



Full wwPDB EM Validation Report ⓘ

Mar 26, 2025 – 02:24 PM JST

PDB ID : 9IUC
EMDB ID : EMD-60897
Title : Cryo-EM structure of human XPR1 in complex with InsP6 in closed state - in the presence of KIDINS220-1-432 without substrate KH2PO4
Authors : Zuo, P.; Liang, L.; Yin, Y.
Deposited on : 2024-07-20
Resolution : 3.80 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

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>.

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

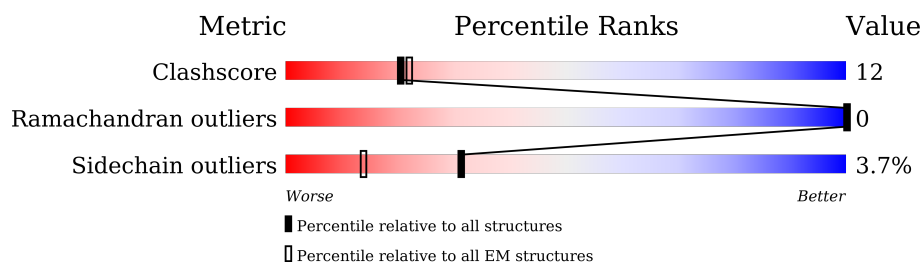
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	704	<div> <div>11%</div> <div>56%</div> <div>24%</div> <div>•</div> <div>19%</div> </div>
1	B	704	<div> <div>12%</div> <div>57%</div> <div>23%</div> <div>•</div> <div>19%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10360 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.

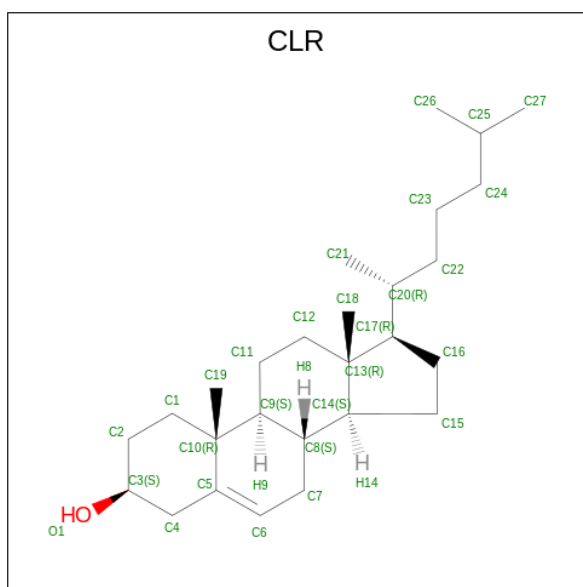
- Molecule 1 is a protein called Solute carrier family 53 member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	570	Total	C	N	O	S	0	0
			4765	3155	780	810	20		
1	B	570	Total	C	N	O	S	0	0
			4765	3155	780	810	20		

There are 16 discrepancies between the modelled and reference sequences:

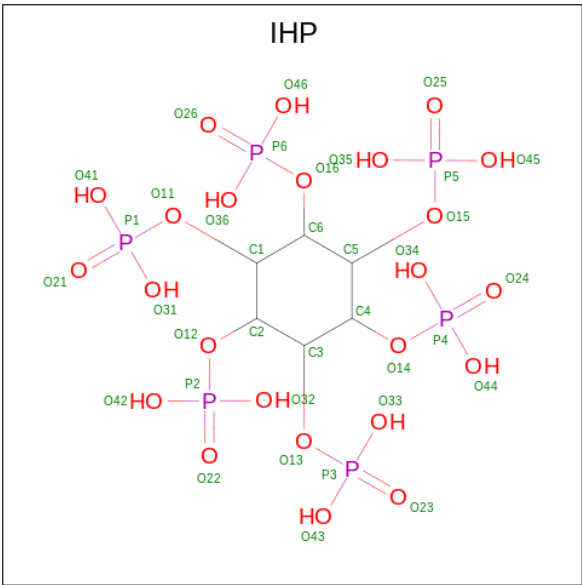
Chain	Residue	Modelled	Actual	Comment	Reference
A	697	SER	-	expression tag	UNP Q9UBH6
A	698	ARG	-	expression tag	UNP Q9UBH6
A	699	GLU	-	expression tag	UNP Q9UBH6
A	700	ASN	-	expression tag	UNP Q9UBH6
A	701	LEU	-	expression tag	UNP Q9UBH6
A	702	TYR	-	expression tag	UNP Q9UBH6
A	703	PHE	-	expression tag	UNP Q9UBH6
A	704	GLN	-	expression tag	UNP Q9UBH6
B	697	SER	-	expression tag	UNP Q9UBH6
B	698	ARG	-	expression tag	UNP Q9UBH6
B	699	GLU	-	expression tag	UNP Q9UBH6
B	700	ASN	-	expression tag	UNP Q9UBH6
B	701	LEU	-	expression tag	UNP Q9UBH6
B	702	TYR	-	expression tag	UNP Q9UBH6
B	703	PHE	-	expression tag	UNP Q9UBH6
B	704	GLN	-	expression tag	UNP Q9UBH6

- Molecule 2 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).



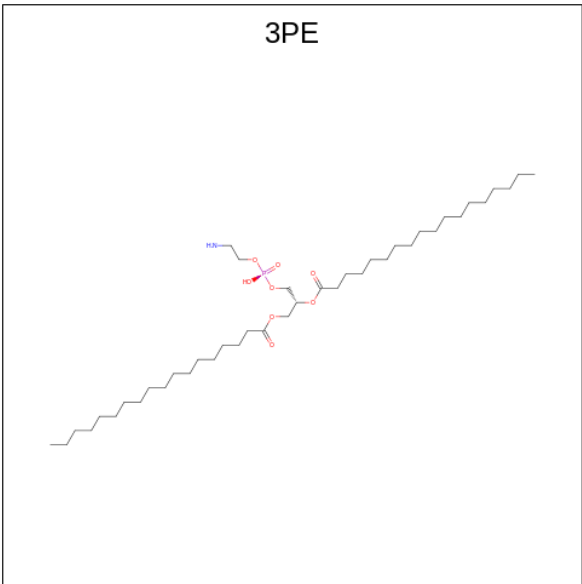
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	A	1	Total	C	O	0
			28	27	1	
2	B	1	Total	C	O	0
			28	27	1	
2	B	1	Total	C	O	0
			28	27	1	
2	B	1	Total	C	O	0
			28	27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

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			36	6	24	6	
3	B	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 4 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



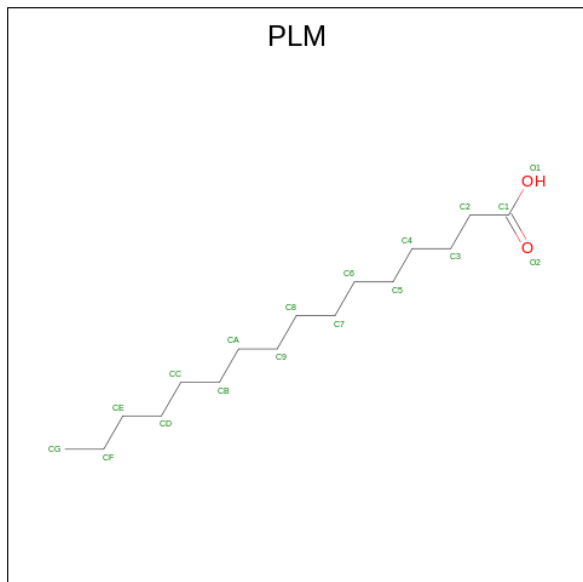
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

Continued on next page...

Continued from previous page...

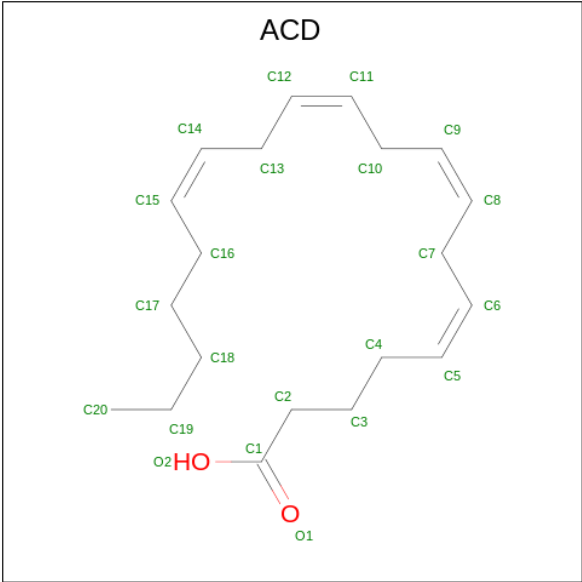
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	B	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			18	16	2	
5	A	1	Total	C	O	0
			18	16	2	
5	B	1	Total	C	O	0
			18	16	2	
5	B	1	Total	C	O	0
			18	16	2	

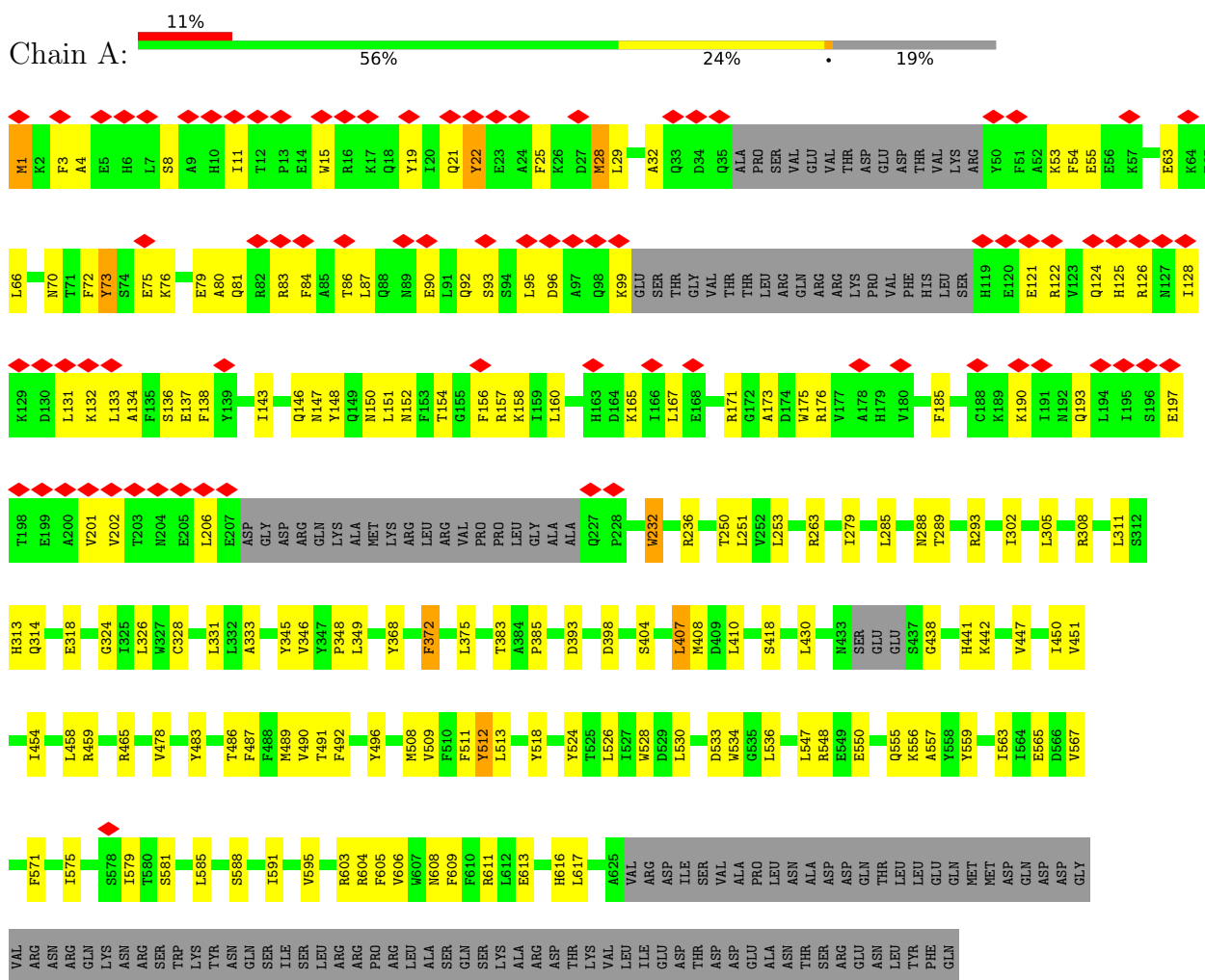
- Molecule 6 is ARACHIDONIC ACID (three-letter code: ACD) (formula: $C_{20}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



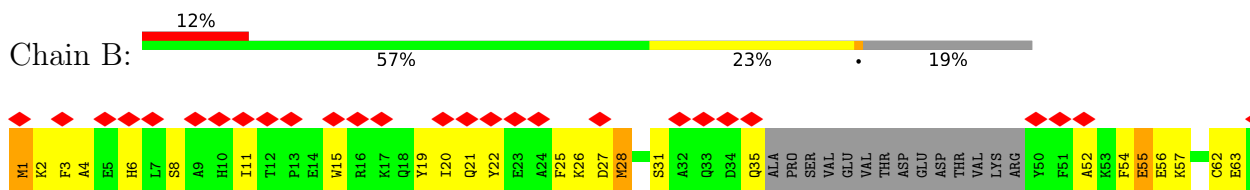
3 Residue-property plots

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

• Molecule 1: Solute carrier family 53 member 1



• Molecule 1: Solute carrier family 53 member 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88082	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)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.663	Depositor
Minimum map value	-0.472	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	296.0, 296.0, 296.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	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: PLM, CLR, IHP, 3PE, ACD

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	0.27	0/4905	0.50	0/6646
1	B	0.26	0/4905	0.47	0/6646
All	All	0.27	0/9810	0.48	0/13292

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	4765	0	4733	118	0
1	B	4765	0	4733	122	0
2	A	196	0	322	11	0
2	B	140	0	230	3	0
3	A	36	0	6	0	0
3	B	36	0	6	3	0
4	A	153	0	246	8	0
4	B	153	0	246	7	0
5	A	36	0	62	0	0
5	B	36	0	62	0	0
6	A	22	0	31	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	22	0	31	1	0
All	All	10360	0	10708	250	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.

All (250) 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:B:514:TRP:HE1	1:B:578:SER:HG	1.12	0.90
1:B:143:ILE:HA	1:B:146:GLN:HE22	1.48	0.77
1:A:548:ARG:NH1	1:A:613:GLU:OE2	2.25	0.69
1:B:491:THR:HG22	2:B:905:CLR:H71	1.73	0.68
1:A:368:TYR:HD2	1:A:372:PHE:HE2	1.42	0.68
1:A:132:LYS:HG2	1:A:206:LEU:HD22	1.74	0.68
1:A:533:ASP:OD1	1:A:611:ARG:NH1	2.27	0.68
1:B:534:TRP:O	1:B:548:ARG:NH1	2.27	0.66
1:B:533:ASP:OD1	1:B:611:ARG:NH1	2.29	0.66
1:B:526:LEU:HD21	1:B:567:VAL:HG22	1.77	0.66
1:A:143:ILE:O	1:A:147:ASN:ND2	2.28	0.66
1:B:202:VAL:HG22	1:B:206:LEU:HD12	1.76	0.66
1:A:171:ARG:O	1:A:175:TRP:N	2.30	0.65
1:B:161:LYS:HA	1:B:164:ASP:HB2	1.78	0.64
1:A:19:TYR:O	1:A:21:GLN:NE2	2.30	0.64
1:A:202:VAL:HG22	1:A:206:LEU:HD12	1.80	0.64
1:A:438:GLY:O	1:A:441:HIS:ND1	2.29	0.63
1:A:550:GLU:N	1:A:550:GLU:OE2	2.32	0.62
1:A:143:ILE:HA	1:A:146:GLN:HE21	1.65	0.62
1:A:575:ILE:O	1:A:579:ILE:HG12	2.00	0.62
1:A:3:PHE:HD1	1:A:308:ARG:HE	1.48	0.62
1:A:492:PHE:HE2	1:A:513:LEU:HD12	1.64	0.62
1:B:92:GLN:O	1:B:96:ASP:N	2.28	0.61
1:B:154:THR:HA	1:B:157:ARG:HE	1.64	0.61
1:A:63:GLU:HA	1:A:66:LEU:HB3	1.82	0.61
1:B:1:MET:N	3:B:903:IHP:O41	2.34	0.61
1:A:534:TRP:HB3	1:A:536:LEU:HD23	1.82	0.61
1:A:263:ARG:NH2	1:A:430:LEU:O	2.35	0.60
1:A:385:PRO:O	1:A:465:ARG:NH1	2.35	0.60
1:B:263:ARG:NH2	1:B:430:LEU:O	2.36	0.59
1:A:550:GLU:HB2	1:A:617:LEU:HD21	1.84	0.59
1:A:491:THR:HG22	2:A:804:CLR:H71	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:VAL:O	1:A:451:VAL:HG12	2.03	0.58
4:B:901:3PE:H371	4:B:901:3PE:H2A2	1.85	0.57
1:B:161:LYS:C	1:B:165:LYS:HZ3	2.08	0.57
1:B:132:LYS:HG2	1:B:206:LEU:HD22	1.85	0.57
1:B:156:PHE:O	1:B:160:LEU:HG	2.04	0.56
1:B:125:HIS:HA	1:B:128:ILE:HB	1.87	0.56
1:A:63:GLU:HG3	1:A:175:TRP:HZ2	1.71	0.56
1:B:548:ARG:NH2	1:B:613:GLU:OE2	2.39	0.56
1:A:125:HIS:HA	1:A:128:ILE:HB	1.88	0.55
1:B:171:ARG:O	1:B:175:TRP:N	2.40	0.55
1:A:154:THR:O	1:A:158:LYS:HG2	2.07	0.54
2:A:806:CLR:H151	4:B:901:3PE:H372	1.89	0.54
1:B:138:PHE:HA	1:B:141:SER:HB3	1.89	0.54
1:A:404:SER:HA	1:A:407:LEU:HD12	1.89	0.54
1:A:509:VAL:HA	1:A:512:TYR:CD2	2.42	0.54
1:A:8:SER:HA	1:A:11:ILE:HD12	1.89	0.54
2:A:806:CLR:H6	4:B:901:3PE:H331	1.90	0.54
1:A:55:GLU:HG3	1:A:167:LEU:HD12	1.89	0.53
1:B:157:ARG:O	1:B:161:LYS:HG2	2.07	0.53
1:B:550:GLU:HB2	1:B:617:LEU:HD21	1.91	0.53
1:B:28:MET:HA	1:B:31:SER:HB3	1.90	0.53
1:B:81:GLN:HA	1:B:84:PHE:HB2	1.90	0.53
4:A:813:3PE:H331	2:A:814:CLR:H6	1.90	0.53
1:A:148:TYR:O	1:A:152:ASN:ND2	2.42	0.52
1:B:121:GLU:HA	1:B:124:GLN:HB3	1.92	0.52
1:B:2:LYS:NZ	3:B:903:IHP:O21	2.42	0.52
1:A:126:ARG:NH1	1:B:27:ASP:OD2	2.42	0.52
1:B:8:SER:HA	1:B:11:ILE:HD12	1.90	0.52
1:B:19:TYR:O	1:B:21:GLN:NE2	2.42	0.52
1:B:202:VAL:HA	1:B:206:LEU:HB2	1.92	0.52
1:B:63:GLU:HG3	1:B:175:TRP:HZ2	1.74	0.52
1:A:128:ILE:O	1:A:132:LYS:HG3	2.10	0.52
1:B:138:PHE:O	1:B:142:LEU:N	2.33	0.52
1:A:81:GLN:HA	1:A:84:PHE:HB2	1.92	0.51
1:A:450:ILE:HD13	2:A:804:CLR:H181	1.91	0.51
1:A:73:TYR:CD2	1:A:185:PHE:HA	2.45	0.51
1:B:308:ARG:O	1:B:308:ARG:NE	2.36	0.51
1:A:588:SER:HA	1:A:591:ILE:HG22	1.92	0.51
1:B:73:TYR:CD2	1:B:185:PHE:HA	2.45	0.51
1:A:346:VAL:HA	1:A:349:LEU:HD13	1.92	0.51
1:A:398:ASP:OD2	1:A:483:TYR:OH	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLN:H	1:A:92:GLN:CD	2.13	0.51
1:A:232:TRP:HZ3	4:B:908:3PE:H2	1.75	0.51
1:A:279:ILE:HD13	1:A:324:GLY:HA2	1.93	0.51
1:B:148:TYR:O	1:B:152:ASN:ND2	2.44	0.51
1:A:526:LEU:HD21	1:A:567:VAL:HG22	1.92	0.51
4:A:813:3PE:H3B1	1:B:333:ALA:HB2	1.93	0.50
1:B:302:ILE:HD11	1:B:616:HIS:HB2	1.93	0.50
1:B:534:TRP:HB3	1:B:536:LEU:HD23	1.94	0.50
1:B:536:LEU:HD12	1:B:547:LEU:HA	1.93	0.50
1:A:146:GLN:O	1:A:150:ASN:ND2	2.43	0.50
1:A:250:THR:HG21	4:B:901:3PE:H281	1.94	0.50
1:A:486:THR:O	1:A:490:VAL:HG23	2.11	0.50
1:A:1:MET:CE	1:A:3:PHE:H	2.25	0.50
1:A:534:TRP:O	1:A:548:ARG:NH2	2.41	0.50
1:B:569:LEU:HD11	1:B:599:LEU:HD22	1.94	0.50
1:A:32:ALA:HB2	1:A:54:PHE:CE2	2.47	0.50
1:B:96:ASP:HA	1:B:99:LYS:HD2	1.92	0.49
1:A:313:HIS:CD2	1:A:314:GLN:HG3	2.48	0.49
1:B:349:LEU:HD11	1:B:417:TYR:HE2	1.78	0.49
1:B:410:LEU:HD11	2:B:910:CLR:H273	1.94	0.49
1:B:438:GLY:H	1:B:441:HIS:CE1	2.31	0.49
1:B:146:GLN:O	1:B:150:ASN:N	2.31	0.49
1:A:288:ASN:HD21	1:A:608:ASN:HB3	1.78	0.49
1:B:506:ASP:OD1	1:B:506:ASP:N	2.36	0.49
1:A:122:ARG:HA	1:A:125:HIS:NE2	2.27	0.49
1:B:570:ARG:HE	1:B:603:ARG:NH1	2.10	0.49
1:A:80:ALA:O	1:A:84:PHE:N	2.44	0.48
1:A:92:GLN:O	1:A:96:ASP:N	2.35	0.48
1:A:372:PHE:HA	1:A:375:LEU:HD12	1.94	0.48
1:A:90:GLU:O	1:A:93:SER:OG	2.29	0.48
1:B:52:ALA:HA	1:B:55:GLU:HG3	1.95	0.48
1:A:345:TYR:O	1:A:348:PRO:HD2	2.14	0.47
4:A:813:3PE:H391	4:A:813:3PE:H2A2	1.95	0.47
1:A:492:PHE:CE2	1:A:513:LEU:HD12	2.46	0.47
1:A:15:TRP:HZ2	1:A:76:LYS:HE3	1.79	0.47
1:B:128:ILE:O	1:B:132:LYS:HG3	2.13	0.47
1:B:174:ASP:O	1:B:178:ALA:N	2.38	0.47
1:B:349:LEU:HD12	1:B:349:LEU:H	1.80	0.47
1:B:525:THR:HG23	1:B:570:ARG:HH11	1.80	0.47
1:A:19:TYR:CE1	1:A:148:TYR:HA	2.50	0.47
1:B:6:HIS:CD2	1:B:308:ARG:HD3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:LYS:HA	1:A:559:TYR:HD2	1.79	0.47
1:A:96:ASP:HA	1:A:99:LYS:HD2	1.96	0.47
1:A:496:TYR:CZ	1:A:511:PHE:HD2	2.32	0.47
1:A:508:MET:HG3	1:A:512:TYR:CZ	2.50	0.47
1:B:176:ARG:O	1:B:181:GLU:N	2.45	0.47
1:B:412:TYR:CZ	1:B:441:HIS:HB3	2.50	0.46
1:A:92:GLN:HA	1:A:95:LEU:HB2	1.97	0.46
1:A:555:GLN:HG3	1:A:557:ALA:H	1.80	0.46
4:A:813:3PE:H272	4:A:813:3PE:H371	1.98	0.46
1:B:251:LEU:HD11	1:B:331:LEU:HG	1.97	0.46
1:B:55:GLU:OE1	1:B:56:GLU:HG3	2.15	0.46
1:A:333:ALA:HB2	4:B:901:3PE:H3B1	1.98	0.46
1:B:408:MET:SD	1:B:448:ARG:NE	2.79	0.46
1:B:488:PHE:HB3	1:B:517:PHE:HD2	1.81	0.46
1:B:520:ILE:O	1:B:524:TYR:HB2	2.15	0.46
1:B:585:LEU:HB3	1:B:588:SER:HB3	1.96	0.46
1:B:1:MET:SD	1:B:2:LYS:N	2.89	0.46
1:B:398:ASP:OD2	1:B:483:TYR:OH	2.33	0.46
1:B:550:GLU:N	1:B:550:GLU:OE1	2.49	0.46
2:A:810:CLR:H162	2:A:810:CLR:H221	1.78	0.46
1:A:173:ALA:HA	1:A:176:ARG:HE	1.81	0.45
1:A:251:LEU:HD11	1:A:331:LEU:HG	1.98	0.45
1:B:266:TRP:HB2	1:B:267:PRO:HD3	1.97	0.45
1:B:588:SER:HA	1:B:591:ILE:HG22	1.98	0.45
2:B:910:CLR:H162	2:B:910:CLR:H221	1.74	0.45
1:A:134:ALA:HA	1:A:137:GLU:OE1	2.16	0.45
1:A:121:GLU:HA	1:A:124:GLN:HB3	1.98	0.45
1:A:190:LYS:O	1:A:193:GLN:HG2	2.15	0.45
4:A:813:3PE:H361	1:B:336:PHE:HD2	1.80	0.45
1:A:3:PHE:CG	1:A:3:PHE:O	2.70	0.45
1:B:4:ALA:HA	1:B:22:TYR:CD2	2.51	0.45
1:B:612:LEU:HD23	1:B:612:LEU:HA	1.69	0.45
1:A:285:LEU:HA	1:A:288:ASN:HB2	1.98	0.45
1:A:410:LEU:HD11	2:A:810:CLR:H273	1.99	0.45
1:A:236:ARG:NH1	1:A:318:GLU:OE1	2.49	0.45
1:A:530:LEU:HD11	1:A:563:ILE:HG12	1.99	0.45
1:A:536:LEU:HD12	1:A:547:LEU:HA	1.98	0.45
1:A:92:GLN:OE1	1:A:92:GLN:N	2.31	0.45
1:A:197:GLU:O	1:A:201:VAL:HG12	2.17	0.45
4:A:813:3PE:H2C1	4:A:813:3PE:H292	1.73	0.45
1:A:90:GLU:HB3	1:A:131:LEU:HD21	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:THR:O	1:A:383:THR:OG1	2.34	0.45
1:B:1:MET:CE	1:B:3:PHE:H	2.30	0.45
1:B:538:ASP:OD1	1:B:539:LYS:N	2.50	0.45
1:A:173:ALA:HA	1:A:176:ARG:NE	2.31	0.44
1:B:54:PHE:HA	1:B:57:LYS:HG2	1.99	0.44
1:B:292:TRP:CZ2	1:B:612:LEU:HD12	2.52	0.44
1:A:603:ARG:O	1:A:606:VAL:HG12	2.17	0.44
1:B:31:SER:O	1:B:35:GLN:N	2.48	0.44
1:B:156:PHE:O	1:B:159:ILE:HG22	2.16	0.44
1:A:143:ILE:HG23	1:A:146:GLN:NE2	2.32	0.44
1:A:591:ILE:O	1:A:595:VAL:HG23	2.18	0.44
1:B:549:GLU:HB3	1:B:550:GLU:OE1	2.16	0.44
1:A:285:LEU:O	1:A:289:THR:HG23	2.18	0.44
1:A:585:LEU:HB3	1:A:588:SER:HB3	1.99	0.44
1:B:20:ILE:HG13	1:B:25:PHE:HE2	1.81	0.44
1:B:308:ARG:HE	1:B:308:ARG:C	2.18	0.44
1:B:383:THR:O	1:B:383:THR:OG1	2.36	0.44
1:B:555:GLN:HG3	1:B:557:ALA:H	1.82	0.44
1:B:521:SER:O	1:B:525:THR:HG22	2.18	0.44
1:A:83:ARG:HA	1:A:86:THR:HB	2.00	0.43
2:A:801:CLR:H211	2:A:801:CLR:H232	1.80	0.43
1:B:541:ALA:HB1	1:B:545:THR:HA	2.00	0.43
1:A:53:LYS:HD3	1:A:53:LYS:N	2.32	0.43
1:A:487:PHE:HD2	2:A:804:CLR:H221	1.84	0.43
1:A:28:MET:SD	1:A:29:LEU:HD23	2.59	0.43
1:B:54:PHE:HD1	1:B:167:LEU:HD11	1.83	0.43
1:B:122:ARG:HA	1:B:125:HIS:CD2	2.53	0.43
1:A:489:MET:CE	1:A:518:TYR:HA	2.48	0.43
1:B:162:LYS:HG3	1:B:166:ILE:HD12	2.00	0.43
1:A:147:ASN:HB2	1:A:151:LEU:HG	2.00	0.43
1:B:526:LEU:HD11	1:B:567:VAL:HG13	1.99	0.43
1:A:311:LEU:HD23	1:A:311:LEU:HA	1.83	0.43
1:A:565:GLU:HB2	2:A:801:CLR:H242	2.01	0.43
1:B:359:LEU:HD11	1:B:374:LEU:HD23	2.00	0.43
1:B:472:ARG:HE	1:B:472:ARG:HB3	1.68	0.43
1:B:565:GLU:OE1	1:B:606:VAL:HG11	2.19	0.43
1:A:518:TYR:OH	1:A:571:PHE:O	2.37	0.43
1:B:126:ARG:O	1:B:129:LYS:HG2	2.19	0.43
1:B:143:ILE:HA	1:B:146:GLN:NE2	2.27	0.43
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.79	0.42
1:A:454:ILE:O	1:A:458:LEU:HG	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:ARG:O	1:B:574:THR:HG23	2.18	0.42
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.87	0.42
1:A:311:LEU:HB2	4:A:803:3PE:H32	2.01	0.42
1:A:478:VAL:HB	1:A:528:TRP:HZ3	1.84	0.42
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.85	0.42
1:B:151:LEU:O	1:B:155:GLY:N	2.51	0.42
1:B:617:LEU:HD12	1:B:617:LEU:HA	1.91	0.42
1:A:441:HIS:HE1	1:A:442:LYS:HE3	1.85	0.42
1:B:385:PRO:O	1:B:465:ARG:NH1	2.48	0.42
1:A:1:MET:HE1	1:A:3:PHE:H	1.83	0.42
1:B:62:CYS:HB3	1:B:175:TRP:CH2	2.55	0.42
1:B:137:GLU:O	1:B:141:SER:N	2.40	0.42
1:B:150:ASN:OD1	1:B:151:LEU:N	2.53	0.42
1:A:87:LEU:HA	1:A:90:GLU:HB2	2.01	0.42
1:A:408:MET:HE2	1:A:408:MET:HB2	1.91	0.42
1:B:279:ILE:HD13	1:B:324:GLY:HA2	2.00	0.42
1:B:459:ARG:HB3	1:B:483:TYR:CE2	2.55	0.42
1:A:157:ARG:HG3	1:A:158:LYS:HD2	2.02	0.42
1:B:4:ALA:HB1	1:B:26:LYS:HD2	2.02	0.42
1:A:66:LEU:HD12	1:A:185:PHE:CE2	2.55	0.41
1:B:80:ALA:O	1:B:84:PHE:N	2.50	0.41
1:B:96:ASP:OD1	1:B:99:LYS:NZ	2.44	0.41
1:B:266:TRP:CH2	6:B:911:ACD:H42	2.54	0.41
1:A:418:SER:HA	2:A:810:CLR:H6	2.03	0.41
1:B:15:TRP:HZ2	1:B:76:LYS:HE3	1.84	0.41
1:B:19:TYR:CE2	1:B:148:TYR:HA	2.55	0.41
1:A:302:ILE:HD11	1:A:616:HIS:HB2	2.01	0.41
1:B:70:ASN:OD1	1:B:185:PHE:N	2.53	0.41
1:B:131:LEU:HD23	1:B:131:LEU:HA	1.89	0.41
1:B:161:LYS:O	1:B:164:ASP:N	2.51	0.41
1:A:293:ARG:HH21	1:A:313:HIS:CE1	2.39	0.41
1:B:255:ALA:HB2	1:B:335:PHE:HE2	1.84	0.41
1:B:2:LYS:HZ3	3:B:903:IHP:P1	2.43	0.41
1:A:4:ALA:HA	1:A:22:TYR:CD2	2.55	0.41
1:A:75:GLU:O	1:A:79:GLU:HG2	2.21	0.41
1:B:555:GLN:OE1	1:B:556:LYS:N	2.54	0.41
1:B:292:TRP:CE2	1:B:612:LEU:HD12	2.56	0.41
1:A:66:LEU:HA	1:A:185:PHE:HE2	1.86	0.41
1:A:156:PHE:O	1:A:160:LEU:HG	2.21	0.41
1:A:447:VAL:HA	1:A:450:ILE:HG22	2.02	0.41
4:A:803:3PE:H3D2	4:A:803:3PE:H3G1	1.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:TYR:OH	1:B:571:PHE:O	2.30	0.41
1:A:70:ASN:OD1	1:A:185:PHE:N	2.54	0.41
1:A:133:LEU:HD12	1:A:136:SER:OG	2.20	0.41
1:B:429:LEU:HD12	1:B:429:LEU:HA	1.95	0.41
1:B:439:ILE:HA	1:B:442:LYS:HD2	2.03	0.40
1:B:496:TYR:CZ	1:B:511:PHE:HD2	2.38	0.40
1:A:398:ASP:OD1	1:A:604:ARG:NH1	2.54	0.40
1:A:459:ARG:HB3	1:A:483:TYR:CD2	2.57	0.40
1:B:84:PHE:HE2	1:B:142:LEU:HD21	1.86	0.40
1:B:228:PRO:HA	4:B:908:3PE:H121	2.03	0.40
1:B:83:ARG:HD3	1:B:86:THR:HB	2.03	0.40
1:B:585:LEU:O	1:B:589:GLY:N	2.54	0.40
1:B:395:TRP:HZ2	1:B:608:ASN:HD21	1.67	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	560/704 (80%)	544 (97%)	16 (3%)	0	100	100
1	B	560/704 (80%)	539 (96%)	21 (4%)	0	100	100
All	All	1120/1408 (80%)	1083 (97%)	37 (3%)	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	508/629 (81%)	489 (96%)	19 (4%)	29	53
1	B	508/629 (81%)	489 (96%)	19 (4%)	29	53
All	All	1016/1258 (81%)	978 (96%)	38 (4%)	31	53

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	22	TYR
1	A	25	PHE
1	A	28	MET
1	A	72	PHE
1	A	73	TYR
1	A	138	PHE
1	A	165	LYS
1	A	232	TRP
1	A	326	LEU
1	A	328	CYS
1	A	372	PHE
1	A	393	ASP
1	A	407	LEU
1	A	512	TYR
1	A	524	TYR
1	A	581	SER
1	A	605	PHE
1	A	609	PHE
1	B	1	MET
1	B	28	MET
1	B	55	GLU
1	B	72	PHE
1	B	73	TYR
1	B	87	LEU
1	B	161	LYS
1	B	165	LYS
1	B	185	PHE
1	B	334	CYS
1	B	372	PHE
1	B	408	MET
1	B	466	ARG
1	B	524	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	532	MET
1	B	576	GLN
1	B	581	SER
1	B	603	ARG
1	B	615	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	HIS
1	B	147	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CLR	A	801	-	31,31,31	0.36	0	48,48,48	0.68	0
2	CLR	A	814	-	31,31,31	0.36	0	48,48,48	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CLR	B	902	-	31,31,31	0.37	0	48,48,48	0.66	0
5	PLM	B	909	-	17,17,17	0.87	1 (5%)	17,17,17	0.74	2 (11%)
2	CLR	A	810	-	31,31,31	0.34	0	48,48,48	0.47	0
2	CLR	A	804	-	31,31,31	0.39	0	48,48,48	0.50	0
4	3PE	B	904	-	50,50,50	0.51	0	53,55,55	0.53	1 (1%)
3	IHP	B	903	-	36,36,36	1.51	6 (16%)	54,60,60	0.86	3 (5%)
2	CLR	B	910	-	31,31,31	0.35	0	48,48,48	0.46	0
2	CLR	A	805	-	31,31,31	0.37	0	48,48,48	0.65	0
5	PLM	A	812	-	17,17,17	0.91	1 (5%)	17,17,17	0.75	2 (11%)
2	CLR	A	807	-	31,31,31	0.37	0	48,48,48	0.51	0
5	PLM	A	809	-	17,17,17	0.88	1 (5%)	17,17,17	0.75	2 (11%)
4	3PE	A	803	-	50,50,50	0.51	0	53,55,55	0.53	1 (1%)
4	3PE	A	808	-	50,50,50	0.51	0	53,55,55	0.55	1 (1%)
3	IHP	A	802	-	36,36,36	1.51	6 (16%)	54,60,60	0.86	2 (3%)
4	3PE	B	901	-	50,50,50	0.51	0	53,55,55	0.57	2 (3%)
6	ACD	B	911	-	21,21,21	0.57	0	21,21,21	0.55	0
4	3PE	A	813	-	50,50,50	0.51	0	53,55,55	0.54	1 (1%)
2	CLR	A	806	-	31,31,31	0.37	0	48,48,48	0.58	0
2	CLR	B	907	-	31,31,31	0.37	0	48,48,48	0.52	0
2	CLR	B	906	-	31,31,31	0.37	0	48,48,48	0.65	0
5	PLM	B	912	-	17,17,17	0.90	1 (5%)	17,17,17	0.74	2 (11%)
2	CLR	B	905	-	31,31,31	0.39	0	48,48,48	0.48	0
6	ACD	A	811	-	21,21,21	0.57	0	21,21,21	0.59	0
4	3PE	B	908	-	50,50,50	0.52	0	53,55,55	0.58	1 (1%)

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
2	CLR	A	801	-	-	6/10/68/68	0/4/4/4
2	CLR	A	814	-	-	4/10/68/68	0/4/4/4
2	CLR	B	902	-	-	5/10/68/68	0/4/4/4
5	PLM	B	909	-	-	4/15/15/15	-
2	CLR	A	810	-	-	7/10/68/68	0/4/4/4
2	CLR	A	804	-	-	2/10/68/68	0/4/4/4
4	3PE	B	904	-	-	27/54/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IHP	B	903	-	-	9/30/54/54	0/1/1/1
2	CLR	B	910	-	-	7/10/68/68	0/4/4/4
2	CLR	A	805	-	-	6/10/68/68	0/4/4/4
5	PLM	A	812	-	-	2/15/15/15	-
2	CLR	A	807	-	-	7/10/68/68	0/4/4/4
5	PLM	A	809	-	-	5/15/15/15	-
4	3PE	A	803	-	-	27/54/54/54	-
4	3PE	A	808	-	-	19/54/54/54	-
3	IHP	A	802	-	-	10/30/54/54	0/1/1/1
4	3PE	B	901	-	-	22/54/54/54	-
6	ACD	B	911	-	-	5/19/19/19	-
4	3PE	A	813	-	-	19/54/54/54	-
2	CLR	A	806	-	-	4/10/68/68	0/4/4/4
2	CLR	B	907	-	-	8/10/68/68	0/4/4/4
2	CLR	B	906	-	-	6/10/68/68	0/4/4/4
5	PLM	B	912	-	-	2/15/15/15	-
2	CLR	B	905	-	-	1/10/68/68	0/4/4/4
6	ACD	A	811	-	-	4/19/19/19	-
4	3PE	B	908	-	-	21/54/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	IHP	P4-O14	3.45	1.65	1.59
3	B	903	IHP	P4-O14	3.42	1.65	1.59
3	B	903	IHP	P2-O12	3.26	1.65	1.59
3	A	802	IHP	P5-O15	3.25	1.65	1.59
3	A	802	IHP	P1-O11	3.24	1.65	1.59
3	B	903	IHP	P6-O16	3.22	1.65	1.59
3	B	903	IHP	P1-O11	3.21	1.65	1.59
3	A	802	IHP	P2-O12	3.19	1.65	1.59
3	A	802	IHP	P6-O16	3.16	1.65	1.59
3	B	903	IHP	P5-O15	3.16	1.65	1.59
3	B	903	IHP	P3-O13	3.12	1.65	1.59
3	A	802	IHP	P3-O13	3.09	1.65	1.59
5	A	812	PLM	C2-C1	2.93	1.57	1.50
5	B	912	PLM	C2-C1	2.91	1.57	1.50
5	A	809	PLM	C2-C1	2.79	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	909	PLM	C2-C1	2.74	1.57	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	IHP	C6-C5-C4	2.63	116.17	110.41
3	B	903	IHP	C6-C5-C4	2.50	115.89	110.41
3	A	802	IHP	C5-C6-C1	2.44	115.76	110.41
3	B	903	IHP	C5-C6-C1	2.38	115.62	110.41
4	B	904	3PE	O12-P-O14	2.34	123.80	112.24
4	A	803	3PE	O12-P-O14	2.33	123.74	112.24
4	A	813	3PE	O12-P-O14	2.32	123.73	112.24
4	A	808	3PE	O12-P-O14	2.32	123.73	112.24
4	B	901	3PE	O12-P-O14	2.31	123.66	112.24
4	B	908	3PE	O12-P-O14	2.29	123.56	112.24
5	A	809	PLM	O1-C1-O2	2.24	128.88	123.30
5	B	909	PLM	O1-C1-O2	2.23	128.86	123.30
5	A	812	PLM	O1-C1-O2	2.21	128.81	123.30
5	B	912	PLM	O1-C1-O2	2.20	128.79	123.30
3	B	903	IHP	C6-C1-C2	2.12	115.05	110.41
5	A	809	PLM	O2-C1-C2	-2.03	116.57	123.08
4	B	901	3PE	C2-O21-C21	2.02	122.76	117.79
5	B	909	PLM	O2-C1-C2	-2.01	116.61	123.08
5	A	812	PLM	O2-C1-C2	-2.00	116.65	123.08
5	B	912	PLM	O2-C1-C2	-2.00	116.65	123.08

There are no chirality outliers.

All (239) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	IHP	C5-C4-O14-P4
3	B	903	IHP	C2-C3-O13-P3
3	B	903	IHP	C4-C3-O13-P3
3	B	903	IHP	C5-C4-O14-P4
3	B	903	IHP	C4-O14-P4-O44
4	A	803	3PE	C1-O11-P-O14
4	A	803	3PE	C11-O13-P-O14
4	A	803	3PE	O11-C1-C2-O21
4	A	803	3PE	C22-C21-O21-C2
4	A	808	3PE	C1-O11-P-O14
4	A	808	3PE	O13-C11-C12-N
4	A	808	3PE	O22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	808	3PE	C22-C21-O21-C2
4	A	813	3PE	C1-O11-P-O13
4	A	813	3PE	C1-O11-P-O14
4	A	813	3PE	O13-C11-C12-N
4	A	813	3PE	C22-C21-O21-C2
4	B	901	3PE	C1-O11-P-O14
4	B	901	3PE	O13-C11-C12-N
4	B	901	3PE	C22-C21-O21-C2
4	B	904	3PE	C1-O11-P-O14
4	B	904	3PE	C11-O13-P-O14
4	B	904	3PE	O11-C1-C2-O21
4	B	904	3PE	C22-C21-O21-C2
4	B	908	3PE	C1-O11-P-O14
4	B	908	3PE	O13-C11-C12-N
4	B	908	3PE	C22-C21-O21-C2
4	A	803	3PE	O32-C31-O31-C3
4	B	904	3PE	O32-C31-O31-C3
4	A	803	3PE	O22-C21-O21-C2
4	A	813	3PE	O22-C21-O21-C2
4	B	901	3PE	O22-C21-O21-C2
4	B	904	3PE	O22-C21-O21-C2
4	B	908	3PE	O22-C21-O21-C2
2	B	910	CLR	C13-C17-C20-C22
4	A	803	3PE	C32-C31-O31-C3
4	B	904	3PE	C32-C31-O31-C3
2	A	805	CLR	C17-C20-C22-C23
2	A	810	CLR	C17-C20-C22-C23
2	B	906	CLR	C17-C20-C22-C23
2	A	814	CLR	C21-C20-C22-C23
2	B	910	CLR	C21-C20-C22-C23
2	A	814	CLR	C17-C20-C22-C23
2	B	910	CLR	C17-C20-C22-C23
4	B	908	3PE	C32-C31-O31-C3
4	B	908	3PE	C27-C28-C29-C2A
4	A	803	3PE	C29-C2A-C2B-C2C
2	A	805	CLR	C21-C20-C22-C23
2	B	906	CLR	C21-C20-C22-C23
2	B	910	CLR	C13-C17-C20-C21
4	B	908	3PE	O32-C31-O31-C3
2	A	806	CLR	C17-C20-C22-C23
2	A	810	CLR	C22-C23-C24-C25
2	B	902	CLR	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	806	CLR	C22-C23-C24-C25
2	A	814	CLR	C22-C23-C24-C25
4	A	808	3PE	C27-C28-C29-C2A
4	B	904	3PE	C29-C2A-C2B-C2C
4	A	803	3PE	C1-O11-P-O13
4	B	904	3PE	C1-O11-P-O13
2	B	910	CLR	C16-C17-C20-C22
2	A	810	CLR	C21-C20-C22-C23
2	A	810	CLR	C13-C17-C20-C22
4	A	813	3PE	C22-C23-C24-C25
4	B	908	3PE	C25-C26-C27-C28
2	A	807	CLR	C13-C17-C20-C22
4	B	908	3PE	C34-C35-C36-C37
3	A	802	IHP	C1-C2-O12-P2
3	A	802	IHP	C3-C2-O12-P2
4	A	813	3PE	C27-C28-C29-C2A
4	B	904	3PE	C33-C34-C35-C36
2	B	910	CLR	C16-C17-C20-C21
2	B	910	CLR	C22-C23-C24-C25
5	B	909	PLM	C3-C4-C5-C6
4	B	901	3PE	C21-C22-C23-C24
4	B	904	3PE	C31-C32-C33-C34
4	A	803	3PE	C33-C34-C35-C36
2	B	905	CLR	C17-C20-C22-C23
4	A	803	3PE	C32-C33-C34-C35
4	A	803	3PE	C31-C32-C33-C34
4	B	908	3PE	C35-C36-C37-C38
4	A	803	3PE	C24-C25-C26-C27
4	A	803	3PE	C27-C28-C29-C2A
4	B	901	3PE	C2B-C2C-C2D-C2E
4	A	808	3PE	C34-C35-C36-C37
4	B	901	3PE	C22-C23-C24-C25
4	A	808	3PE	C32-C31-O31-C3
2	A	804	CLR	C17-C20-C22-C23
2	B	907	CLR	C21-C20-C22-C23
4	B	904	3PE	C3C-C3D-C3E-C3F
4	A	803	3PE	C3C-C3D-C3E-C3F
4	A	803	3PE	C35-C36-C37-C38
2	A	810	CLR	C13-C17-C20-C21
4	B	904	3PE	C27-C28-C29-C2A
2	A	807	CLR	C16-C17-C20-C21
2	A	805	CLR	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	813	3PE	C2E-C2F-C2G-C2H
2	B	907	CLR	C13-C17-C20-C22
4	A	803	3PE	C11-O13-P-O11
4	B	904	3PE	C11-O13-P-O11
4	A	803	3PE	O11-C1-C2-C3
4	B	904	3PE	O11-C1-C2-C3
2	A	807	CLR	C13-C17-C20-C21
4	A	808	3PE	C26-C27-C28-C29
4	B	904	3PE	C21-C22-C23-C24
4	A	808	3PE	O32-C31-O31-C3
4	B	904	3PE	C32-C33-C34-C35
4	A	808	3PE	C1-C2-C3-O31
4	A	808	3PE	C25-C26-C27-C28
2	A	807	CLR	C16-C17-C20-C22
2	A	810	CLR	C16-C17-C20-C22
4	A	808	3PE	C2F-C2G-C2H-C2I
4	B	908	3PE	C2F-C2G-C2H-C2I
4	B	901	3PE	C3F-C3G-C3H-C3I
4	B	908	3PE	C26-C27-C28-C29
2	A	810	CLR	C16-C17-C20-C21
2	A	807	CLR	C21-C20-C22-C23
4	A	813	3PE	C3C-C3D-C3E-C3F
2	B	906	CLR	C23-C24-C25-C26
4	A	803	3PE	C22-C23-C24-C25
2	B	907	CLR	C16-C17-C20-C21
2	A	801	CLR	C13-C17-C20-C21
4	B	901	3PE	C35-C36-C37-C38
2	B	907	CLR	C13-C17-C20-C21
2	B	907	CLR	C16-C17-C20-C22
2	A	801	CLR	C13-C17-C20-C22
5	A	809	PLM	C1-C2-C3-C4
4	B	904	3PE	C36-C37-C38-C39
2	A	801	CLR	C16-C17-C20-C21
4	A	803	3PE	C21-C22-C23-C24
4	B	901	3PE	C2D-C2E-C2F-C2G
4	A	808	3PE	C2B-C2C-C2D-C2E
4	A	808	3PE	C35-C36-C37-C38
4	B	904	3PE	C24-C25-C26-C27
2	B	902	CLR	C13-C17-C20-C21
4	B	901	3PE	C2C-C2D-C2E-C2F
2	B	902	CLR	C13-C17-C20-C22
4	A	813	3PE	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	805	CLR	C23-C24-C25-C27
2	B	907	CLR	C20-C22-C23-C24
4	B	904	3PE	C22-C23-C24-C25
2	A	801	CLR	C16-C17-C20-C22
2	B	906	CLR	C23-C24-C25-C27
2	A	801	CLR	C22-C23-C24-C25
3	B	903	IHP	C3-O13-P3-O23
4	B	908	3PE	C2B-C2C-C2D-C2E
2	B	906	CLR	C20-C22-C23-C24
2	A	805	CLR	C20-C22-C23-C24
4	A	808	3PE	O21-C2-C3-O31
4	B	908	3PE	O21-C2-C3-O31
3	A	802	IHP	C4-O14-P4-O44
3	B	903	IHP	C6-O16-P6-O46
4	A	813	3PE	C28-C29-C2A-C2B
4	B	901	3PE	C1-O11-P-O13
4	B	908	3PE	C1-O11-P-O13
4	A	803	3PE	C1-O11-P-O12
4	A	803	3PE	C11-O13-P-O12
4	B	904	3PE	C1-O11-P-O12
4	B	904	3PE	C11-O13-P-O12
2	B	902	CLR	C16-C17-C20-C22
2	B	902	CLR	C16-C17-C20-C21
4	B	901	3PE	C27-C28-C29-C2A
4	A	813	3PE	C37-C38-C39-C3A
4	A	803	3PE	C2A-C2B-C2C-C2D
2	B	906	CLR	C22-C23-C24-C25
2	A	806	CLR	C21-C20-C22-C23
4	A	813	3PE	C29-C2A-C2B-C2C
2	A	807	CLR	C23-C24-C25-C26
4	A	808	3PE	C1-O11-P-O13
4	A	813	3PE	C11-O13-P-O11
4	B	901	3PE	C11-O13-P-O11
3	A	802	IHP	C2-C3-O13-P3
3	B	903	IHP	C3-C2-O12-P2
4	B	908	3PE	C1-C2-C3-O31
2	A	805	CLR	C22-C23-C24-C25
2	B	907	CLR	C23-C24-C25-C26
4	A	813	3PE	C33-C34-C35-C36
5	B	909	PLM	O2-C1-C2-C3
6	A	811	ACD	O2-C1-C2-C3
4	B	901	3PE	C2F-C2G-C2H-C2I

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	811	ACD	O1-C1-C2-C3
4	A	803	3PE	C3E-C3F-C3G-C3H
4	B	904	3PE	C3E-C3F-C3G-C3H
5	B	912	PLM	O1-C1-C2-C3
2	A	807	CLR	C23-C24-C25-C27
5	A	812	PLM	O1-C1-C2-C3
4	B	901	3PE	C3-C2-O21-C21
6	B	911	ACD	C5-C6-C7-C8
6	B	911	ACD	C6-C7-C8-C9
6	B	911	ACD	C12-C13-C14-C15
5	A	812	PLM	O2-C1-C2-C3
5	B	912	PLM	O2-C1-C2-C3
4	B	908	3PE	C3B-C3C-C3D-C3E
5	B	909	PLM	O1-C1-C2-C3
5	B	909	PLM	C4-C5-C6-C7
5	A	809	PLM	C3-C4-C5-C6
3	A	802	IHP	C2-C1-O11-P1
3	B	903	IHP	C2-C1-O11-P1
2	A	801	CLR	C21-C20-C22-C23
2	B	907	CLR	C23-C24-C25-C27
2	A	806	CLR	C20-C22-C23-C24
4	B	904	3PE	C2A-C2B-C2C-C2D
4	B	901	3PE	O11-C1-C2-O21
4	A	808	3PE	C21-C22-C23-C24
4	B	901	3PE	C25-C26-C27-C28
6	B	911	ACD	O2-C1-C2-C3
3	A	802	IHP	C3-O13-P3-O23
6	A	811	ACD	C2-C3-C4-C5
4	A	813	3PE	C35-C36-C37-C38
4	A	813	3PE	O31-C31-C32-C33
4	B	901	3PE	O31-C31-C32-C33
4	B	908	3PE	O21-C21-C22-C23
5	A	809	PLM	O1-C1-C2-C3
5	A	809	PLM	O2-C1-C2-C3
4	A	803	3PE	C36-C37-C38-C39
4	A	803	3PE	C28-C29-C2A-C2B
4	B	901	3PE	C2A-C2B-C2C-C2D
5	A	809	PLM	CC-CD-CE-CF
6	B	911	ACD	O1-C1-C2-C3
4	A	808	3PE	O21-C21-C22-C23
4	B	904	3PE	C28-C29-C2A-C2B
6	A	811	ACD	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	802	IHP	C4-C3-O13-P3
3	A	802	IHP	C2-O12-P2-O32
3	A	802	IHP	C3-O13-P3-O33
3	B	903	IHP	C2-O12-P2-O32
2	A	804	CLR	C23-C24-C25-C26
4	A	813	3PE	C3F-C3G-C3H-C3I
4	B	908	3PE	O22-C21-C22-C23
4	A	813	3PE	O32-C31-C32-C33
4	A	808	3PE	O22-C21-C22-C23
4	B	901	3PE	O32-C31-C32-C33
4	B	908	3PE	C3-C2-O21-C21
4	B	901	3PE	C2E-C2F-C2G-C2H
4	B	908	3PE	C29-C2A-C2B-C2C
4	B	904	3PE	O31-C31-C32-C33
4	A	803	3PE	O31-C31-C32-C33
4	B	904	3PE	O32-C31-C32-C33
2	A	814	CLR	C13-C17-C20-C21

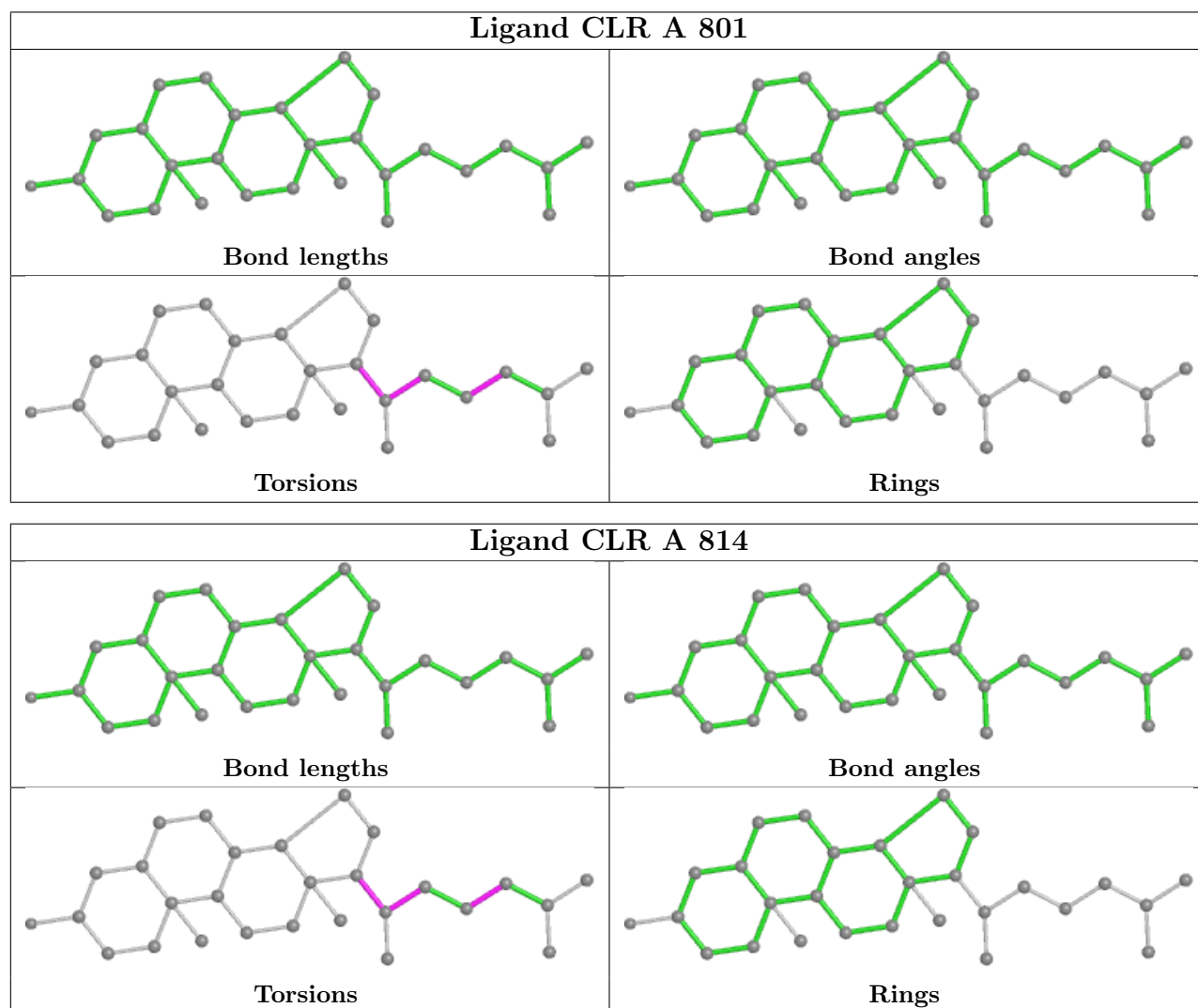
There are no ring outliers.

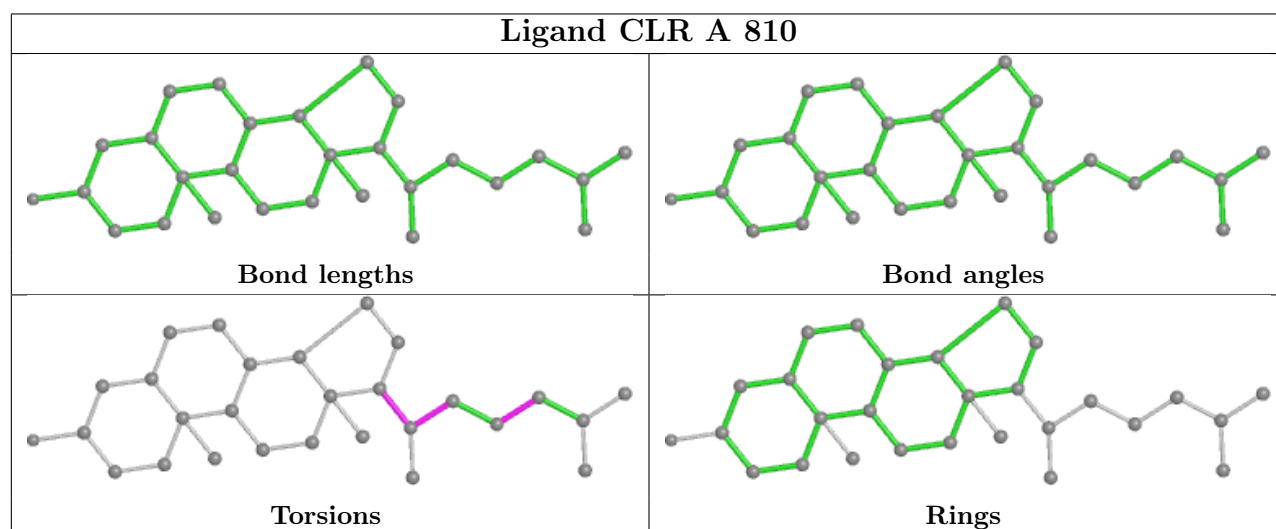
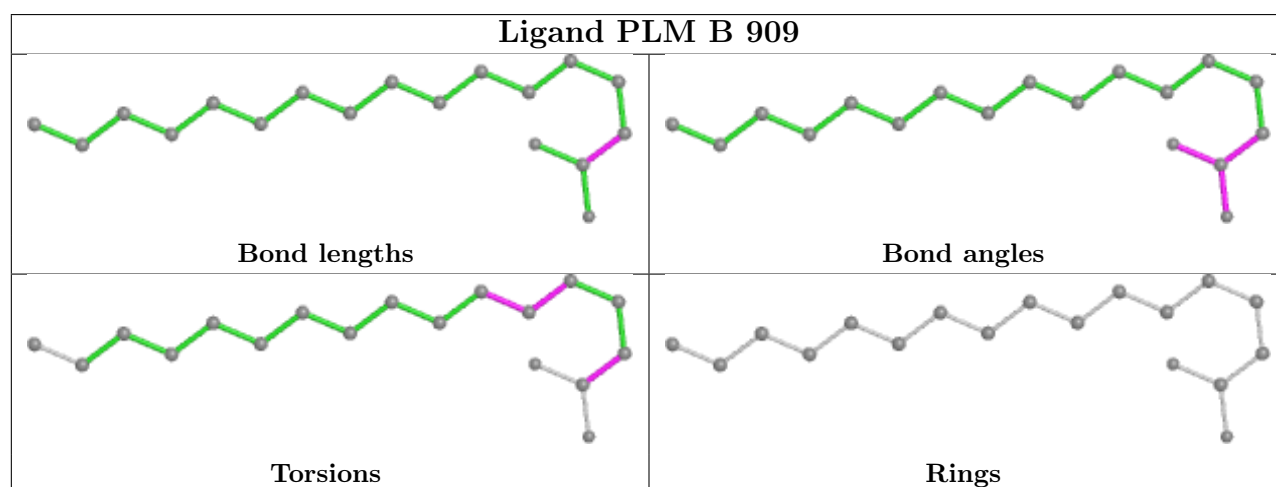
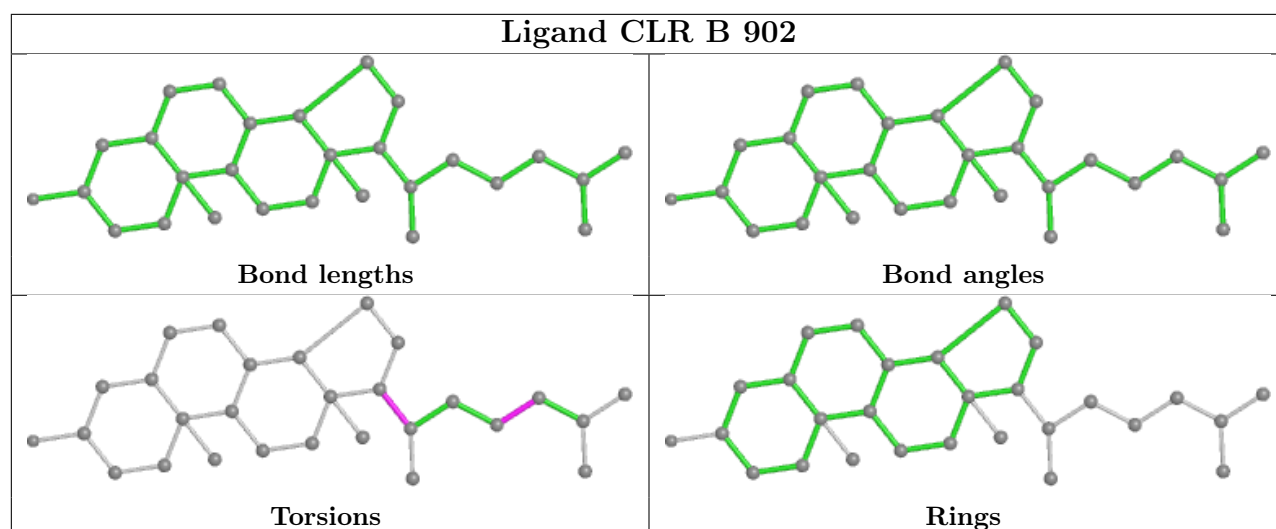
13 monomers are involved in 30 short contacts:

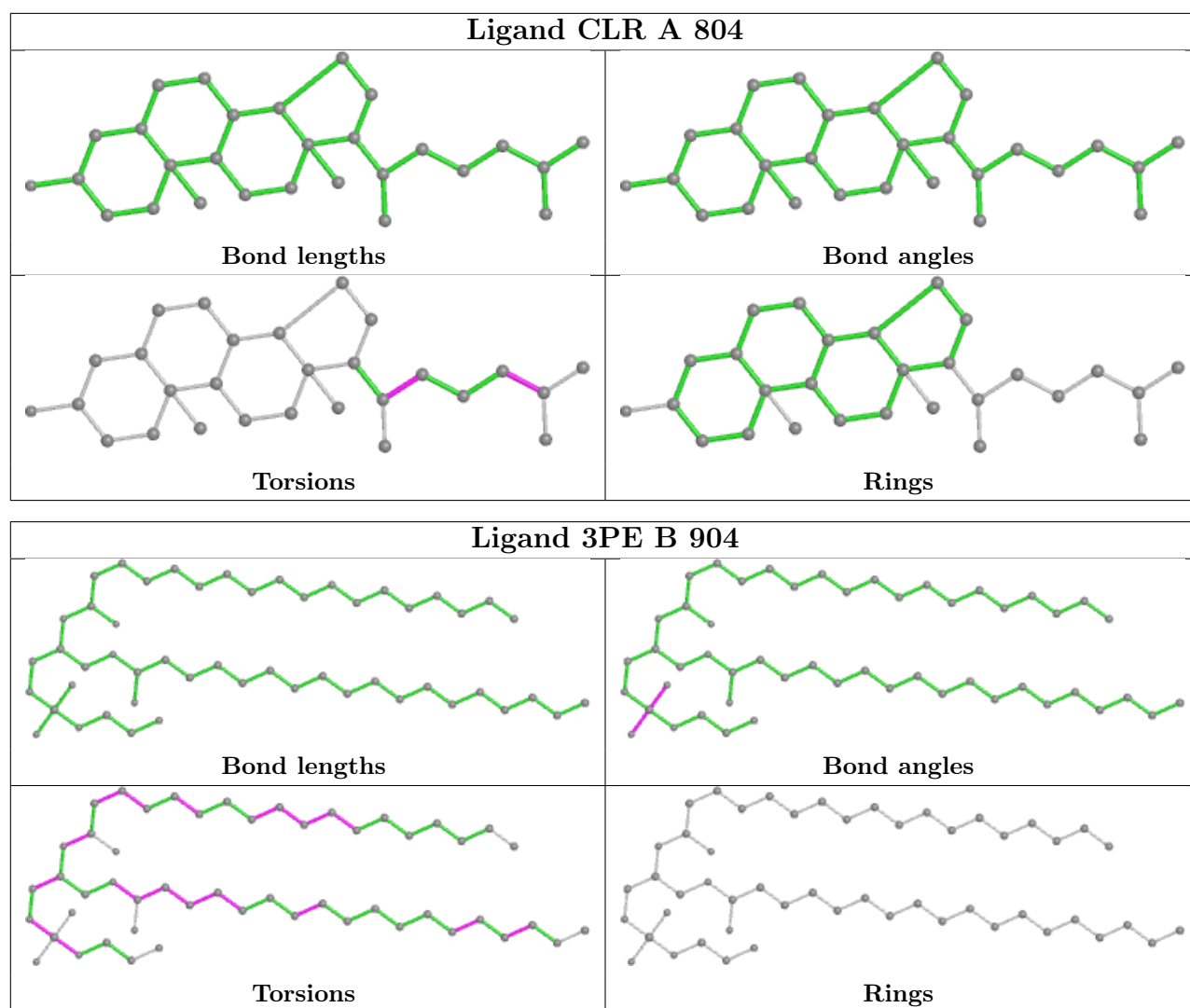
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	CLR	2	0
2	A	814	CLR	1	0
2	A	810	CLR	3	0
2	A	804	CLR	3	0
3	B	903	IHP	3	0
2	B	910	CLR	2	0
4	A	803	3PE	2	0
4	B	901	3PE	5	0
6	B	911	ACD	1	0
4	A	813	3PE	6	0
2	A	806	CLR	2	0
2	B	905	CLR	1	0
4	B	908	3PE	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

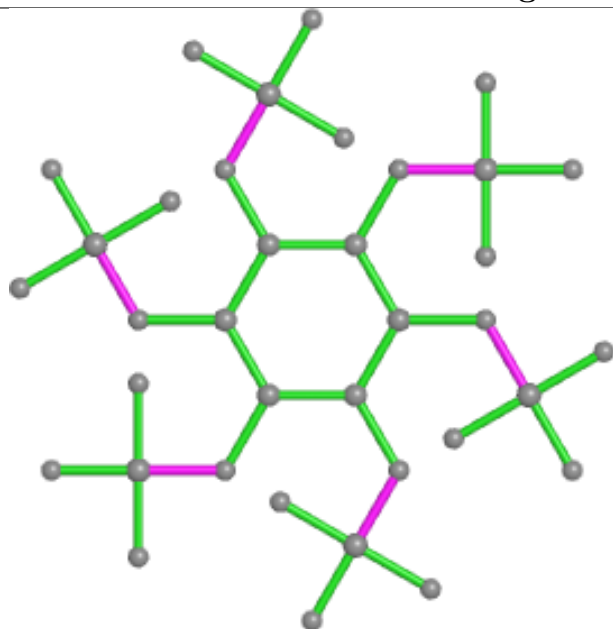
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



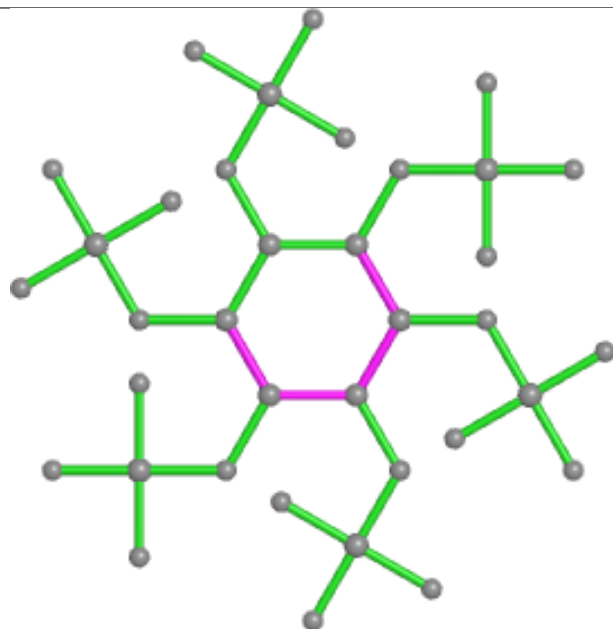




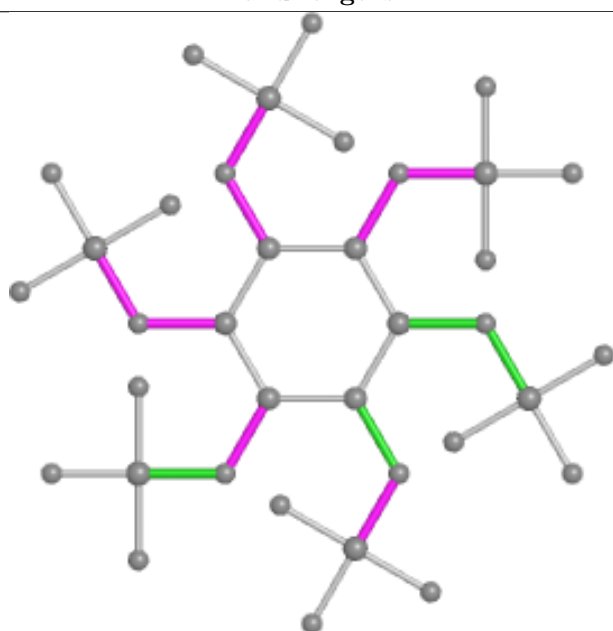
Ligand IHP B 903



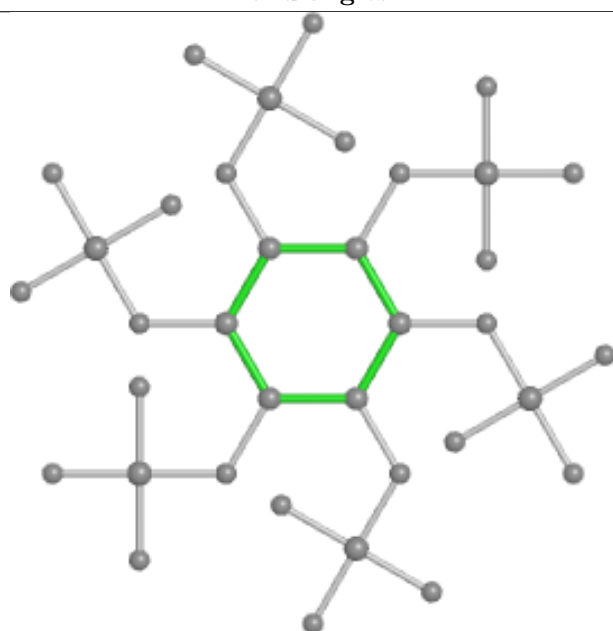
Bond lengths



Bond angles

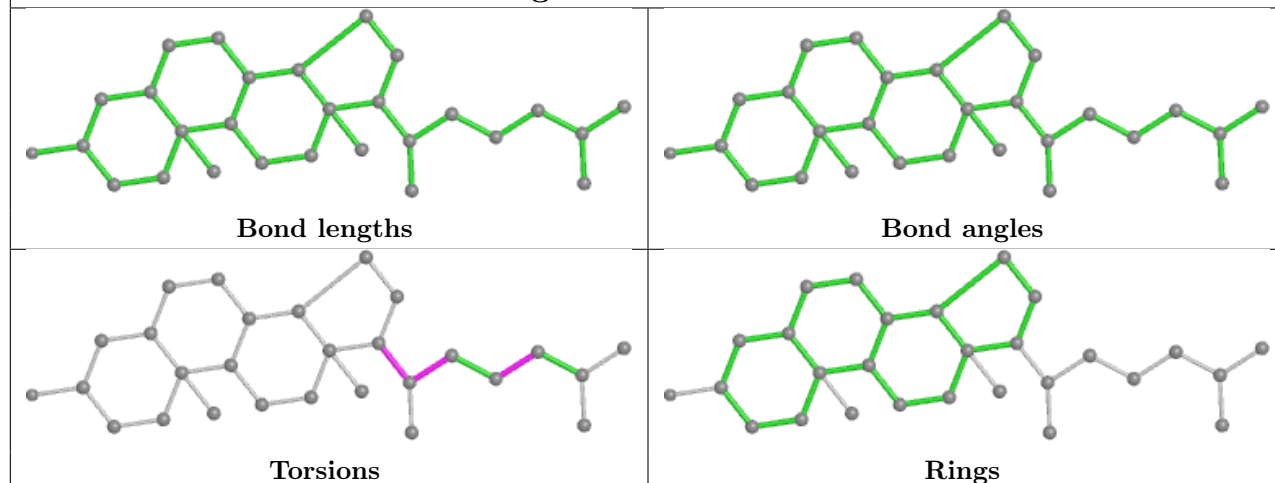


Torsions

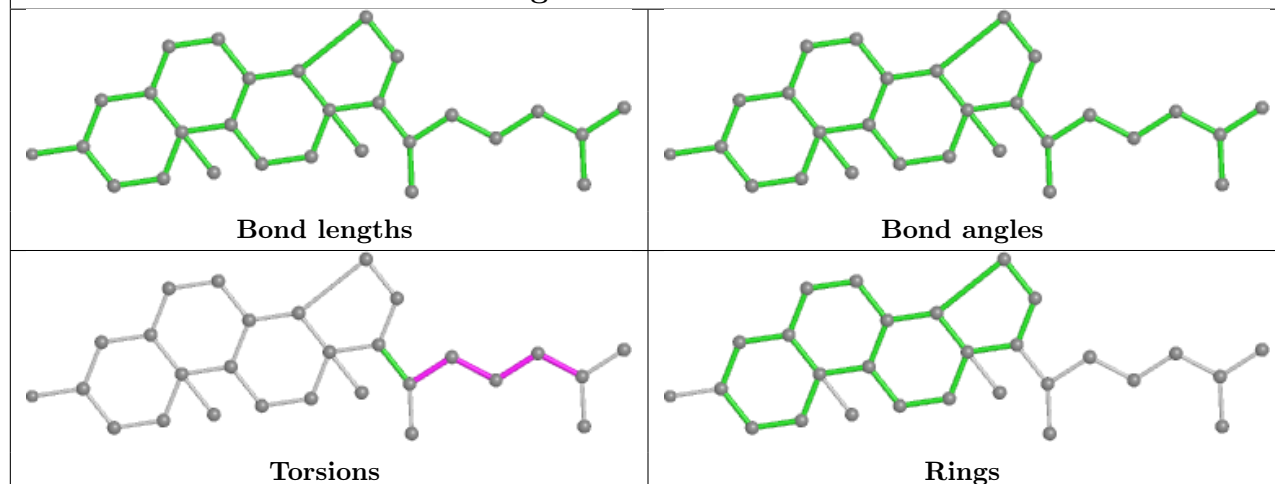


Rings

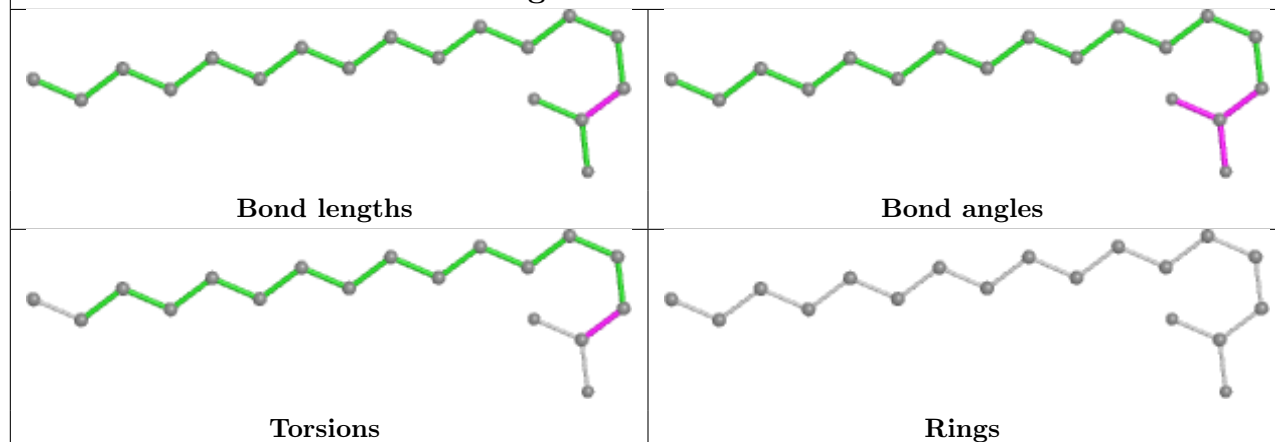
Ligand CLR B 910

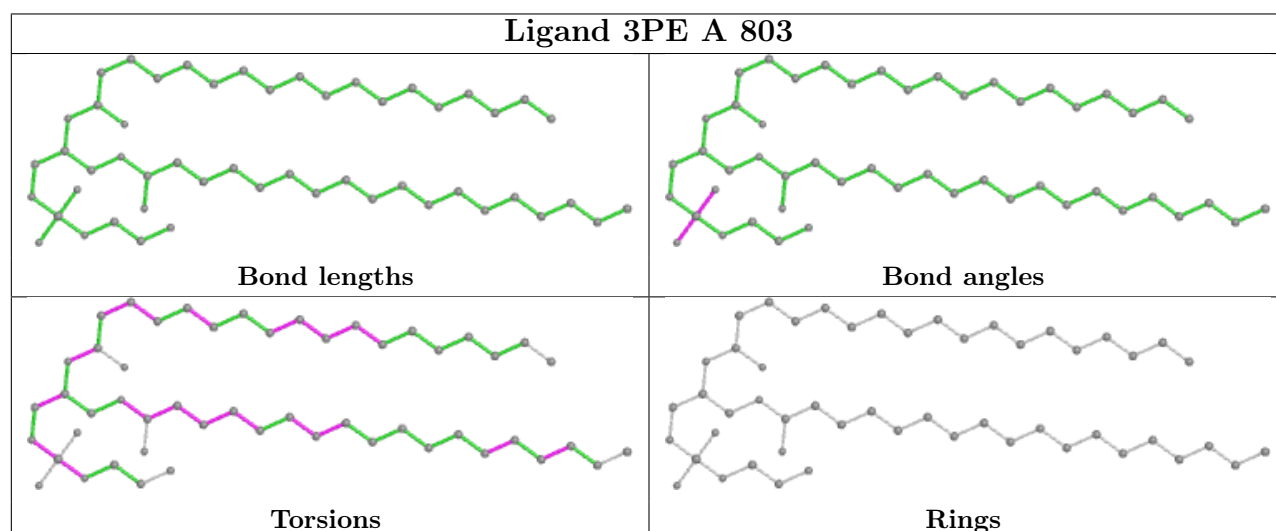
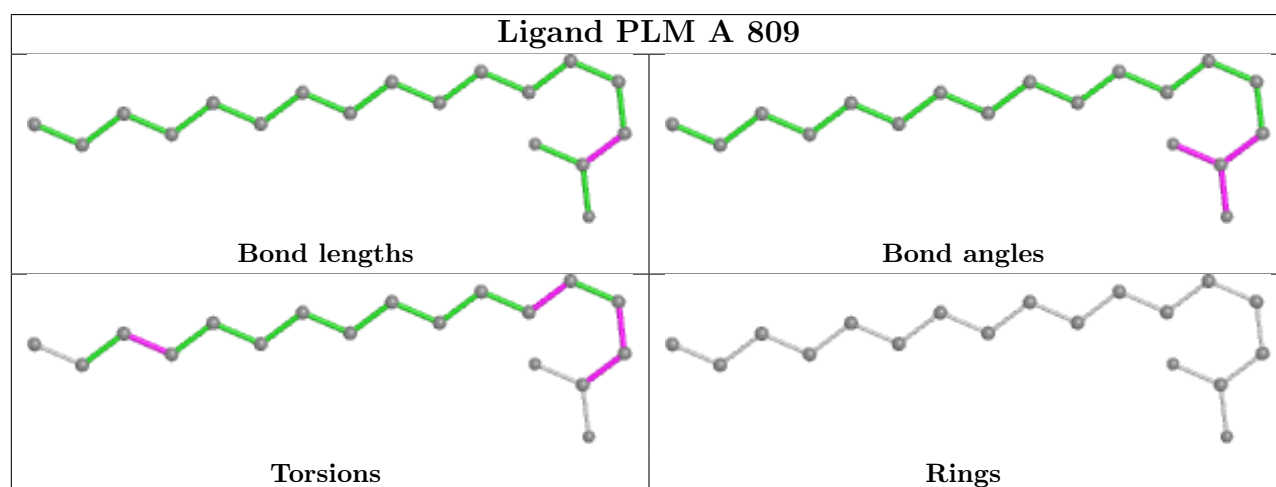
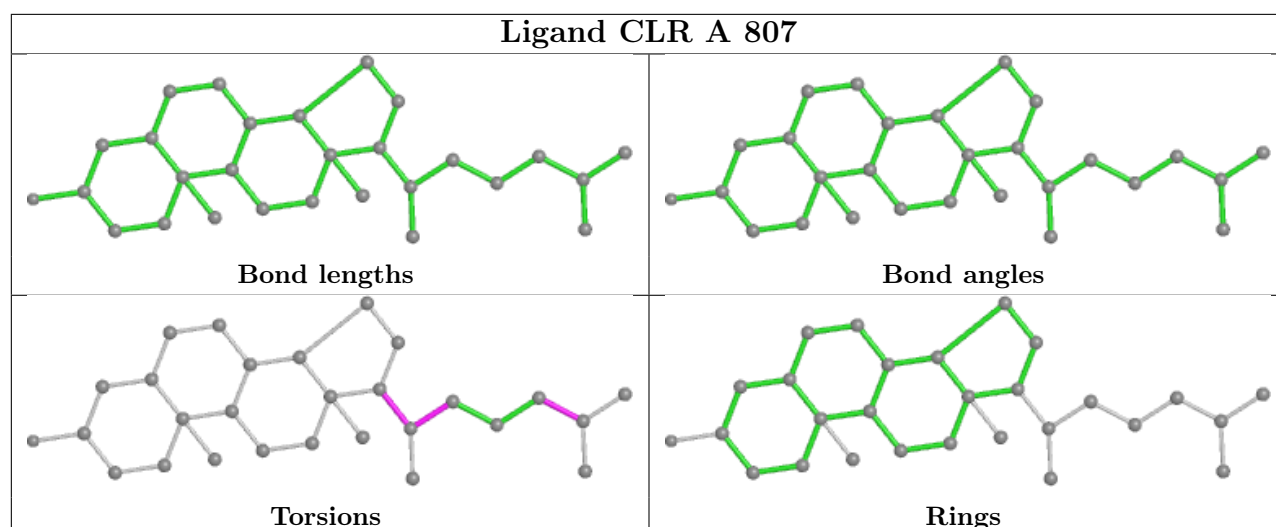


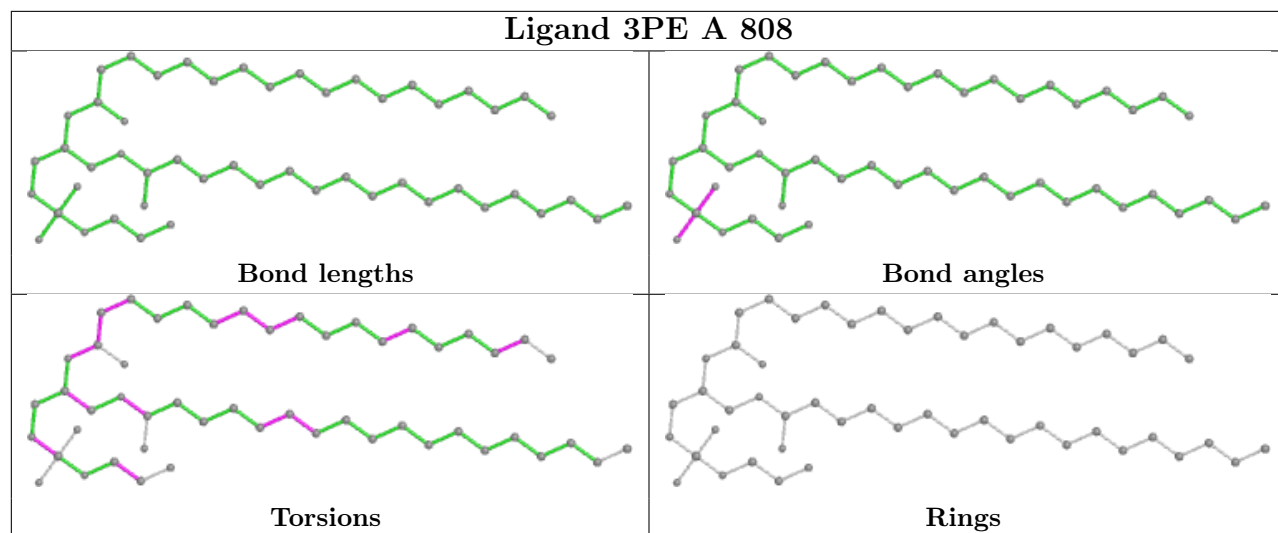
Ligand CLR A 805



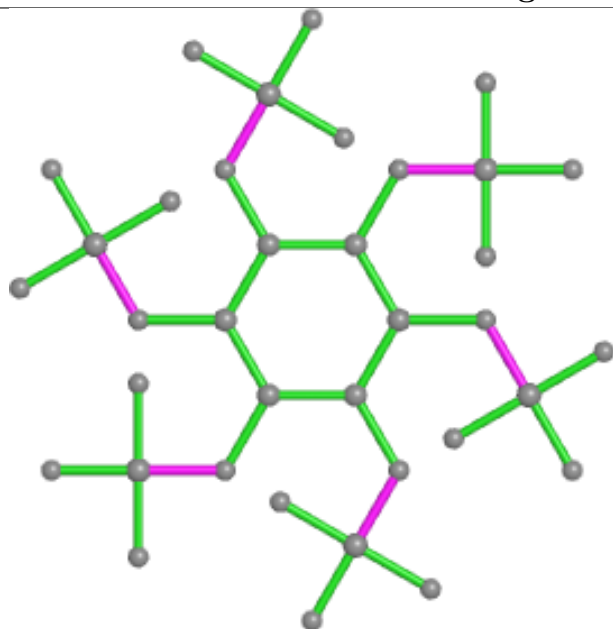
Ligand PLM A 812



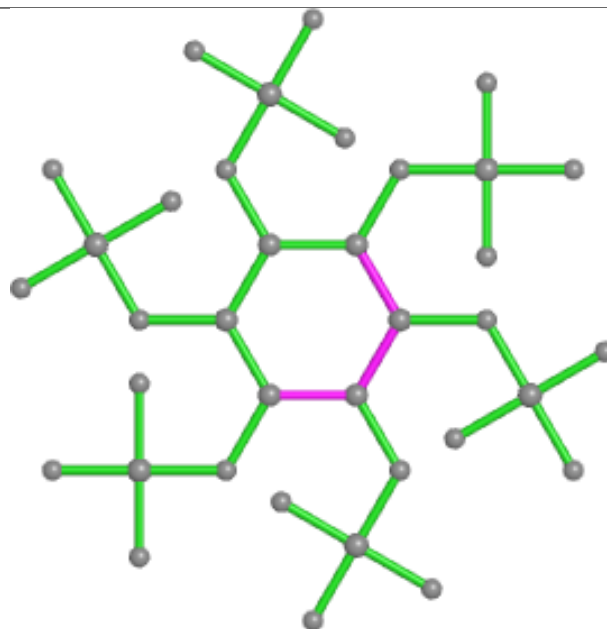




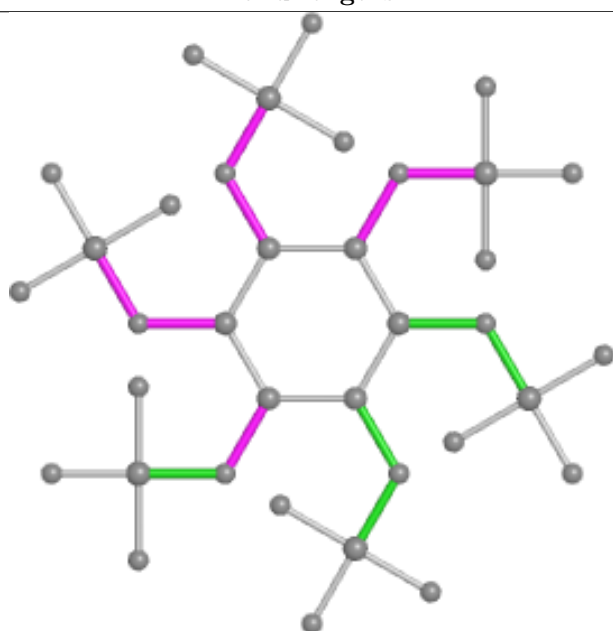
Ligand IHP A 802



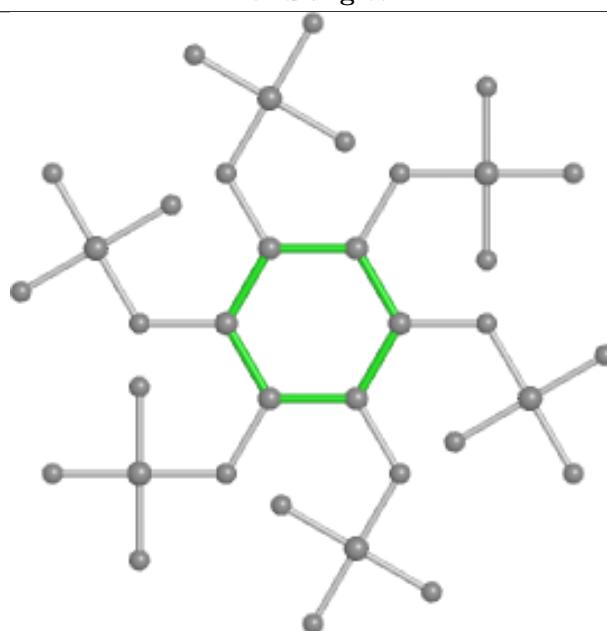
Bond lengths



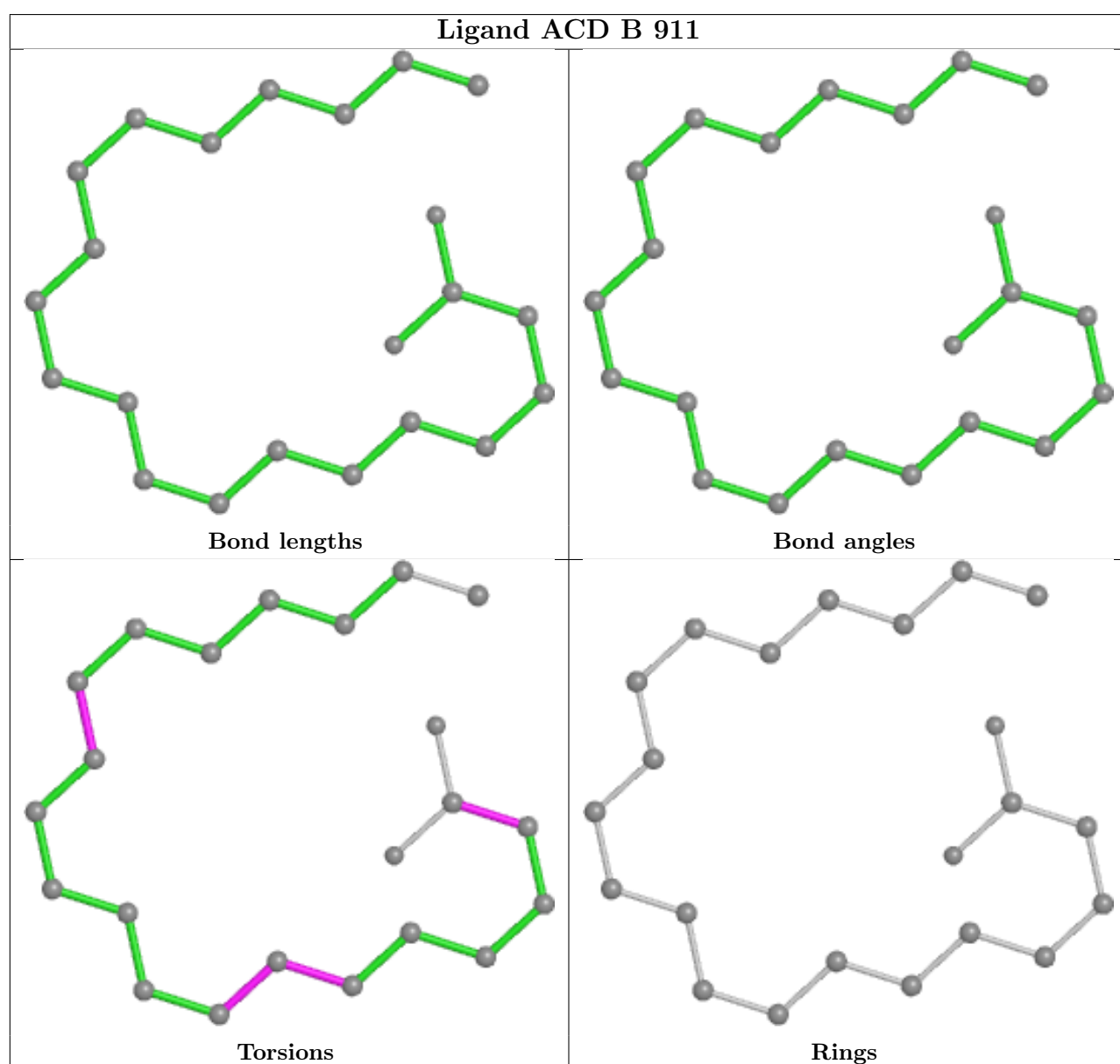
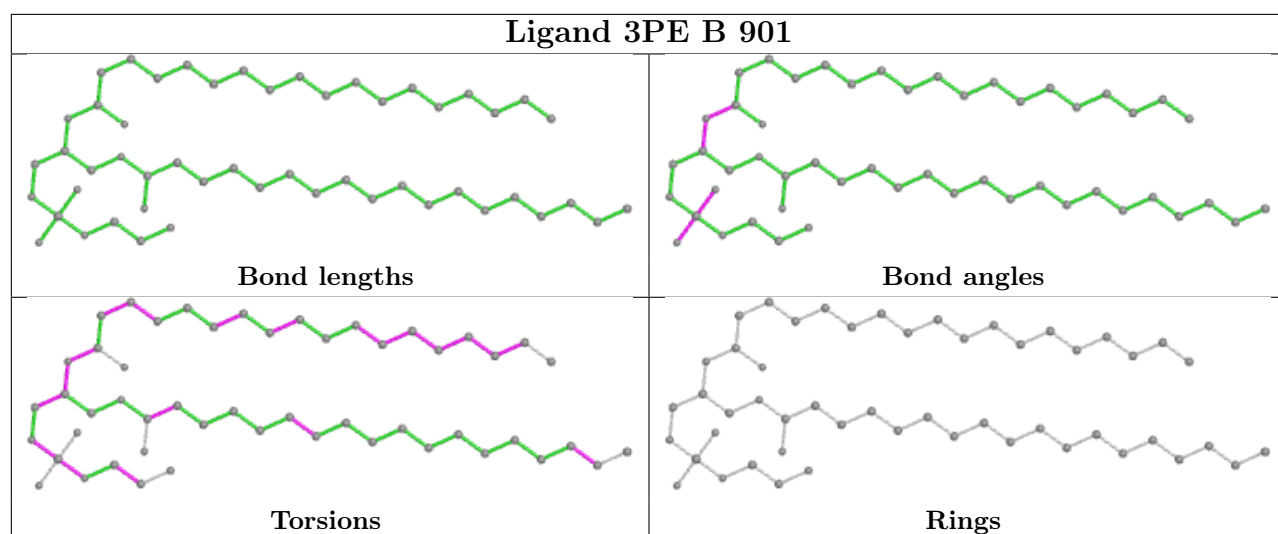
Bond angles



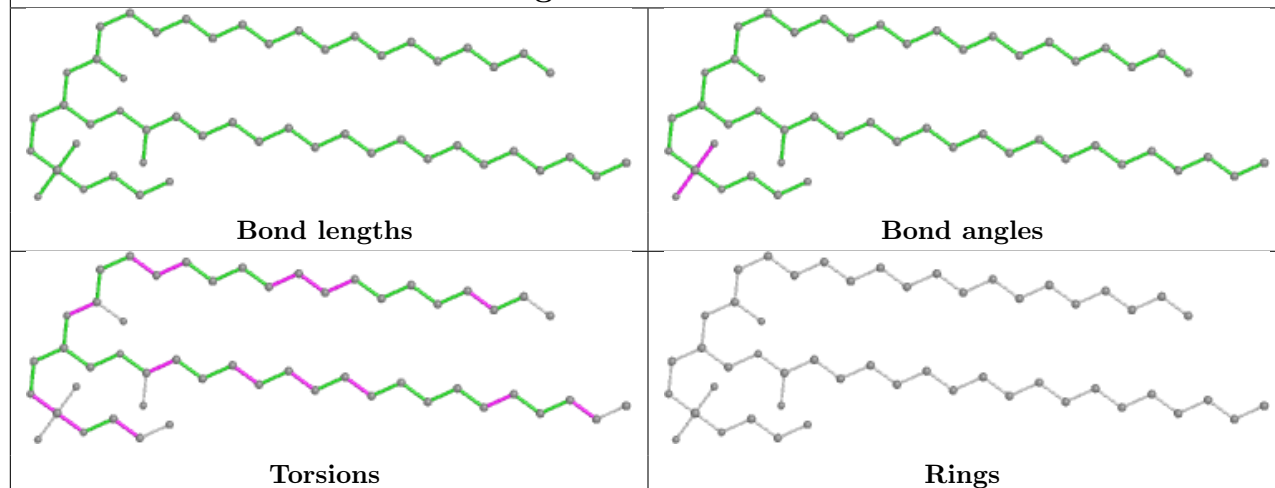
Torsions



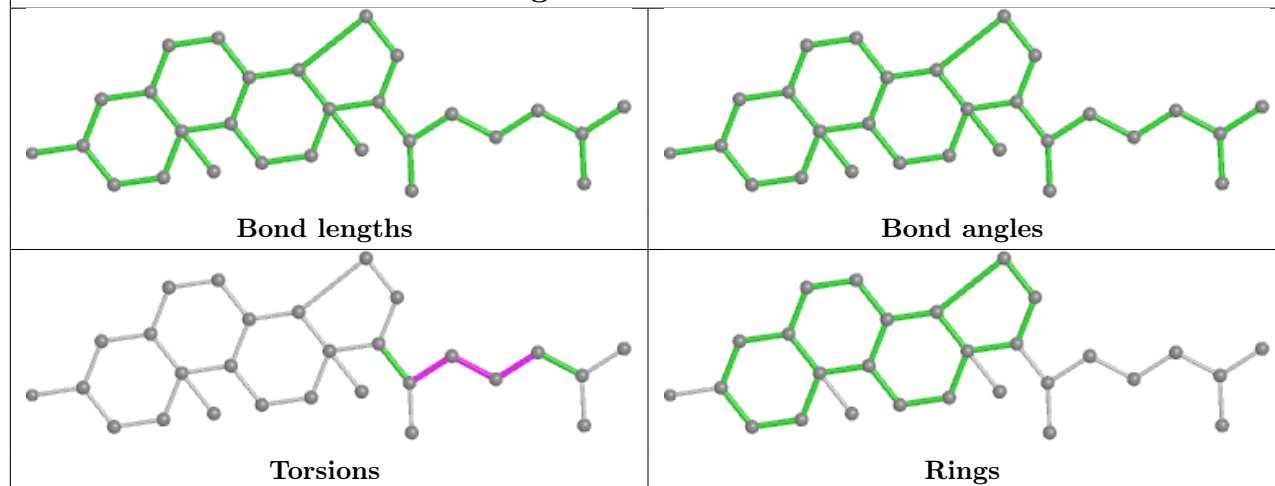
Rings



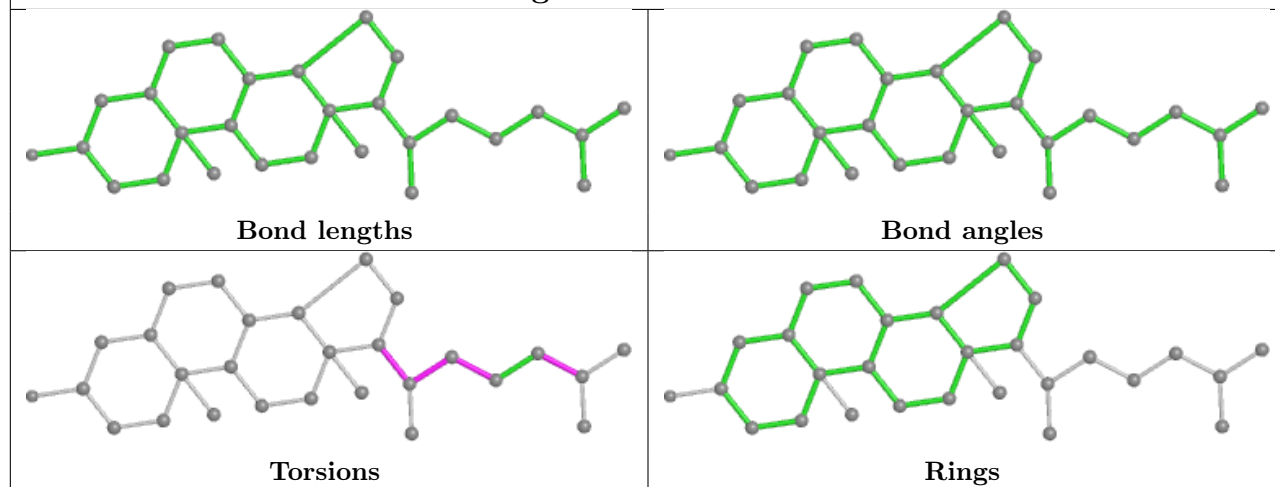
Ligand 3PE A 813

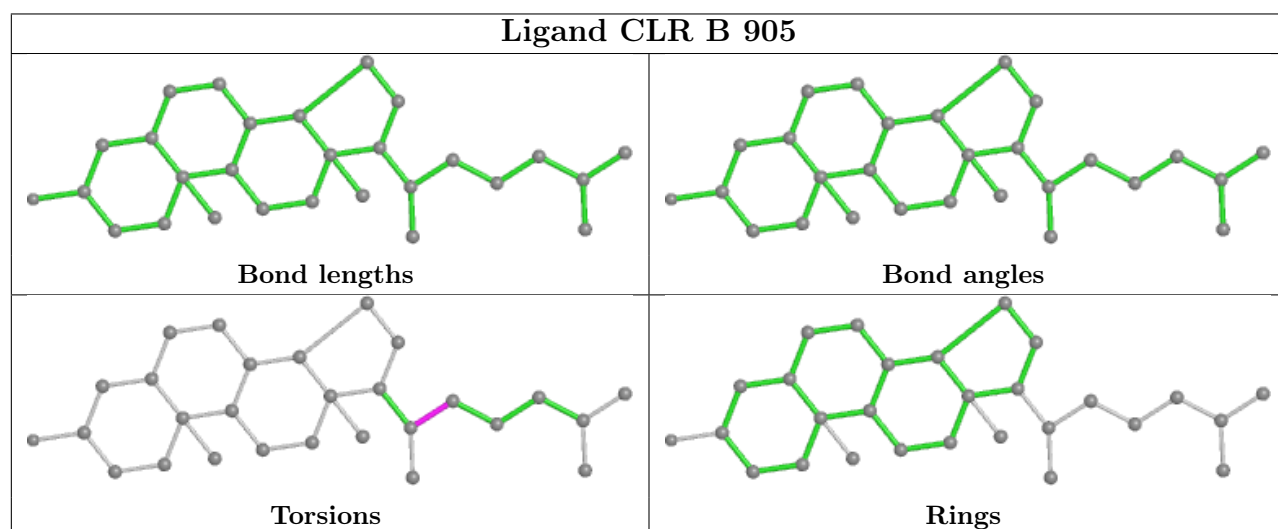
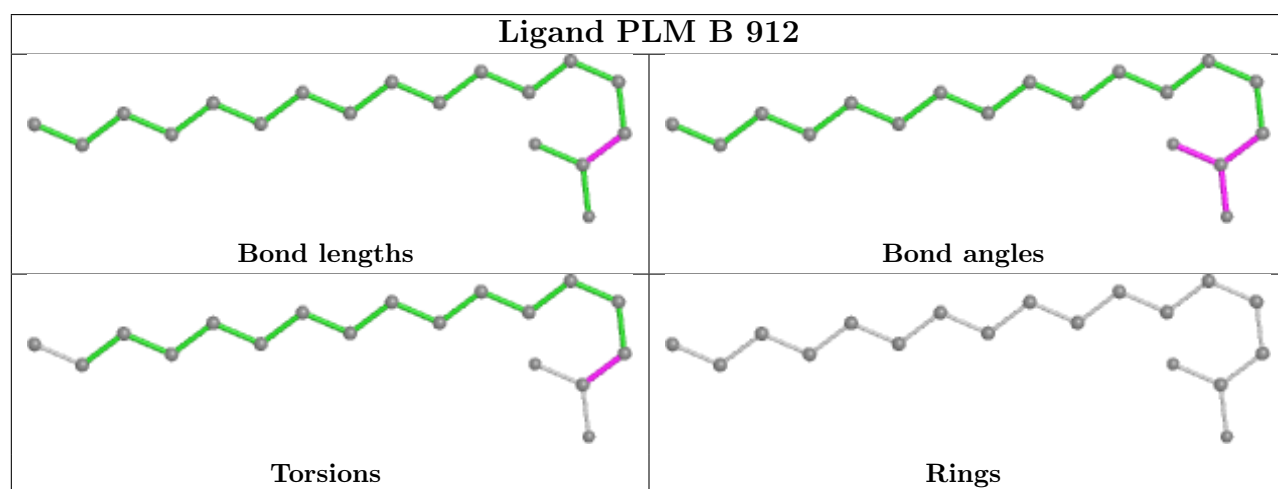
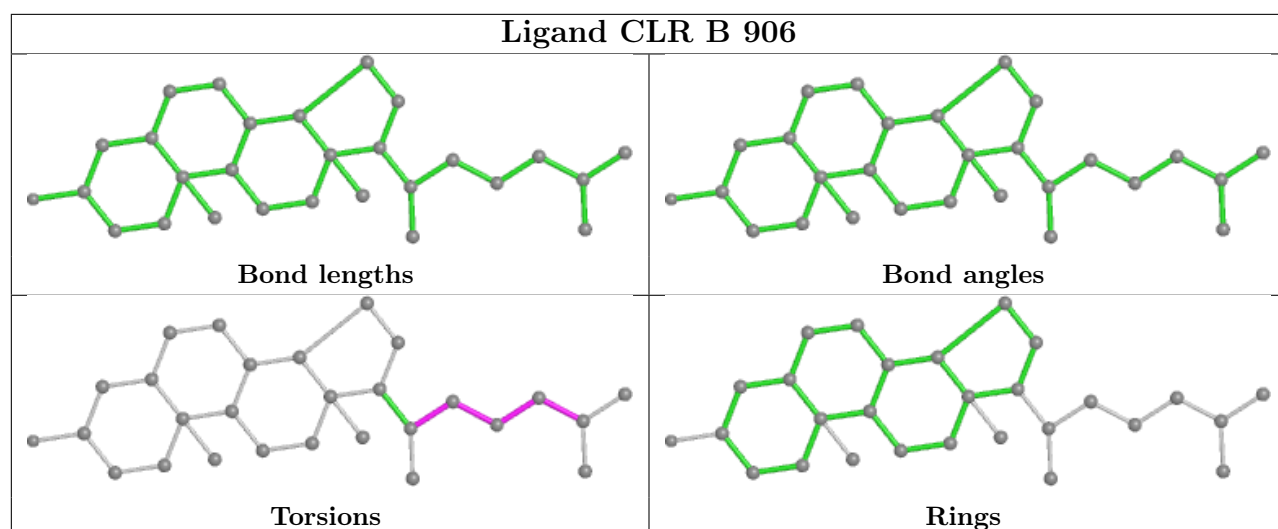


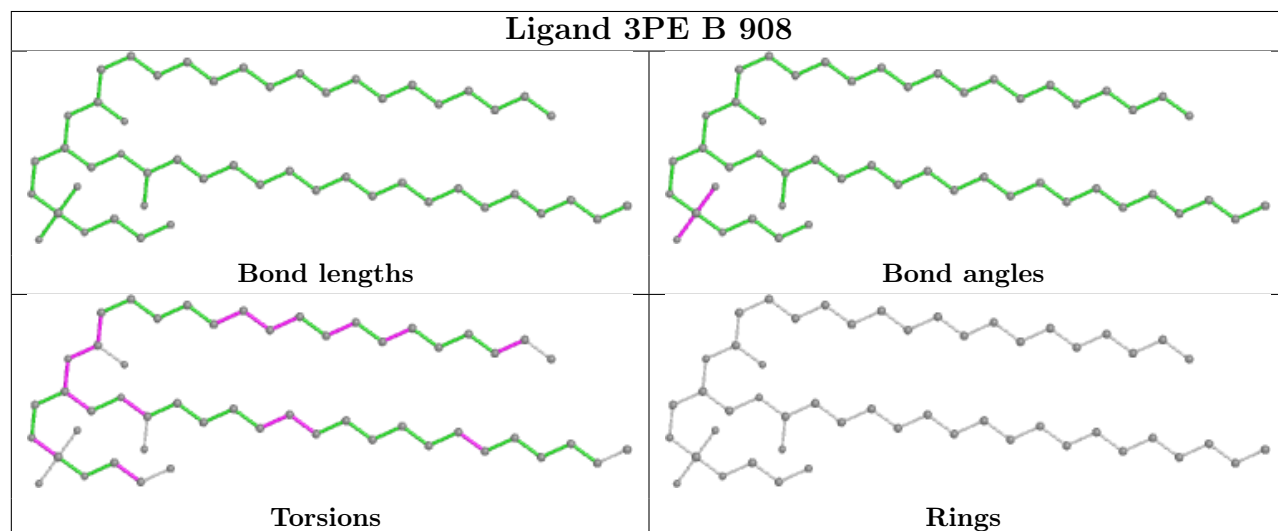
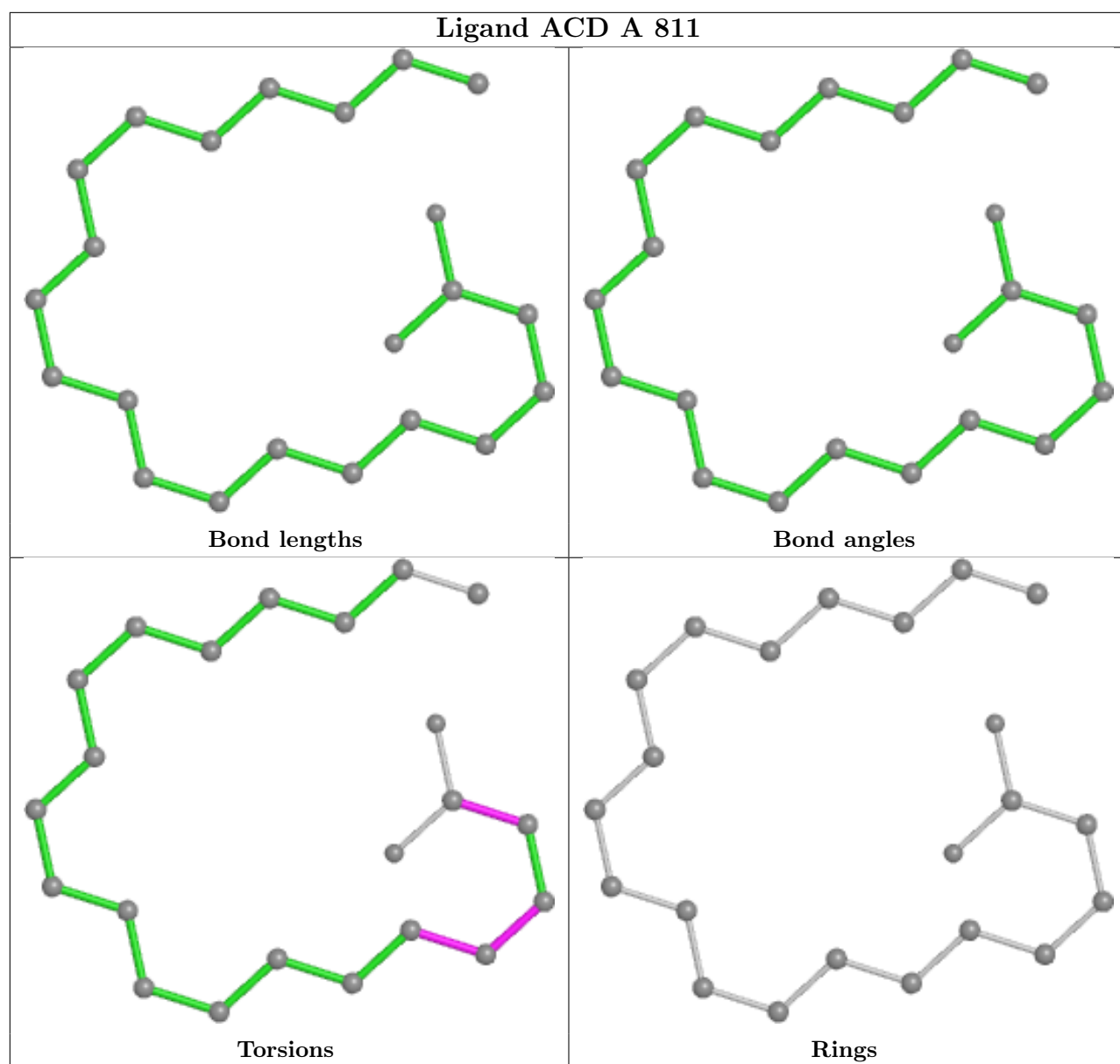
Ligand CLR A 806



Ligand CLR B 907







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.

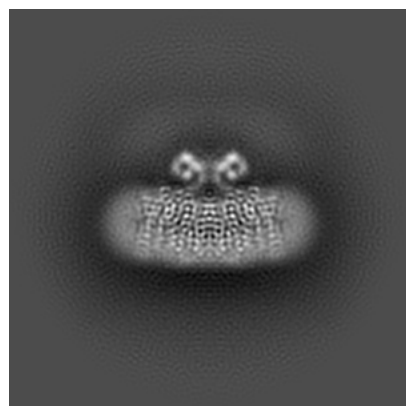
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60897. These allow visual inspection of the internal detail of the map and identification of artifacts.

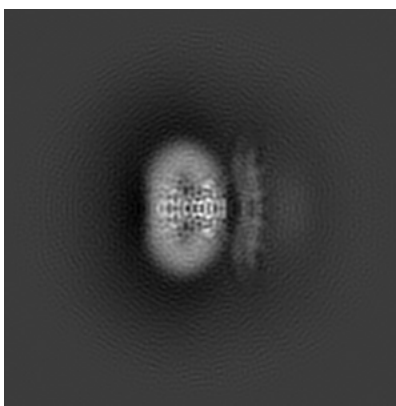
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

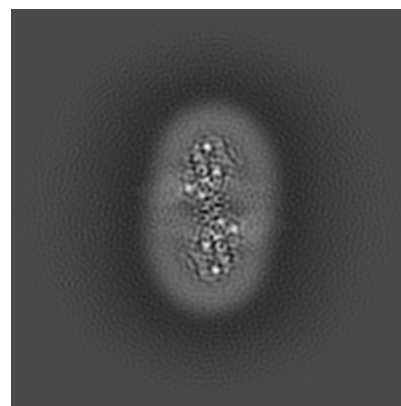
6.1.1 Primary map



X

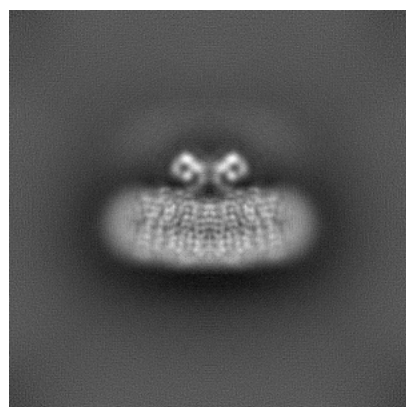


Y

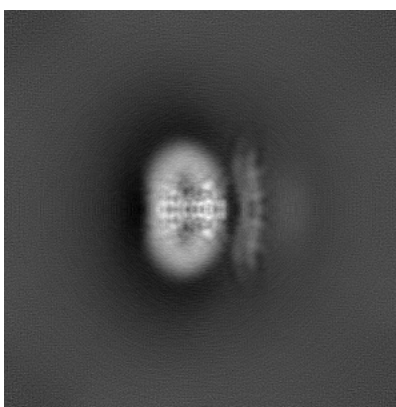


Z

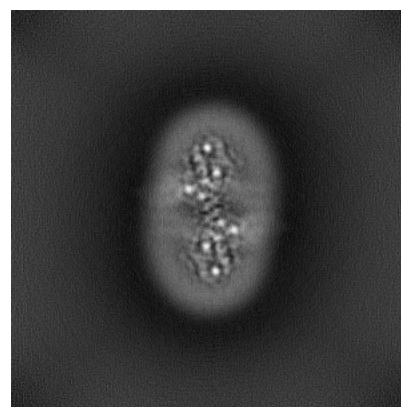
6.1.2 Raw map



X



Y

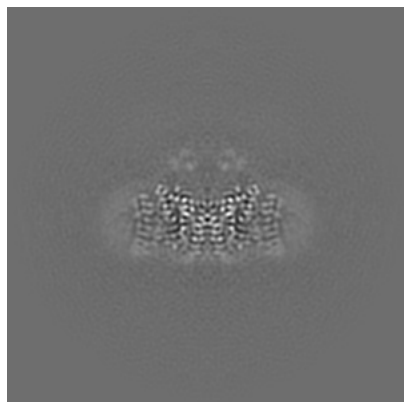


Z

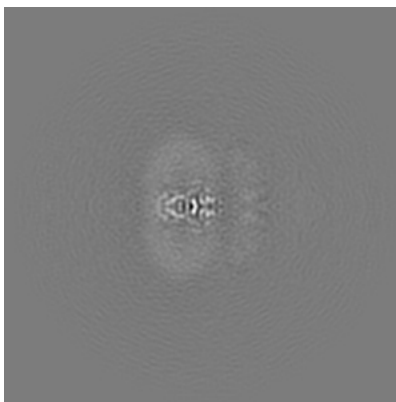
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

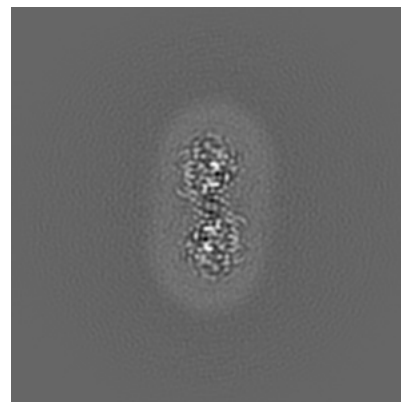
6.2.1 Primary map



X Index: 200

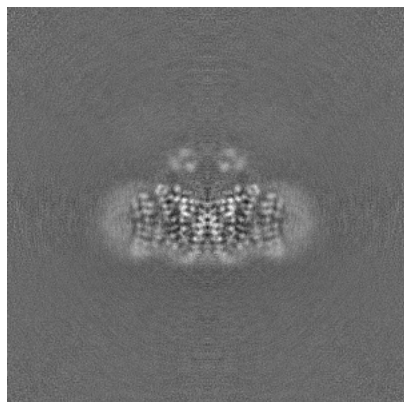


Y Index: 200

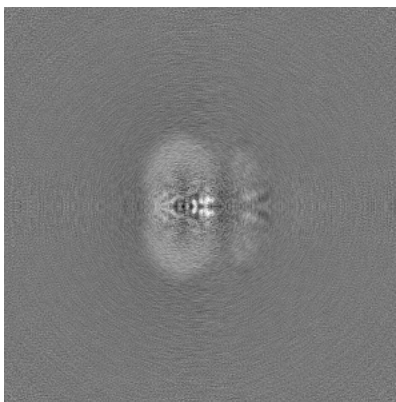


Z Index: 200

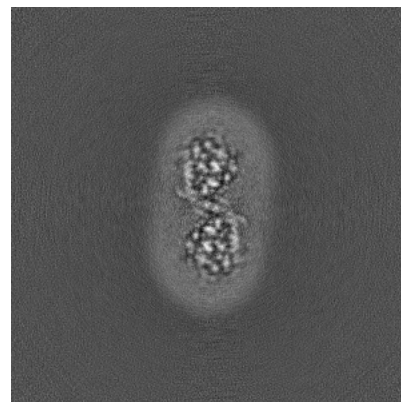
6.2.2 Raw map



X Index: 200



Y Index: 200

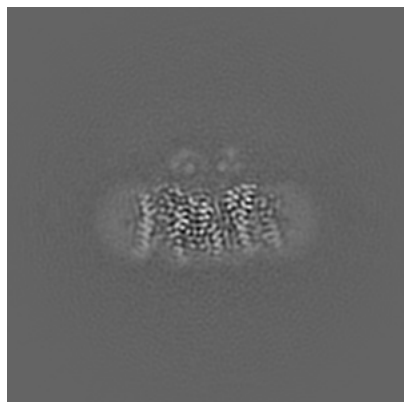


Z Index: 200

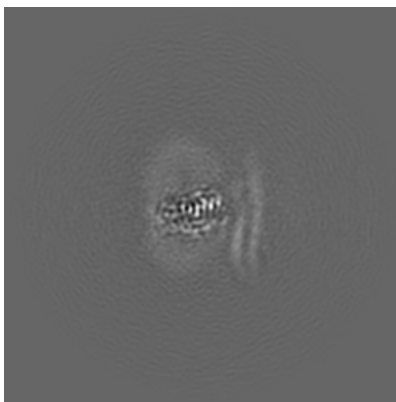
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

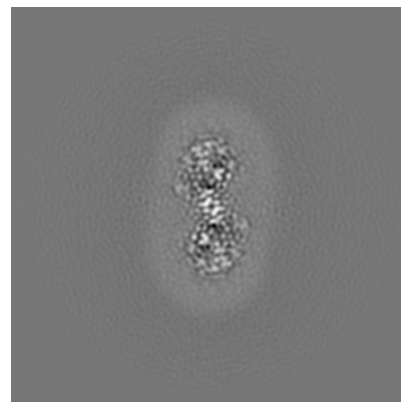
6.3.1 Primary map



X Index: 204

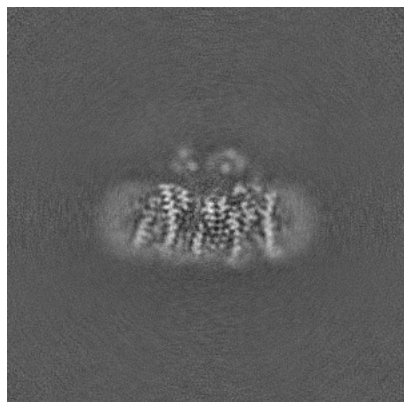


Y Index: 223

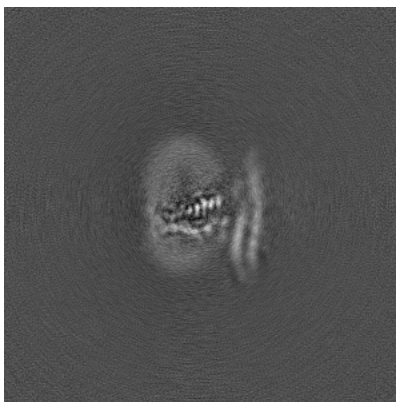


Z Index: 196

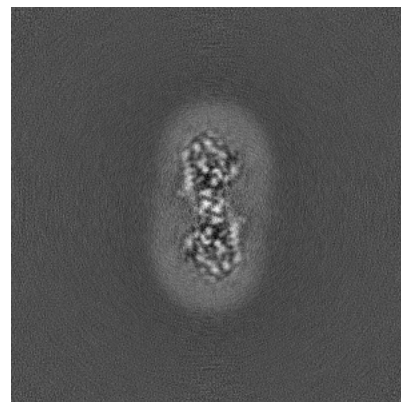
6.3.2 Raw map



X Index: 195



Y Index: 222

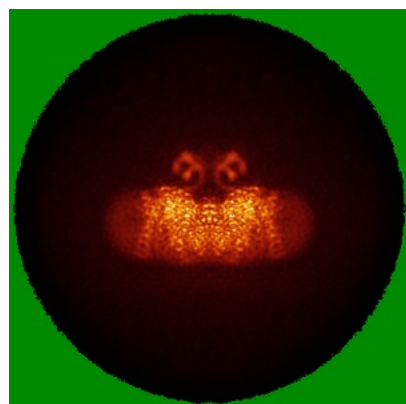


Z Index: 203

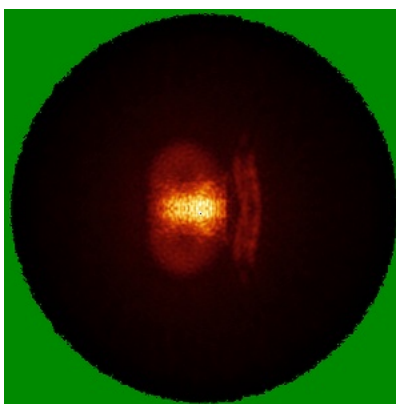
The images above show the largest variance slices of the map in three orthogonal directions.

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

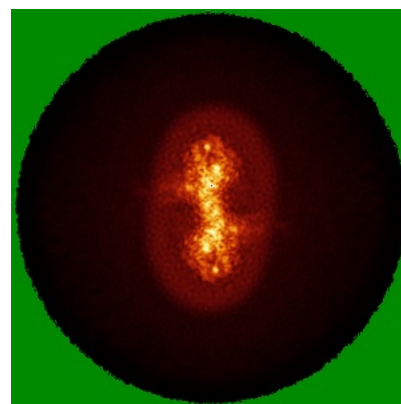
6.4.1 Primary map



X



Y

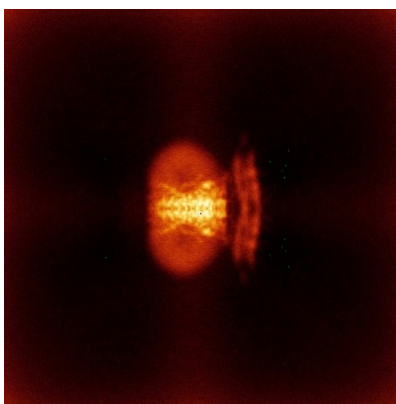


Z

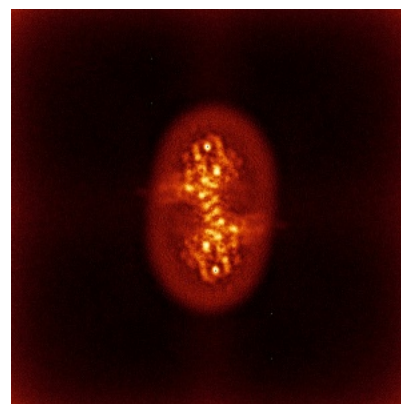
6.4.2 Raw map



X



Y

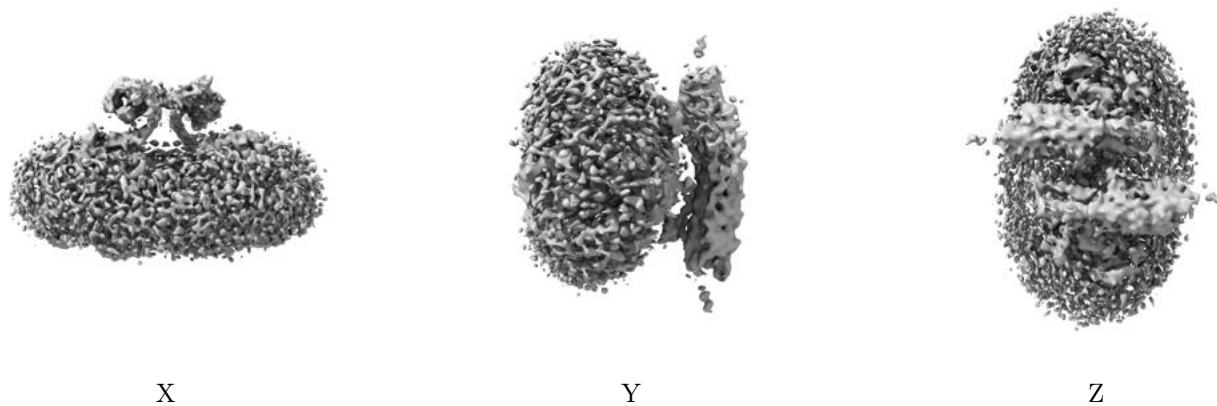


Z

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.

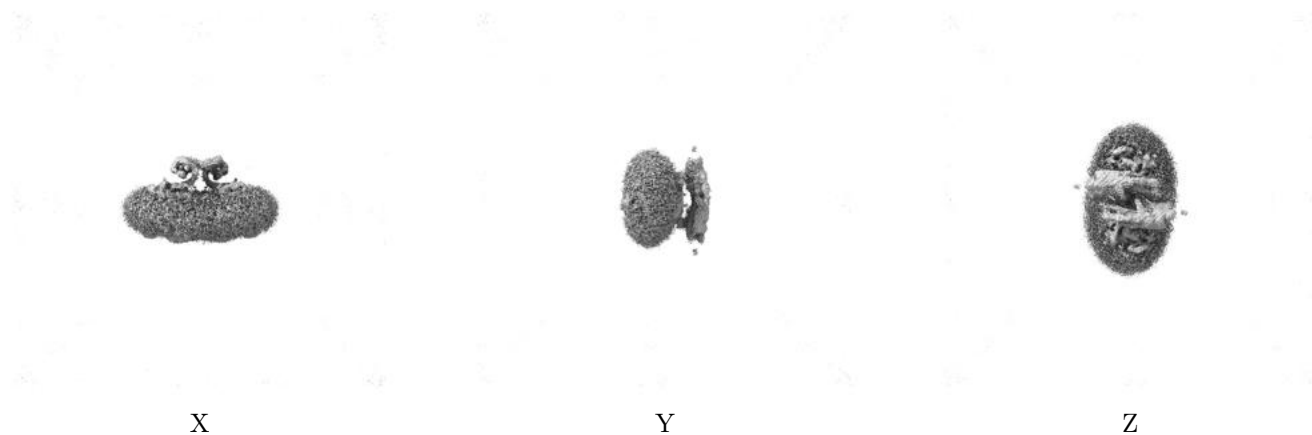
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. 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.

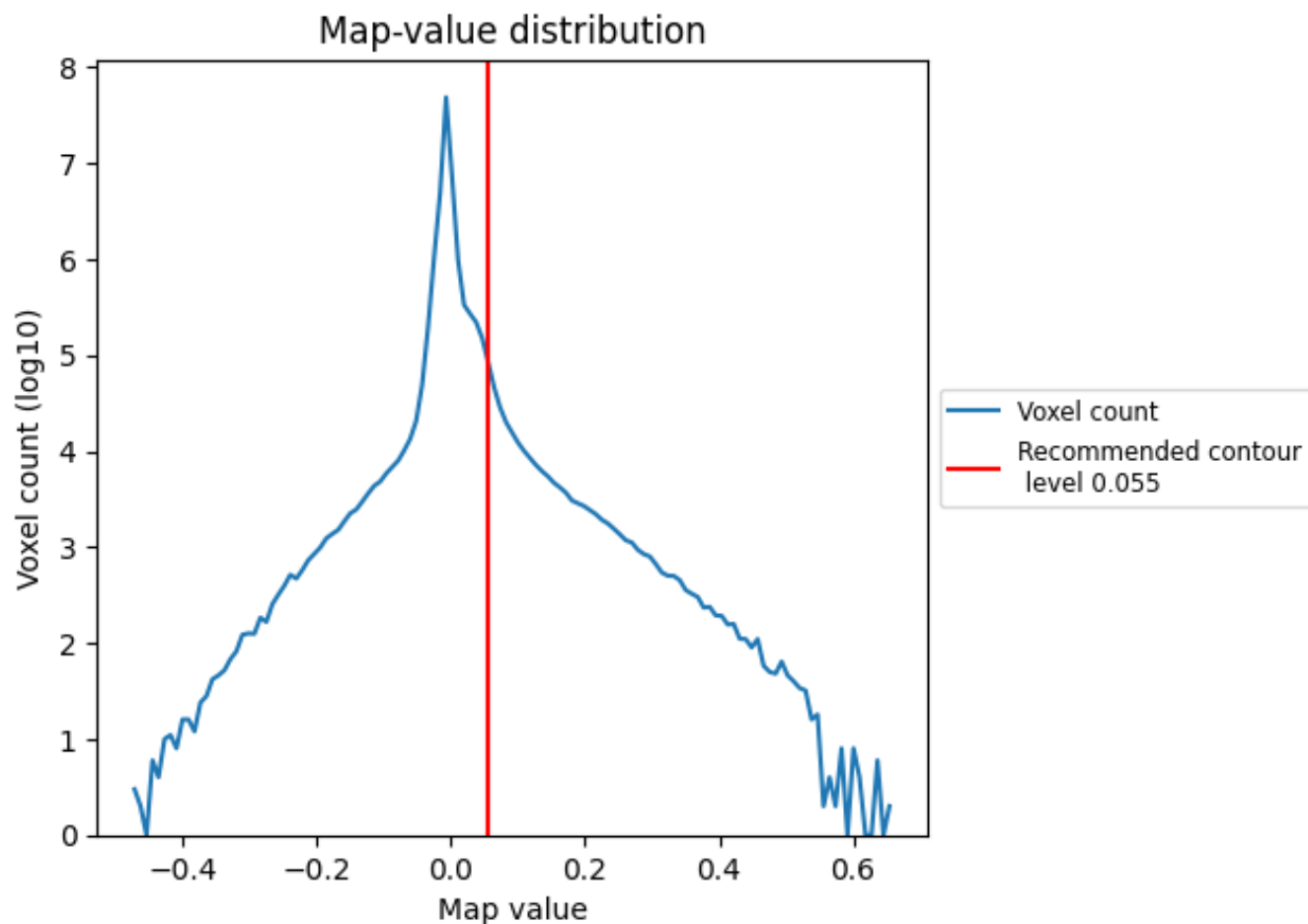
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

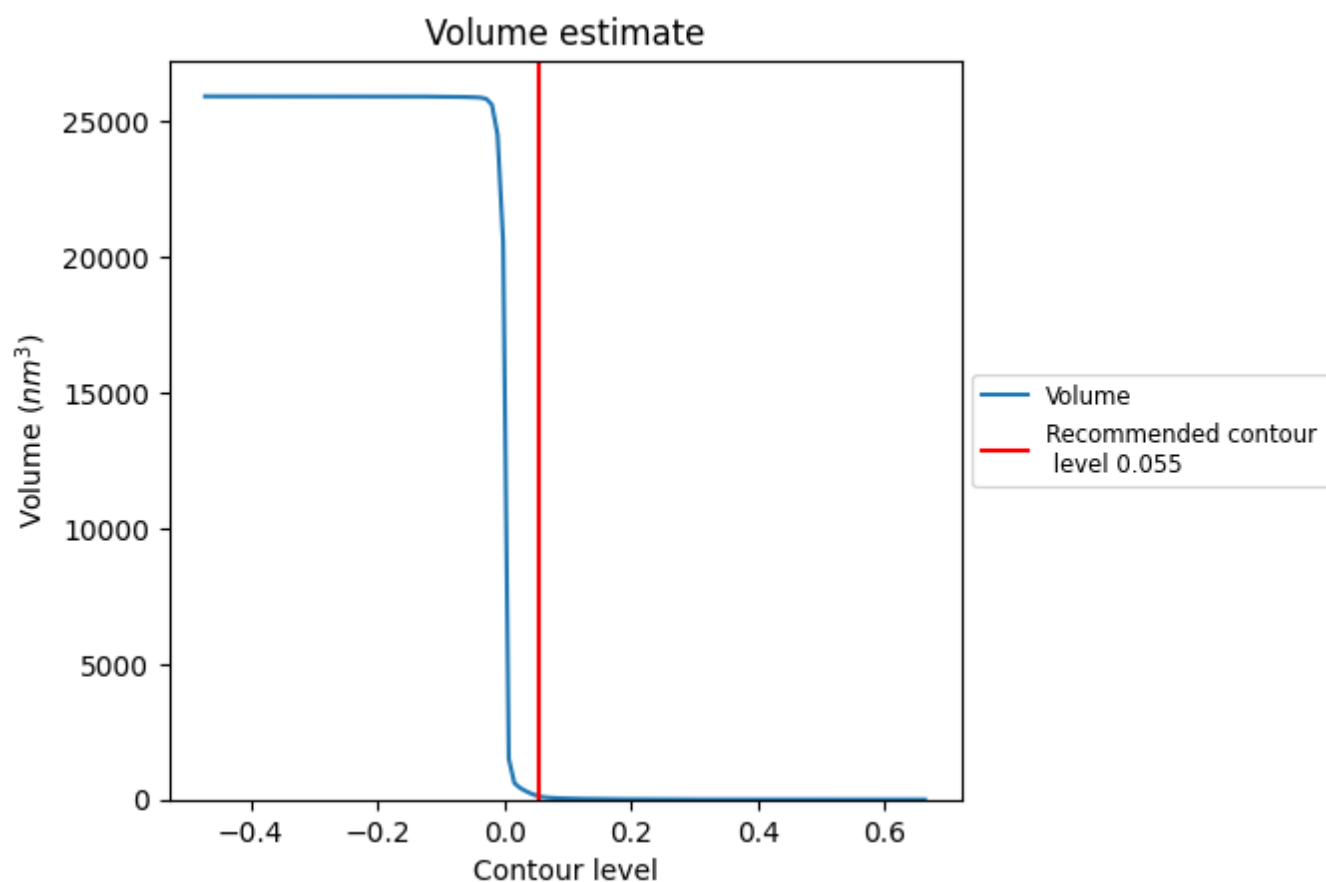
This section contains the results of statistical analysis of the map.

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.

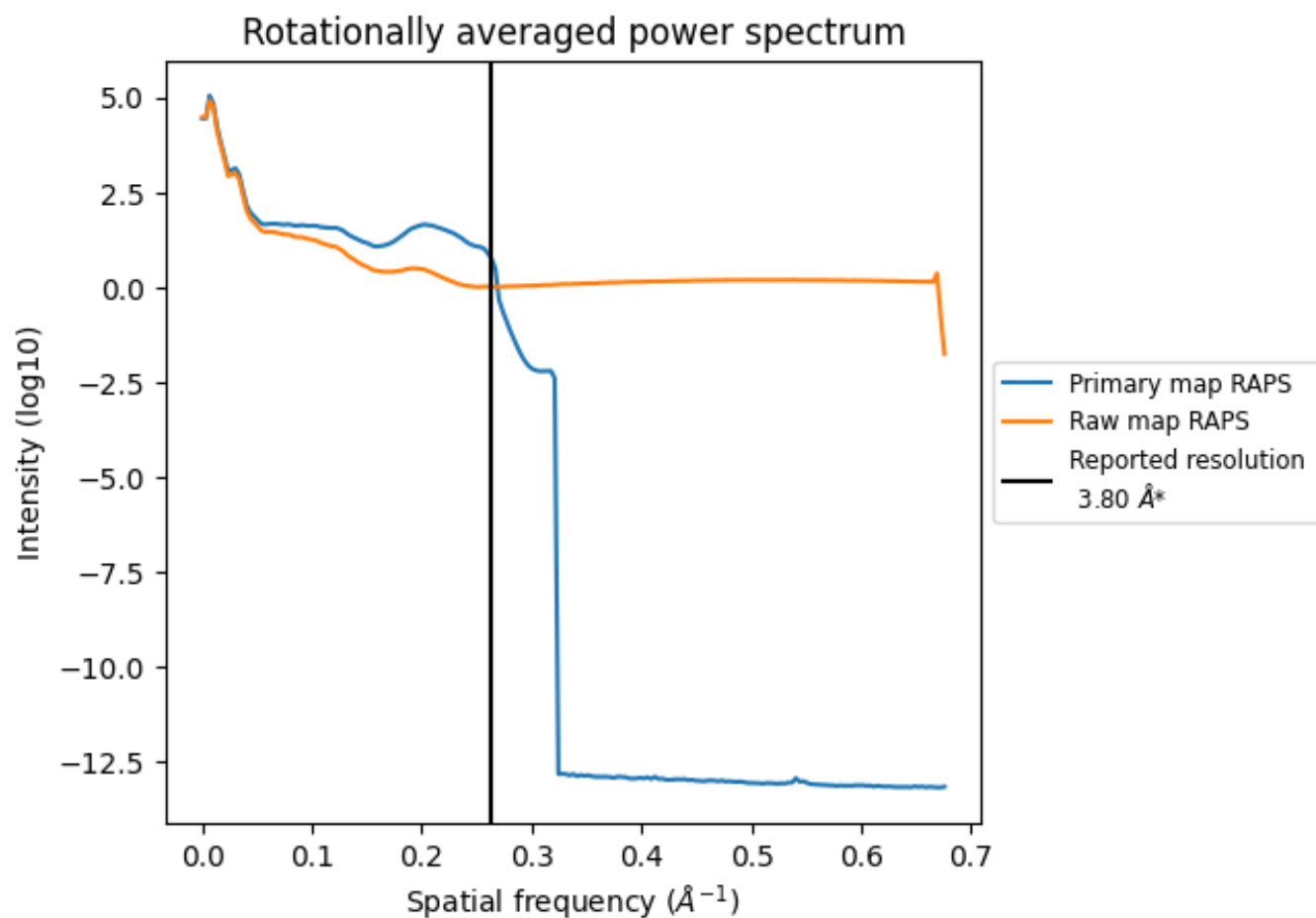
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 121 nm³; this corresponds to an approximate mass of 109 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 ⓘ

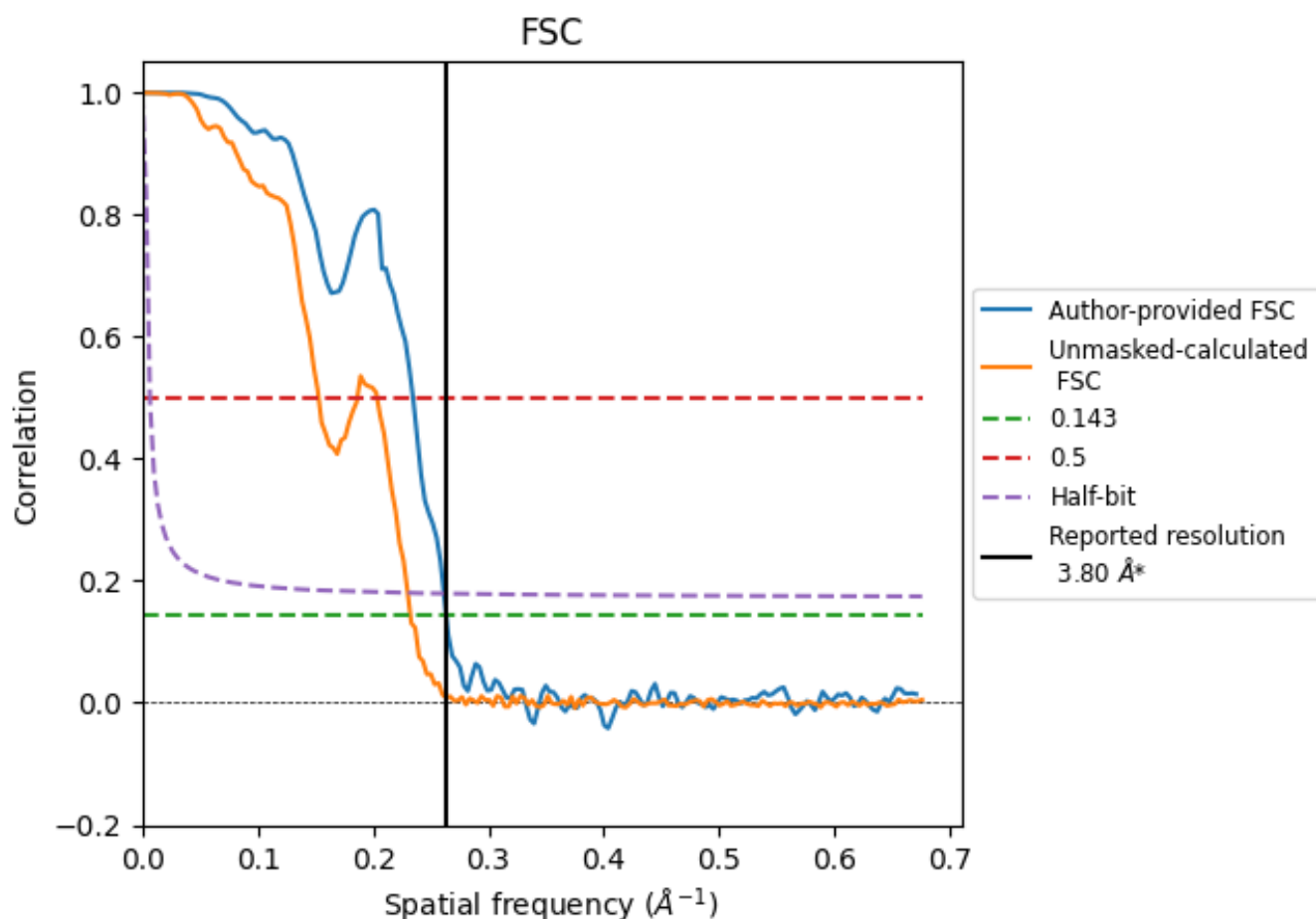


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 \AA^{-1}

8.2 Resolution estimates [i](#)

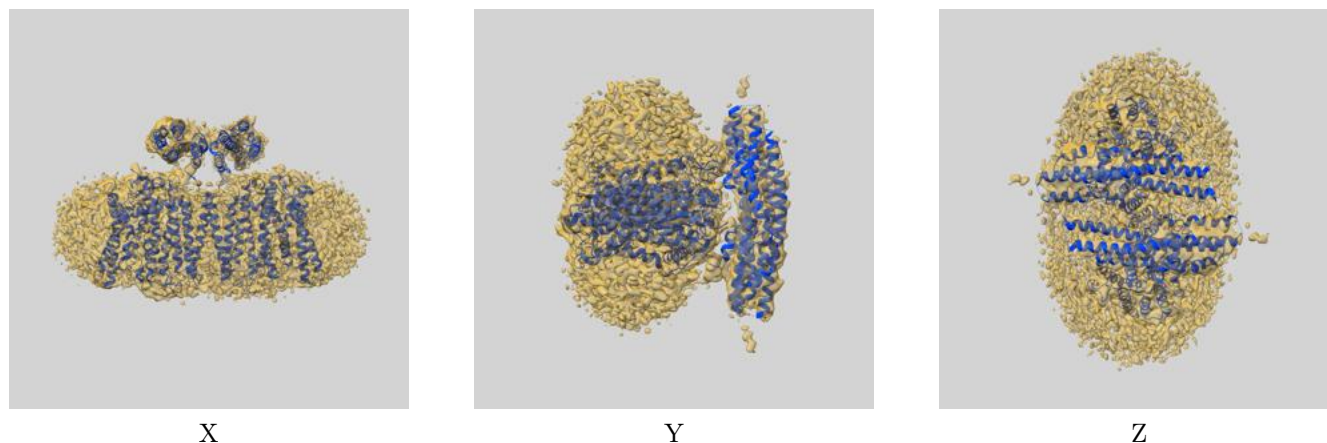
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.80	4.26	3.83
Unmasked-calculated*	4.30	6.54	4.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.30 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

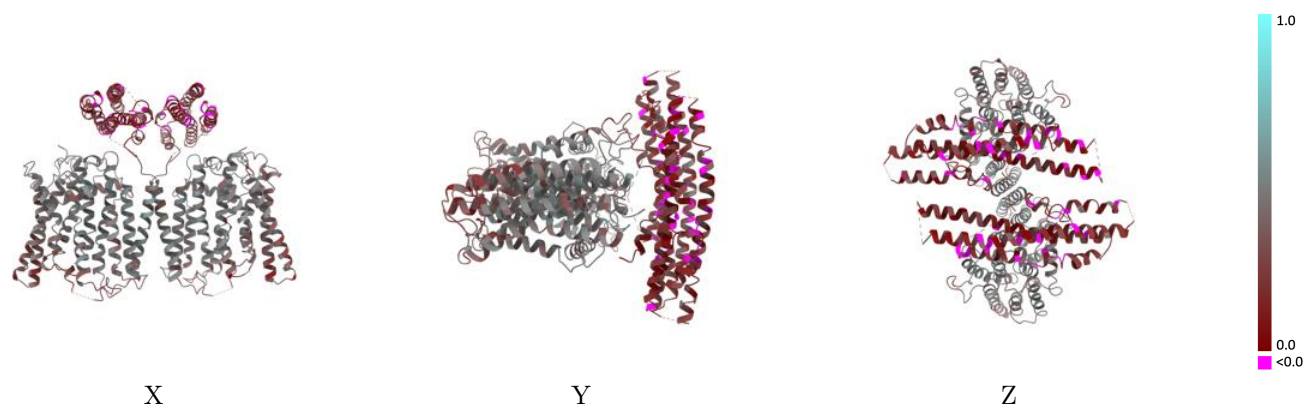
This section contains information regarding the fit between EMDB map EMD-60897 and PDB model 9IUC. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



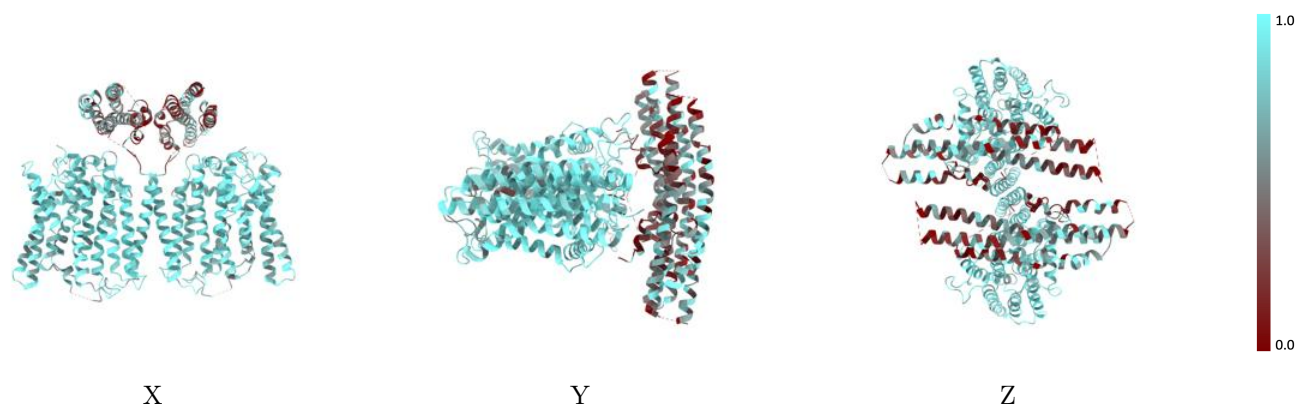
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



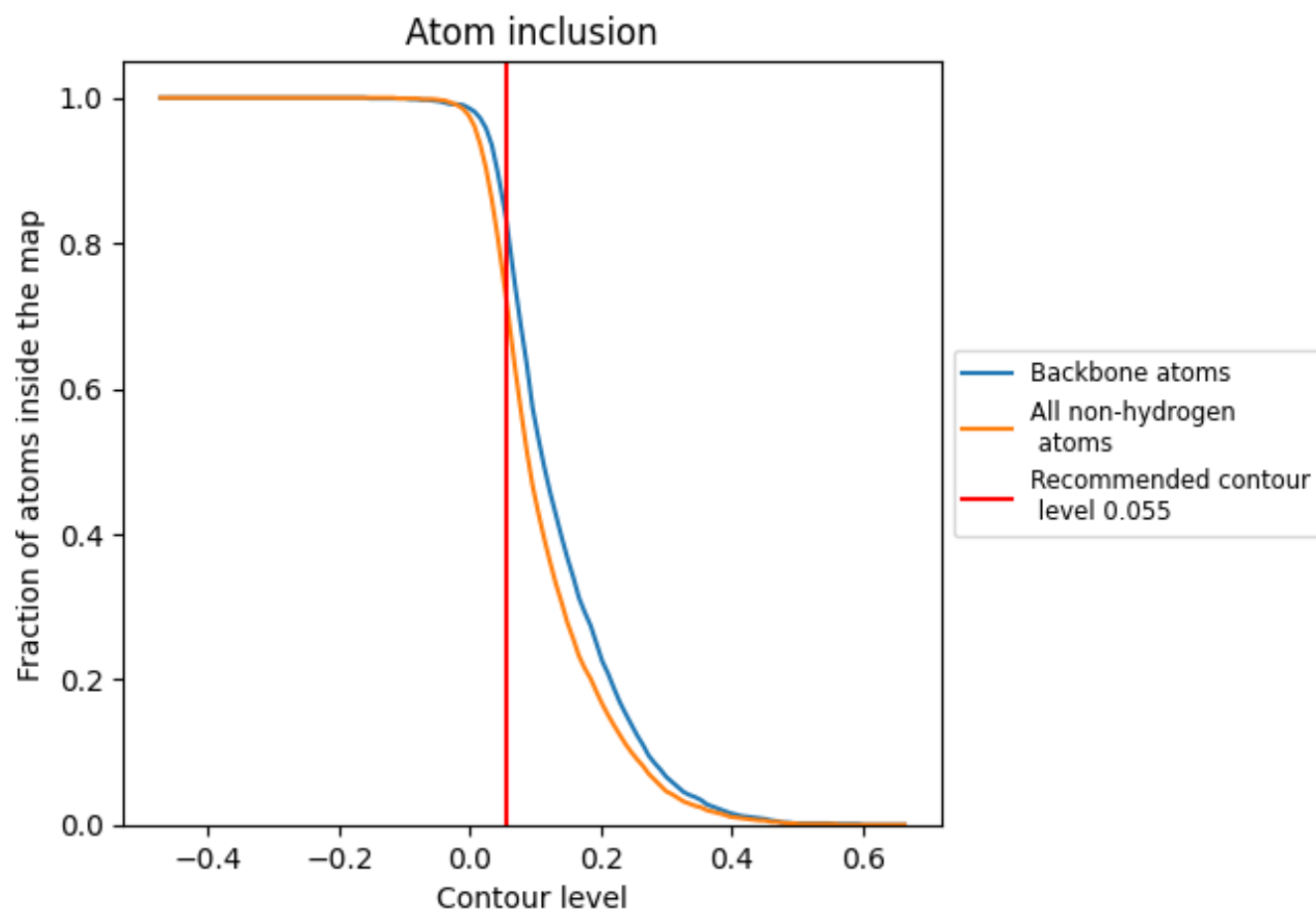
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.055).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 73% 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 (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7260	<div></div> 0.3480
A	<div></div> 0.7220	<div></div> 0.3440
B	<div></div> 0.7300	<div></div> 0.3510

