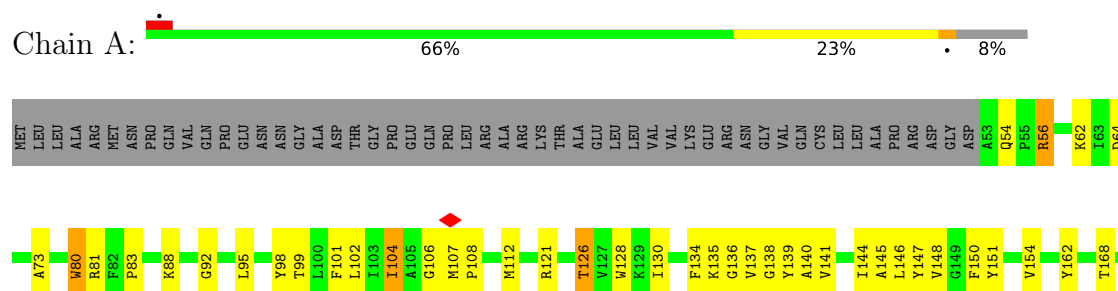
### 3 Residue-property plots [i](#)

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.

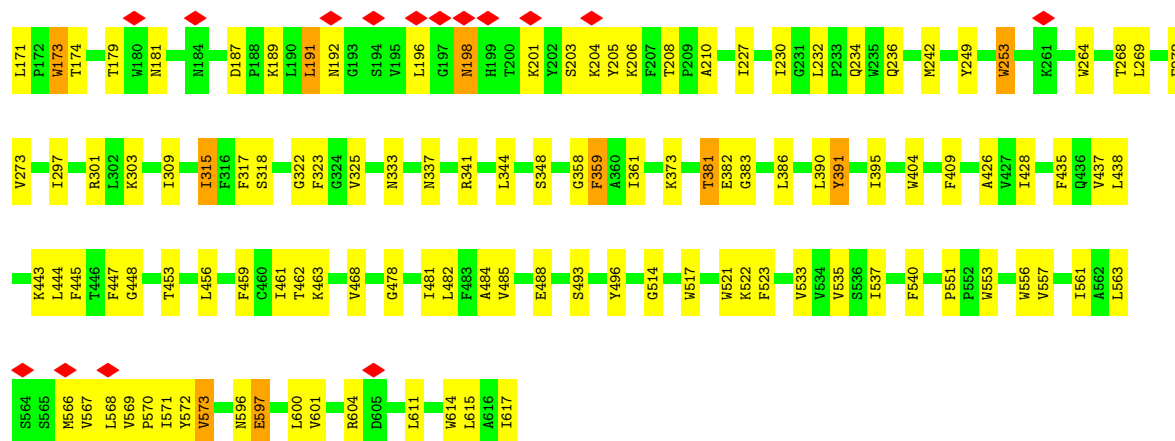
- Molecule 1: Sodium-dependent noradrenaline transporter



- Molecule 1: Sodium-dependent noradrenaline transporter







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	209365	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.781	Depositor
Minimum map value	-1.115	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	186.88, 186.88, 186.88	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	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: CL, NA, 4IU, CLR, PIO, A1LX7

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	0.25	0/4663	0.39	0/6361
1	B	0.25	0/4663	0.39	0/6361
All	All	0.25	0/9326	0.39	0/12722

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	4516	0	4500	179	0
1	B	4516	0	4501	185	0
2	A	20	0	21	6	0
2	B	20	0	21	5	0
3	A	47	0	44	7	0
3	B	47	0	44	5	0
4	A	2	0	0	1	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	252	0	410	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	308	0	505	125	0
7	A	78	0	0	4	0
7	B	78	0	0	5	0
8	A	3	0	0	0	0
8	B	3	0	0	0	0
All	All	9894	0	10046	423	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 21.

All (423) 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:566:MET:O	6:A:713:CLR:C27	1.71	1.39
1:B:351:CYS:SG	6:B:717:CLR:C24	2.21	1.29
1:B:566:MET:CG	6:B:718:CLR:H241	1.58	1.24
1:B:566:MET:CE	6:B:718:CLR:H213	1.67	1.20
1:B:566:MET:O	6:B:718:CLR:C27	1.90	1.18
1:A:107:MET:CE	6:A:715:CLR:H12	1.73	1.17
1:B:351:CYS:SG	6:B:717:CLR:H242	1.82	1.17
1:A:566:MET:O	6:A:713:CLR:H271	1.40	1.14
1:A:107:MET:CE	6:A:715:CLR:C1	2.25	1.12
1:B:566:MET:HE1	6:B:718:CLR:H213	1.13	1.12
1:A:563:LEU:HD11	6:A:713:CLR:H151	1.28	1.11
1:A:566:MET:O	6:A:713:CLR:H272	1.49	1.11
1:A:107:MET:HE1	6:A:715:CLR:H11	1.33	1.10
1:B:351:CYS:HB2	6:B:717:CLR:H241	1.29	1.07
1:B:351:CYS:CB	6:B:717:CLR:H241	1.83	1.07
1:B:268:THR:HB	6:B:716:CLR:H122	1.36	1.07
1:A:107:MET:HE1	6:A:715:CLR:C1	1.83	1.06
1:B:230:ILE:HD13	6:B:709:CLR:H21	1.37	1.06
1:B:561:ILE:HG12	6:B:710:CLR:H262	1.35	1.05
1:B:566:MET:HG3	6:B:718:CLR:H241	1.40	1.01
1:A:107:MET:HE2	6:A:715:CLR:H9	1.44	1.00
1:B:227:ILE:O	6:B:709:CLR:O1	1.79	0.99
1:B:351:CYS:SG	6:B:717:CLR:H241	2.00	0.99
1:B:566:MET:HG3	6:B:718:CLR:C24	1.92	0.99
1:A:563:LEU:HD11	6:A:713:CLR:C15	1.91	0.99
1:A:438:LEU:CD2	6:A:706:CLR:H71	1.93	0.98
1:A:272:PHE:CD1	6:A:714:CLR:H273	1.99	0.97
1:B:107:MET:HE1	6:B:717:CLR:H192	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:MET:CG	6:B:718:CLR:C24	2.43	0.96
1:A:268:THR:HG21	6:A:716:CLR:H191	1.45	0.96
1:B:566:MET:CE	6:B:718:CLR:C21	2.44	0.96
1:B:269:LEU:HD13	6:B:716:CLR:H242	1.48	0.95
1:A:438:LEU:HD23	6:A:706:CLR:H71	1.47	0.94
1:B:107:MET:CE	6:B:717:CLR:H9	1.99	0.93
1:A:437:VAL:HG21	6:A:707:CLR:H42	1.49	0.93
1:B:268:THR:CB	6:B:716:CLR:H122	1.99	0.93
1:B:107:MET:HE2	6:B:717:CLR:H191	1.49	0.92
1:A:269:LEU:CD1	6:A:716:CLR:H222	1.99	0.92
1:B:107:MET:CE	6:B:717:CLR:C19	2.48	0.92
1:A:107:MET:HE2	6:A:715:CLR:H12	1.50	0.92
1:A:272:PHE:HD1	6:A:714:CLR:H273	1.34	0.91
1:B:566:MET:HE1	6:B:718:CLR:C21	1.99	0.89
1:B:566:MET:O	6:B:718:CLR:H271	1.71	0.89
1:B:566:MET:O	6:B:718:CLR:C25	2.21	0.89
1:A:269:LEU:HD13	6:A:716:CLR:H222	1.51	0.88
1:B:107:MET:CE	6:B:717:CLR:H192	2.04	0.88
1:B:269:LEU:CD1	6:B:716:CLR:H242	2.02	0.88
1:A:268:THR:HB	6:A:716:CLR:H152	1.57	0.87
1:B:568:LEU:HD11	7:B:713:A1LX7:C01	2.06	0.85
1:B:557:VAL:HG22	6:B:710:CLR:H121	1.57	0.85
1:A:107:MET:SD	6:A:715:CLR:H12	2.16	0.85
1:A:249:TYR:OH	3:A:702:PIO:H2C	1.78	0.84
1:A:557:VAL:HG22	6:A:710:CLR:H121	1.59	0.84
1:B:566:MET:O	6:B:718:CLR:H25	1.77	0.83
1:B:444:LEU:CD2	3:B:702:PIO:H2AA	2.08	0.82
1:B:107:MET:HE2	6:B:717:CLR:H9	1.59	0.82
1:B:566:MET:O	6:B:718:CLR:H272	1.79	0.82
1:B:437:VAL:HG21	6:B:708:CLR:H42	1.61	0.82
1:A:566:MET:C	6:A:713:CLR:H272	2.01	0.80
1:A:107:MET:CE	6:A:715:CLR:H9	2.10	0.80
1:A:107:MET:HE1	6:A:715:CLR:H112	1.63	0.80
1:B:268:THR:CG2	6:B:716:CLR:H122	2.11	0.79
1:B:272:PHE:HB2	6:B:715:CLR:H262	1.62	0.79
1:B:268:THR:HB	6:B:716:CLR:C12	2.10	0.78
1:A:268:THR:CB	6:A:716:CLR:H8	2.15	0.77
1:B:107:MET:CE	6:B:717:CLR:H191	2.12	0.77
1:A:556:TRP:HB3	6:A:710:CLR:H193	1.66	0.77
1:B:559:TRP:CZ2	6:B:718:CLR:H12	2.20	0.76
1:A:566:MET:HG3	6:A:713:CLR:H272	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:TRP:CZ3	6:B:718:CLR:H122	2.21	0.75
1:B:563:LEU:HD11	6:B:718:CLR:C15	2.16	0.75
1:A:272:PHE:HD1	6:A:714:CLR:C27	1.99	0.75
1:B:556:TRP:HB3	6:B:710:CLR:H193	1.69	0.74
1:A:563:LEU:HD11	6:A:713:CLR:C16	2.17	0.74
6:B:711:CLR:H241	6:A:707:CLR:H213	1.69	0.74
6:B:707:CLR:H241	6:B:708:CLR:H213	1.70	0.73
1:B:107:MET:HE1	6:B:717:CLR:H9	1.71	0.73
1:B:351:CYS:SG	6:B:717:CLR:C23	2.77	0.73
1:B:268:THR:HB	6:B:716:CLR:H17	1.71	0.72
1:A:566:MET:HB2	6:A:713:CLR:H25	1.69	0.72
1:A:107:MET:SD	6:A:715:CLR:C1	2.77	0.72
1:A:268:THR:HB	6:A:716:CLR:H8	1.72	0.72
1:A:203:SER:O	1:A:206:LYS:NZ	2.24	0.71
1:A:107:MET:CE	6:A:715:CLR:C9	2.69	0.70
1:A:563:LEU:CD1	6:A:713:CLR:H151	2.15	0.70
1:B:566:MET:HB2	6:B:718:CLR:H25	1.74	0.70
1:B:563:LEU:HD11	6:B:718:CLR:H151	1.74	0.70
1:A:572:TYR:HE1	7:A:711:A1LX7:O38	1.75	0.69
1:B:203:SER:O	1:B:206:LYS:NZ	2.24	0.69
1:A:563:LEU:HD11	6:A:713:CLR:H161	1.75	0.69
1:A:447:PHE:HZ	3:A:702:PIO:H5BA	1.59	0.68
6:B:715:CLR:H263	6:B:715:CLR:H162	1.75	0.67
1:B:268:THR:CB	6:B:716:CLR:H17	2.25	0.66
1:A:272:PHE:CD1	6:A:714:CLR:C27	2.75	0.66
1:A:438:LEU:HD11	6:A:707:CLR:H182	1.76	0.66
6:B:707:CLR:H9	7:B:713:A1LX7:O38	1.96	0.66
1:A:268:THR:OG1	6:A:716:CLR:H182	1.95	0.65
1:A:73:ALA:O	4:A:703:NA:NA	1.71	0.64
1:A:88:LYS:O	1:A:301:ARG:NH1	2.31	0.64
1:B:563:LEU:HA	1:B:566:MET:HG2	1.79	0.64
1:A:268:THR:HB	6:A:716:CLR:C8	2.27	0.64
1:B:482:LEU:HB3	1:B:533:VAL:HG22	1.79	0.64
1:A:272:PHE:CD2	6:A:716:CLR:H241	2.33	0.64
1:B:88:LYS:O	1:B:301:ARG:NH1	2.31	0.63
1:B:348:SER:OG	6:B:717:CLR:H151	1.98	0.63
1:A:99:THR:HA	1:A:102:LEU:HB3	1.81	0.63
1:A:482:LEU:HB3	1:A:533:VAL:HG22	1.79	0.63
1:A:102:LEU:O	1:A:106:GLY:N	2.32	0.63
1:B:102:LEU:O	1:B:106:GLY:N	2.32	0.63
1:A:563:LEU:HA	1:A:566:MET:HG2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:CD1	6:A:716:CLR:H242	2.29	0.62
1:B:444:LEU:HB3	6:B:706:CLR:H122	1.81	0.62
6:B:707:CLR:H242	7:B:713:A1LX7:C06	2.28	0.62
1:A:269:LEU:HD12	6:A:716:CLR:H222	1.77	0.62
1:A:596:ASN:ND2	1:A:597:GLU:OE1	2.33	0.62
1:B:107:MET:HE1	6:B:717:CLR:C19	2.17	0.62
1:B:99:THR:HA	1:B:102:LEU:HB3	1.81	0.62
1:B:596:ASN:ND2	1:B:597:GLU:OE1	2.33	0.61
1:A:323:PHE:HD2	2:A:701:41U:H20	1.65	0.61
1:A:107:MET:HE1	6:A:715:CLR:C11	2.30	0.61
1:B:99:THR:OG1	6:B:717:CLR:H213	2.01	0.61
1:A:443:LYS:NZ	3:A:702:PIO:O41	2.33	0.61
1:A:323:PHE:CD2	2:A:701:41U:H20	2.36	0.60
1:B:323:PHE:HD2	2:B:701:41U:H20	1.66	0.60
1:B:438:LEU:HD11	6:B:708:CLR:H182	1.84	0.59
1:A:230:ILE:HD13	6:A:709:CLR:H21	1.83	0.59
1:A:107:MET:HE2	6:A:715:CLR:C9	2.24	0.59
1:A:447:PHE:CZ	3:A:702:PIO:H3BA	2.37	0.59
1:B:561:ILE:CG1	6:B:710:CLR:H262	2.22	0.59
1:A:107:MET:HB2	1:A:108:PRO:HD3	1.85	0.59
1:A:264:TRP:HZ3	6:A:716:CLR:H42	1.68	0.59
1:B:323:PHE:CD2	2:B:701:41U:H20	2.38	0.58
1:B:107:MET:HB2	1:B:108:PRO:HD3	1.85	0.58
1:A:107:MET:CE	6:A:715:CLR:H11	2.05	0.58
1:A:566:MET:HG3	6:A:713:CLR:C27	2.33	0.58
1:B:269:LEU:CD1	6:B:716:CLR:C24	2.78	0.58
1:A:438:LEU:CD2	6:A:706:CLR:C7	2.77	0.58
1:B:447:PHE:HZ	3:B:702:PIO:H5BA	1.68	0.58
1:B:447:PHE:CZ	3:B:702:PIO:H3BA	2.39	0.58
1:B:601:VAL:O	1:B:604:ARG:NH2	2.37	0.57
1:A:268:THR:HB	6:A:716:CLR:C15	2.31	0.57
1:A:154:VAL:HG13	1:A:461:ILE:HG22	1.87	0.57
1:A:318:SER:O	2:A:701:41U:H1	2.04	0.57
1:A:444:LEU:HB3	6:A:706:CLR:H122	1.87	0.57
1:B:318:SER:O	2:B:701:41U:H1	2.05	0.56
1:B:567:VAL:O	1:B:571:ILE:N	2.31	0.56
1:A:141:VAL:HA	1:A:144:ILE:HD12	1.87	0.56
1:A:148:VAL:HA	1:A:151:TYR:CE2	2.41	0.56
1:A:563:LEU:CD1	6:A:713:CLR:H161	2.35	0.56
1:B:141:VAL:HA	1:B:144:ILE:HD12	1.87	0.56
1:A:601:VAL:O	1:A:604:ARG:NH2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:LEU:HA	1:A:571:ILE:HB	1.87	0.56
1:A:80:TRP:HB2	1:A:383:GLY:H	1.71	0.55
1:B:154:VAL:HG13	1:B:461:ILE:HG22	1.87	0.55
1:A:567:VAL:O	1:A:571:ILE:N	2.30	0.55
1:B:148:VAL:HA	1:B:151:TYR:CE2	2.41	0.55
1:B:566:MET:HG3	6:B:718:CLR:C25	2.36	0.55
1:A:201:LYS:HB2	1:A:204:LYS:HB2	1.89	0.55
1:B:566:MET:CB	6:B:718:CLR:H241	2.33	0.55
1:A:92:GLY:HA3	1:A:297:ILE:HG12	1.89	0.55
1:B:80:TRP:HB2	1:B:383:GLY:H	1.71	0.54
1:B:92:GLY:HA3	1:B:297:ILE:HG12	1.88	0.54
1:B:63:ILE:HD13	6:B:715:CLR:O1	2.07	0.54
1:B:568:LEU:HA	1:B:571:ILE:HB	1.88	0.54
1:B:141:VAL:HG12	1:B:484:ALA:HB1	1.90	0.54
1:A:107:MET:HB3	1:A:517:TRP:HZ3	1.72	0.54
1:B:134:PHE:O	1:B:137:VAL:HB	2.08	0.54
1:B:171:LEU:HB2	1:B:174:THR:HG23	1.89	0.54
1:A:107:MET:HE1	6:A:715:CLR:C9	2.37	0.54
1:A:566:MET:O	6:A:713:CLR:C25	2.51	0.54
1:B:201:LYS:HB2	1:B:204:LYS:HB2	1.89	0.53
1:B:227:ILE:HD11	1:B:551:PRO:HD2	1.90	0.53
1:A:272:PHE:HD2	6:A:716:CLR:H241	1.71	0.53
1:A:141:VAL:HG12	1:A:484:ALA:HB1	1.90	0.53
1:A:171:LEU:HB2	1:A:174:THR:HG23	1.89	0.53
1:A:234:GLN:NE2	1:A:236:GLN:OE1	2.42	0.53
1:A:134:PHE:O	1:A:137:VAL:HB	2.08	0.53
1:B:107:MET:HB3	1:B:517:TRP:HZ3	1.73	0.53
1:A:268:THR:OG1	6:A:716:CLR:C18	2.56	0.53
6:B:708:CLR:H41	6:A:707:CLR:H41	1.91	0.52
1:A:322:GLY:HA3	1:A:485:VAL:HG12	1.91	0.52
1:B:99:THR:OG1	6:B:717:CLR:C21	2.58	0.52
1:B:322:GLY:HA3	1:B:485:VAL:HG12	1.91	0.52
1:A:437:VAL:CG2	6:A:707:CLR:H192	2.39	0.52
1:B:234:GLN:NE2	1:B:236:GLN:OE1	2.42	0.52
1:A:56:ARG:HG3	1:A:121:ARG:HG2	1.92	0.52
1:B:563:LEU:HD11	6:B:718:CLR:H14	1.92	0.52
1:A:227:ILE:HD11	1:A:551:PRO:HD2	1.90	0.52
1:B:559:TRP:CE2	6:B:718:CLR:H12	2.44	0.51
1:B:56:ARG:HG3	1:B:121:ARG:HG2	1.92	0.51
1:B:444:LEU:HD21	3:B:702:PIO:H2AA	1.89	0.51
1:A:104:ILE:O	1:A:108:PRO:HD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:VAL:HA	1:B:426:ALA:HB2	1.93	0.51
1:A:269:LEU:HD12	6:A:716:CLR:H242	1.92	0.51
1:B:556:TRP:CB	6:B:710:CLR:H193	2.38	0.51
6:B:707:CLR:C19	6:A:706:CLR:H11	2.41	0.51
1:A:438:LEU:HD23	6:A:706:CLR:C7	2.32	0.51
1:B:104:ILE:O	1:B:108:PRO:HD2	2.10	0.51
1:B:566:MET:CB	6:B:718:CLR:H25	2.40	0.51
1:A:135:LYS:NZ	1:A:139:TYR:OH	2.44	0.51
1:A:107:MET:CE	6:A:715:CLR:H112	2.39	0.50
1:A:268:THR:CG2	6:A:716:CLR:H8	2.41	0.50
1:B:135:LYS:NZ	1:B:139:TYR:OH	2.44	0.50
1:B:438:LEU:CD2	6:B:706:CLR:H71	2.42	0.50
1:B:456:LEU:HD13	6:B:709:CLR:C21	2.41	0.50
1:B:523:PHE:HE2	1:B:617:ILE:HG12	1.75	0.50
1:A:325:VAL:HA	1:A:426:ALA:HB2	1.93	0.50
1:B:563:LEU:HD11	6:B:718:CLR:C14	2.40	0.50
1:A:523:PHE:HE2	1:A:617:ILE:HG12	1.75	0.50
1:A:448:GLY:HA3	6:A:706:CLR:H221	1.94	0.50
1:B:566:MET:C	6:B:718:CLR:H272	2.32	0.50
1:A:64:ASP:OD1	1:A:264:TRP:NE1	2.44	0.50
1:A:205:TYR:HD2	1:A:208:THR:HG23	1.76	0.50
1:B:64:ASP:OD1	1:B:264:TRP:NE1	2.44	0.50
1:B:437:VAL:CG2	6:B:708:CLR:H192	2.41	0.50
6:B:706:CLR:H72	6:B:708:CLR:H6	1.93	0.50
1:A:597:GLU:O	1:A:600:LEU:HG	2.11	0.49
1:B:428:ILE:HA	1:B:445:PHE:HE2	1.77	0.49
1:A:230:ILE:HB	1:A:462:THR:HG21	1.94	0.49
1:B:268:THR:HG21	6:B:716:CLR:H9	1.95	0.49
1:A:264:TRP:HE3	6:A:716:CLR:H192	1.78	0.49
1:B:264:TRP:CZ3	6:B:716:CLR:H3	2.48	0.49
1:B:597:GLU:O	1:B:600:LEU:HG	2.11	0.49
1:B:230:ILE:HB	1:B:462:THR:HG21	1.94	0.49
6:B:706:CLR:H232	6:B:706:CLR:H211	1.44	0.49
1:A:121:ARG:NH1	1:A:333:ASN:O	2.34	0.49
1:A:438:LEU:HD21	6:A:706:CLR:H71	1.85	0.49
1:B:205:TYR:HD2	1:B:208:THR:HG23	1.77	0.49
6:B:707:CLR:H193	6:A:706:CLR:H11	1.95	0.48
1:A:144:ILE:HG21	1:A:481:ILE:HD13	1.95	0.48
1:A:196:LEU:HD13	1:A:373:LYS:HE3	1.95	0.48
1:A:428:ILE:HA	1:A:445:PHE:HE2	1.77	0.48
1:B:395:ILE:HG23	1:B:404:TRP:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:MET:CE	6:A:715:CLR:C11	2.91	0.48
6:B:712:CLR:H273	6:B:712:CLR:H231	1.63	0.48
1:B:112:MET:HB2	1:B:521:TRP:NE1	2.29	0.48
1:A:101:PHE:O	1:A:104:ILE:HG13	2.14	0.48
1:B:101:PHE:O	1:B:104:ILE:HG13	2.14	0.48
1:B:144:ILE:HG21	1:B:481:ILE:HD13	1.96	0.48
1:B:268:THR:OG1	6:B:716:CLR:H14	2.14	0.48
1:B:196:LEU:HD13	1:B:373:LYS:HE3	1.95	0.47
6:B:710:CLR:H183	6:B:710:CLR:H20	1.73	0.47
1:A:447:PHE:CZ	3:A:702:PIO:H5BA	2.45	0.47
1:A:456:LEU:HD13	6:A:709:CLR:C21	2.44	0.47
1:B:268:THR:HB	6:B:716:CLR:C17	2.42	0.47
1:A:242:MET:HE1	7:A:712:A1LX7:C02	2.44	0.47
1:B:95:LEU:O	1:B:99:THR:HG22	2.15	0.47
1:A:112:MET:HB2	1:A:521:TRP:NE1	2.29	0.47
1:A:561:ILE:HG12	6:A:710:CLR:H272	1.97	0.47
1:B:559:TRP:CZ3	6:B:718:CLR:H9	2.50	0.47
1:A:95:LEU:O	1:A:99:THR:HG22	2.15	0.47
1:A:268:THR:HG21	6:A:716:CLR:H8	1.95	0.47
1:A:395:ILE:HG23	1:A:404:TRP:HB2	1.96	0.47
1:B:563:LEU:HD21	6:B:718:CLR:H151	1.95	0.47
1:A:83:PRO:HG3	1:A:358:GLY:HA2	1.96	0.47
1:B:268:THR:OG1	6:B:716:CLR:H17	2.15	0.47
6:B:707:CLR:H263	7:B:713:A1LX7:C05	2.45	0.47
1:B:80:TRP:CD1	1:B:81:ARG:HG3	2.50	0.46
1:A:80:TRP:CD1	1:A:81:ARG:HG3	2.50	0.46
6:B:708:CLR:H162	6:B:708:CLR:H222	1.58	0.46
1:A:62:LYS:HZ3	1:A:337:ASN:HB2	1.80	0.46
1:B:559:TRP:CE3	6:B:718:CLR:H9	2.50	0.46
1:A:468:VAL:HG13	6:A:709:CLR:H193	1.97	0.46
1:B:569:VAL:HB	1:B:570:PRO:HD3	1.97	0.46
1:B:83:PRO:HG3	1:B:358:GLY:HA2	1.96	0.46
1:B:566:MET:SD	6:B:718:CLR:H17	2.56	0.46
6:B:706:CLR:H11	6:B:711:CLR:C19	2.46	0.46
6:B:717:CLR:H162	6:B:717:CLR:H221	1.46	0.46
1:A:569:VAL:HB	1:A:570:PRO:HD3	1.97	0.46
1:B:272:PHE:HB2	6:B:715:CLR:C26	2.42	0.46
1:A:435:PHE:CG	6:A:707:CLR:H193	2.51	0.46
1:B:361:ILE:HG13	1:B:391:TYR:HE1	1.81	0.46
2:B:701:41U:H7	2:B:701:41U:H3	1.66	0.46
1:A:348:SER:OG	6:A:715:CLR:H151	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:ILE:HG12	6:A:710:CLR:C27	2.45	0.46
6:A:706:CLR:H193	6:A:706:CLR:H111	1.85	0.46
1:B:98:TYR:CE1	1:B:315:ILE:HG12	2.51	0.46
1:B:268:THR:HG21	6:B:716:CLR:H122	1.94	0.46
1:B:449:VAL:HG22	6:B:708:CLR:H25	1.98	0.45
6:B:710:CLR:H232	6:B:710:CLR:H211	1.42	0.45
1:B:107:MET:HE1	6:B:717:CLR:C9	2.45	0.45
1:B:269:LEU:HD12	6:B:716:CLR:C24	2.46	0.45
6:B:716:CLR:H183	6:B:716:CLR:H20	1.77	0.45
1:B:107:MET:HB3	1:B:517:TRP:CZ3	2.52	0.45
1:B:268:THR:O	6:B:716:CLR:H213	2.17	0.45
6:B:712:CLR:H232	6:B:712:CLR:H211	1.58	0.45
1:B:444:LEU:HD12	6:B:706:CLR:H121	1.97	0.45
1:A:481:ILE:HD12	1:A:481:ILE:HA	1.83	0.45
1:B:563:LEU:HD11	6:B:718:CLR:C16	2.46	0.45
1:A:98:TYR:CE1	1:A:315:ILE:HG12	2.51	0.45
1:A:361:ILE:HG13	1:A:391:TYR:HE1	1.81	0.45
1:B:317:PHE:HZ	1:B:478:GLY:HA2	1.82	0.45
6:B:706:CLR:H111	6:B:706:CLR:H193	1.76	0.45
1:A:514:GLY:H	1:A:517:TRP:HD1	1.65	0.45
1:A:553:TRP:CH2	6:A:709:CLR:H42	2.51	0.45
1:B:121:ARG:NH1	1:B:333:ASN:O	2.34	0.44
1:B:268:THR:HG21	6:B:716:CLR:H14	1.99	0.44
6:B:717:CLR:H213	6:B:717:CLR:H231	1.65	0.44
1:A:187:ASP:HB3	1:A:189:LYS:HE3	1.99	0.44
1:A:344:LEU:HD12	6:A:715:CLR:H71	1.97	0.44
1:B:187:ASP:HB3	1:B:189:LYS:HE3	2.00	0.44
1:B:62:LYS:HD3	1:B:62:LYS:HA	1.83	0.44
6:B:709:CLR:H213	6:B:709:CLR:H232	1.71	0.44
1:A:179:THR:O	1:A:181:ASN:ND2	2.51	0.44
1:A:572:TYR:HB2	7:A:711:A1LX7:O21	2.17	0.44
2:A:701:41U:H3	2:A:701:41U:H7	1.65	0.44
6:B:706:CLR:H191	6:B:706:CLR:H8	1.79	0.44
1:A:62:LYS:HA	1:A:62:LYS:HD3	1.84	0.44
1:A:150:PHE:HD1	1:A:453:THR:HG23	1.83	0.44
1:B:344:LEU:HD12	6:B:717:CLR:H71	1.99	0.44
6:B:706:CLR:H183	6:B:706:CLR:H20	1.62	0.43
1:B:150:PHE:HD1	1:B:453:THR:HG23	1.84	0.43
1:B:112:MET:HB2	1:B:521:TRP:HE1	1.83	0.43
1:B:136:GLY:O	1:B:139:TYR:HB2	2.19	0.43
6:B:718:CLR:H183	6:B:718:CLR:H20	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:TYR:HH	3:A:702:PIO:H2C	1.78	0.43
6:A:707:CLR:H193	6:A:707:CLR:H111	1.73	0.43
1:A:493:SER:HB2	1:A:522:LYS:HA	2.00	0.43
1:B:179:THR:O	1:B:181:ASN:ND2	2.51	0.43
1:B:514:GLY:H	1:B:517:TRP:HD1	1.65	0.43
6:A:706:CLR:H183	6:A:706:CLR:H20	1.75	0.43
6:A:716:CLR:H273	6:A:716:CLR:H231	1.74	0.43
1:A:146:LEU:HG	1:A:150:PHE:CZ	2.53	0.43
6:A:706:CLR:H162	6:A:706:CLR:H222	1.65	0.43
1:B:481:ILE:HD12	1:B:481:ILE:HA	1.83	0.43
6:B:716:CLR:H111	6:B:716:CLR:H193	1.77	0.43
1:A:112:MET:HB2	1:A:521:TRP:HE1	1.83	0.43
1:A:269:LEU:O	1:A:273:VAL:HG23	2.19	0.43
1:A:317:PHE:HZ	1:A:478:GLY:HA2	1.82	0.43
1:B:191:LEU:HD12	1:B:192:ASN:H	1.84	0.43
1:B:373:LYS:HE2	1:B:373:LYS:HB2	1.89	0.43
6:B:712:CLR:H14	6:A:710:CLR:H122	2.01	0.43
1:A:126:THR:HA	1:A:135:LYS:HE2	2.00	0.43
1:A:264:TRP:CE3	6:A:716:CLR:H192	2.53	0.43
1:A:268:THR:O	6:A:716:CLR:H152	2.19	0.43
1:A:553:TRP:HH2	6:A:709:CLR:H42	1.82	0.43
6:A:715:CLR:H231	6:A:715:CLR:H262	1.38	0.43
1:B:130:ILE:HD12	1:B:496:TYR:CG	2.54	0.43
1:B:493:SER:HB2	1:B:522:LYS:HA	2.00	0.43
6:A:710:CLR:H112	6:A:710:CLR:H12	1.75	0.43
1:B:351:CYS:SG	6:B:717:CLR:C22	3.07	0.42
1:A:198:ASN:OD1	1:A:198:ASN:N	2.52	0.42
1:A:462:THR:OG1	1:A:463:LYS:N	2.52	0.42
1:B:146:LEU:HG	1:B:150:PHE:CZ	2.53	0.42
1:B:269:LEU:O	1:B:273:VAL:HG23	2.19	0.42
6:B:709:CLR:H221	6:B:709:CLR:H162	1.52	0.42
1:A:130:ILE:HD12	1:A:496:TYR:CG	2.54	0.42
6:A:709:CLR:H232	6:A:709:CLR:H213	1.79	0.42
1:A:381:THR:HG22	1:A:382:GLU:H	1.83	0.42
6:A:714:CLR:H222	6:A:714:CLR:H162	1.35	0.42
1:B:462:THR:OG1	1:B:463:LYS:N	2.52	0.42
1:A:359:PHE:HD1	1:A:359:PHE:HA	1.74	0.42
1:B:381:THR:HG22	1:B:382:GLU:H	1.83	0.42
1:A:128:TRP:HZ2	1:A:488:GLU:HG2	1.85	0.42
1:A:107:MET:HB3	1:A:517:TRP:CZ3	2.52	0.42
1:A:191:LEU:HD12	1:A:192:ASN:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:LEU:HD22	1:A:390:LEU:HD23	2.02	0.42
6:A:710:CLR:H272	6:A:710:CLR:H231	1.61	0.42
1:B:162:TYR:HB3	1:B:409:PHE:CE2	2.55	0.42
6:B:715:CLR:H8	6:B:715:CLR:H182	1.72	0.42
1:A:136:GLY:O	1:A:139:TYR:HB2	2.18	0.42
1:A:438:LEU:HD21	6:A:706:CLR:C7	2.46	0.41
6:A:706:CLR:H272	6:A:706:CLR:H231	1.76	0.41
6:A:708:CLR:H231	6:A:708:CLR:H272	1.65	0.41
1:B:126:THR:HA	1:B:135:LYS:HE2	2.02	0.41
1:B:137:VAL:HA	1:B:569:VAL:HG22	2.02	0.41
1:A:162:TYR:HB3	1:A:409:PHE:CE2	2.55	0.41
1:A:249:TYR:O	1:A:253:TRP:HB3	2.20	0.41
6:A:716:CLR:H183	6:A:716:CLR:H20	1.91	0.41
1:B:198:ASN:N	1:B:198:ASN:OD1	2.53	0.41
1:B:540:PHE:CD2	6:B:718:CLR:H21	2.55	0.41
1:B:570:PRO:O	1:B:573:VAL:HG12	2.20	0.41
6:B:706:CLR:H72	6:B:708:CLR:C6	2.50	0.41
6:B:706:CLR:H192	6:B:706:CLR:H22	1.83	0.41
1:A:137:VAL:HA	1:A:569:VAL:HG22	2.03	0.41
1:B:566:MET:HG3	6:B:718:CLR:H272	2.02	0.41
6:A:710:CLR:H20	6:A:710:CLR:H183	1.64	0.41
1:B:315:ILE:HG23	1:B:319:LEU:HD12	2.02	0.41
1:B:456:LEU:HD13	6:B:709:CLR:H213	2.03	0.41
6:A:709:CLR:H182	6:A:709:CLR:H8	1.78	0.41
1:A:537:ILE:HG23	6:A:713:CLR:H112	2.01	0.41
1:A:611:LEU:HA	1:A:614:TRP:HD1	1.86	0.41
1:B:128:TRP:HZ2	1:B:488:GLU:HG2	1.85	0.41
1:B:611:LEU:HA	1:B:614:TRP:HD1	1.86	0.41
1:A:540:PHE:HD2	6:A:713:CLR:H21	1.86	0.41
2:A:701:41U:H21	2:A:701:41U:H17	1.75	0.41
1:B:323:PHE:CZ	1:B:481:ILE:HG12	2.56	0.41
6:A:707:CLR:H183	6:A:707:CLR:H20	1.76	0.41
1:B:138:GLY:O	1:B:141:VAL:HG22	2.21	0.41
1:B:145:ALA:HA	2:B:701:41U:H22	2.03	0.41
1:B:386:LEU:HD22	1:B:390:LEU:HD23	2.02	0.41
6:B:711:CLR:H182	6:B:711:CLR:H8	1.86	0.41
1:A:309:ILE:HD13	1:A:535:VAL:HG11	2.03	0.41
6:A:708:CLR:H193	6:A:708:CLR:H111	1.84	0.41
1:B:147:TYR:HA	1:B:150:PHE:CD2	2.56	0.41
1:B:268:THR:HG22	6:B:715:CLR:H71	2.01	0.41
6:B:709:CLR:H182	6:B:709:CLR:H8	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:713:CLR:H193	6:A:713:CLR:H111	1.81	0.41
1:B:140:ALA:O	1:B:144:ILE:HG13	2.21	0.40
1:B:589:ALA:O	1:B:593:THR:OG1	2.33	0.40
1:A:147:TYR:HA	1:A:150:PHE:CD2	2.56	0.40
1:A:151:TYR:O	1:A:154:VAL:HB	2.21	0.40
1:B:249:TYR:O	1:B:253:TRP:HB3	2.21	0.40
6:B:715:CLR:H121	6:B:715:CLR:H212	2.02	0.40
1:A:80:TRP:HD1	1:A:81:ARG:N	2.19	0.40
1:A:268:THR:CG2	6:A:716:CLR:H72	2.51	0.40
1:A:456:LEU:HD13	6:A:709:CLR:H213	2.02	0.40
3:A:702:PIO:H3A	3:A:702:PIO:H6AA	1.62	0.40
6:A:714:CLR:H183	6:A:714:CLR:H20	1.72	0.40
6:A:716:CLR:H191	6:A:716:CLR:H8	1.92	0.40
1:B:80:TRP:HD1	1:B:81:ARG:N	2.19	0.40
1:A:138:GLY:O	1:A:141:VAL:HG22	2.21	0.40
1:A:568:LEU:HD22	7:A:711:A1LX7:C14	2.51	0.40
1:B:96:ILE:HB	1:B:97:PRO:HD3	2.04	0.40
1:B:525:SER:HB2	1:B:526:PRO:HD3	2.03	0.40
1:A:173:TRP:HB3	1:A:210:ALA:HA	2.04	0.40
1:B:130:ILE:H	1:B:130:ILE:HG12	1.75	0.40
1:B:151:TYR:O	1:B:154:VAL:HB	2.21	0.40
1:B:572:TYR:HD1	7:B:713:A1LX7:C22	2.35	0.40
3:B:702:PIO:H8AB	3:B:702:PIO:H5AA	1.85	0.40
1:A:140:ALA:O	1:A:144:ILE:HG13	2.21	0.40
1:A:145:ALA:HA	2:A:701:41U:H22	2.04	0.40
1:A:570:PRO:O	1:A:573:VAL:HG12	2.21	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	A	563/617 (91%)	540 (96%)	23 (4%)	0	100	100
1	B	563/617 (91%)	540 (96%)	23 (4%)	0	100	100
All	All	1126/1234 (91%)	1080 (96%)	46 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	476/519 (92%)	455 (96%)	21 (4%)	28	61
1	B	476/519 (92%)	455 (96%)	21 (4%)	28	61
All	All	952/1038 (92%)	910 (96%)	42 (4%)	32	61

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	54	GLN
1	B	56	ARG
1	B	80	TRP
1	B	104	ILE
1	B	126	THR
1	B	168	THR
1	B	173	TRP
1	B	191	LEU
1	B	198	ASN
1	B	232	LEU
1	B	253	TRP
1	B	303	LYS
1	B	315	ILE
1	B	341	ARG
1	B	359	PHE
1	B	381	THR
1	B	391	TYR
1	B	459	PHE

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Mol	Chain	Res	Type
1	B	573	VAL
1	B	597	GLU
1	B	615	LEU
1	A	54	GLN
1	A	56	ARG
1	A	80	TRP
1	A	104	ILE
1	A	126	THR
1	A	168	THR
1	A	173	TRP
1	A	191	LEU
1	A	198	ASN
1	A	232	LEU
1	A	253	TRP
1	A	303	LYS
1	A	315	ILE
1	A	341	ARG
1	A	359	PHE
1	A	381	THR
1	A	391	TYR
1	A	459	PHE
1	A	573	VAL
1	A	597	GLU
1	A	615	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	153	ASN
1	B	181	ASN
1	B	234	GLN
1	B	236	GLN
1	B	350	ASN
1	B	507	GLN
1	B	610	GLN
1	B	612	GLN
1	A	153	ASN
1	A	181	ASN
1	A	234	GLN
1	A	236	GLN
1	A	350	ASN
1	A	507	GLN

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Mol	Chain	Res	Type
1	A	610	GLN
1	A	612	GLN

### 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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 6 are monoatomic - leaving 28 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	$\# Z  > 2$
6	CLR	B	715	-	31,31,31	0.88	2 (6%)	48,48,48	1.55	10 (20%)
6	CLR	A	706	-	31,31,31	0.95	2 (6%)	48,48,48	1.35	7 (14%)
6	CLR	A	716	-	31,31,31	0.87	1 (3%)	48,48,48	1.39	5 (10%)
6	CLR	B	707	-	31,31,31	0.83	1 (3%)	48,48,48	1.38	6 (12%)
2	41U	A	701	-	21,21,21	1.37	2 (9%)	24,26,26	2.52	6 (25%)
6	CLR	B	708	-	31,31,31	0.91	2 (6%)	48,48,48	1.18	3 (6%)
6	CLR	B	717	-	31,31,31	0.90	0	48,48,48	5.24	14 (29%)
6	CLR	A	710	-	31,31,31	1.01	2 (6%)	48,48,48	1.47	9 (18%)
7	A1LX7	B	713	-	39,39,39	1.04	4 (10%)	49,51,51	1.13	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	CLR	A	713	-	31,31,31	0.90	2 (6%)	48,48,48	1.35	6 (12%)
3	PIO	B	702	-	47,47,47	1.17	5 (10%)	61,65,65	1.03	4 (6%)
6	CLR	B	716	-	31,31,31	0.80	2 (6%)	48,48,48	1.18	5 (10%)
6	CLR	A	715	-	31,31,31	0.94	1 (3%)	48,48,48	1.44	8 (16%)
6	CLR	B	718	-	31,31,31	0.96	1 (3%)	48,48,48	1.42	9 (18%)
2	41U	B	701	-	21,21,21	1.34	2 (9%)	24,26,26	2.52	6 (25%)
7	A1LX7	B	714	-	39,39,39	1.07	3 (7%)	49,51,51	1.40	5 (10%)
6	CLR	A	714	-	31,31,31	0.85	2 (6%)	48,48,48	1.28	4 (8%)
6	CLR	A	709	-	31,31,31	1.10	2 (6%)	48,48,48	1.84	13 (27%)
7	A1LX7	A	712	-	39,39,39	1.06	3 (7%)	49,51,51	1.32	5 (10%)
6	CLR	A	708	-	31,31,31	1.10	2 (6%)	48,48,48	1.59	12 (25%)
6	CLR	B	706	-	31,31,31	0.97	2 (6%)	48,48,48	1.76	12 (25%)
6	CLR	B	711	-	31,31,31	0.85	1 (3%)	48,48,48	1.38	9 (18%)
6	CLR	A	707	-	31,31,31	0.88	1 (3%)	48,48,48	1.34	6 (12%)
6	CLR	B	709	-	31,31,31	1.07	2 (6%)	48,48,48	1.48	7 (14%)
7	A1LX7	A	711	-	39,39,39	1.03	4 (10%)	49,51,51	1.19	3 (6%)
6	CLR	B	710	-	31,31,31	0.96	2 (6%)	48,48,48	1.58	9 (18%)
3	PIO	A	702	-	47,47,47	1.19	7 (14%)	61,65,65	1.10	5 (8%)
6	CLR	B	712	-	31,31,31	0.97	2 (6%)	48,48,48	1.28	5 (10%)

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
6	CLR	B	715	-	-	4/10/68/68	0/4/4/4
6	CLR	A	706	-	-	8/10/68/68	0/4/4/4
6	CLR	A	716	-	-	6/10/68/68	0/4/4/4
6	CLR	B	707	-	-	6/10/68/68	0/4/4/4
2	41U	A	701	-	-	4/14/14/14	0/2/2/2
6	CLR	B	708	-	-	7/10/68/68	0/4/4/4
6	CLR	B	717	-	-	9/10/68/68	0/4/4/4
6	CLR	A	710	-	-	8/10/68/68	0/4/4/4
7	A1LX7	B	713	-	-	16/34/58/58	0/1/1/1
6	CLR	A	713	-	-	9/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PIO	B	702	-	-	18/44/68/68	0/1/1/1
6	CLR	B	716	-	-	8/10/68/68	0/4/4/4
6	CLR	A	715	-	-	6/10/68/68	0/4/4/4
6	CLR	B	718	-	-	10/10/68/68	0/4/4/4
2	41U	B	701	-	-	3/14/14/14	0/2/2/2
7	A1LX7	B	714	-	-	15/34/58/58	0/1/1/1
6	CLR	A	714	-	-	9/10/68/68	0/4/4/4
6	CLR	A	709	-	-	7/10/68/68	0/4/4/4
7	A1LX7	A	712	-	-	20/34/58/58	0/1/1/1
6	CLR	A	708	-	-	7/10/68/68	0/4/4/4
6	CLR	B	706	-	-	9/10/68/68	0/4/4/4
6	CLR	B	711	-	-	5/10/68/68	0/4/4/4
6	CLR	A	707	-	-	10/10/68/68	0/4/4/4
6	CLR	B	709	-	-	9/10/68/68	0/4/4/4
7	A1LX7	A	711	-	-	21/34/58/58	0/1/1/1
6	CLR	B	710	-	-	7/10/68/68	0/4/4/4
3	PIO	A	702	-	-	17/44/68/68	0/1/1/1
6	CLR	B	712	-	-	5/10/68/68	0/4/4/4

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	41U	O-C7	-5.06	1.40	1.44
2	B	701	41U	O-C7	-4.92	1.40	1.44
3	A	702	PIO	P4-O4	3.18	1.65	1.59
3	B	702	PIO	P4-O4	3.11	1.65	1.59
6	B	709	CLR	C10-C9	-2.97	1.51	1.56
6	B	718	CLR	C10-C9	-2.93	1.51	1.56
3	A	702	PIO	P5-O5	2.93	1.64	1.59
3	B	702	PIO	P5-O5	2.87	1.64	1.59
6	A	710	CLR	C10-C9	-2.82	1.51	1.56
6	A	708	CLR	C10-C9	-2.81	1.51	1.56
3	B	702	PIO	O2C-C2C	-2.72	1.39	1.46
6	A	713	CLR	C10-C9	-2.70	1.51	1.56
6	B	706	CLR	C10-C9	-2.66	1.51	1.56
7	A	712	A1LX7	O12-C11	-2.65	1.40	1.46
6	B	711	CLR	C10-C9	-2.65	1.51	1.56
6	B	707	CLR	C10-C9	-2.64	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	714	A1LX7	O12-C11	-2.61	1.40	1.46
6	A	706	CLR	C10-C9	-2.59	1.51	1.56
6	A	709	CLR	C10-C9	-2.59	1.51	1.56
6	A	709	CLR	C13-C14	-2.59	1.50	1.55
6	B	712	CLR	C10-C9	-2.58	1.51	1.56
6	A	716	CLR	C10-C9	-2.57	1.51	1.56
7	B	713	A1LX7	O12-C11	-2.55	1.40	1.46
7	A	711	A1LX7	O12-C11	-2.51	1.40	1.46
6	B	710	CLR	C10-C9	-2.47	1.51	1.56
3	A	702	PIO	P1-O1	2.41	1.66	1.60
7	B	714	A1LX7	O09-C08	2.41	1.40	1.33
7	A	712	A1LX7	O09-C08	2.39	1.40	1.33
6	B	709	CLR	C13-C14	-2.37	1.50	1.55
3	A	702	PIO	O2C-C2C	-2.37	1.40	1.46
3	A	702	PIO	O3C-C1B	2.35	1.40	1.33
6	A	707	CLR	C10-C9	-2.35	1.52	1.56
6	A	715	CLR	C10-C9	-2.34	1.52	1.56
6	A	708	CLR	C13-C14	-2.33	1.50	1.55
2	A	701	41U	O-C	2.32	1.41	1.37
6	B	708	CLR	C10-C9	-2.32	1.52	1.56
3	B	702	PIO	O3C-C1B	2.30	1.40	1.33
7	B	713	A1LX7	O09-C10	-2.28	1.40	1.45
2	B	701	41U	O-C	2.28	1.41	1.37
6	B	710	CLR	C13-C14	-2.24	1.50	1.55
6	A	714	CLR	C10-C9	-2.23	1.52	1.56
6	B	706	CLR	C13-C14	-2.23	1.50	1.55
6	B	715	CLR	C13-C14	-2.23	1.50	1.55
6	A	710	CLR	C13-C14	-2.22	1.50	1.55
3	B	702	PIO	O3C-C3C	-2.20	1.40	1.45
7	A	711	A1LX7	O09-C10	-2.18	1.40	1.45
6	B	715	CLR	C10-C9	-2.17	1.52	1.56
6	B	716	CLR	C10-C9	-2.17	1.52	1.56
6	B	712	CLR	C13-C14	-2.17	1.50	1.55
7	A	712	A1LX7	O09-C10	-2.16	1.40	1.45
6	A	706	CLR	C13-C14	-2.14	1.50	1.55
3	A	702	PIO	O3C-C3C	-2.14	1.40	1.45
7	B	714	A1LX7	O09-C10	-2.14	1.40	1.45
7	B	713	A1LX7	O09-C08	2.12	1.39	1.33
7	A	711	A1LX7	O09-C08	2.11	1.39	1.33
3	A	702	PIO	O2C-C1A	2.10	1.40	1.34
7	B	713	A1LX7	O12-C13	2.06	1.40	1.34
6	B	708	CLR	C19-C10	-2.06	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	714	CLR	C13-C14	-2.06	1.51	1.55
6	A	713	CLR	C13-C14	-2.05	1.51	1.55
7	A	711	A1LX7	O12-C13	2.04	1.40	1.34
6	B	716	CLR	C13-C14	-2.00	1.51	1.55

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	717	CLR	C19-C10-C9	-23.89	83.20	111.68
6	B	717	CLR	C19-C10-C1	-17.04	82.51	109.43
6	B	717	CLR	C19-C10-C5	-13.60	86.33	108.34
6	B	717	CLR	C1-C10-C9	10.95	124.02	108.73
2	A	701	41U	O1-C5-C	6.99	125.14	115.41
2	B	701	41U	O1-C5-C	6.95	125.09	115.41
6	A	709	CLR	C4-C5-C10	6.10	124.53	116.42
6	B	717	CLR	C1-C2-C3	5.52	117.56	110.47
2	B	701	41U	O1-C5-C4	-5.26	115.35	124.37
2	A	701	41U	O1-C5-C4	-5.26	115.35	124.37
6	B	706	CLR	C13-C17-C20	-5.02	111.63	119.49
6	B	710	CLR	C4-C5-C10	4.87	122.89	116.42
2	B	701	41U	C14-C7-C8	-4.53	104.43	112.62
2	A	701	41U	C14-C7-C8	-4.53	104.44	112.62
6	B	717	CLR	C1-C10-C5	4.51	117.00	108.75
7	B	714	A1LX7	O12-C13-C14	4.44	121.07	111.50
6	B	715	CLR	C13-C17-C20	-4.43	112.54	119.49
6	A	710	CLR	C13-C17-C20	-4.31	112.73	119.49
7	A	712	A1LX7	O12-C13-C14	4.20	120.55	111.50
6	B	715	CLR	C13-C14-C8	-4.19	108.18	114.38
2	B	701	41U	O-C-C1	-4.17	114.08	123.87
2	A	701	41U	O-C-C1	-4.16	114.10	123.87
7	B	713	A1LX7	O12-C13-C14	4.16	120.46	111.50
6	B	706	CLR	C11-C9-C10	-4.15	107.61	113.08
7	B	714	A1LX7	C30-C28-C27	4.12	119.10	109.68
7	A	711	A1LX7	O12-C13-C14	3.99	120.10	111.50
6	A	716	CLR	C4-C5-C10	3.93	121.64	116.42
7	A	712	A1LX7	C30-C28-C27	3.91	118.60	109.68
6	A	714	CLR	C13-C17-C20	-3.91	113.37	119.49
3	B	702	PIO	O2C-C1A-C2A	3.89	119.89	111.50
6	B	717	CLR	C9-C10-C5	3.84	115.67	109.65
6	B	709	CLR	C14-C8-C9	-3.77	104.04	109.09
6	A	707	CLR	C13-C17-C20	-3.75	113.61	119.49
6	B	716	CLR	C13-C17-C20	-3.70	113.69	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	41U	O-C-C5	3.70	128.00	116.74
6	A	708	CLR	C7-C8-C9	3.68	114.17	109.71
2	A	701	41U	O-C-C5	3.68	127.93	116.74
6	B	710	CLR	C13-C17-C20	-3.68	113.73	119.49
6	A	706	CLR	C13-C17-C20	-3.67	113.74	119.49
6	B	706	CLR	C13-C14-C8	-3.64	108.98	114.38
6	B	711	CLR	C22-C20-C17	3.64	117.81	110.28
6	B	706	CLR	C17-C13-C14	3.61	104.35	100.07
6	A	709	CLR	C8-C7-C6	-3.57	107.61	112.73
6	A	709	CLR	C7-C6-C5	-3.52	118.57	125.06
7	A	712	A1LX7	C36-C27-C28	3.50	115.90	110.85
6	A	709	CLR	C1-C2-C3	-3.50	105.98	110.47
6	A	707	CLR	C11-C9-C10	-3.48	108.49	113.08
7	A	711	A1LX7	P24-O26-C27	-3.46	106.81	119.41
6	B	707	CLR	C22-C20-C17	3.46	117.44	110.28
6	A	706	CLR	C10-C9-C8	-3.45	107.55	112.73
6	A	713	CLR	C11-C9-C10	-3.45	108.54	113.08
6	A	715	CLR	C8-C7-C6	-3.44	107.79	112.73
6	B	717	CLR	C16-C17-C20	-3.42	106.85	112.15
6	A	713	CLR	C21-C20-C17	3.41	118.14	112.92
6	A	706	CLR	C11-C9-C10	-3.38	108.62	113.08
6	B	717	CLR	C7-C8-C9	3.38	113.81	109.71
3	A	702	PIO	O2C-C1A-C2A	3.37	118.77	111.50
6	B	706	CLR	C4-C5-C10	3.35	120.87	116.42
6	A	709	CLR	C13-C14-C8	-3.30	109.49	114.38
6	B	709	CLR	C7-C8-C9	3.25	113.65	109.71
6	B	708	CLR	C11-C9-C10	-3.25	108.80	113.08
6	B	715	CLR	C17-C13-C14	3.23	103.90	100.07
6	B	710	CLR	C23-C22-C20	-3.23	105.76	115.03
6	B	707	CLR	C4-C5-C10	3.22	120.70	116.42
7	B	714	A1LX7	C36-C27-C28	3.21	115.48	110.85
6	B	709	CLR	C13-C14-C8	-3.21	109.63	114.38
7	A	711	A1LX7	O09-C08-C07	3.21	121.97	111.91
6	A	709	CLR	C10-C5-C6	-3.19	118.02	122.90
6	B	707	CLR	C7-C8-C9	3.15	113.53	109.71
7	B	714	A1LX7	O09-C08-C07	3.12	121.69	111.91
6	B	711	CLR	C4-C5-C10	3.12	120.56	116.42
6	B	706	CLR	C10-C9-C8	-3.10	108.09	112.73
6	A	710	CLR	C4-C5-C10	3.09	120.53	116.42
6	A	710	CLR	C10-C9-C8	-3.07	108.12	112.73
6	B	709	CLR	C13-C17-C20	-3.07	114.68	119.49
7	B	713	A1LX7	O09-C08-C07	3.05	121.47	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	710	CLR	C23-C22-C20	-3.03	106.33	115.03
6	A	715	CLR	C16-C17-C20	-3.00	107.50	112.15
6	B	718	CLR	C11-C9-C10	-2.98	109.15	113.08
6	A	715	CLR	C11-C9-C10	-2.97	109.16	113.08
6	A	706	CLR	C17-C13-C14	2.95	103.56	100.07
7	B	714	A1LX7	C32-C30-C28	2.93	115.93	110.82
6	B	716	CLR	C11-C9-C10	-2.91	109.25	113.08
6	B	717	CLR	C10-C9-C8	-2.87	108.43	112.73
6	A	715	CLR	C19-C10-C9	-2.86	108.27	111.68
6	B	709	CLR	C4-C5-C10	2.85	120.20	116.42
6	B	712	CLR	C3-C4-C5	-2.82	107.25	112.03
3	A	702	PIO	P1-O1-C1	2.81	129.64	119.41
6	B	711	CLR	C18-C13-C14	-2.80	106.48	111.71
7	A	712	A1LX7	C32-C30-C28	2.78	115.68	110.82
6	B	708	CLR	C13-C17-C20	-2.78	115.14	119.49
6	A	710	CLR	C11-C9-C10	-2.76	109.45	113.08
6	B	711	CLR	C7-C8-C9	2.71	113.00	109.71
6	B	706	CLR	C10-C5-C6	-2.70	118.77	122.90
6	B	718	CLR	C10-C9-C8	-2.69	108.70	112.73
6	B	718	CLR	C11-C12-C13	-2.69	108.17	112.78
7	A	712	A1LX7	O09-C08-C07	2.68	120.32	111.91
6	B	715	CLR	C7-C6-C5	-2.67	120.13	125.06
6	B	710	CLR	C21-C20-C22	-2.66	106.19	110.36
6	B	718	CLR	C1-C10-C9	2.65	112.43	108.73
6	A	710	CLR	C17-C13-C14	2.65	103.21	100.07
6	B	718	CLR	C8-C7-C6	-2.65	108.93	112.73
6	A	708	CLR	C11-C9-C10	-2.64	109.60	113.08
6	A	708	CLR	C13-C17-C20	-2.63	115.37	119.49
3	B	702	PIO	C5-C6-C1	2.62	114.40	108.96
6	A	713	CLR	C3-C4-C5	-2.61	107.59	112.03
6	A	708	CLR	C4-C5-C10	2.60	119.88	116.42
6	A	709	CLR	C2-C1-C10	-2.60	107.10	112.74
6	B	708	CLR	C19-C10-C5	-2.60	104.13	108.34
6	A	715	CLR	C23-C22-C20	-2.59	107.58	115.03
3	A	702	PIO	C5-C6-C1	2.58	114.31	108.96
6	B	709	CLR	C11-C9-C10	-2.58	109.69	113.08
6	A	708	CLR	C14-C8-C9	-2.57	105.65	109.09
6	B	717	CLR	C3-C4-C5	-2.57	107.67	112.03
6	A	708	CLR	C19-C10-C9	-2.56	108.63	111.68
3	B	702	PIO	O3C-C1B-C2B	2.56	119.93	111.91
6	A	708	CLR	C3-C4-C5	-2.56	107.69	112.03
3	A	702	PIO	O3C-C1B-C2B	2.55	119.92	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	716	CLR	C19-C10-C5	2.55	112.46	108.34
6	B	706	CLR	C19-C10-C9	-2.53	108.66	111.68
6	B	718	CLR	C3-C4-C5	-2.53	107.74	112.03
6	B	710	CLR	C11-C9-C10	-2.53	109.75	113.08
6	B	707	CLR	C18-C13-C14	-2.51	107.02	111.71
6	B	717	CLR	C13-C17-C20	-2.50	115.56	119.49
6	A	709	CLR	C2-C3-C4	-2.50	106.87	110.31
6	A	707	CLR	C14-C8-C9	-2.48	105.77	109.09
6	B	715	CLR	C10-C5-C6	-2.48	119.11	122.90
2	B	701	41U	C6-O1-C5	-2.47	113.80	117.53
6	A	715	CLR	C11-C12-C13	-2.47	108.54	112.78
6	A	709	CLR	C13-C17-C20	-2.45	115.64	119.49
6	A	708	CLR	C13-C14-C8	-2.45	110.75	114.38
6	B	715	CLR	C4-C5-C10	2.44	119.67	116.42
2	A	701	41U	C6-O1-C5	-2.44	113.84	117.53
6	A	714	CLR	C13-C14-C8	-2.44	110.77	114.38
6	A	706	CLR	C4-C5-C10	2.44	119.66	116.42
6	B	718	CLR	C13-C17-C20	-2.43	115.69	119.49
6	A	708	CLR	C8-C7-C6	-2.40	109.28	112.73
6	B	706	CLR	C1-C10-C9	2.39	112.07	108.73
6	B	712	CLR	C11-C9-C10	-2.39	109.93	113.08
6	A	710	CLR	C18-C13-C17	-2.38	107.27	111.71
6	B	711	CLR	C1-C10-C5	2.38	113.11	108.75
6	A	708	CLR	C1-C10-C9	2.38	112.05	108.73
6	B	710	CLR	C10-C5-C6	-2.37	119.27	122.90
7	B	713	A1LX7	C22-C11-C10	-2.37	106.18	111.79
6	A	707	CLR	C13-C14-C8	-2.36	110.89	114.38
6	B	715	CLR	C11-C12-C13	-2.34	108.76	112.78
6	B	706	CLR	C2-C1-C10	-2.32	107.72	112.74
6	B	710	CLR	C3-C4-C5	2.31	115.94	112.03
6	B	712	CLR	C4-C5-C10	2.30	119.48	116.42
6	A	715	CLR	C4-C5-C10	2.30	119.48	116.42
6	B	716	CLR	C17-C13-C14	2.30	102.80	100.07
6	A	709	CLR	C16-C17-C20	-2.29	108.60	112.15
6	B	717	CLR	C14-C8-C9	-2.29	106.03	109.09
6	A	716	CLR	C19-C10-C9	-2.28	108.97	111.68
6	B	711	CLR	C11-C9-C10	-2.26	110.10	113.08
6	A	710	CLR	C10-C5-C6	-2.26	119.45	122.90
6	A	706	CLR	C13-C14-C8	-2.25	111.05	114.38
6	A	706	CLR	C18-C13-C17	-2.24	107.53	111.71
6	B	712	CLR	C1-C10-C9	2.24	111.85	108.73
6	B	711	CLR	C13-C17-C20	2.23	122.98	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	710	CLR	C13-C14-C8	-2.20	111.13	114.38
6	A	708	CLR	C23-C22-C20	-2.20	108.72	115.03
6	A	715	CLR	C13-C17-C20	-2.20	116.05	119.49
6	A	709	CLR	C4-C5-C6	-2.19	117.45	120.61
6	B	718	CLR	C19-C10-C9	-2.19	109.07	111.68
6	B	707	CLR	C13-C17-C20	2.19	122.92	119.49
6	A	708	CLR	C21-C20-C22	-2.18	106.94	110.36
3	A	702	PIO	O11-P1-O1	2.18	115.39	106.78
6	A	707	CLR	C19-C10-C9	-2.18	109.08	111.68
6	A	713	CLR	C16-C17-C20	-2.18	108.78	112.15
6	B	715	CLR	C7-C8-C9	2.17	112.34	109.71
6	A	709	CLR	C11-C9-C10	-2.15	110.25	113.08
6	A	716	CLR	C7-C8-C9	2.14	112.31	109.71
6	B	710	CLR	C18-C13-C17	-2.14	107.73	111.71
6	A	709	CLR	C14-C8-C9	-2.14	106.23	109.09
6	A	707	CLR	C8-C7-C6	-2.13	109.67	112.73
6	B	716	CLR	C10-C9-C8	-2.12	109.55	112.73
6	B	716	CLR	C13-C14-C8	-2.12	111.24	114.38
6	B	715	CLR	C1-C10-C9	2.11	111.67	108.73
6	B	711	CLR	C10-C5-C6	-2.11	119.68	122.90
6	B	706	CLR	C18-C13-C17	-2.10	107.79	111.71
6	B	712	CLR	C10-C5-C6	-2.10	119.69	122.90
6	B	706	CLR	C23-C22-C20	-2.10	109.01	115.03
6	B	710	CLR	C13-C14-C8	-2.08	111.30	114.38
6	B	707	CLR	C19-C10-C9	-2.07	109.21	111.68
6	B	711	CLR	C19-C10-C9	-2.07	109.22	111.68
6	A	714	CLR	C1-C10-C9	2.06	111.60	108.73
6	A	713	CLR	C13-C17-C20	2.05	122.70	119.49
6	A	713	CLR	C19-C10-C9	-2.04	109.24	111.68
6	B	718	CLR	C18-C13-C17	-2.04	107.90	111.71
6	B	709	CLR	C7-C6-C5	-2.04	121.30	125.06
6	A	714	CLR	C7-C6-C5	-2.03	121.32	125.06
6	B	717	CLR	C23-C22-C20	-2.02	109.22	115.03
3	B	702	PIO	C3C-C2C-C1C	-2.02	107.01	111.79
6	B	715	CLR	C3-C4-C5	-2.01	108.61	112.03
6	A	716	CLR	C15-C14-C13	2.00	106.25	103.84

There are no chirality outliers.

All (263) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	41U	C7-C14-C15-N

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Mol	Chain	Res	Type	Atoms
2	A	701	41U	C7-C14-C15-N
3	B	702	PIO	C1C-O13-P1-O11
3	B	702	PIO	C1C-O13-P1-O12
3	B	702	PIO	C5-C4-O4-P4
3	A	702	PIO	C6-C1-O1-P1
3	A	702	PIO	C4-O4-P4-O42
6	B	707	CLR	C13-C17-C20-C22
6	B	707	CLR	C16-C17-C20-C21
6	B	710	CLR	C13-C17-C20-C21
6	B	711	CLR	C13-C17-C20-C22
6	B	711	CLR	C16-C17-C20-C21
6	B	711	CLR	C16-C17-C20-C22
7	B	713	A1LX7	C14-C13-O12-C11
7	B	713	A1LX7	C22-O23-P24-O38
7	B	714	A1LX7	C27-O26-P24-O25
7	A	711	A1LX7	C14-C13-O12-C11
7	A	711	A1LX7	O21-C13-O12-C11
7	A	711	A1LX7	C22-O23-P24-O25
7	A	711	A1LX7	C22-O23-P24-O26
7	A	711	A1LX7	C22-O23-P24-O38
7	A	712	A1LX7	C27-O26-P24-O25
6	A	709	CLR	C21-C20-C22-C23
7	B	714	A1LX7	O39-C08-O09-C10
6	B	710	CLR	C16-C17-C20-C21
6	A	707	CLR	C16-C17-C20-C21
6	A	710	CLR	C16-C17-C20-C21
6	A	714	CLR	C16-C17-C20-C21
6	B	707	CLR	C13-C17-C20-C21
6	B	711	CLR	C13-C17-C20-C21
6	A	707	CLR	C13-C17-C20-C21
6	A	710	CLR	C13-C17-C20-C21
6	A	714	CLR	C13-C17-C20-C21
6	A	716	CLR	C13-C17-C20-C21
6	B	707	CLR	C16-C17-C20-C22
6	B	716	CLR	C13-C17-C20-C22
3	B	702	PIO	O1A-C1A-O2C-C2C
7	B	713	A1LX7	O21-C13-O12-C11
7	B	714	A1LX7	C07-C08-O09-C10
7	A	712	A1LX7	C07-C08-O09-C10
6	B	709	CLR	C21-C20-C22-C23
6	B	718	CLR	C21-C20-C22-C23
6	A	710	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
6	A	716	CLR	C21-C20-C22-C23
6	B	716	CLR	C16-C17-C20-C21
6	A	716	CLR	C16-C17-C20-C21
6	B	716	CLR	C13-C17-C20-C21
6	B	718	CLR	C13-C17-C20-C21
6	B	706	CLR	C13-C17-C20-C22
6	B	710	CLR	C13-C17-C20-C22
6	B	718	CLR	C13-C17-C20-C22
6	A	707	CLR	C13-C17-C20-C22
6	A	710	CLR	C13-C17-C20-C22
6	A	714	CLR	C13-C17-C20-C22
6	A	716	CLR	C13-C17-C20-C22
6	A	708	CLR	C21-C20-C22-C23
7	A	712	A1LX7	O39-C08-O09-C10
6	B	706	CLR	C13-C17-C20-C21
6	B	710	CLR	C16-C17-C20-C22
6	A	707	CLR	C16-C17-C20-C22
6	A	714	CLR	C16-C17-C20-C22
3	B	702	PIO	C2A-C1A-O2C-C2C
3	A	702	PIO	C3A-C4A-C5A-C6A
6	A	713	CLR	C16-C17-C20-C22
6	A	713	CLR	C17-C20-C22-C23
6	A	716	CLR	C17-C20-C22-C23
7	B	713	A1LX7	C04-C05-C06-C07
2	B	701	41U	C1-C-O-C7
2	A	701	41U	C1-C-O-C7
6	A	715	CLR	C21-C20-C22-C23
3	B	702	PIO	C4B-C5B-C6B-C7B
3	A	702	PIO	C4B-C5B-C6B-C7B
6	B	717	CLR	C17-C20-C22-C23
6	A	715	CLR	C17-C20-C22-C23
7	A	712	A1LX7	C02-C03-C04-C05
6	B	710	CLR	C21-C20-C22-C23
6	B	708	CLR	C13-C17-C20-C21
6	A	710	CLR	C16-C17-C20-C22
6	B	718	CLR	C20-C22-C23-C24
6	A	715	CLR	C22-C23-C24-C25
6	B	717	CLR	C21-C20-C22-C23
6	A	713	CLR	C20-C22-C23-C24
3	A	702	PIO	C2A-C1A-O2C-C2C
6	B	716	CLR	C16-C17-C20-C22
7	A	711	A1LX7	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
6	A	707	CLR	C17-C20-C22-C23
6	A	708	CLR	C17-C20-C22-C23
6	A	710	CLR	C17-C20-C22-C23
6	A	714	CLR	C21-C20-C22-C23
7	A	712	A1LX7	C05-C06-C07-C08
6	B	715	CLR	C20-C22-C23-C24
6	A	714	CLR	C22-C23-C24-C25
6	A	716	CLR	C16-C17-C20-C22
6	B	708	CLR	C13-C17-C20-C22
3	A	702	PIO	C1B-C2B-C3B-C4B
6	B	709	CLR	C17-C20-C22-C23
6	B	718	CLR	C17-C20-C22-C23
6	A	709	CLR	C17-C20-C22-C23
6	B	712	CLR	C22-C23-C24-C25
6	B	716	CLR	C20-C22-C23-C24
6	A	713	CLR	C13-C17-C20-C21
6	B	712	CLR	C20-C22-C23-C24
6	A	714	CLR	C17-C20-C22-C23
6	A	707	CLR	C21-C20-C22-C23
6	A	713	CLR	C21-C20-C22-C23
3	A	702	PIO	O1A-C1A-O2C-C2C
6	B	717	CLR	C22-C23-C24-C25
7	B	713	A1LX7	C05-C06-C07-C08
6	A	706	CLR	C22-C23-C24-C25
7	B	714	A1LX7	C14-C13-O12-C11
7	A	712	A1LX7	C14-C13-O12-C11
6	B	706	CLR	C22-C23-C24-C25
6	A	706	CLR	C20-C22-C23-C24
6	A	707	CLR	C22-C23-C24-C25
3	B	702	PIO	C1C-O13-P1-O1
6	B	708	CLR	C22-C23-C24-C25
7	B	714	A1LX7	O21-C13-O12-C11
7	A	712	A1LX7	O21-C13-O12-C11
6	B	718	CLR	C22-C23-C24-C25
3	B	702	PIO	C1A-C2A-C3A-C4A
7	A	712	A1LX7	C15-C16-C17-C18
7	B	714	A1LX7	C13-C14-C15-C16
7	B	714	A1LX7	C05-C06-C07-C08
2	B	701	41U	C5-C-O-C7
2	A	701	41U	C5-C-O-C7
6	B	708	CLR	C16-C17-C20-C21
6	A	706	CLR	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
3	B	702	PIO	C1B-C2B-C3B-C4B
7	B	714	A1LX7	C16-C17-C18-C19
6	B	708	CLR	C23-C24-C25-C26
6	B	715	CLR	C23-C24-C25-C26
6	B	717	CLR	C23-C24-C25-C27
6	B	706	CLR	C16-C17-C20-C21
6	B	715	CLR	C23-C24-C25-C27
7	B	714	A1LX7	C01-C02-C03-C04
6	B	718	CLR	C16-C17-C20-C21
6	A	708	CLR	C22-C23-C24-C25
6	A	706	CLR	C13-C17-C20-C21
7	B	713	A1LX7	C01-C02-C03-C04
6	B	710	CLR	C23-C24-C25-C27
6	B	716	CLR	C23-C24-C25-C27
6	A	706	CLR	C23-C24-C25-C26
6	A	710	CLR	C23-C24-C25-C26
6	B	706	CLR	C16-C17-C20-C22
6	B	718	CLR	C23-C24-C25-C27
6	A	707	CLR	C23-C24-C25-C27
3	B	702	PIO	C5A-C6A-C7A-C8A
6	B	716	CLR	C23-C24-C25-C26
6	B	717	CLR	C23-C24-C25-C26
7	B	714	A1LX7	C04-C05-C06-C07
7	B	713	A1LX7	C22-O23-P24-O26
7	B	713	A1LX7	C10-C11-C22-O23
6	B	712	CLR	C23-C24-C25-C26
6	B	718	CLR	C16-C17-C20-C22
6	B	716	CLR	C22-C23-C24-C25
7	A	712	A1LX7	C04-C05-C06-C07
6	B	706	CLR	C23-C24-C25-C27
6	B	709	CLR	C13-C17-C20-C21
7	B	713	A1LX7	O09-C10-C11-C22
6	B	708	CLR	C16-C17-C20-C22
7	A	711	A1LX7	C17-C18-C19-C20
6	B	706	CLR	C20-C22-C23-C24
7	B	714	A1LX7	C27-O26-P24-O23
7	A	712	A1LX7	C27-O26-P24-O23
3	A	702	PIO	C5A-C6A-C7A-C8A
6	B	709	CLR	C22-C23-C24-C25
6	B	709	CLR	C13-C17-C20-C22
7	A	712	A1LX7	C17-C18-C19-C20
6	A	706	CLR	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
6	A	713	CLR	C16-C17-C20-C21
6	B	717	CLR	C13-C17-C20-C21
6	A	708	CLR	C13-C17-C20-C21
7	B	713	A1LX7	C16-C17-C18-C19
3	A	702	PIO	C2B-C1B-O3C-C3C
3	A	702	PIO	O13-C1C-C2C-C3C
3	A	702	PIO	C2A-C3A-C4A-C5A
6	B	709	CLR	C16-C17-C20-C21
3	A	702	PIO	C1A-C2A-C3A-C4A
3	A	702	PIO	C4A-C5A-C6A-C7A
7	A	711	A1LX7	C07-C08-O09-C10
7	B	714	A1LX7	C27-O26-P24-O38
7	A	712	A1LX7	C27-O26-P24-O38
6	B	706	CLR	C23-C24-C25-C26
6	A	707	CLR	C23-C24-C25-C26
6	B	712	CLR	C21-C20-C22-C23
7	A	711	A1LX7	O12-C11-C22-O23
6	B	712	CLR	C23-C24-C25-C27
6	B	706	CLR	C21-C20-C22-C23
7	A	711	A1LX7	O09-C10-C11-O12
6	A	706	CLR	C16-C17-C20-C22
6	B	718	CLR	C23-C24-C25-C26
6	A	706	CLR	C23-C24-C25-C27
6	A	710	CLR	C23-C24-C25-C27
6	A	713	CLR	C23-C24-C25-C26
3	A	702	PIO	O1B-C1B-O3C-C3C
6	B	708	CLR	C23-C24-C25-C27
6	B	710	CLR	C23-C24-C25-C26
7	A	711	A1LX7	C10-C11-C22-O23
3	B	702	PIO	C4A-C5A-C6A-C7A
7	B	713	A1LX7	C15-C16-C17-C18
3	A	702	PIO	C1C-C2C-O2C-C1A
6	A	707	CLR	C20-C22-C23-C24
3	B	702	PIO	C1C-C2C-C3C-O3C
7	A	711	A1LX7	O09-C10-C11-C22
7	B	714	A1LX7	O12-C11-C22-O23
6	A	715	CLR	C23-C24-C25-C26
6	B	717	CLR	C13-C17-C20-C22
6	A	709	CLR	C22-C23-C24-C25
3	B	702	PIO	C3A-C4A-C5A-C6A
7	A	711	A1LX7	O39-C08-O09-C10
7	A	711	A1LX7	C06-C07-C08-O09

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Mol	Chain	Res	Type	Atoms
6	B	709	CLR	C16-C17-C20-C22
7	B	713	A1LX7	C11-C22-O23-P24
7	A	711	A1LX7	C11-C22-O23-P24
6	A	714	CLR	C23-C24-C25-C27
7	B	714	A1LX7	C10-C11-C22-O23
6	A	713	CLR	C13-C17-C20-C22
3	A	702	PIO	O13-C1C-C2C-O2C
3	B	702	PIO	O2C-C2C-C3C-O3C
7	B	713	A1LX7	O09-C10-C11-O12
7	B	714	A1LX7	C17-C18-C19-C20
6	A	708	CLR	C13-C17-C20-C22
6	A	708	CLR	C16-C17-C20-C21
6	A	709	CLR	C13-C17-C20-C21
7	B	713	A1LX7	O12-C11-C22-O23
7	A	711	A1LX7	C01-C02-C03-C04
6	A	713	CLR	C23-C24-C25-C27
7	B	713	A1LX7	C03-C04-C05-C06
6	B	709	CLR	C23-C24-C25-C26
3	A	702	PIO	O2C-C2C-C3C-O3C
6	A	708	CLR	C23-C24-C25-C27
6	A	715	CLR	C23-C24-C25-C27
6	B	717	CLR	C16-C17-C20-C21
6	A	714	CLR	C23-C24-C25-C26
3	B	702	PIO	C2C-C1C-O13-P1
6	A	709	CLR	C23-C24-C25-C26
7	A	712	A1LX7	C10-C11-C22-O23
7	B	713	A1LX7	C13-C14-C15-C16
7	A	712	A1LX7	C16-C17-C18-C19
7	A	711	A1LX7	C04-C05-C06-C07
7	A	711	A1LX7	C16-C17-C18-C19
3	B	702	PIO	C6-C1-O1-P1
7	A	711	A1LX7	C15-C16-C17-C18
6	B	709	CLR	C23-C24-C25-C27
7	A	712	A1LX7	O12-C11-C22-O23
3	B	702	PIO	C5-O5-P5-O53
7	A	712	A1LX7	C06-C07-C08-O09
6	A	709	CLR	C23-C24-C25-C27
7	A	711	A1LX7	O12-C13-C14-C15
7	A	712	A1LX7	C01-C02-C03-C04
3	B	702	PIO	C4-O4-P4-O41
6	B	717	CLR	C16-C17-C20-C22
7	A	712	A1LX7	O12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
6	A	709	CLR	C13-C17-C20-C22
6	A	715	CLR	C13-C17-C20-C21
7	A	712	A1LX7	C06-C07-C08-O39
6	B	715	CLR	C13-C17-C20-C21
2	A	701	41U	C14-C15-N-C16
7	A	711	A1LX7	O21-C13-C14-C15
6	B	711	CLR	C20-C22-C23-C24
6	B	707	CLR	C23-C24-C25-C27
7	A	712	A1LX7	O21-C13-C14-C15
6	B	707	CLR	C20-C22-C23-C24

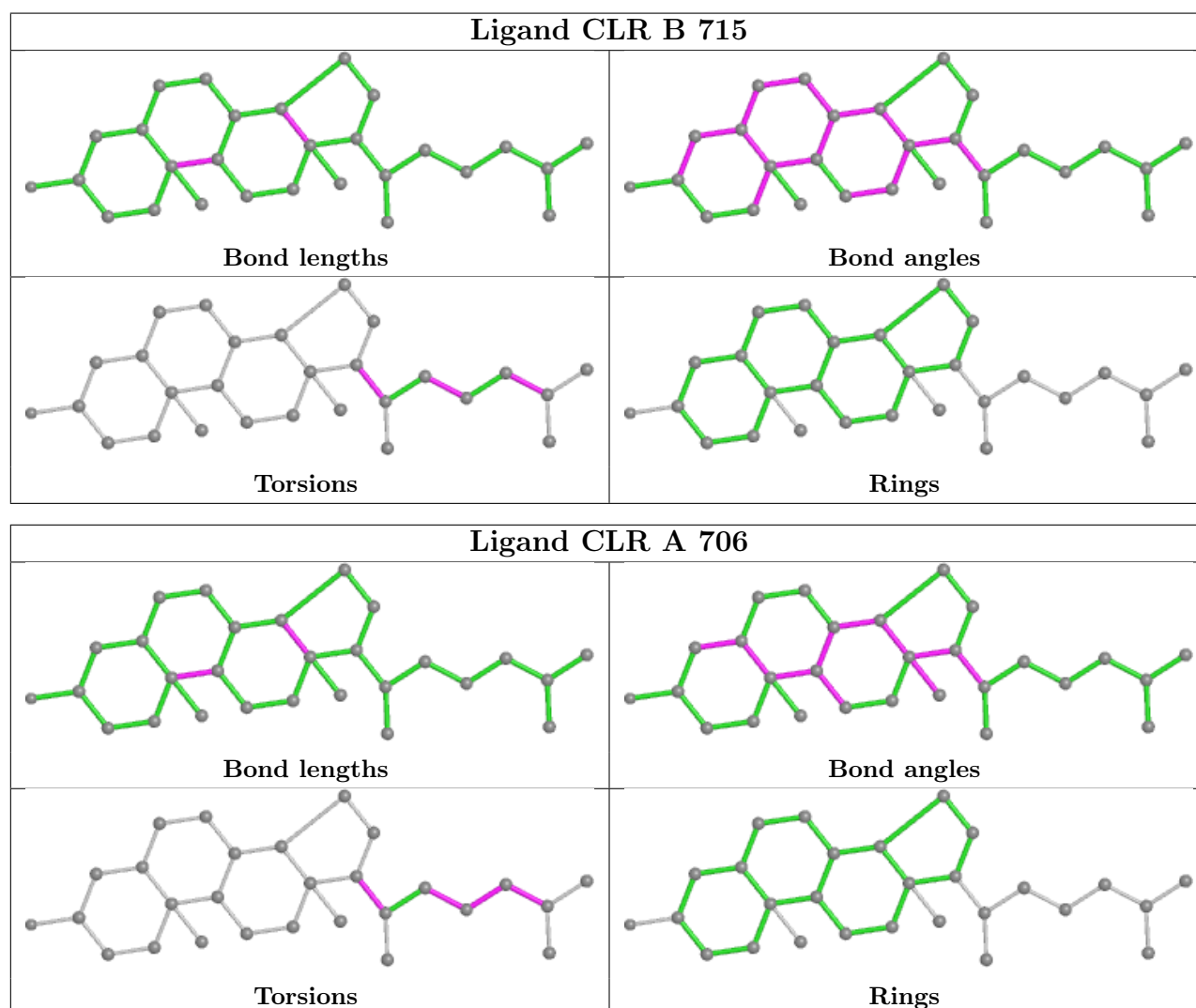
There are no ring outliers.

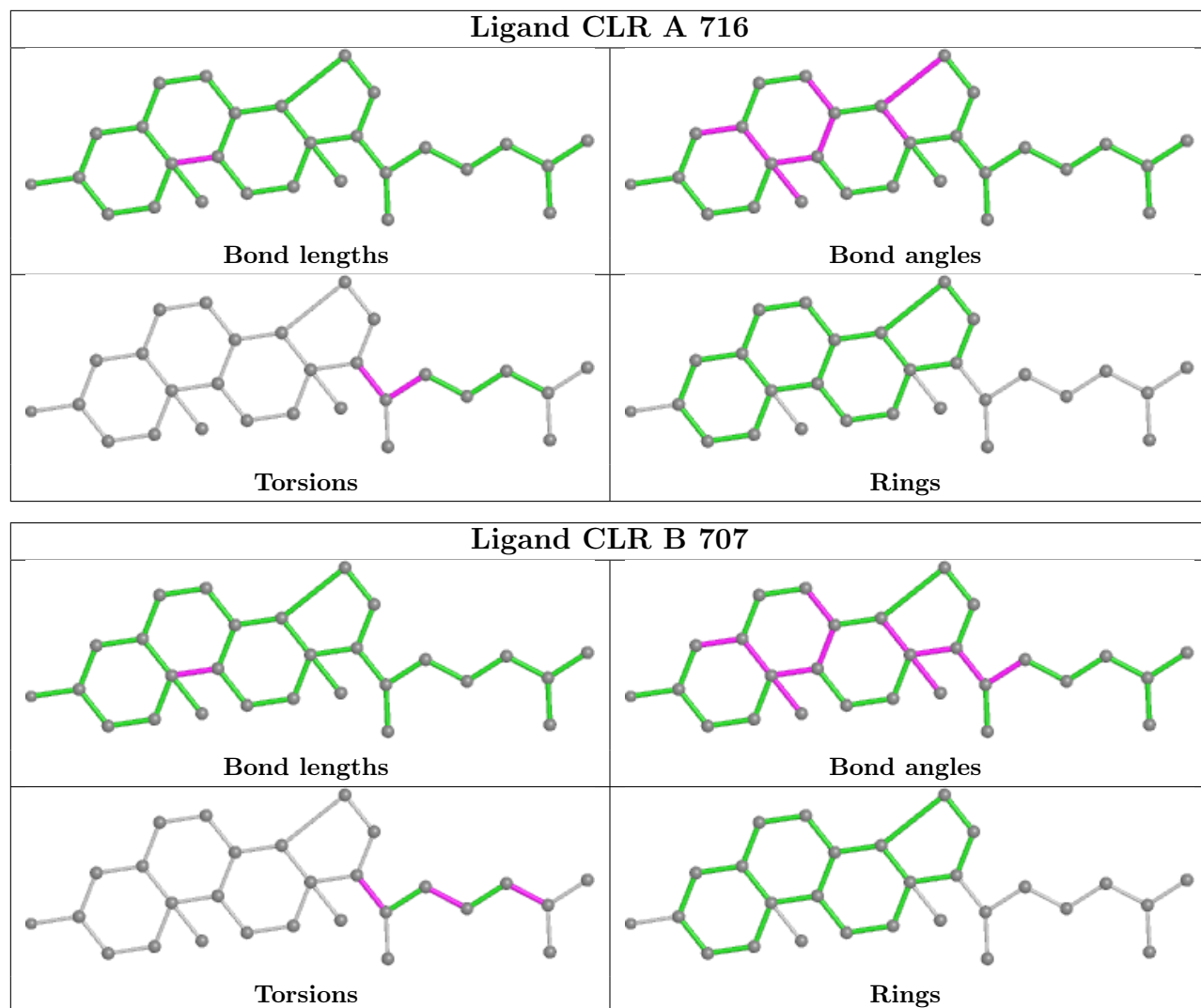
27 monomers are involved in 257 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	715	CLR	7	0
6	A	706	CLR	14	0
6	A	716	CLR	25	0
6	B	707	CLR	6	0
2	A	701	41U	6	0
6	B	708	CLR	9	0
6	B	717	CLR	23	0
6	A	710	CLR	8	0
7	B	713	A1LX7	5	0
6	A	713	CLR	17	0
3	B	702	PIO	5	0
6	B	716	CLR	20	0
6	A	715	CLR	20	0
6	B	718	CLR	33	0
2	B	701	41U	5	0
6	A	714	CLR	6	0
6	A	709	CLR	8	0
7	A	712	A1LX7	1	0
6	A	708	CLR	2	0
6	B	706	CLR	11	0
6	B	711	CLR	3	0
6	A	707	CLR	8	0
6	B	709	CLR	7	0
7	A	711	A1LX7	3	0
6	B	710	CLR	7	0
3	A	702	PIO	7	0
6	B	712	CLR	3	0

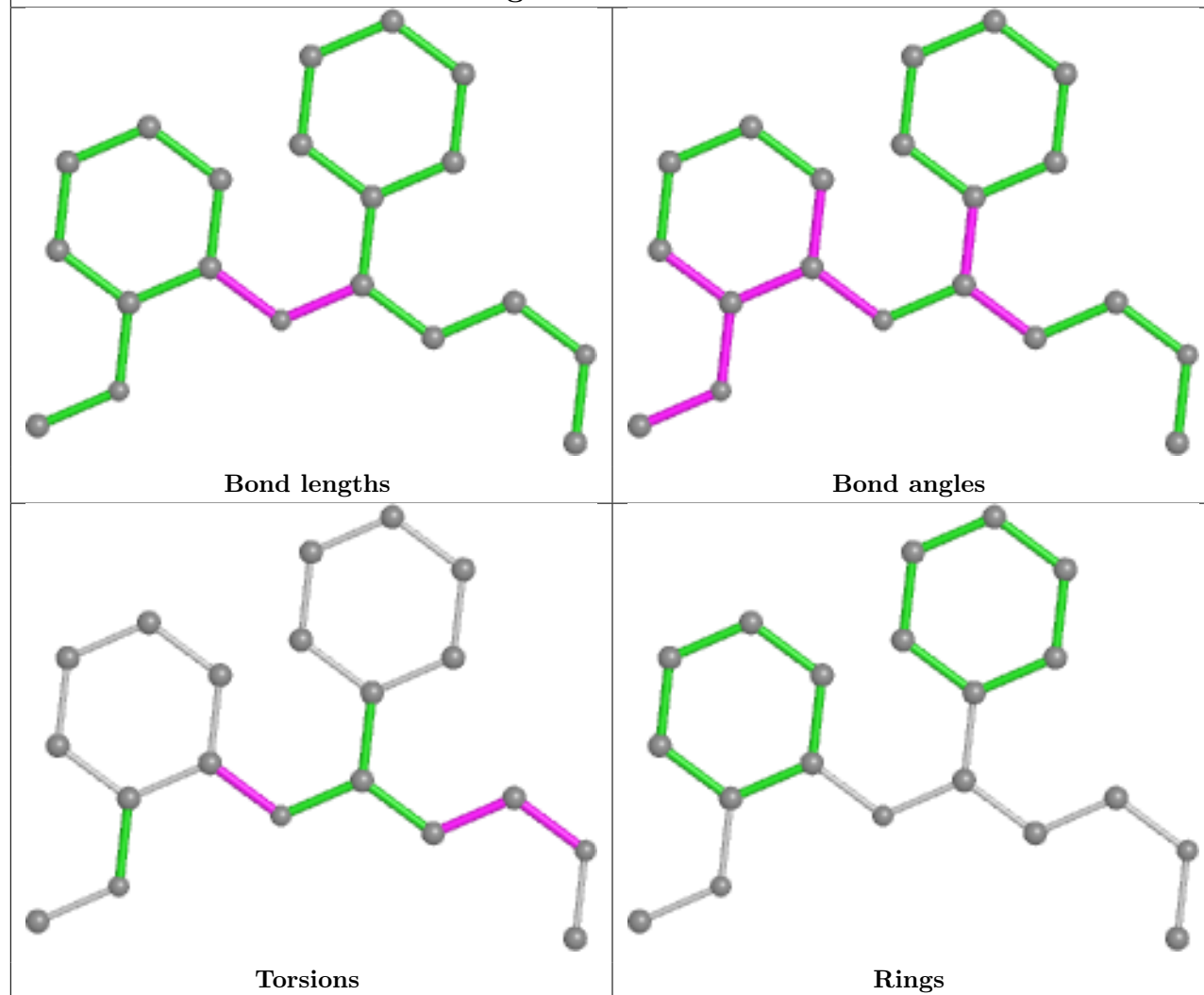


The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

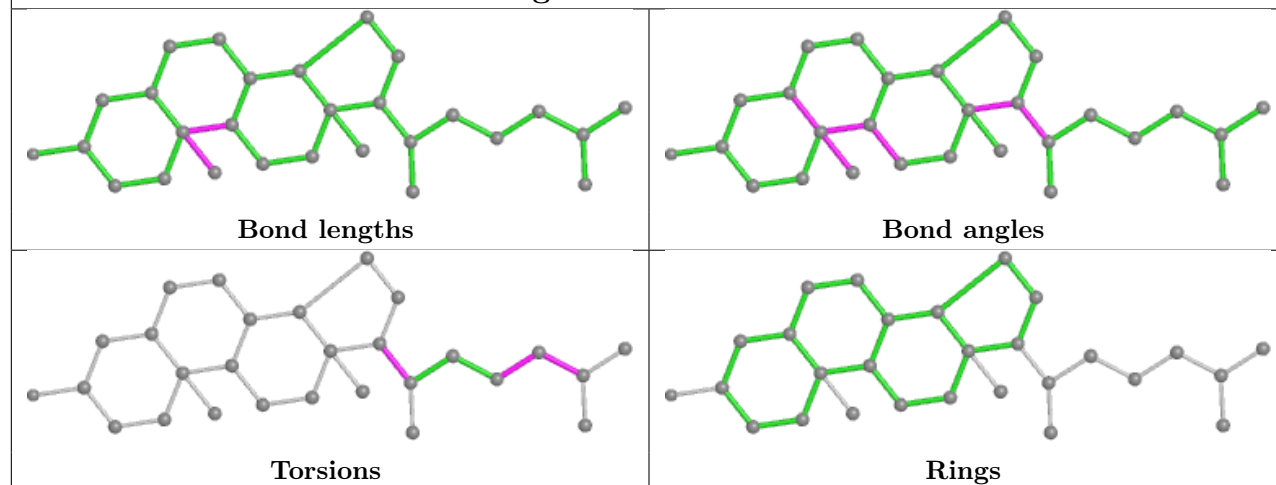


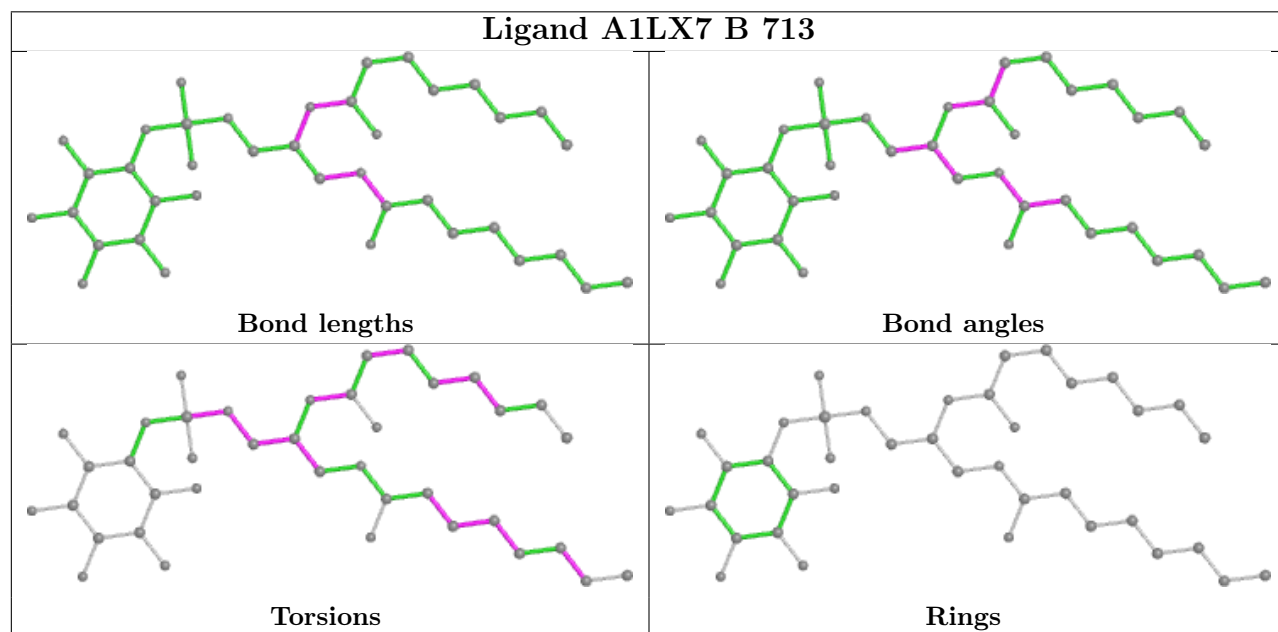
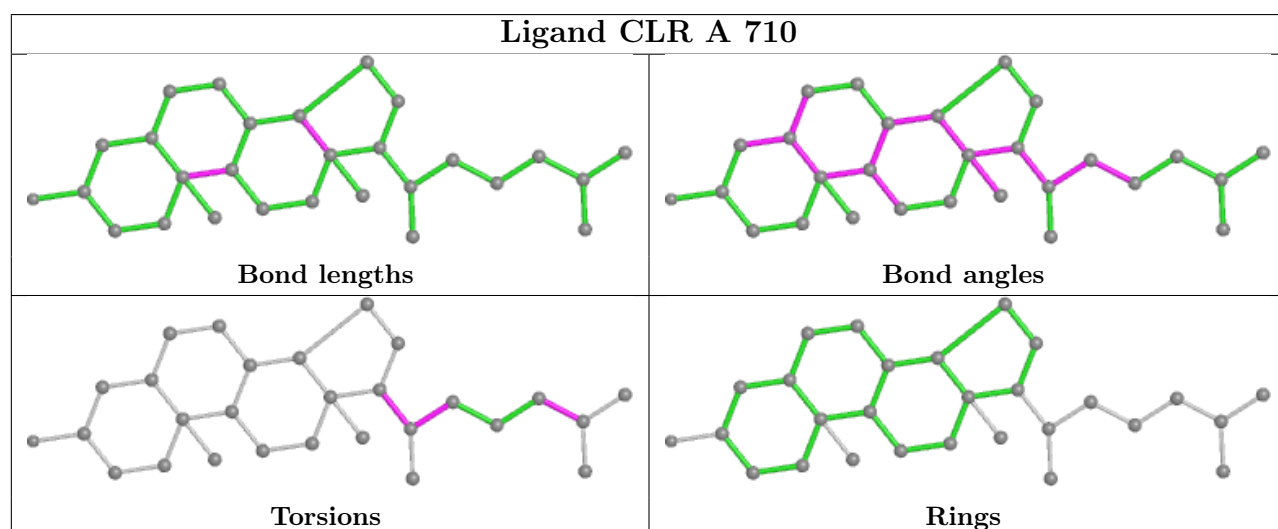
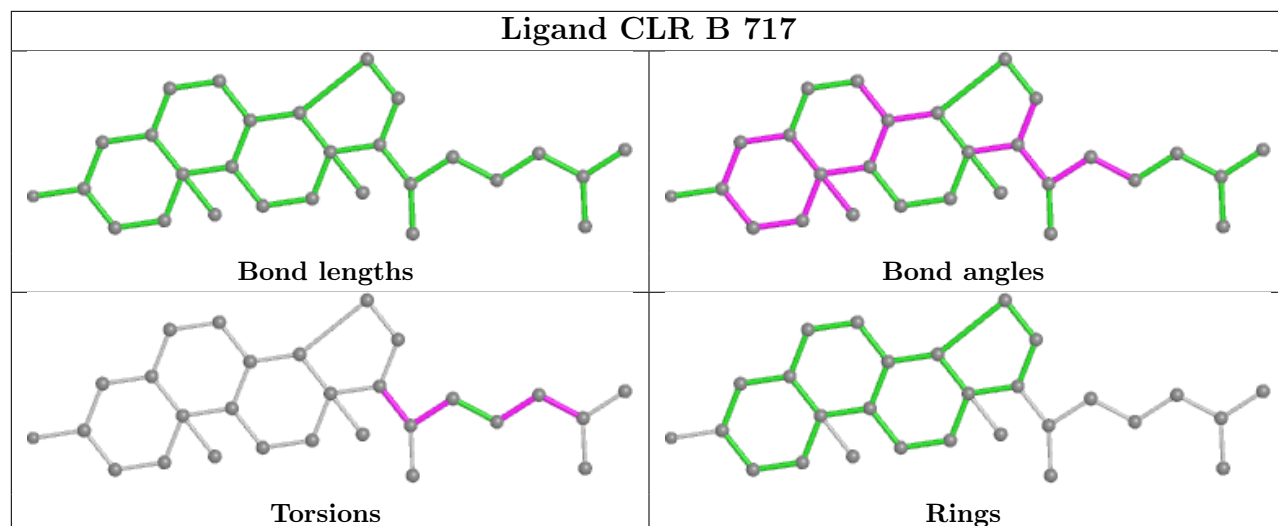


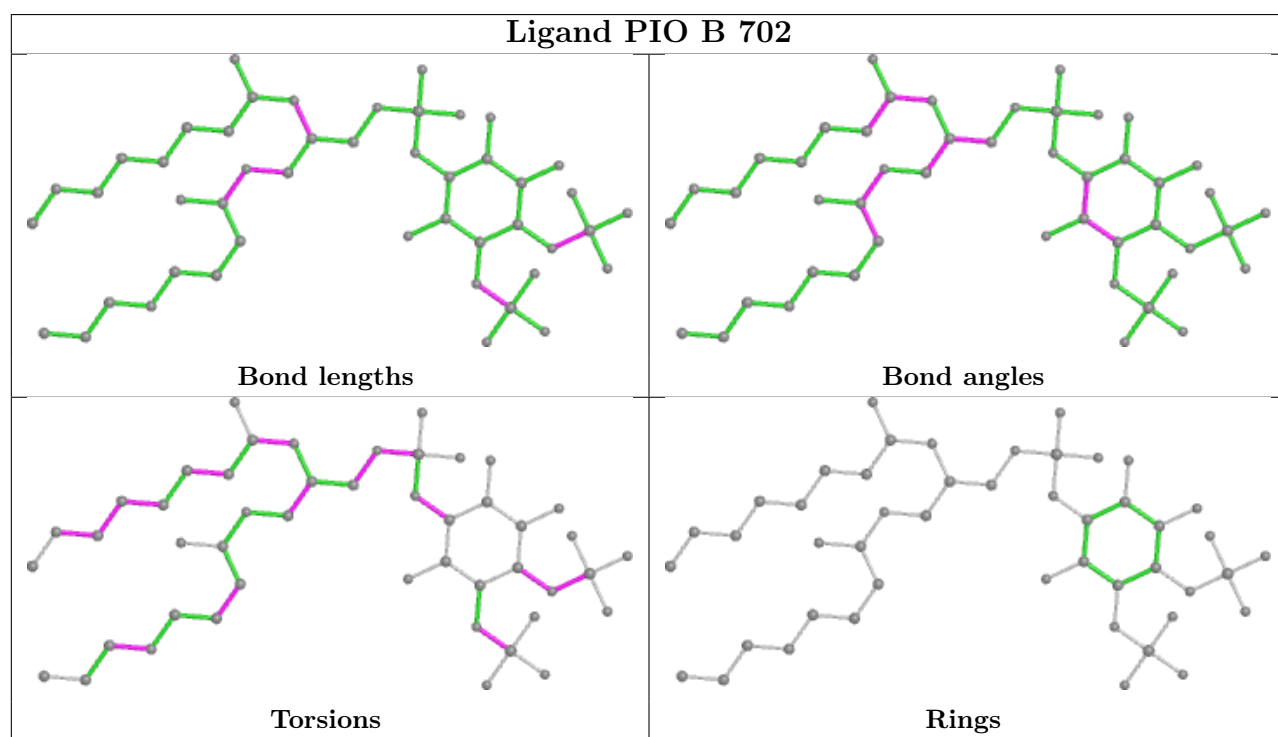
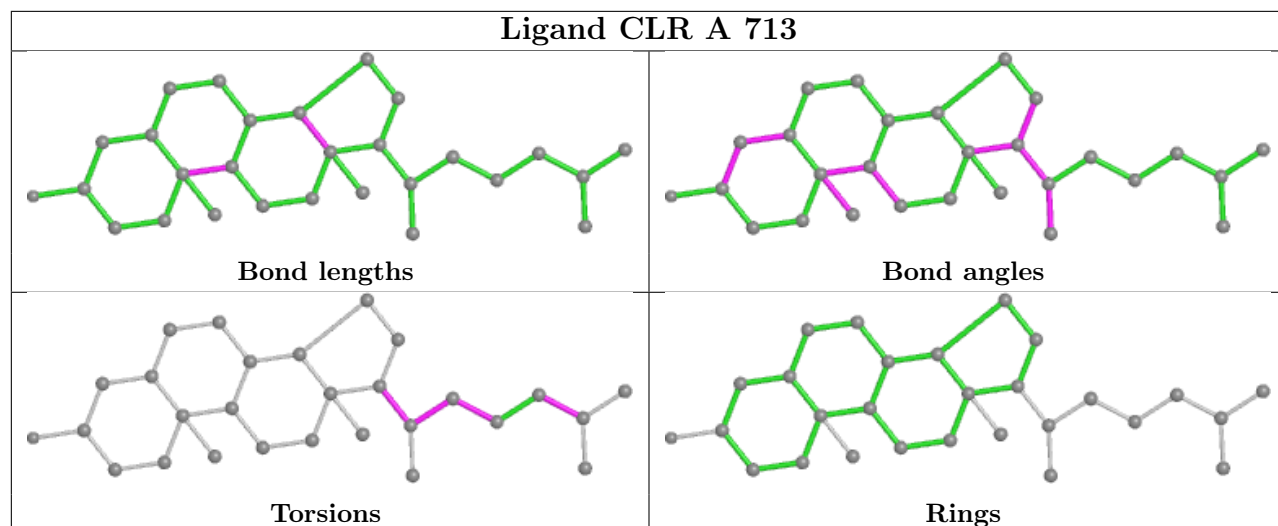
## Ligand 41U A 701



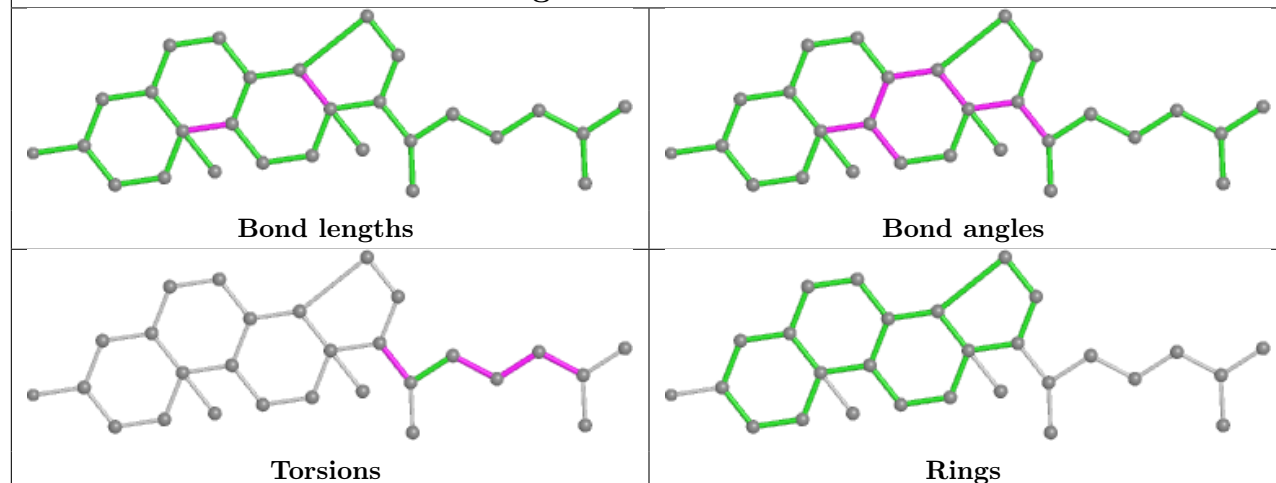
## Ligand CLR B 708



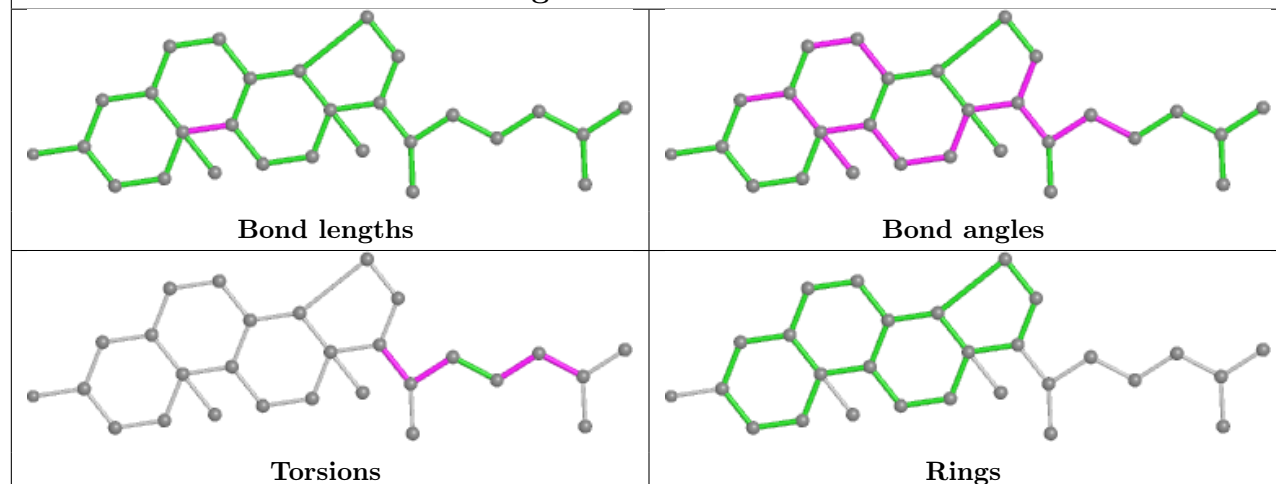




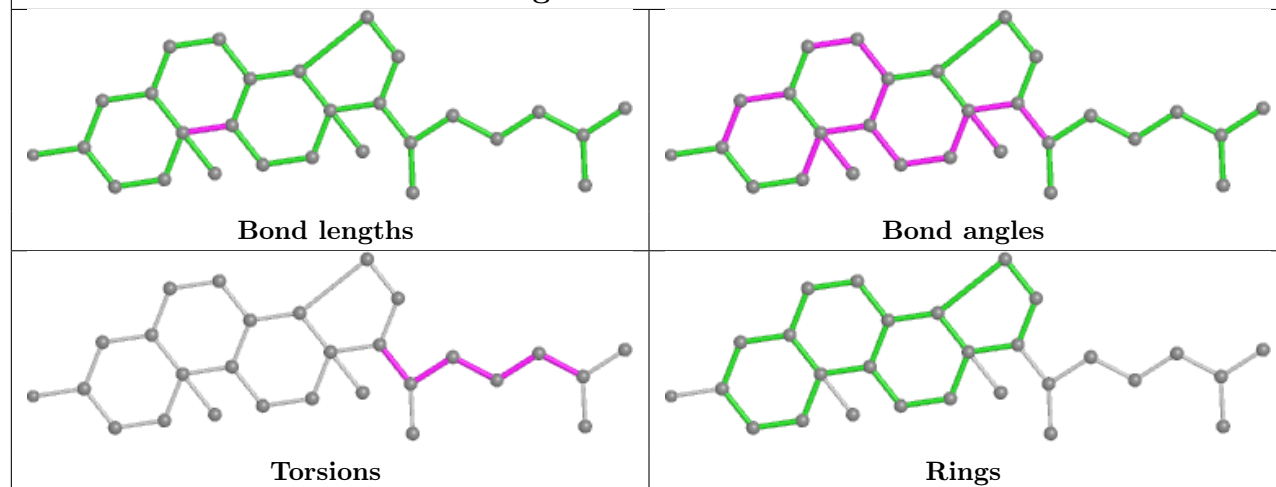
## Ligand CLR B 716



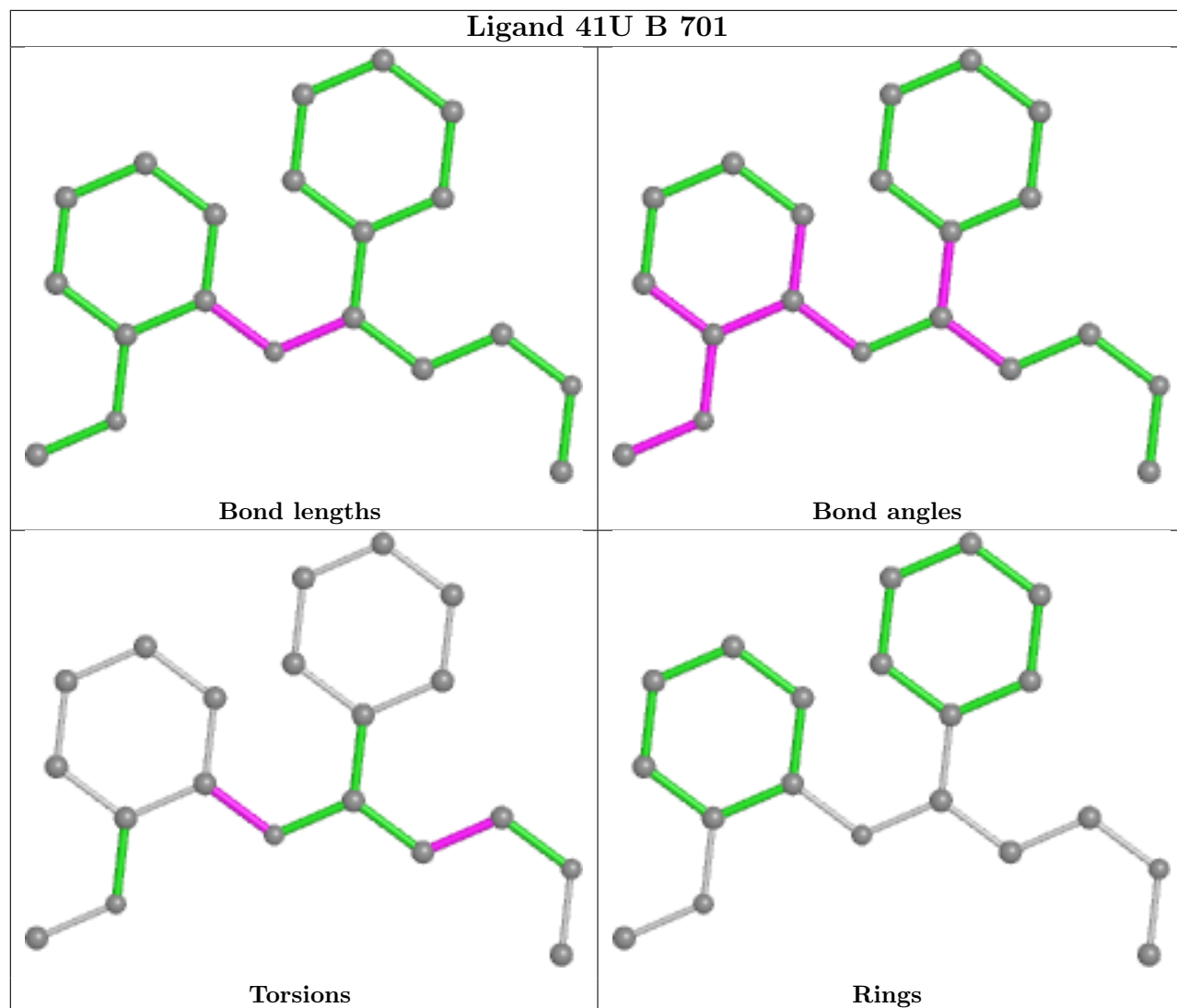
## Ligand CLR A 715



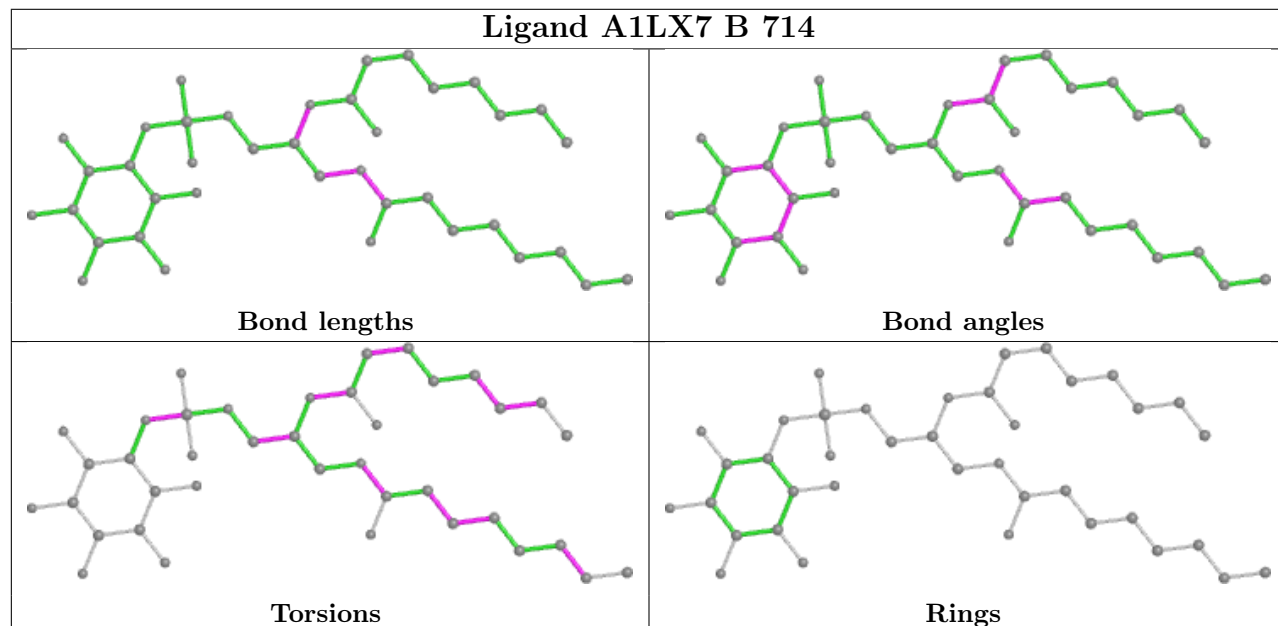
## Ligand CLR B 718

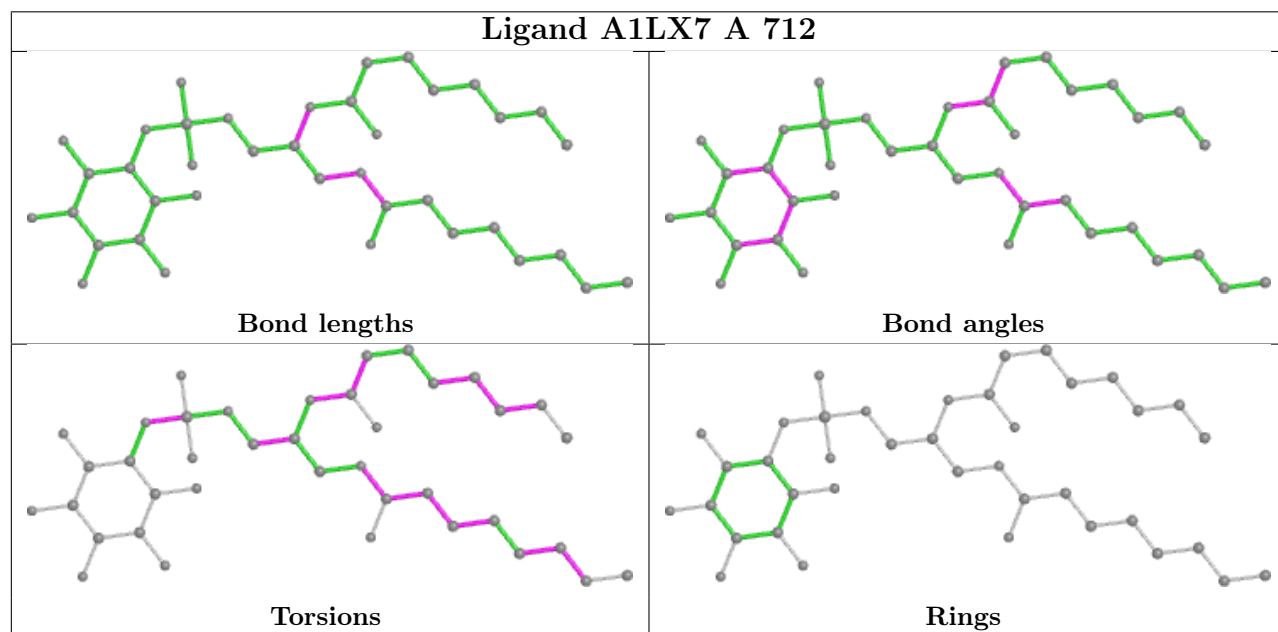
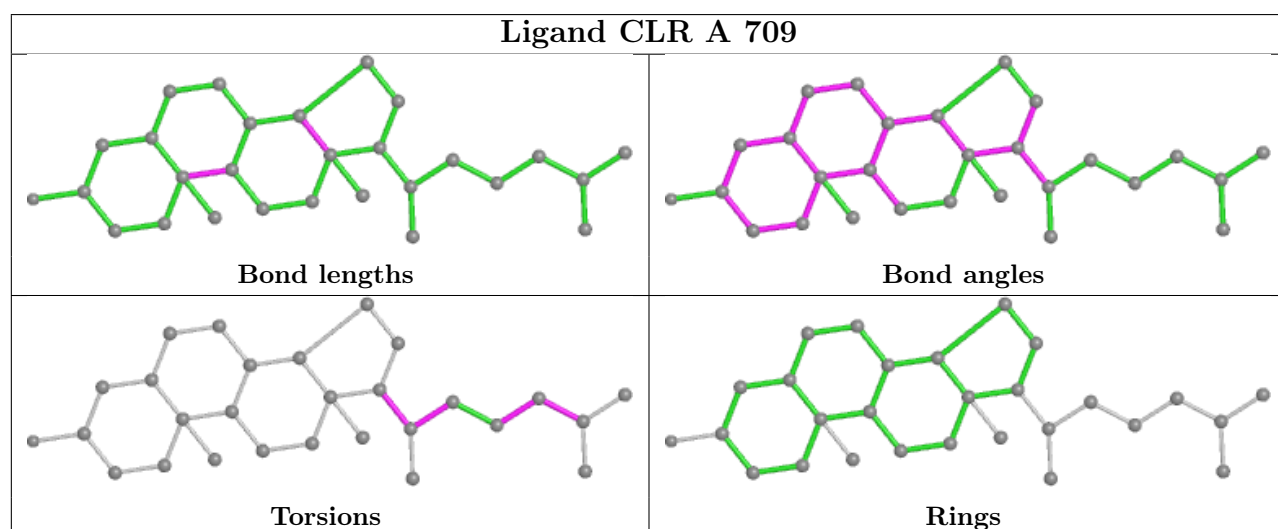
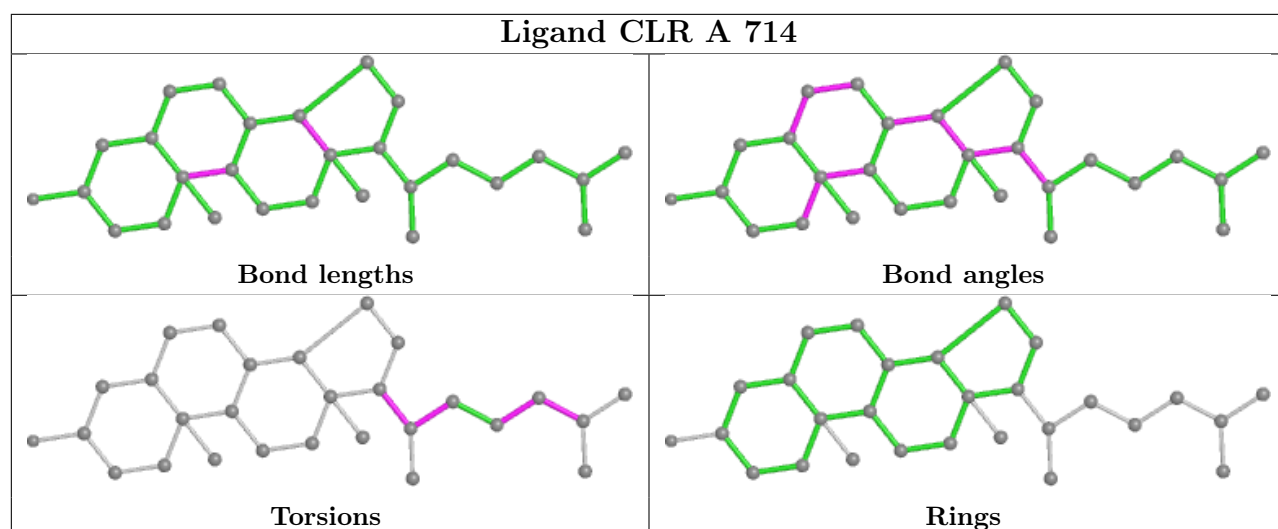


## Ligand 41U B 701



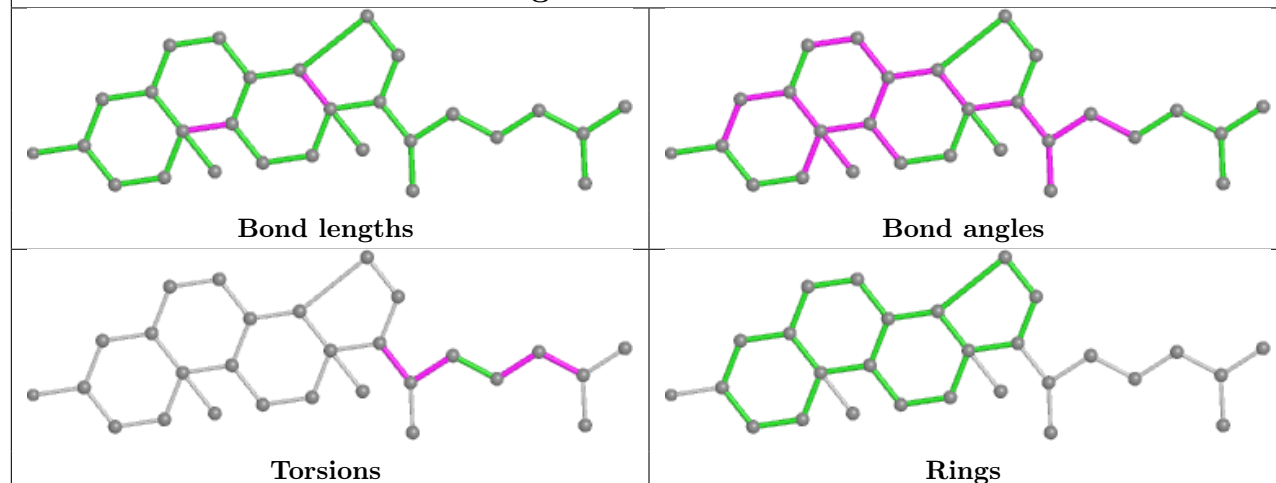
## Ligand A1LX7 B 714



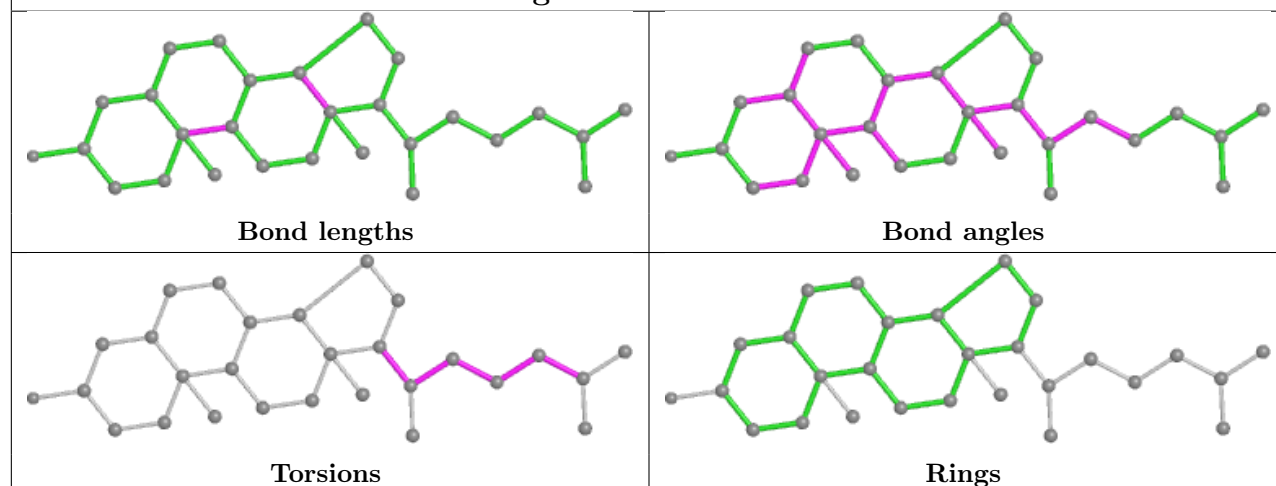




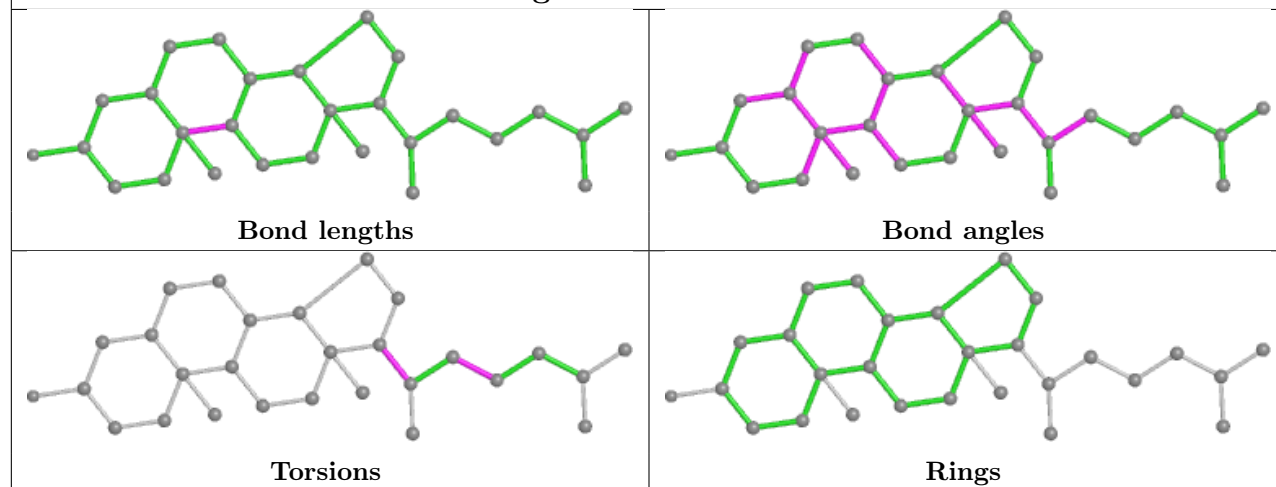
## Ligand CLR A 708

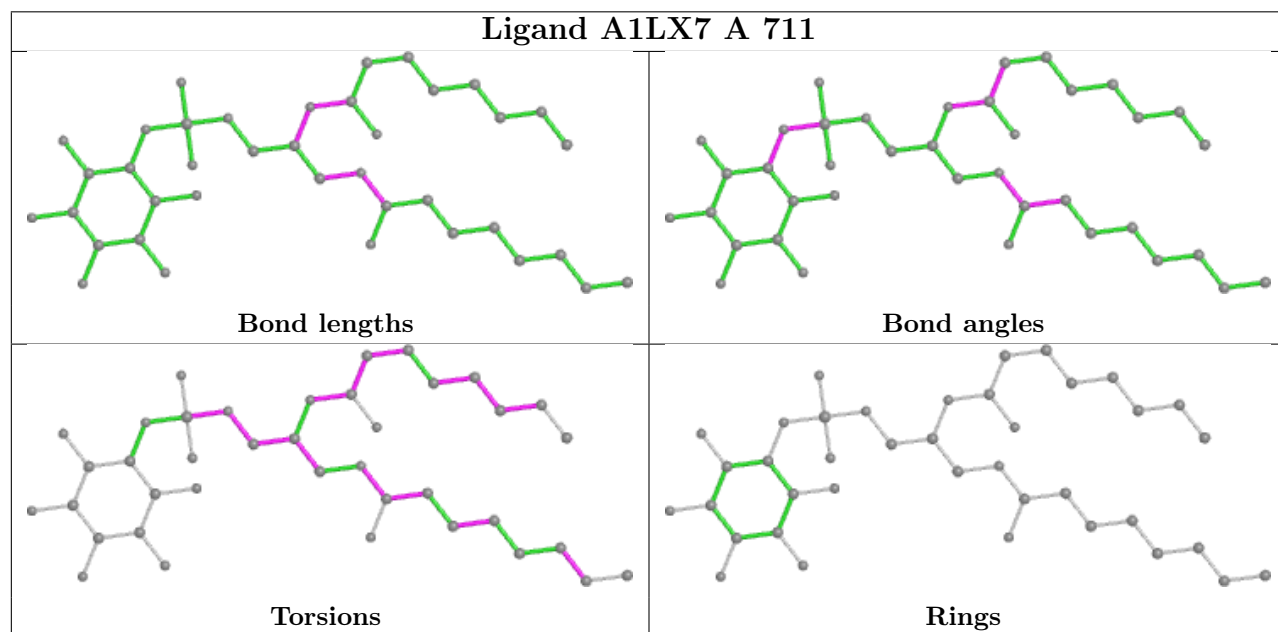
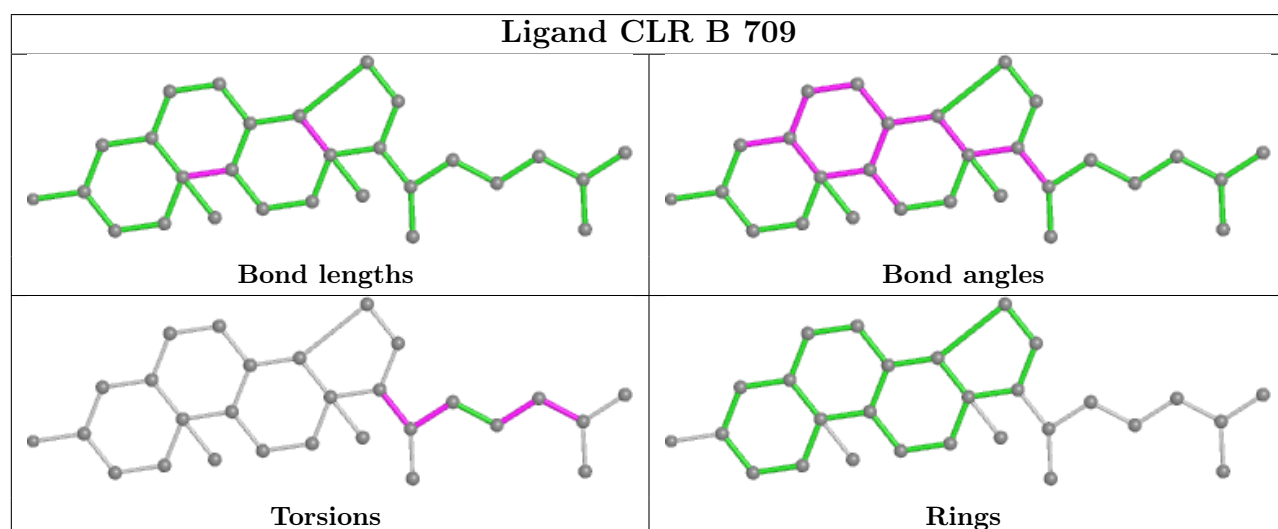
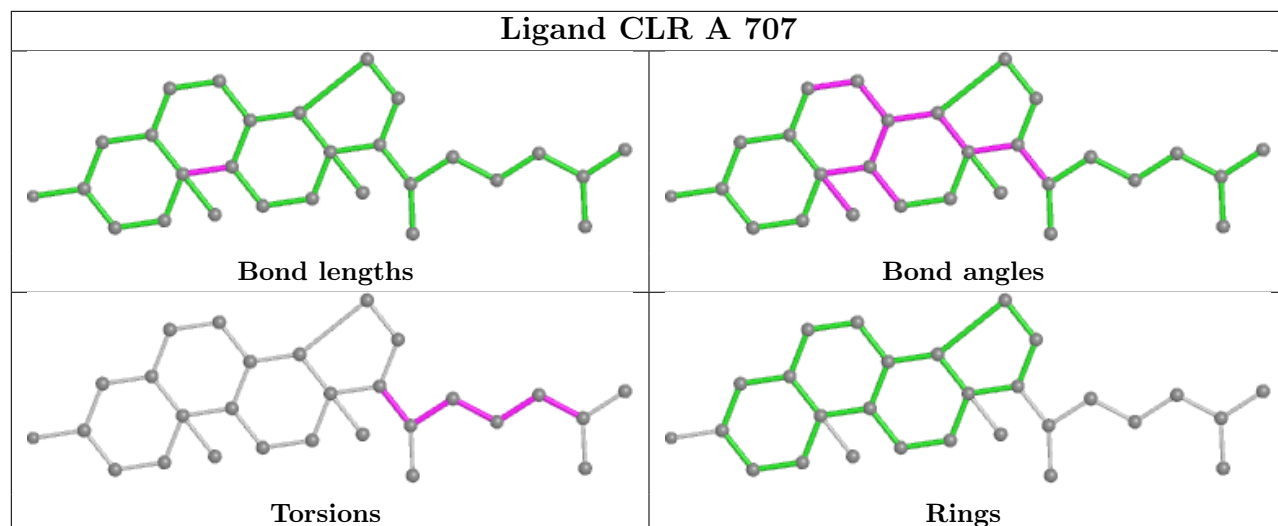


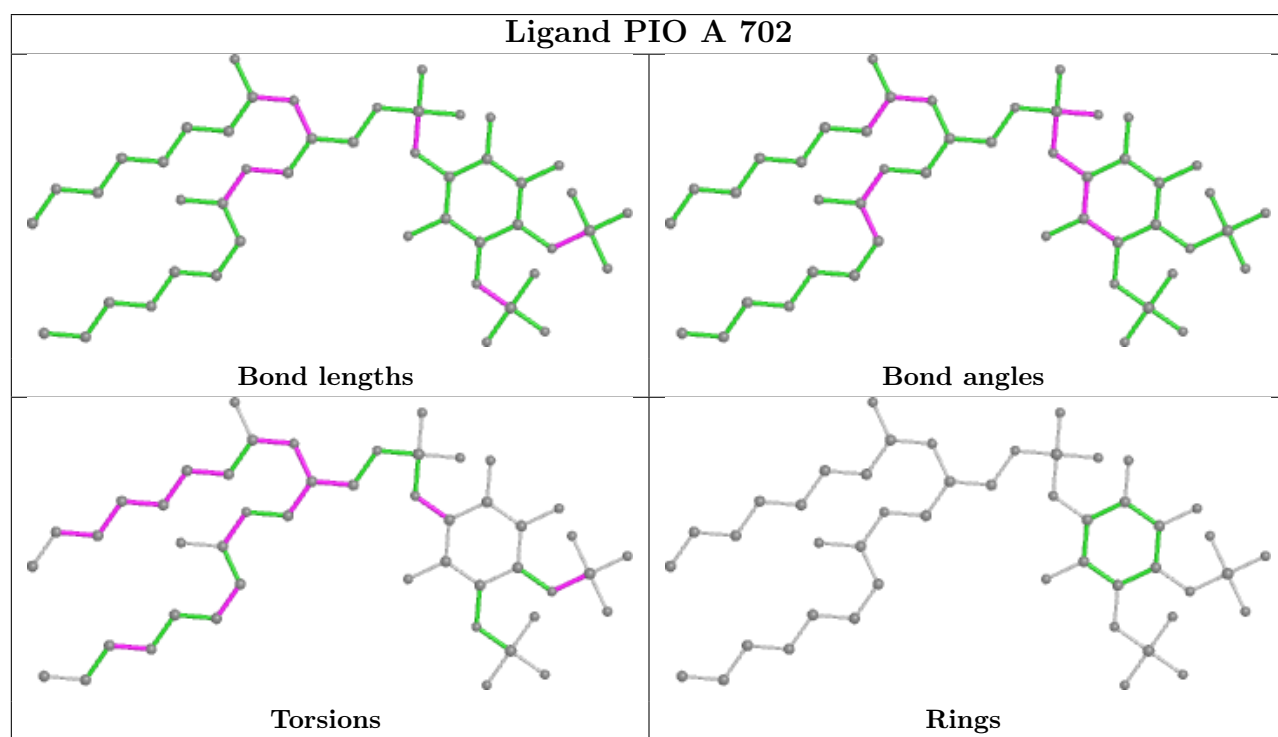
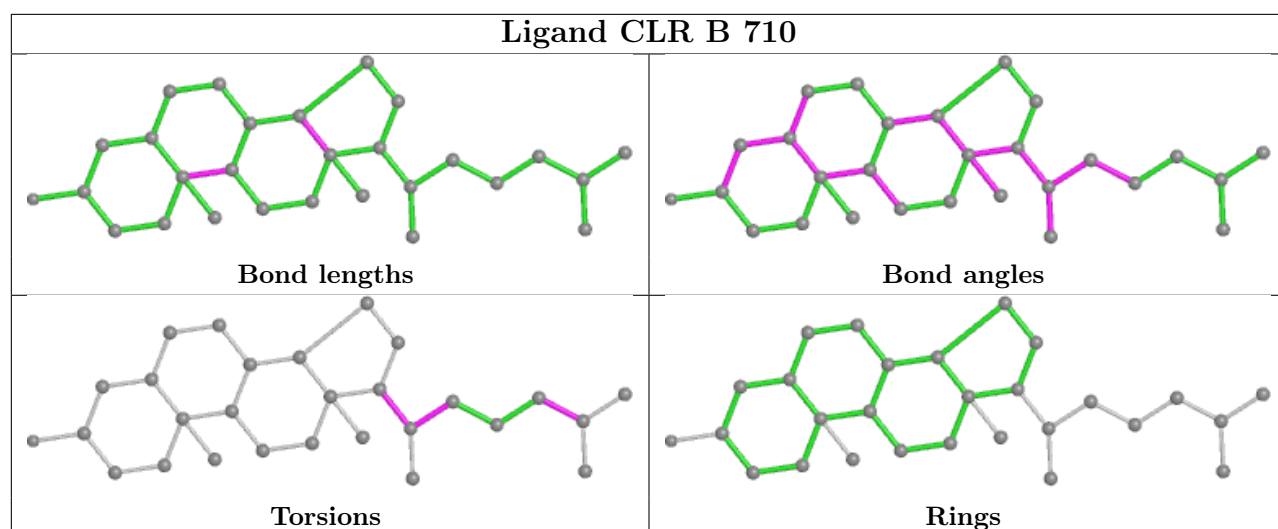
## Ligand CLR B 706

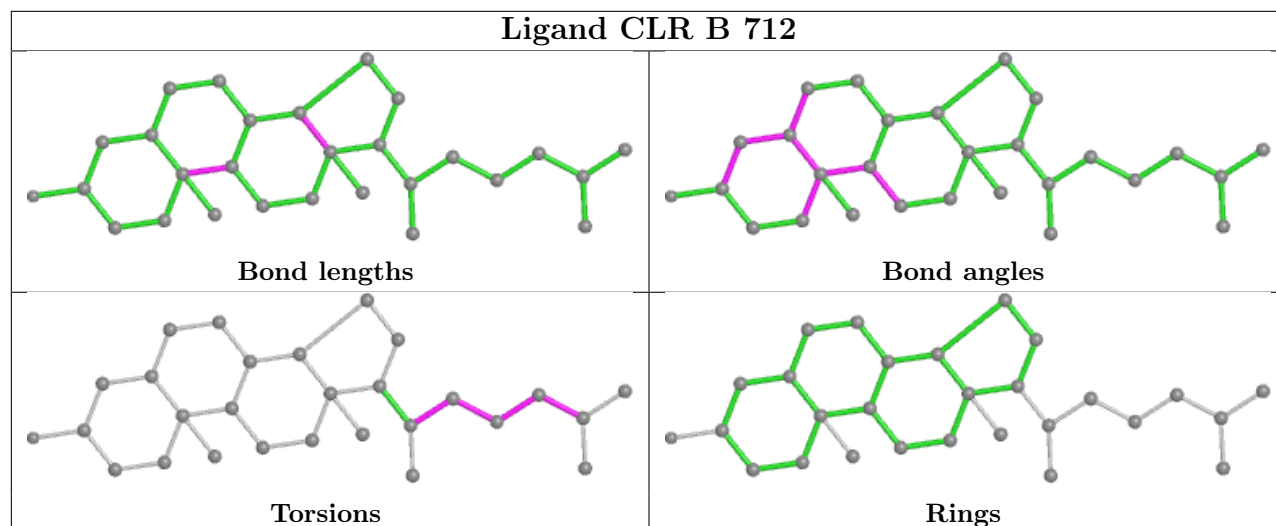


## Ligand CLR B 711









## 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.

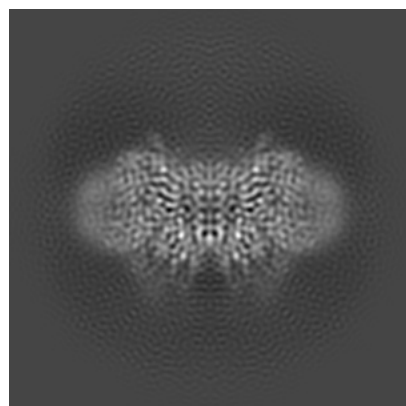
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39533. These allow visual inspection of the internal detail of the map and identification of artifacts.

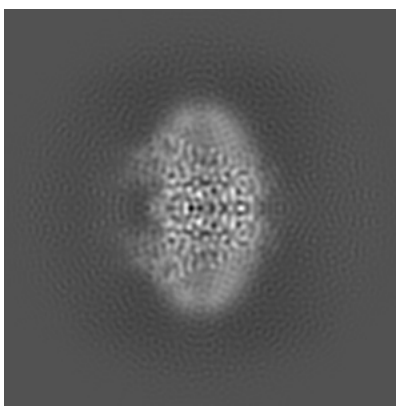
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

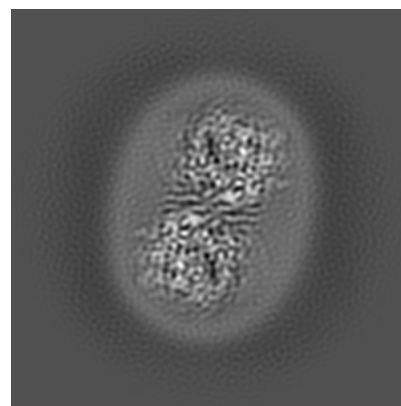
#### 6.1.1 Primary map



X

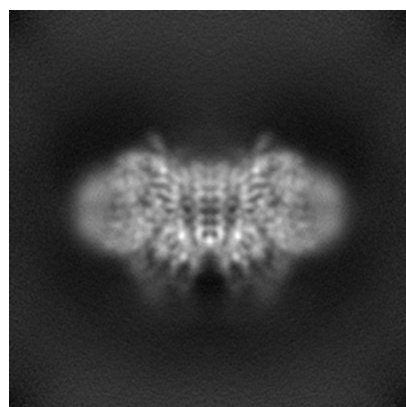


Y

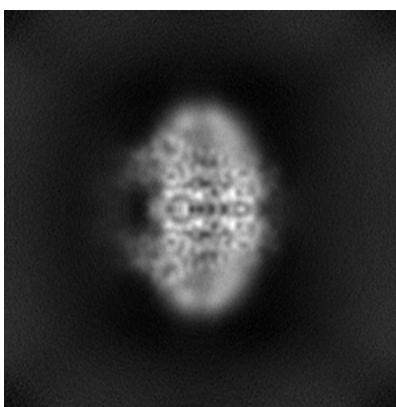


Z

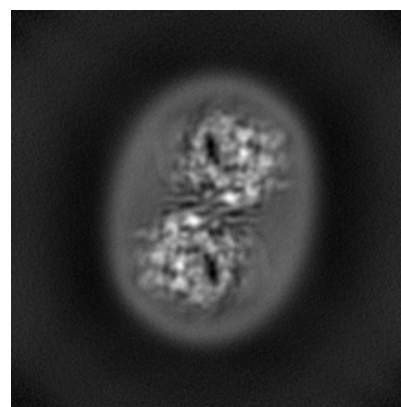
#### 6.1.2 Raw map



X



Y

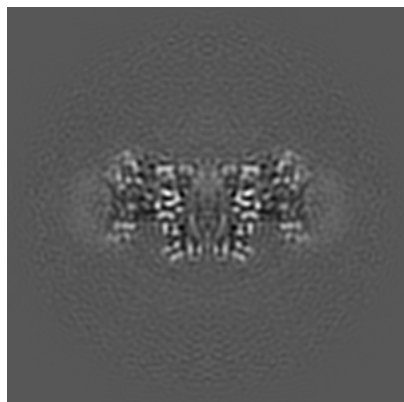


Z

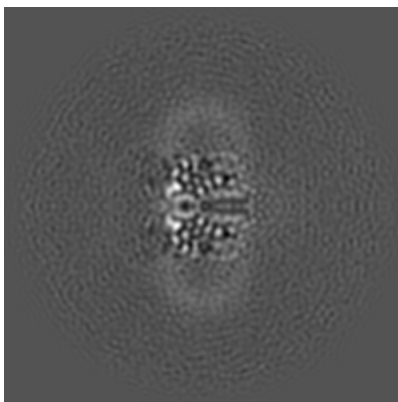
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

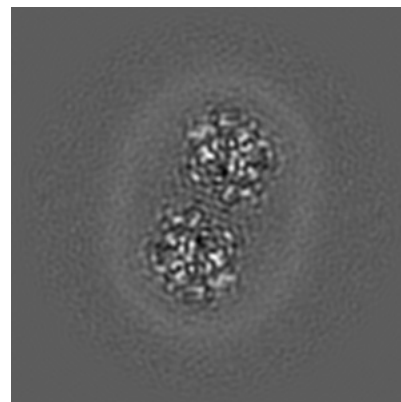
### 6.2.1 Primary map



X Index: 128

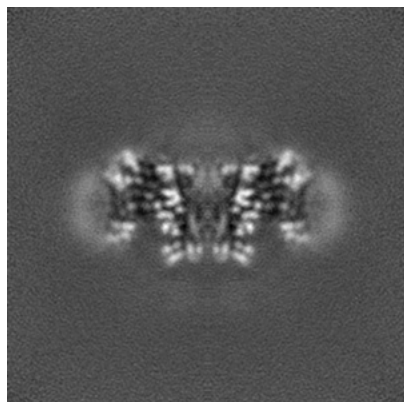


Y Index: 128

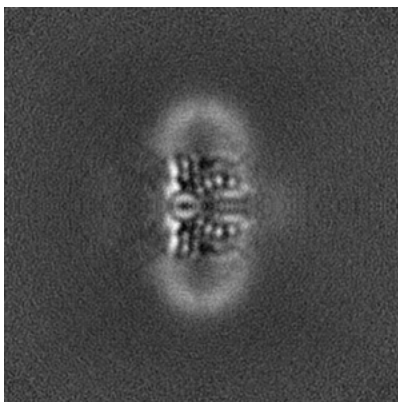


Z Index: 128

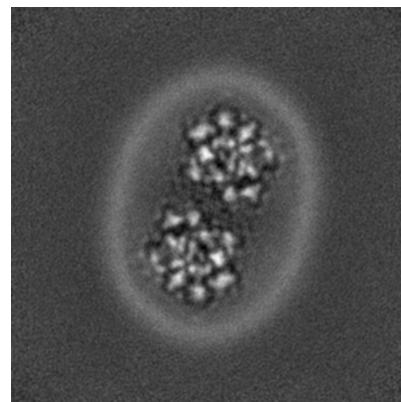
### 6.2.2 Raw map



X Index: 128



Y Index: 128

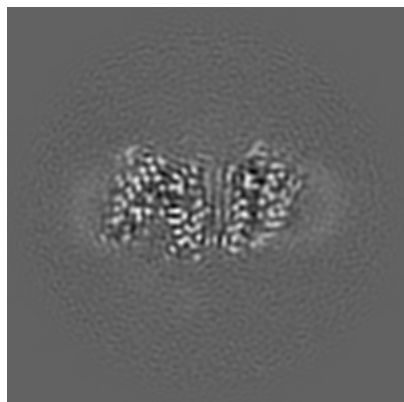


Z Index: 128

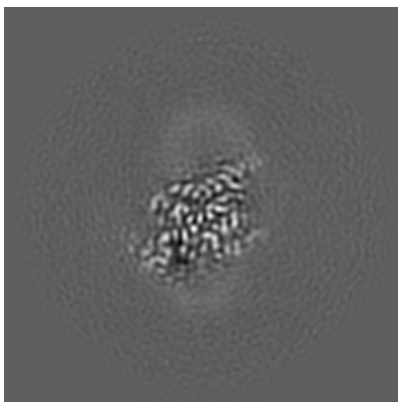
The images above show central slices of the map in three orthogonal directions.

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

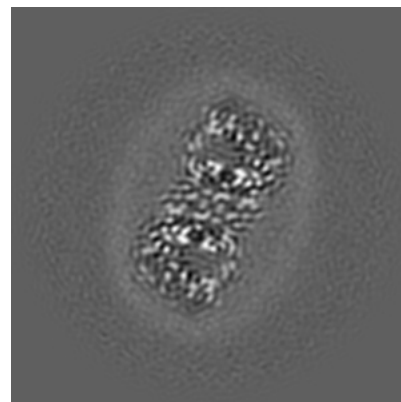
### 6.3.1 Primary map



X Index: 119

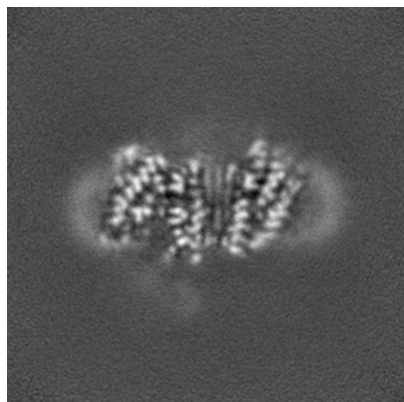


Y Index: 107

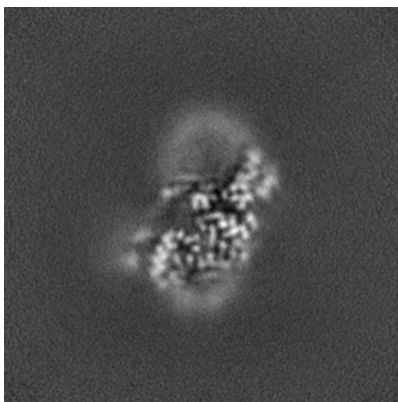


Z Index: 115

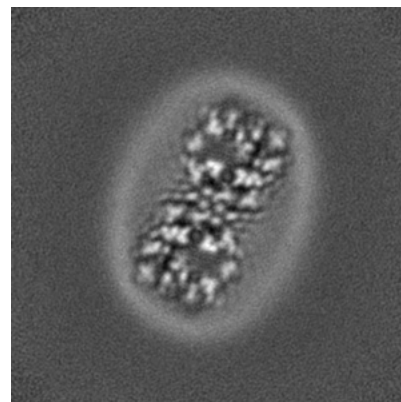
### 6.3.2 Raw map



X Index: 119



Y Index: 97



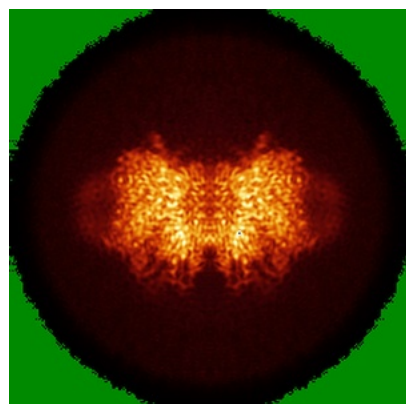
Z Index: 115

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

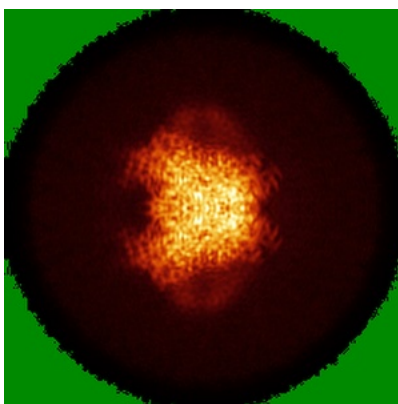


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

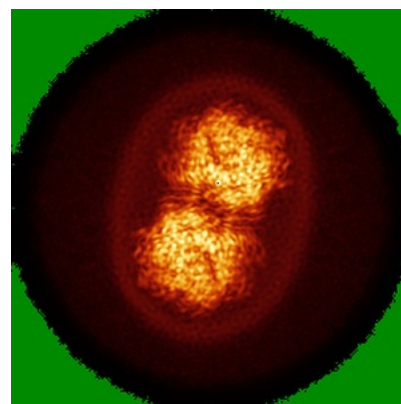
### 6.4.1 Primary map



X

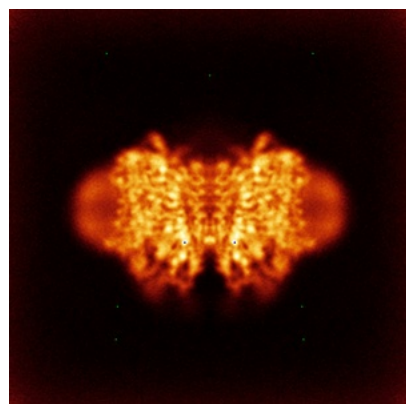


Y

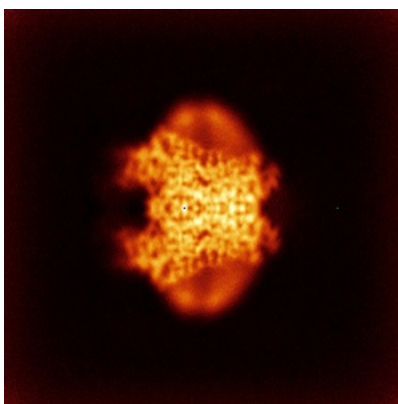


Z

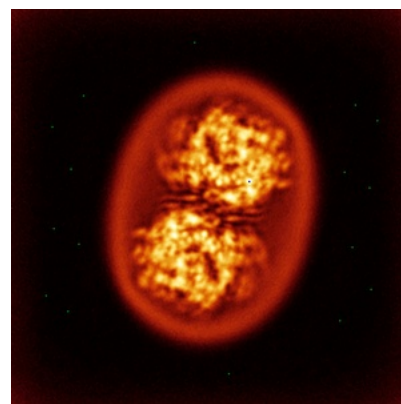
### 6.4.2 Raw map



X



Y



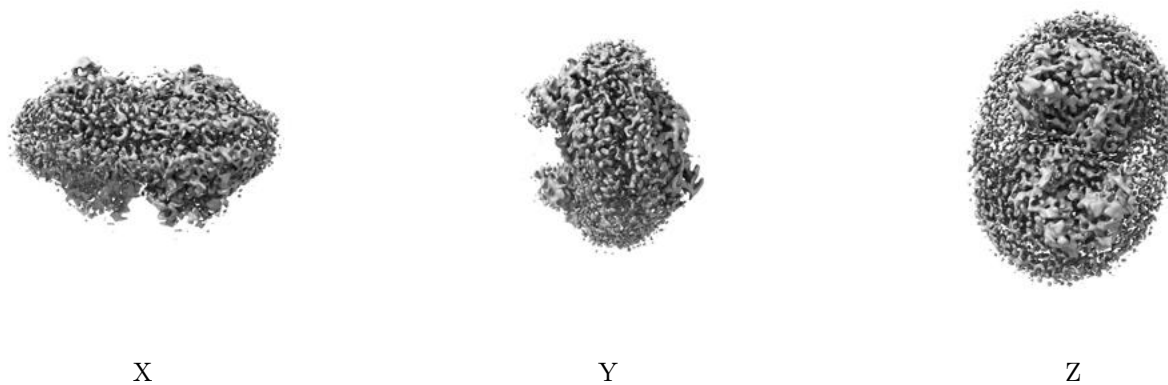
Z

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.



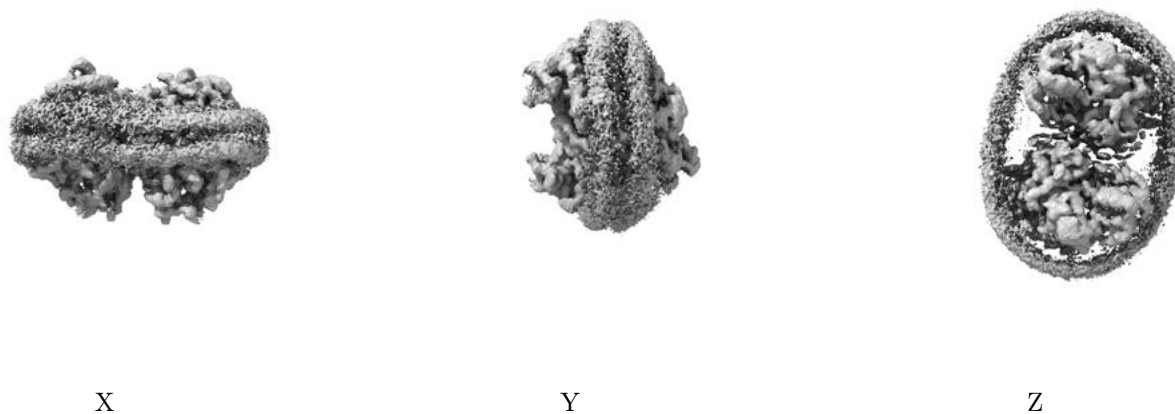
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

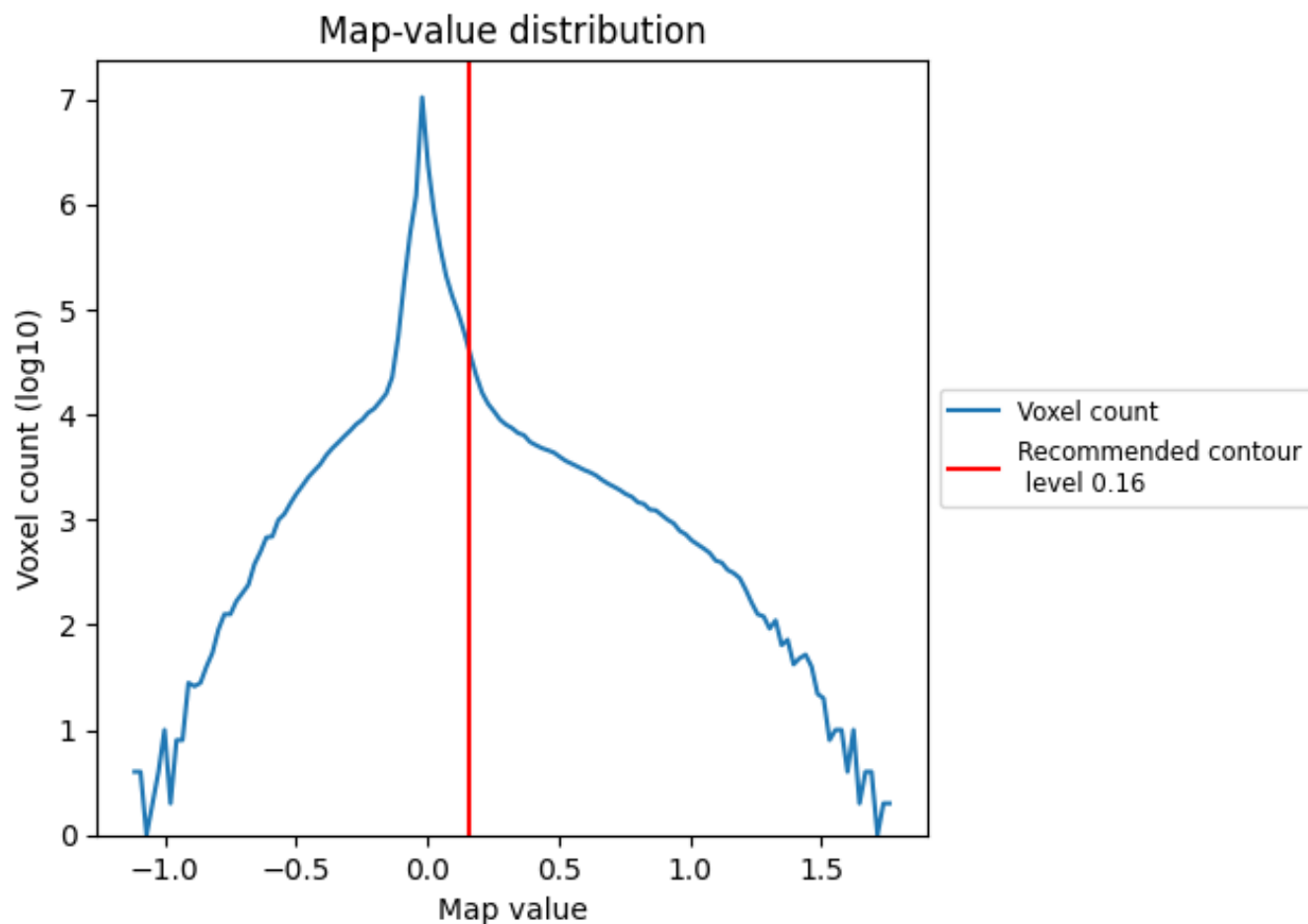
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

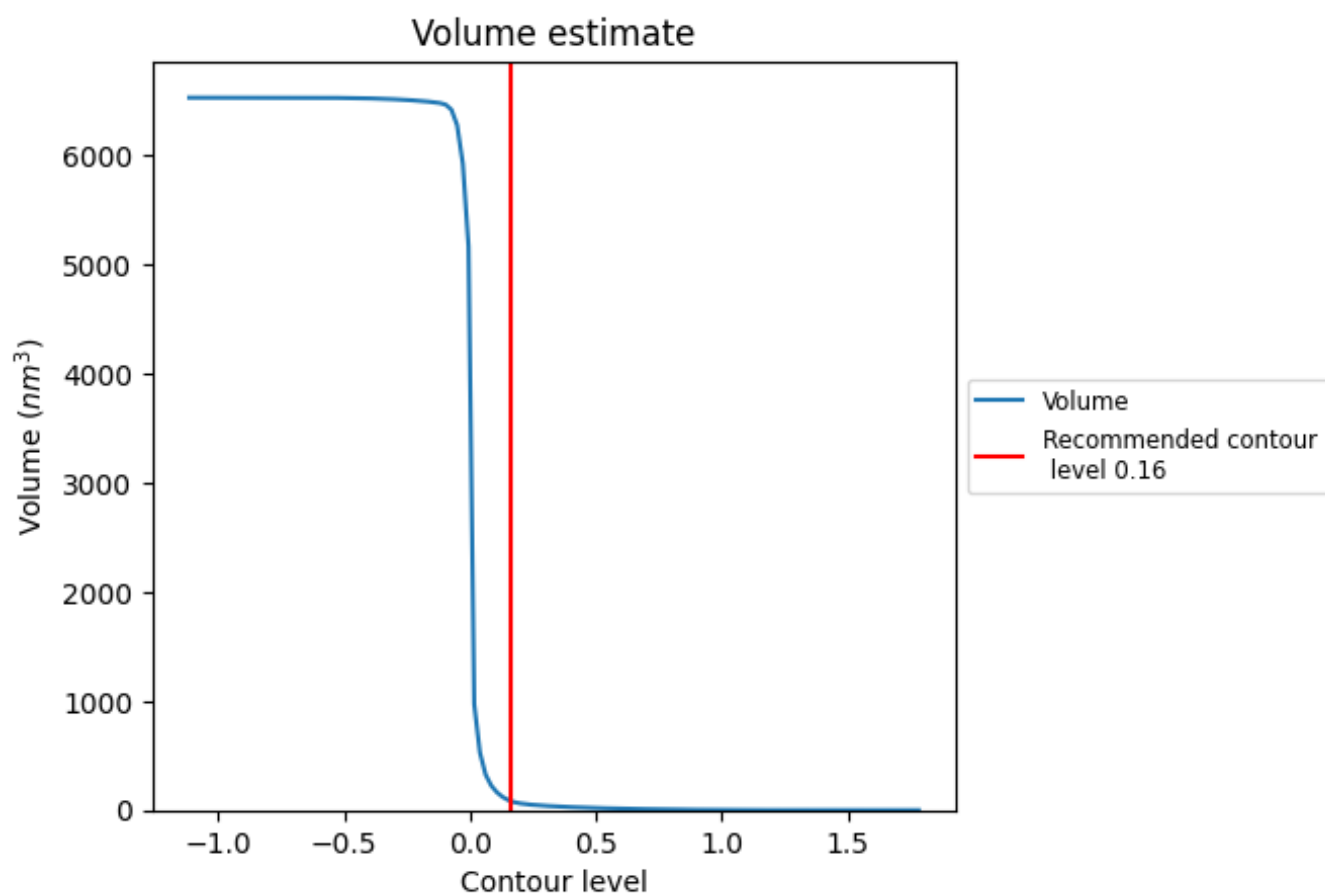
This section contains the results of statistical analysis of the map.

### 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.

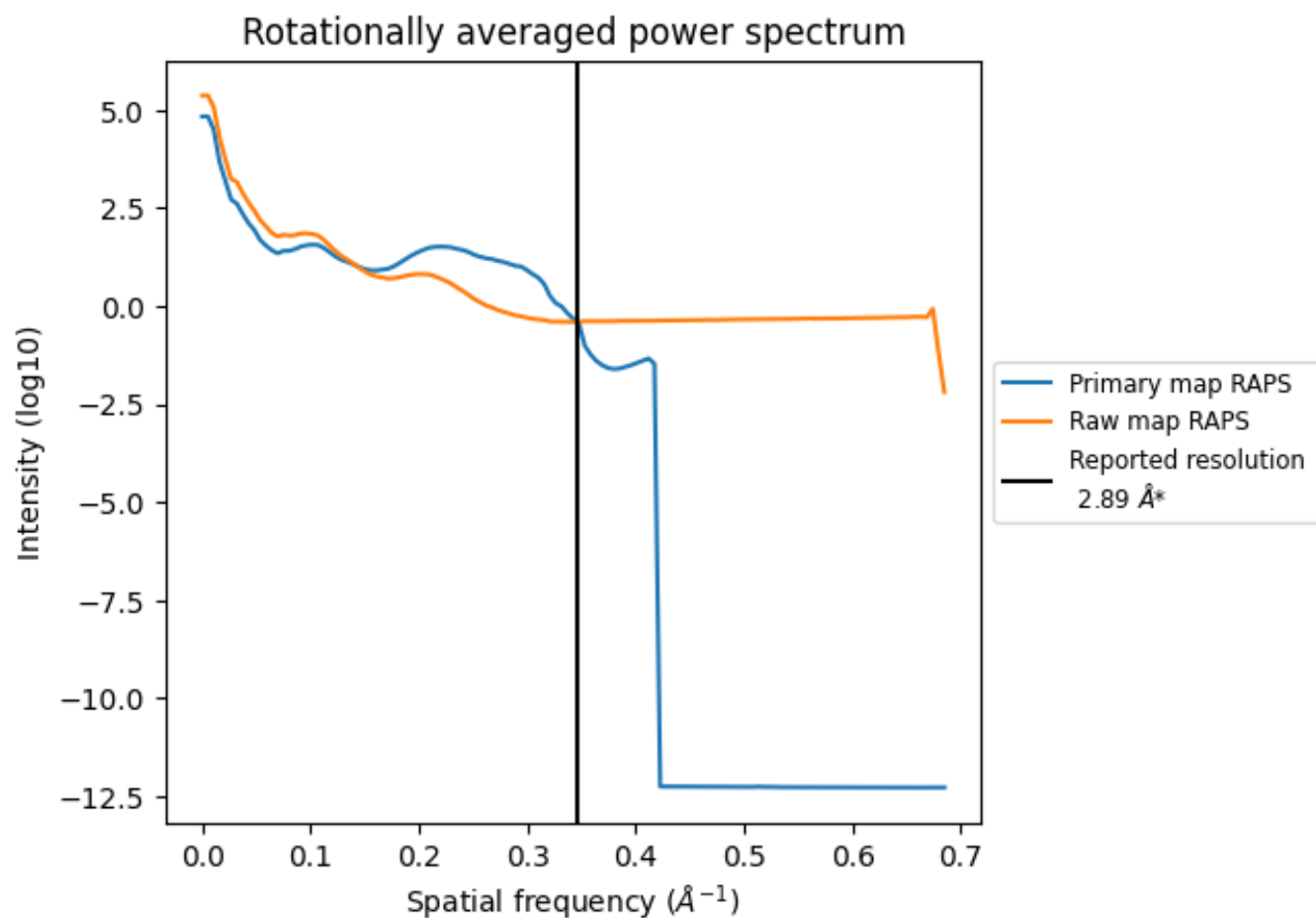
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 85  $\text{nm}^3$ ; this corresponds to an approximate mass of 77 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 ⓘ

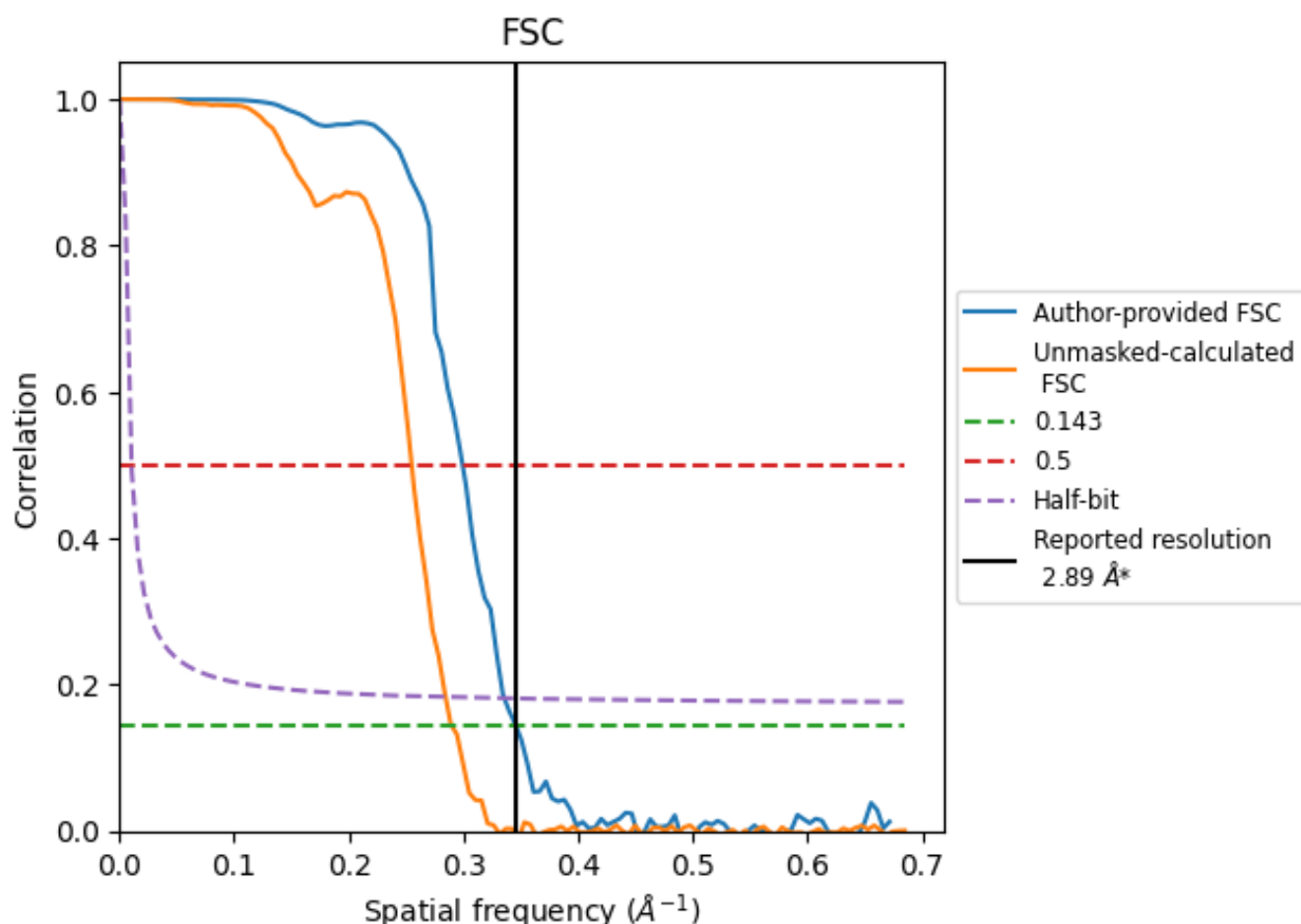


\*Reported resolution corresponds to spatial frequency of 0.346  $\text{\AA}^{-1}$

## 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 0.346 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

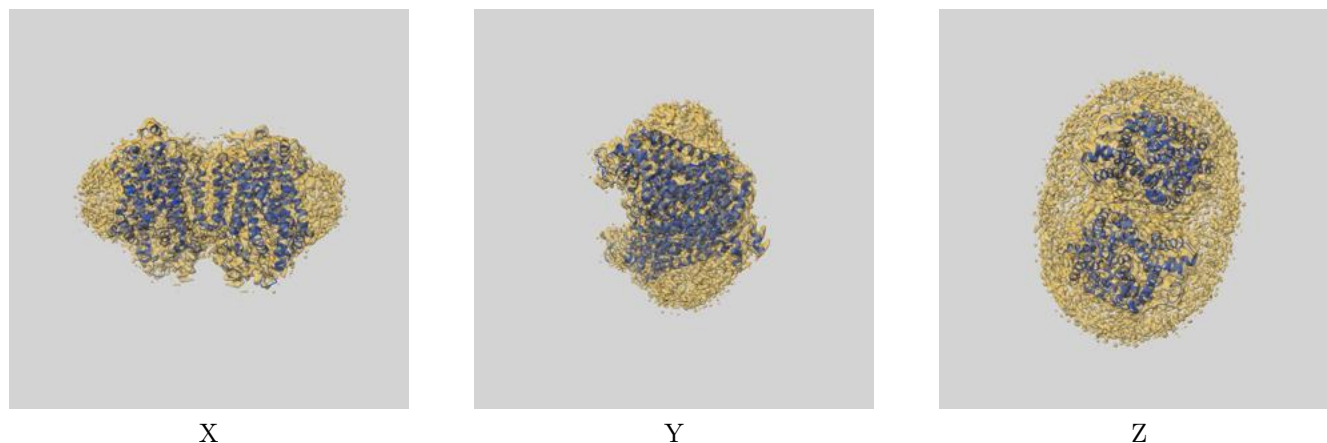
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	2.89	3.34	2.98
Unmasked-calculated*	3.45	3.92	3.52

\*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 3.45 differs from the reported value 2.89 by more than 10 %

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

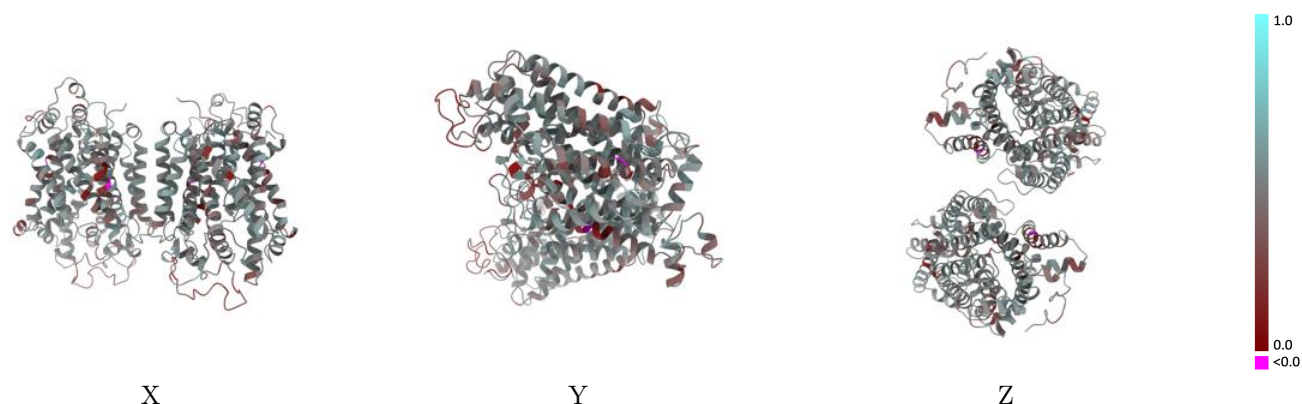
This section contains information regarding the fit between EMDB map EMD-39533 and PDB model 8YR2. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



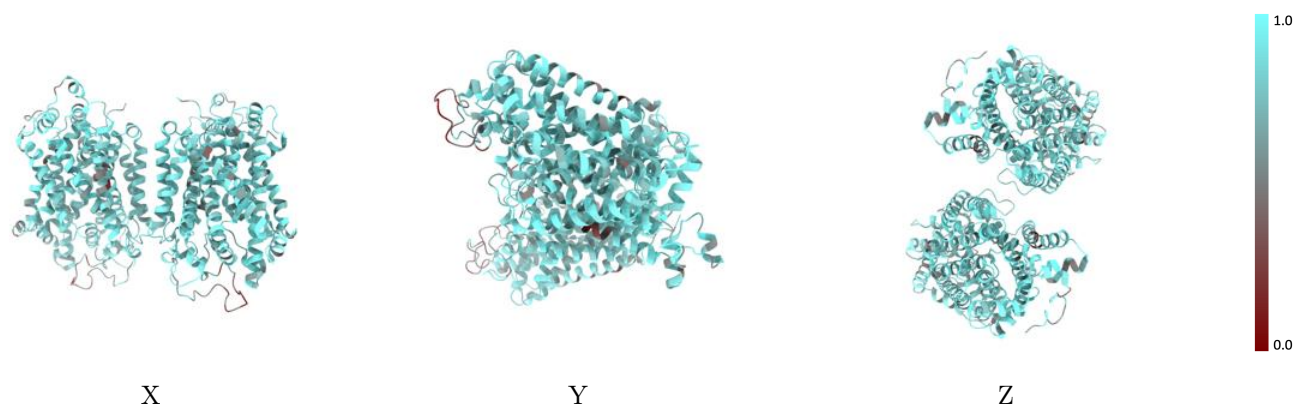
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

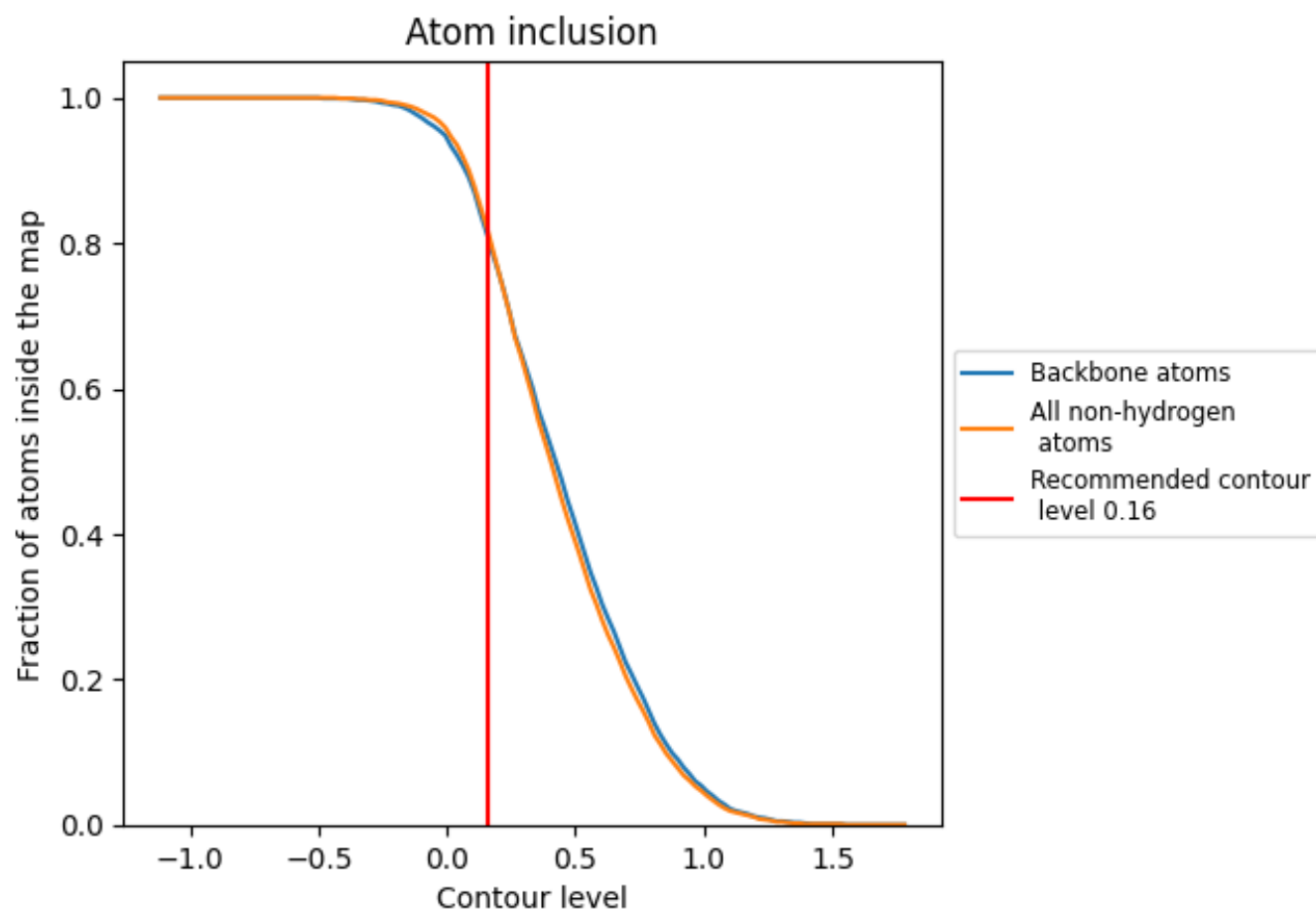
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.16).



## 9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 82% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8160	<div></div> 0.4700
A	<div></div> 0.8190	<div></div> 0.4700
B	<div></div> 0.8200	<div></div> 0.4690

