



Full wwPDB EM Validation Report ⓘ

Jul 8, 2025 – 06:20 PM JST

PDB ID : 9JBF / pdb_00009jbf
EMDB ID : EMD-61312
Title : Cryo-EM structure of the human LYCHOS Y57A mutant in complex with
cholesteryl hemisuccinate in the contracted state
Authors : Yu, S.; Liang, L.
Deposited on : 2024-08-27
Resolution : 3.21 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

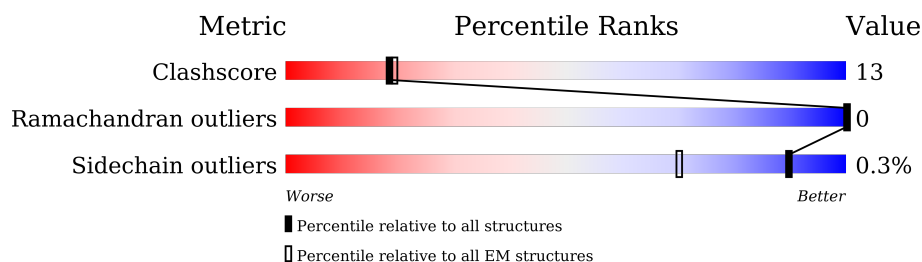
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.21 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	878	<div> <div>12%</div> <div>58%</div> <div>21%</div> <div>21%</div> </div>
1	B	878	<div> <div>12%</div> <div>57%</div> <div>21%</div> <div>21%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11718 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 Lysosomal cholesterol signaling protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	691	Total	C	N	O	S	0	0
			5443	3598	867	941	37		
1	B	691	Total	C	N	O	S	0	0
			5443	3598	867	941	37		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ALA	TYR	engineered mutation	UNP Q7Z3F1
A	871	SER	-	expression tag	UNP Q7Z3F1
A	872	ARG	-	expression tag	UNP Q7Z3F1
A	873	GLU	-	expression tag	UNP Q7Z3F1
A	874	ASN	-	expression tag	UNP Q7Z3F1
A	875	LEU	-	expression tag	UNP Q7Z3F1
A	876	TYR	-	expression tag	UNP Q7Z3F1
A	877	PHE	-	expression tag	UNP Q7Z3F1
A	878	GLN	-	expression tag	UNP Q7Z3F1
B	57	ALA	TYR	engineered mutation	UNP Q7Z3F1
B	871	SER	-	expression tag	UNP Q7Z3F1
B	872	ARG	-	expression tag	UNP Q7Z3F1
B	873	GLU	-	expression tag	UNP Q7Z3F1
B	874	ASN	-	expression tag	UNP Q7Z3F1
B	875	LEU	-	expression tag	UNP Q7Z3F1
B	876	TYR	-	expression tag	UNP Q7Z3F1
B	877	PHE	-	expression tag	UNP Q7Z3F1
B	878	GLN	-	expression tag	UNP Q7Z3F1

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$) (labeled as "Ligand of Interest" by depositor).



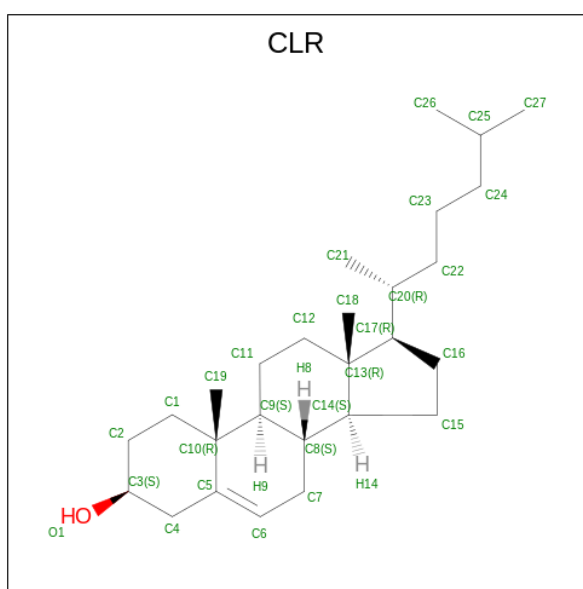
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total 35	C 31	O 4	0
2	A	1	Total 35	C 31	O 4	0
2	B	1	Total 35	C 31	O 4	0
2	B	1	Total 35	C 31	O 4	0

- Molecule 3 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



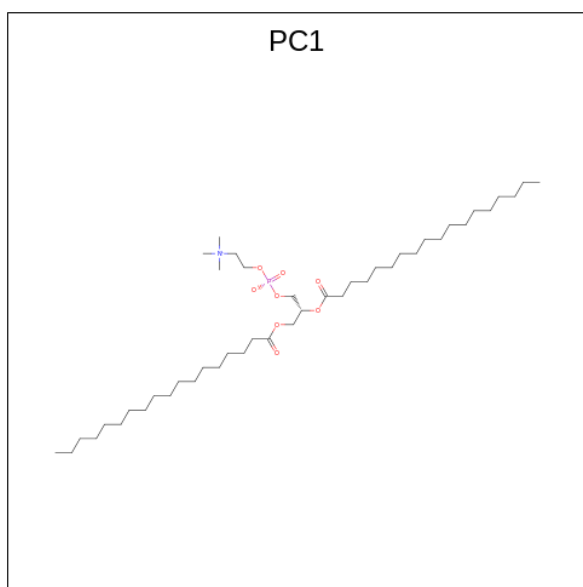
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	B	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



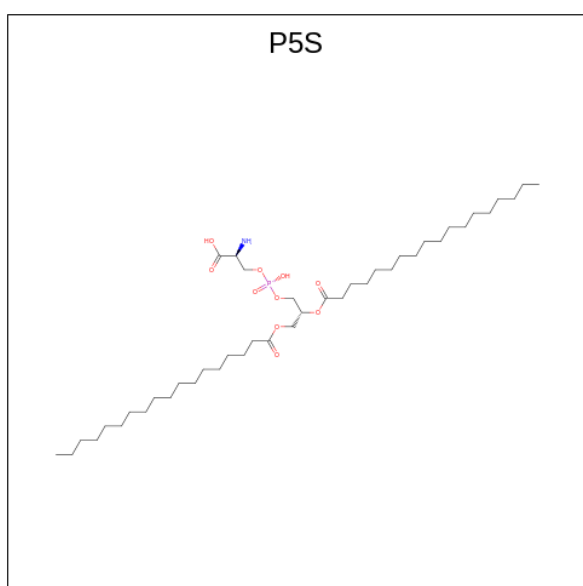
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	

- Molecule 5 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	B	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 6 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: $C_{42}H_{82}NO_{10}P$) (labeled as "Ligand of Interest" by depositor).

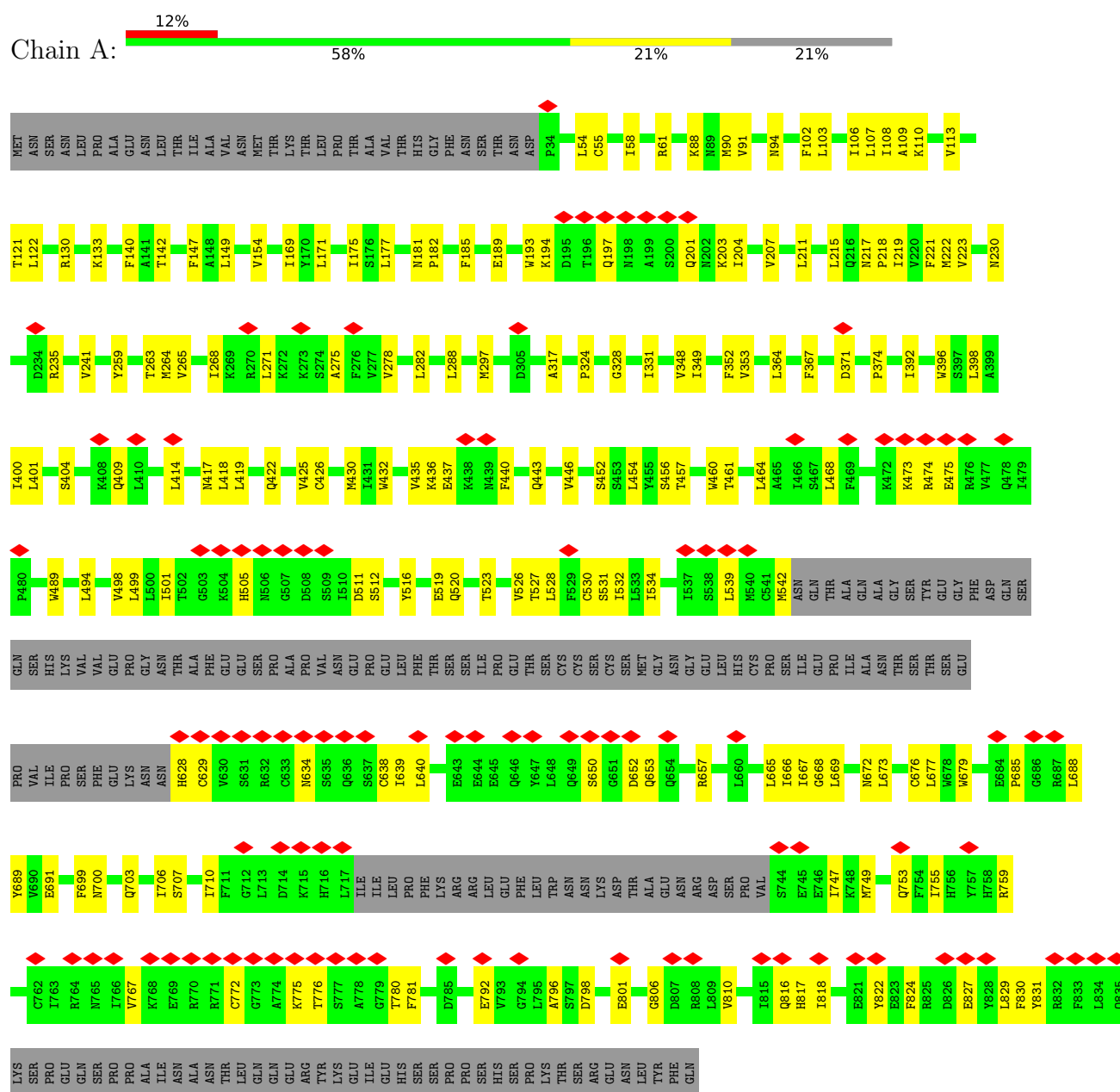


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			54	42	1	10	1	
6	A	1	Total	C	N	O	P	0
			54	42	1	10	1	
6	B	1	Total	C	N	O	P	0
			54	42	1	10	1	
6	B	1	Total	C	N	O	P	0
			54	42	1	10	1	

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: Lysosomal cholesterol signaling protein



Chain B:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96240	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 ($e^-/\text{\AA}^2$)	49.90	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.595	Depositor
Minimum map value	-0.903	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.23	Depositor
Map size (\AA)	323.2, 323.2, 323.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.808, 0.808, 0.808	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: Y01, PC1, CLR, P5S, 3PE

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	0.15	0/5568	0.34	0/7554
1	B	0.17	0/5568	0.37	0/7554
All	All	0.16	0/11136	0.36	0/15108

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	5443	0	5615	132	0
1	B	5443	0	5615	141	0
2	A	70	0	98	8	0
2	B	70	0	98	6	0
3	A	102	0	164	9	0
3	B	102	0	164	9	0
4	A	28	0	46	0	0
4	B	28	0	46	0	0
5	A	108	0	176	13	0
5	B	108	0	176	9	0
6	A	108	0	160	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	108	0	160	6	0
All	All	11718	0	12518	309	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 13.

All (309) 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:752:GLN:HA	1:B:755:ILE:HG22	1.74	0.69
1:B:108:ILE:HG21	1:B:297:MET:HE2	1.73	0.69
1:A:264:MET:HE3	1:A:352:PHE:HE1	1.58	0.68
1:B:390:SER:O	1:B:394:LEU:HB2	1.94	0.68
1:A:241:VAL:HG21	6:A:909:P5S:H50	1.76	0.67
2:B:903:Y01:HAI	2:B:904:Y01:HB ^F	1.77	0.66
1:B:822:TYR:HB3	1:B:825:ARG:HH12	1.58	0.66
1:A:264:MET:HG3	1:A:348:VAL:HG22	1.79	0.65
1:B:747:ILE:HD12	1:B:747:ILE:H	1.60	0.65
1:A:829:LEU:HB2	1:A:831:TYR:HE1	1.63	0.64
1:B:295:ARG:HD3	1:B:318:PHE:HB2	1.78	0.64
2:B:903:Y01:HAK1	2:B:904:Y01:HAU1	1.79	0.64
1:A:749:MET:HG2	1:A:753:GLN:HE21	1.63	0.63
1:B:772:CYS:H	1:B:776:THR:HB	1.64	0.63
1:A:747:ILE:HD12	1:A:747:ILE:H	1.64	0.62
1:A:110:LYS:NZ	1:A:142:THR:O	2.34	0.61
5:B:901:PC1:H3G1	5:B:901:PC1:H2H2	1.82	0.61
1:B:483:ILE:HA	1:B:486:ILE:HD12	1.81	0.60
1:B:769:GLU:HB3	1:B:778:ALA:HA	1.83	0.60
1:A:796:ALA:HB1	1:A:801:GLU:HB2	1.84	0.60
1:B:528:LEU:O	1:B:532:ILE:HG13	2.01	0.59
1:A:519:GLU:O	1:A:523:THR:HG23	2.02	0.59
6:A:906:P5S:H28	1:B:222:MET:HE1	1.83	0.59
1:B:646:GLN:HA	1:B:649:GLN:NE2	2.18	0.59
1:B:452:SER:O	1:B:456:SER:OG	2.20	0.59
1:A:417:ASN:HD21	1:A:489:TRP:HE1	1.51	0.59
1:B:117:VAL:O	1:B:121:THR:HG22	2.02	0.59
1:B:780:THR:HB	1:B:830:PHE:HB3	1.84	0.59
1:B:110:LYS:NZ	1:B:142:THR:O	2.35	0.58
1:A:268:ILE:HD11	3:A:907:3PE:H12	1.85	0.58
1:A:530:CYS:O	1:A:534:ILE:HG12	2.04	0.58
1:A:772:CYS:H	1:A:776:THR:HB	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:TRP:CE2	1:A:400:ILE:HD11	2.39	0.57
1:A:700:ASN:O	1:A:703:GLN:NE2	2.37	0.57
1:A:516:TYR:HB2	1:A:520:GLN:HE21	1.70	0.57
1:B:364:LEU:HA	1:B:367:PHE:HB2	1.86	0.57
1:A:417:ASN:ND2	1:A:489:TRP:HE1	2.02	0.56
1:B:459:LEU:O	1:B:463:LEU:HG	2.05	0.56
1:A:401:LEU:HD11	1:A:419:LEU:HD13	1.88	0.56
1:A:222:MET:HE1	6:B:908:P5S:H28	1.87	0.56
1:A:364:LEU:HA	1:A:367:PHE:HD2	1.71	0.56
1:A:54:LEU:HD23	6:B:902:P5S:H31A	1.88	0.56
1:B:817:HIS:HD2	1:B:822:TYR:HB2	1.71	0.56
1:A:268:ILE:HG23	2:A:902:Y01:HAM1	1.88	0.55
1:A:528:LEU:O	1:A:532:ILE:HG13	2.05	0.55
2:A:901:Y01:HAQ1	2:A:902:Y01:HAC2	1.87	0.55
1:B:755:ILE:HA	1:B:759:ARG:HD2	1.86	0.55
1:A:474:ARG:NH2	1:A:475:GLU:O	2.38	0.55
1:B:412:HIS:HA	1:B:415:THR:HG22	1.88	0.55
5:A:908:PC1:H242	6:A:909:P5S:H54A	1.89	0.55
2:B:904:Y01:HAE3	3:B:909:3PE:H262	1.88	0.55
1:B:432:TRP:HA	1:B:435:VAL:HG12	1.89	0.55
1:B:797:SER:OG	1:B:798:ASP:OD1	2.25	0.55
1:A:90:MET:HE1	1:A:223:VAL:HG13	1.89	0.55
1:A:511:ASP:OD1	1:A:512:SER:N	2.40	0.55
1:A:349:ILE:O	1:A:353:VAL:HG23	2.07	0.54
1:A:392:ILE:HG21	5:B:901:PC1:H2A1	1.88	0.54
1:A:806:GLY:HA3	1:A:824:PHE:CE2	2.42	0.54
1:A:264:MET:HE3	1:A:352:PHE:CE1	2.42	0.54
1:A:102:PHE:CZ	1:A:106:ILE:HD11	2.42	0.54
1:B:279:LEU:O	1:B:283:ILE:HG12	2.08	0.54
1:B:324:PRO:HB3	1:B:351:THR:HA	1.90	0.54
1:A:452:SER:O	1:A:456:SER:OG	2.23	0.54
1:B:367:PHE:HE1	1:B:375:LEU:HG	1.72	0.54
1:A:207:VAL:O	1:A:211:LEU:HD12	2.08	0.53
1:B:822:TYR:HB3	1:B:825:ARG:NH1	2.23	0.53
1:A:103:LEU:HD21	1:A:171:LEU:HB3	1.91	0.53
1:A:419:LEU:HD21	1:A:707:SER:HB2	1.90	0.53
1:A:767:VAL:HG12	1:A:781:PHE:HB3	1.91	0.53
1:B:139:ILE:HG13	1:B:329:VAL:HG13	1.90	0.53
1:A:61:ARG:NH1	2:A:901:Y01:OAH	2.42	0.53
5:A:908:PC1:H352	6:A:909:P5S:H56A	1.91	0.53
1:B:375:LEU:HD11	1:B:690:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:908:PC1:H292	6:A:909:P5S:H36B	1.91	0.52
3:A:907:3PE:H231	3:A:907:3PE:H322	1.92	0.52
6:A:909:P5S:H21A	6:B:908:P5S:H2	1.91	0.52
1:B:283:ILE:HD12	1:B:350:SER:HB3	1.92	0.52
1:B:470:LEU:HB3	1:B:479:ILE:HD11	1.91	0.52
1:B:280:ILE:HD13	3:B:909:3PE:H382	1.92	0.52
1:A:91:VAL:O	1:A:230:ASN:ND2	2.42	0.52
1:B:102:PHE:HE1	1:B:317:ALA:HB2	1.74	0.51
1:A:432:TRP:HA	1:A:435:VAL:HG12	1.91	0.51
1:B:297:MET:HE3	1:B:301:LEU:HD11	1.92	0.51
1:B:641:ALA:O	1:B:644:GLU:HG3	2.11	0.51
1:B:810:VAL:HG21	1:B:824:PHE:HB2	1.92	0.51
1:A:516:TYR:HB2	1:A:520:GLN:HB2	1.91	0.51
1:A:673:LEU:HA	1:A:676:CYS:SG	2.51	0.51
1:B:818:ILE:HA	1:B:832:ARG:HD3	1.92	0.51
1:B:641:ALA:HB2	1:B:818:ILE:HD13	1.93	0.51
1:B:394:LEU:HD21	1:B:422:GLN:HB3	1.93	0.50
1:A:499:LEU:HD21	1:A:520:GLN:HG3	1.92	0.50
1:A:780:THR:HG21	1:A:818:ILE:HD12	1.94	0.50
1:A:679:TRP:CD1	1:A:689:TYR:HH	2.30	0.50
1:B:463:LEU:HD13	1:B:484:ILE:HG23	1.93	0.50
1:B:519:GLU:HA	1:B:522:ILE:HD12	1.92	0.50
1:B:754:PHE:O	1:B:759:ARG:HG3	2.11	0.50
6:A:906:P5S:H53A	5:B:901:PC1:H291	1.94	0.50
1:A:90:MET:SD	1:A:223:VAL:HG22	2.52	0.50
1:B:349:ILE:HG21	3:B:909:3PE:H342	1.94	0.50
1:B:817:HIS:CD2	1:B:822:TYR:HB2	2.47	0.50
1:A:109:ALA:O	1:A:113:VAL:HG23	2.12	0.49
1:A:221:PHE:HZ	6:A:909:P5S:H3A	1.77	0.49
1:B:532:ILE:HD12	1:B:673:LEU:HD22	1.93	0.49
1:B:146:ASP:HB2	1:B:169:ILE:HG23	1.94	0.49
1:B:399:ALA:O	1:B:403:LEU:HG	2.13	0.49
1:B:769:GLU:OE1	1:B:780:THR:OG1	2.29	0.49
1:A:639:ILE:HG22	1:A:772:CYS:HB3	1.94	0.49
1:B:744:SER:HA	1:B:747:ILE:HD13	1.94	0.49
1:B:746:GLU:HG2	1:B:747:ILE:HD12	1.94	0.49
1:B:749:MET:HG2	1:B:753:GLN:HE21	1.78	0.49
1:A:824:PHE:HA	1:A:831:TYR:CE2	2.47	0.48
5:A:908:PC1:H3E1	5:B:907:PC1:H3E2	1.95	0.48
1:A:398:LEU:HD23	1:A:401:LEU:HD12	1.95	0.48
1:B:271:LEU:HD13	1:B:275:ALA:HB1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:673:LEU:HA	1:B:676:CYS:SG	2.52	0.48
1:B:817:HIS:HE2	1:B:829:LEU:HD23	1.78	0.48
1:A:417:ASN:CG	1:A:489:TRP:HE1	2.21	0.48
1:B:154:VAL:HG11	1:B:169:ILE:HD11	1.95	0.48
1:B:349:ILE:HD13	3:B:909:3PE:H321	1.96	0.48
1:B:823:GLU:HG2	1:B:824:PHE:H	1.79	0.48
1:A:154:VAL:HG11	1:A:169:ILE:HD11	1.94	0.48
1:A:532:ILE:HD12	1:A:673:LEU:HD22	1.95	0.48
1:A:816:GLN:OE1	1:A:816:GLN:N	2.47	0.48
1:A:121:THR:HG21	1:A:133:LYS:C	2.38	0.48
2:A:901:Y01:HAB1	2:A:901:Y01:HAJ1	1.73	0.48
6:B:902:P5S:H42	6:B:902:P5S:H27A	1.96	0.48
1:A:107:LEU:HD11	1:A:175:ILE:HG22	1.95	0.48
1:B:373:LYS:HB3	1:B:374:PRO:HD3	1.96	0.48
1:B:798:ASP:OD1	1:B:798:ASP:N	2.47	0.48
2:A:901:Y01:HAK1	2:A:902:Y01:HAU1	1.95	0.47
5:A:908:PC1:H2A1	1:B:392:ILE:HG21	1.96	0.47
1:B:816:GLN:HE21	1:B:832:ARG:CZ	2.27	0.47
1:A:409:GLN:NE2	1:A:652:ASP:O	2.43	0.47
1:B:628:HIS:CD2	1:B:771:ARG:HH12	2.31	0.47
1:B:480:PRO:HB2	1:B:483:ILE:HG12	1.96	0.47
1:A:523:THR:O	1:A:527:THR:HG22	2.15	0.47
1:B:529:PHE:O	1:B:533:LEU:HG	2.14	0.47
1:A:203:LYS:HD2	1:A:204:ILE:HD13	1.97	0.47
1:A:494:LEU:O	1:A:498:VAL:HG13	2.14	0.47
1:B:83:PRO:HB3	1:B:222:MET:HG2	1.96	0.47
1:B:189:GLU:HB2	1:B:206:ILE:HG23	1.97	0.47
1:A:706:ILE:HG22	1:A:710:ILE:HD11	1.97	0.47
5:A:908:PC1:H272	6:A:909:P5S:H36B	1.96	0.47
1:A:454:LEU:O	1:A:457:THR:OG1	2.27	0.47
1:B:67:SER:O	1:B:71:LYS:HG2	2.15	0.47
1:B:505:HIS:HD1	1:B:516:TYR:HE1	1.62	0.47
1:B:827:GLU:HB2	1:B:829:LEU:CD1	2.45	0.47
1:A:755:ILE:HA	1:A:759:ARG:HB2	1.97	0.47
1:B:367:PHE:CE1	1:B:375:LEU:HG	2.49	0.47
1:B:394:LEU:HD12	1:B:394:LEU:HA	1.76	0.47
1:A:288:LEU:HG	3:A:907:3PE:H3C2	1.97	0.47
6:B:908:P5S:H20	6:B:908:P5S:H39	1.97	0.47
1:A:218:PRO:HG3	6:A:909:P5S:H3	1.97	0.47
1:A:426:CYS:O	1:A:430:MET:HG3	2.15	0.46
5:A:905:PC1:H3E2	5:B:901:PC1:H3E1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:816:GLN:HE21	1:B:832:ARG:NH2	2.13	0.46
1:A:461:THR:OG1	1:A:665:LEU:HD13	2.15	0.46
1:B:288:LEU:HD13	3:B:909:3PE:H3F2	1.97	0.46
1:B:780:THR:HG21	1:B:818:ILE:HD12	1.96	0.46
1:A:657:ARG:HG2	1:A:710:ILE:HG22	1.97	0.46
1:B:473:LYS:HD3	1:B:474:ARG:H	1.80	0.46
1:A:634:ASN:O	1:A:638:CYS:N	2.49	0.46
1:A:685:PRO:HA	1:A:689:TYR:HB3	1.97	0.46
1:A:817:HIS:HD2	1:A:822:TYR:HB2	1.81	0.46
1:A:829:LEU:HB2	1:A:831:TYR:CE1	2.49	0.46
1:B:455:TYR:HB2	1:B:492:PRO:HB3	1.98	0.46
1:A:810:VAL:HG21	1:A:824:PHE:HB2	1.97	0.46
5:A:905:PC1:H3C1	5:B:901:PC1:H3A1	1.98	0.46
1:B:374:PRO:HA	1:B:377:TYR:HD2	1.80	0.46
1:B:806:GLY:HA3	1:B:824:PHE:CE2	2.50	0.46
1:A:218:PRO:HA	1:A:221:PHE:CZ	2.50	0.46
1:B:279:LEU:HD12	1:B:279:LEU:HA	1.78	0.46
1:B:220:VAL:O	1:B:223:VAL:HG22	2.15	0.46
1:B:102:PHE:CZ	1:B:106:ILE:HD11	2.51	0.45
1:A:94:ASN:HA	1:A:235:ARG:HD3	1.98	0.45
2:A:902:Y01:HAQ1	3:A:907:3PE:H252	1.97	0.45
1:B:288:LEU:CD1	3:B:909:3PE:H3F2	2.46	0.45
1:B:393:SER:HB3	6:B:908:P5S:H53	1.97	0.45
1:A:400:ILE:O	1:A:404:SER:HB3	2.16	0.45
3:A:907:3PE:H2D2	3:A:907:3PE:H3E1	1.98	0.45
5:A:908:PC1:H3G1	5:A:908:PC1:H2H2	1.97	0.45
1:B:275:ALA:HA	1:B:278:VAL:HG22	1.97	0.45
1:A:140:PHE:CE2	1:A:282:LEU:HB3	2.52	0.45
1:A:629:CYS:HB2	1:A:775:LYS:HE2	1.99	0.45
1:B:181:ASN:N	1:B:182:PRO:HD2	2.32	0.45
6:A:906:P5S:H20	6:A:906:P5S:H39	1.99	0.45
5:A:908:PC1:H2C1	6:A:909:P5S:H50A	1.99	0.45
1:B:412:HIS:O	1:B:416:THR:OG1	2.22	0.45
1:A:417:ASN:OD1	1:A:489:TRP:NE1	2.50	0.45
1:A:665:LEU:HD23	1:A:665:LEU:HA	1.77	0.45
1:B:211:LEU:O	1:B:215:LEU:HB2	2.17	0.45
1:A:193:TRP:HZ2	1:A:201:GLN:HA	1.81	0.45
1:B:364:LEU:HD23	1:B:367:PHE:CD2	2.52	0.45
1:B:469:PHE:CD2	1:B:470:LEU:HD12	2.52	0.45
2:A:901:Y01:HAA1	2:A:902:Y01:HAA2	1.98	0.44
1:A:265:VAL:HG23	2:A:901:Y01:CAX	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:PHE:HZ	1:A:505:HIS:HB2	1.82	0.44
1:B:442:GLY:O	1:B:446:VAL:HG12	2.17	0.44
1:A:792:GLU:OE2	1:B:757:TYR:OH	2.28	0.44
3:A:907:3PE:H271	3:A:907:3PE:H242	1.81	0.44
1:B:371:ASP:HB3	1:B:374:PRO:HD2	1.99	0.44
1:B:396:TRP:CH2	1:B:400:ILE:HD11	2.53	0.44
1:B:352:PHE:CZ	2:B:903:Y01:HBC	2.53	0.44
2:B:904:Y01:HAK1	3:B:909:3PE:H221	1.99	0.44
1:A:688:LEU:O	1:A:688:LEU:HD12	2.18	0.44
1:A:328:GLY:HA2	1:A:331:ILE:HG12	2.00	0.44
1:A:443:GLN:HA	1:A:446:VAL:HG12	2.00	0.44
1:B:418:LEU:HD12	1:B:460:TRP:HB3	2.00	0.44
1:B:646:GLN:NE2	1:B:650:SER:OG	2.51	0.44
1:B:817:HIS:HB3	1:B:820:ASN:H	1.82	0.44
1:A:436:LYS:O	1:A:437:GLU:HG2	2.17	0.44
1:A:528:LEU:HD21	1:A:672:ASN:HB3	1.99	0.43
1:B:218:PRO:HA	1:B:221:PHE:CZ	2.53	0.43
1:B:454:LEU:O	1:B:457:THR:OG1	2.26	0.43
1:B:638:CYS:HA	1:B:772:CYS:HB3	1.99	0.43
1:A:371:ASP:HB3	1:A:374:PRO:HD2	1.99	0.43
1:A:666:ILE:HA	1:A:669:LEU:HD12	2.00	0.43
1:B:663:LEU:HD13	1:B:666:ILE:HD12	2.00	0.43
1:B:328:GLY:HA2	1:B:331:ILE:HG12	2.00	0.43
1:B:465:ALA:HB1	1:B:538:SER:HB2	2.00	0.43
1:B:675:SER:HB2	1:B:692:LEU:HD12	2.00	0.43
1:A:194:LYS:O	1:A:197:GLN:HG3	2.18	0.43
1:B:505:HIS:ND1	1:B:516:TYR:HE1	2.17	0.43
1:A:241:VAL:HG23	6:A:909:P5S:H36	2.01	0.43
5:A:908:PC1:H322	5:A:908:PC1:H351	1.75	0.43
5:A:908:PC1:H3A1	5:B:907:PC1:H3C1	2.01	0.43
1:B:523:THR:O	1:B:527:THR:HG22	2.18	0.43
1:A:473:LYS:HD2	1:A:473:LYS:HA	1.82	0.43
1:B:668:GLY:HA3	1:B:699:PHE:CE2	2.54	0.43
1:A:102:PHE:HE1	1:A:317:ALA:HB2	1.83	0.43
1:B:54:LEU:HD13	2:B:903:Y01:HAD2	1.99	0.43
1:B:210:GLY:O	1:B:214:VAL:HG12	2.18	0.43
1:B:521:MET:HE2	1:B:521:MET:HA	2.00	0.43
3:B:909:3PE:H282	3:B:909:3PE:H361	2.00	0.43
1:A:241:VAL:HG11	6:A:909:P5S:H51A	2.00	0.43
3:A:907:3PE:H231	3:A:907:3PE:H342	2.01	0.43
1:B:140:PHE:CE1	1:B:282:LEU:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:PHE:CZ	1:B:388:ILE:HD11	2.54	0.43
1:B:436:LYS:O	1:B:437:GLU:HG2	2.19	0.43
1:A:749:MET:HG2	1:A:753:GLN:NE2	2.33	0.42
1:A:798:ASP:H	1:A:801:GLU:HG2	1.84	0.42
1:A:177:LEU:HD21	1:A:217:ASN:ND2	2.33	0.42
1:A:364:LEU:HD22	1:A:691:GLU:HG2	2.00	0.42
1:B:175:ILE:O	1:B:179:MET:HG3	2.19	0.42
1:A:422:GLN:HA	1:A:425:VAL:HG12	2.01	0.42
1:B:751:CYS:SG	1:B:812:GLY:HA3	2.59	0.42
1:A:414:LEU:HD22	1:A:460:TRP:CH2	2.54	0.42
1:A:464:LEU:O	1:A:468:LEU:HD13	2.19	0.42
1:A:650:SER:O	1:A:653:GLN:NE2	2.53	0.42
1:B:93:LEU:O	1:B:230:ASN:ND2	2.47	0.42
1:B:662:CYS:O	1:B:666:ILE:HG13	2.19	0.42
1:A:181:ASN:N	1:A:182:PRO:HD2	2.35	0.42
1:A:259:TYR:O	1:A:263:THR:HG23	2.20	0.42
1:A:275:ALA:HA	1:A:278:VAL:HG22	2.00	0.42
1:B:435:VAL:HG11	1:B:446:VAL:HG11	2.02	0.42
1:B:519:GLU:O	1:B:523:THR:HG23	2.19	0.42
1:A:193:TRP:CZ2	1:A:201:GLN:HA	2.55	0.42
1:A:817:HIS:CD2	1:A:822:TYR:HB2	2.54	0.42
3:A:903:3PE:H3F2	3:A:903:3PE:H3C2	1.93	0.42
1:B:282:LEU:HD23	1:B:282:LEU:HA	1.92	0.42
1:B:456:SER:O	1:B:460:TRP:HB2	2.20	0.42
1:A:122:LEU:HA	1:A:130:ARG:HD3	2.02	0.41
1:A:673:LEU:O	1:A:677:LEU:HG	2.20	0.41
1:B:360:VAL:HG11	3:B:909:3PE:H2I1	2.01	0.41
1:B:464:LEU:HD23	1:B:464:LEU:HA	1.89	0.41
1:A:501:ILE:HD13	1:A:501:ILE:HA	1.86	0.41
1:B:349:ILE:O	1:B:353:VAL:HG23	2.20	0.41
1:B:518:LYS:HG2	1:B:522:ILE:HD11	2.03	0.41
3:A:907:3PE:H3C2	3:A:907:3PE:H3F2	1.86	0.41
1:B:41:ARG:HH12	1:B:160:THR:HG23	1.85	0.41
1:B:174:PRO:O	1:B:178:MET:HG3	2.20	0.41
1:A:398:LEU:HA	1:A:401:LEU:HD12	2.02	0.41
1:A:628:HIS:HB2	1:A:629:CYS:H	1.71	0.41
6:A:906:P5S:H34A	5:B:901:PC1:H3B1	2.03	0.41
1:B:685:PRO:HA	1:B:689:TYR:HB3	2.02	0.41
1:A:185:PHE:O	1:A:189:GLU:HG2	2.20	0.41
1:B:803:VAL:HA	1:B:824:PHE:HE2	1.85	0.41
1:A:102:PHE:CE1	1:A:106:ILE:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ILE:HG21	1:A:297:MET:HE2	2.03	0.41
5:A:908:PC1:H281	5:A:908:PC1:H252	1.84	0.41
1:B:516:TYR:HB2	1:B:520:GLN:HE21	1.86	0.41
1:B:648:LEU:HD23	1:B:648:LEU:N	2.36	0.41
1:B:758:HIS:CE1	1:B:795:LEU:HD21	2.55	0.41
1:B:716:HIS:N	1:B:716:HIS:CD2	2.88	0.41
1:A:528:LEU:O	1:A:531:SER:OG	2.33	0.41
1:A:827:GLU:O	1:A:829:LEU:HD12	2.19	0.41
1:B:797:SER:H	1:B:801:GLU:CD	2.25	0.41
1:A:88:LYS:HE2	1:A:88:LYS:HB3	1.86	0.41
1:A:147:PHE:HE2	1:A:219:ILE:HD13	1.85	0.41
1:A:215:LEU:HD23	1:A:215:LEU:HA	1.92	0.41
1:A:665:LEU:HD23	1:A:699:PHE:CZ	2.56	0.41
6:A:906:P5S:H33A	5:B:901:PC1:H3G2	2.03	0.41
1:B:394:LEU:HD23	1:B:423:SER:HA	2.02	0.41
1:A:55:CYS:O	1:A:58:ILE:HG12	2.21	0.41
1:A:523:THR:HA	1:A:526:VAL:HG12	2.02	0.41
1:A:640:LEU:HD12	1:A:830:PHE:HE1	1.86	0.41
6:A:909:P5S:H33	6:A:909:P5S:H30A	1.68	0.41
1:B:218:PRO:O	1:B:222:MET:HB2	2.20	0.41
1:A:364:LEU:HD23	1:A:367:PHE:CD2	2.56	0.40
1:A:668:GLY:HA3	1:A:699:PHE:CE2	2.56	0.40
1:B:354:SER:OG	1:B:358:MET:HE2	2.21	0.40
1:B:834:LEU:HB3	1:B:835:GLN:H	1.67	0.40
1:A:418:LEU:HD12	1:A:460:TRP:HB3	2.04	0.40
1:A:271:LEU:HB3	1:A:275:ALA:HB3	2.02	0.40
1:B:661:LEU:HD12	1:B:661:LEU:O	2.22	0.40
1:A:539:LEU:HA	1:A:542:MET:HG2	2.04	0.40
1:A:149:LEU:HD23	1:A:324:PRO:HG3	2.03	0.40
1:B:88:LYS:HB3	1:B:88:LYS:HE2	1.80	0.40
1:B:532:ILE:HG13	1:B:532:ILE:H	1.68	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	685/878 (78%)	667 (97%)	18 (3%)	0	100	100
1	B	685/878 (78%)	662 (97%)	23 (3%)	0	100	100
All	All	1370/1756 (78%)	1329 (97%)	41 (3%)	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	602/772 (78%)	601 (100%)	1 (0%)	92	96
1	B	602/772 (78%)	599 (100%)	3 (0%)	86	92
All	All	1204/1544 (78%)	1200 (100%)	4 (0%)	90	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	667	ILE
1	B	296	GLU
1	B	663	LEU
1	B	798	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	94	ASN
1	A	335	GLN
1	A	380	GLN
1	A	443	GLN
1	A	520	GLN

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Mol	Chain	Res	Type
1	A	628	HIS
1	A	658	HIS
1	A	672	ASN
1	A	683	GLN
1	A	753	GLN
1	B	69	GLN
1	B	89	ASN
1	B	159	GLN
1	B	216	GLN
1	B	335	GLN
1	B	443	GLN
1	B	506	ASN
1	B	520	GLN
1	B	646	GLN
1	B	672	ASN
1	B	683	GLN
1	B	703	GLN
1	B	716	HIS
1	B	758	HIS
1	B	811	GLN

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](#)

18 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
6	P5S	B	902	-	52,53,53	0.52	0	56,60,60	0.75	1 (1%)
3	3PE	B	909	-	50,50,50	0.51	0	53,55,55	0.52	1 (1%)
5	PC1	B	901	-	53,53,53	0.48	0	59,61,61	0.50	1 (1%)
6	P5S	A	909	-	52,53,53	0.53	0	56,60,60	0.73	1 (1%)
2	Y01	B	903	-	38,38,38	0.57	0	57,57,57	0.91	2 (3%)
2	Y01	B	904	-	38,38,38	0.53	0	57,57,57	0.60	0
5	PC1	B	907	-	53,53,53	0.49	0	59,61,61	0.47	1 (1%)
4	CLR	B	906	-	31,31,31	0.39	0	48,48,48	0.56	0
2	Y01	A	902	-	38,38,38	0.56	0	57,57,57	0.63	0
5	PC1	A	905	-	53,53,53	0.49	0	59,61,61	0.47	1 (1%)
4	CLR	A	904	-	31,31,31	0.40	0	48,48,48	0.57	0
5	PC1	A	908	-	53,53,53	0.48	0	59,61,61	0.51	1 (1%)
6	P5S	B	908	-	52,53,53	0.52	0	56,60,60	0.83	1 (1%)
3	3PE	A	907	-	50,50,50	0.51	0	53,55,55	0.53	1 (1%)
6	P5S	A	906	-	52,53,53	0.52	0	56,60,60	0.83	1 (1%)
3	3PE	A	903	-	50,50,50	0.51	0	53,55,55	0.53	1 (1%)
2	Y01	A	901	-	38,38,38	0.56	0	57,57,57	0.75	0
3	3PE	B	905	-	50,50,50	0.51	0	53,55,55	0.53	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
6	P5S	B	902	-	-	34/59/59/59	-
3	3PE	B	909	-	-	23/54/54/54	-
5	PC1	B	901	-	-	22/57/57/57	-
6	P5S	A	909	-	-	32/59/59/59	-
2	Y01	B	903	-	-	9/19/77/77	0/4/4/4
2	Y01	B	904	-	-	12/19/77/77	0/4/4/4
5	PC1	B	907	-	-	16/57/57/57	-
4	CLR	B	906	-	-	7/10/68/68	0/4/4/4
2	Y01	A	902	-	-	5/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PC1	A	905	-	-	15/57/57/57	-
4	CLR	A	904	-	-	4/10/68/68	0/4/4/4
5	PC1	A	908	-	-	24/57/57/57	-
6	P5S	B	908	-	-	35/59/59/59	-
3	3PE	A	907	-	-	16/54/54/54	-
6	P5S	A	906	-	-	36/59/59/59	-
3	3PE	A	903	-	-	15/54/54/54	-
2	Y01	A	901	-	-	8/19/77/77	0/4/4/4
3	3PE	B	905	-	-	17/54/54/54	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	908	P5S	OG-CB-CA	4.44	111.93	108.06
6	A	906	P5S	OG-CB-CA	4.36	111.86	108.06
6	B	902	P5S	OG-CB-CA	3.59	111.18	108.06
6	A	909	P5S	OG-CB-CA	3.36	110.99	108.06
2	B	903	Y01	CBI-CBE-CBB	2.64	123.63	119.49
3	B	909	3PE	O12-P-O14	2.36	123.89	112.24
3	A	907	3PE	O12-P-O14	2.34	123.81	112.24
5	A	908	PC1	O12-P-O14	2.33	123.74	112.24
5	B	901	PC1	O12-P-O14	2.32	123.71	112.24
3	A	903	3PE	O12-P-O14	2.32	123.71	112.24
5	B	907	PC1	O12-P-O14	2.32	123.70	112.24
3	B	905	3PE	O12-P-O14	2.32	123.69	112.24
5	A	905	PC1	O12-P-O14	2.32	123.69	112.24
2	B	903	Y01	CAC-CBB-CBE	2.23	116.34	112.92

There are no chirality outliers.

All (330) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	902	Y01	OAG-CAY-OAW-CBC
2	B	904	Y01	CAV-CBC-OAW-CAY
3	A	903	3PE	C1-O11-P-O14
3	A	903	3PE	C11-O13-P-O11
3	A	903	3PE	C11-O13-P-O14
3	A	907	3PE	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
3	B	905	3PE	C1-O11-P-O14
3	B	909	3PE	C11-O13-P-O11
3	B	909	3PE	C11-O13-P-O14
3	B	909	3PE	O13-C11-C12-N
5	A	905	PC1	C11-O13-P-O14
5	A	905	PC1	C1-O11-P-O12
5	A	905	PC1	C1-O11-P-O13
5	A	908	PC1	C1-O11-P-O14
5	B	901	PC1	C1-O11-P-O14
5	B	907	PC1	C11-O13-P-O14
5	B	907	PC1	C1-O11-P-O12
5	B	907	PC1	O22-C21-O21-C2
5	B	907	PC1	C22-C21-O21-C2
6	A	906	P5S	CB-OG-P12-O13
6	A	906	P5S	CB-OG-P12-O15
6	A	906	P5S	CB-OG-P12-O16
6	A	906	P5S	C3-O16-P12-O13
6	A	906	P5S	O47-C38-O37-C2
6	A	909	P5S	O-C-CA-N
6	A	909	P5S	CB-OG-P12-O13
6	A	909	P5S	CB-OG-P12-O15
6	A	909	P5S	CB-OG-P12-O16
6	B	902	P5S	O-C-CA-N
6	B	902	P5S	O-C-CA-CB
6	B	902	P5S	OXT-C-CA-CB
6	B	902	P5S	C-CA-CB-OG
6	B	902	P5S	N-CA-CB-OG
6	B	902	P5S	C3-O16-P12-O13
6	B	902	P5S	C3-O16-P12-O15
6	B	908	P5S	CB-OG-P12-O15
6	B	908	P5S	CB-OG-P12-O16
6	B	908	P5S	C3-O16-P12-O13
6	B	908	P5S	O47-C38-O37-C2
3	A	903	3PE	O32-C31-O31-C3
3	B	905	3PE	O32-C31-O31-C3
6	A	909	P5S	O18-C17-O19-C1
6	B	902	P5S	O18-C17-O19-C1
3	B	905	3PE	O22-C21-O21-C2
5	A	905	PC1	O22-C21-O21-C2
3	B	905	3PE	C32-C31-O31-C3
2	A	902	Y01	CAM-CAY-OAW-CBC
3	B	905	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
5	A	905	PC1	C22-C21-O21-C2
6	A	906	P5S	C39-C38-O37-C2
6	B	908	P5S	C39-C38-O37-C2
3	A	903	3PE	C32-C31-O31-C3
6	A	909	P5S	C20-C17-O19-C1
6	B	902	P5S	C20-C17-O19-C1
6	B	908	P5S	C20-C17-O19-C1
3	A	903	3PE	O22-C21-O21-C2
2	B	904	Y01	CAJ-CAO-CBB-CAC
2	B	904	Y01	CAM-CAY-OAW-CBC
3	A	903	3PE	C22-C21-O21-C2
2	B	904	Y01	OAG-CAY-OAW-CBC
4	B	906	CLR	C21-C20-C22-C23
6	B	908	P5S	O18-C17-O19-C1
6	A	906	P5S	C20-C17-O19-C1
2	B	903	Y01	CAJ-CAO-CBB-CBE
4	B	906	CLR	C17-C20-C22-C23
6	A	909	P5S	OXT-C-CA-N
6	B	902	P5S	OXT-C-CA-N
6	A	906	P5S	O18-C17-O19-C1
3	A	907	3PE	C32-C31-O31-C3
2	B	903	Y01	CAJ-CAO-CBB-CAC
6	A	909	P5S	C26-C27-C28-C29
6	A	909	P5S	C52-C53-C54-C55
5	B	901	PC1	C22-C21-O21-C2
4	B	906	CLR	C13-C17-C20-C22
6	B	908	P5S	C17-C20-C21-C22
6	A	906	P5S	C38-C39-C40-C41
6	B	902	P5S	C17-C20-C21-C22
6	A	906	P5S	C17-C20-C21-C22
6	A	909	P5S	C17-C20-C21-C22
6	B	902	P5S	C38-C39-C40-C41
3	A	907	3PE	O32-C31-O31-C3
6	B	902	P5S	C26-C27-C28-C29
2	A	901	Y01	CAO-CAJ-CAN-CBA
3	B	909	3PE	C3D-C3E-C3F-C3G
3	A	907	3PE	C11-O13-P-O11
3	B	905	3PE	C1-O11-P-O13
5	A	908	PC1	C11-O13-P-O11
5	B	901	PC1	C11-O13-P-O11
5	B	907	PC1	C1-O11-P-O13
6	A	909	P5S	C3-O16-P12-OG

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Mol	Chain	Res	Type	Atoms
6	B	902	P5S	CB-OG-P12-O16
6	B	902	P5S	C3-O16-P12-OG
5	B	901	PC1	O22-C21-O21-C2
2	B	904	Y01	CAO-CBB-CBE-CBI
5	A	908	PC1	C2C-C2D-C2E-C2F
5	B	901	PC1	C2C-C2D-C2E-C2F
3	B	909	3PE	C22-C21-O21-C2
5	A	908	PC1	C22-C21-O21-C2
6	B	902	P5S	C25-C26-C27-C28
6	B	902	P5S	C52-C53-C54-C55
5	B	901	PC1	C33-C34-C35-C36
6	A	906	P5S	C39-C40-C41-C42
6	B	908	P5S	C39-C40-C41-C42
5	A	908	PC1	O22-C21-O21-C2
3	A	903	3PE	C3B-C3C-C3D-C3E
6	A	906	P5S	C27-C28-C29-C30
6	B	902	P5S	C39-C40-C41-C42
6	B	908	P5S	C31-C32-C33-C34
5	A	908	PC1	C27-C28-C29-C2A
5	A	908	PC1	C33-C34-C35-C36
6	A	909	P5S	C39-C40-C41-C42
4	B	906	CLR	C16-C17-C20-C21
3	B	909	3PE	O22-C21-O21-C2
3	A	903	3PE	C21-C22-C23-C24
6	B	908	P5S	C38-C39-C40-C41
6	A	909	P5S	C46-C48-C49-C50
6	A	906	P5S	C31-C32-C33-C34
6	B	902	P5S	C30-C31-C32-C33
6	B	908	P5S	C46-C48-C49-C50
5	B	901	PC1	C27-C28-C29-C2A
6	B	908	P5S	C27-C28-C29-C30
4	B	906	CLR	C13-C17-C20-C21
4	B	906	CLR	C16-C17-C20-C22
3	B	905	3PE	C33-C34-C35-C36
6	A	909	P5S	C49-C50-C51-C52
3	A	907	3PE	C28-C29-C2A-C2B
5	B	901	PC1	C26-C27-C28-C29
3	B	909	3PE	C32-C31-O31-C3
6	A	906	P5S	C32-C33-C34-C35
6	B	902	P5S	C49-C50-C51-C52
5	A	908	PC1	C32-C33-C34-C35
6	B	908	P5S	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
4	A	904	CLR	C13-C17-C20-C22
6	A	909	P5S	C-CA-CB-OG
3	A	907	3PE	C34-C35-C36-C37
3	B	909	3PE	C28-C29-C2A-C2B
5	A	905	PC1	O21-C2-C3-O31
5	A	908	PC1	C2E-C2F-C2G-C2H
2	B	904	Y01	CAC-CBB-CBE-CBI
3	B	905	3PE	C29-C2A-C2B-C2C
6	A	909	P5S	OXT-C-CA-CB
6	B	908	P5S	OXT-C-CA-CB
6	A	906	P5S	C22-C23-C24-C25
3	B	909	3PE	O32-C31-O31-C3
5	A	905	PC1	C11-O13-P-O11
5	B	901	PC1	C1-O11-P-O13
5	B	907	PC1	C11-O13-P-O11
6	A	906	P5S	C3-O16-P12-OG
6	B	908	P5S	C3-O16-P12-OG
6	A	906	P5S	C41-C42-C43-C44
6	B	902	P5S	C41-C42-C43-C44
6	A	906	P5S	C26-C27-C28-C29
6	A	906	P5S	C46-C48-C49-C50
6	B	908	P5S	C22-C23-C24-C25
6	B	908	P5S	C26-C27-C28-C29
4	A	904	CLR	C16-C17-C20-C21
3	B	905	3PE	C28-C29-C2A-C2B
5	A	905	PC1	C1-C2-C3-O31
5	A	908	PC1	C1-C2-C3-O31
4	A	904	CLR	C16-C17-C20-C22
3	A	903	3PE	C29-C2A-C2B-C2C
3	B	905	3PE	C21-C22-C23-C24
6	A	906	P5S	C52-C53-C54-C55
6	A	909	P5S	C51-C52-C53-C54
3	B	909	3PE	C2F-C2G-C2H-C2I
2	B	904	Y01	CAC-CBB-CBE-CAP
3	B	909	3PE	C27-C28-C29-C2A
6	A	909	P5S	C21-C22-C23-C24
6	B	908	P5S	C52-C53-C54-C55
6	B	908	P5S	C41-C42-C43-C44
4	A	904	CLR	C13-C17-C20-C21
5	A	908	PC1	C2D-C2E-C2F-C2G
5	B	907	PC1	O21-C2-C3-O31
6	A	909	P5S	O19-C1-C2-O37

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Mol	Chain	Res	Type	Atoms
6	B	908	P5S	O19-C1-C2-O37
6	A	909	P5S	C41-C42-C43-C44
2	B	904	Y01	CAO-CBB-CBE-CAP
2	A	901	Y01	CAM-CAY-OAW-CBC
5	B	901	PC1	C2E-C2F-C2G-C2H
6	B	908	P5S	C30-C31-C32-C33
2	A	901	Y01	CAJ-CAO-CBB-CBE
5	B	901	PC1	C3C-C3D-C3E-C3F
3	B	909	3PE	C1-C2-C3-O31
5	B	907	PC1	C1-C2-C3-O31
3	B	905	3PE	O11-C1-C2-O21
6	B	908	P5S	O37-C2-C3-O16
3	B	909	3PE	O21-C2-C3-O31
6	A	906	P5S	C29-C30-C31-C32
6	B	902	P5S	C46-C48-C49-C50
6	B	902	P5S	C50-C51-C52-C53
3	B	905	3PE	C32-C33-C34-C35
6	B	902	P5S	C51-C52-C53-C54
2	A	901	Y01	OAG-CAY-OAW-CBC
6	A	906	P5S	C30-C31-C32-C33
3	B	905	3PE	O11-C1-C2-C3
6	A	906	P5S	C1-C2-C3-O16
6	B	902	P5S	C1-C2-C3-O16
6	B	908	P5S	C29-C30-C31-C32
5	A	908	PC1	C3-C2-O21-C21
5	B	901	PC1	C2F-C2G-C2H-C2I
5	A	905	PC1	C32-C33-C34-C35
5	A	908	PC1	C3C-C3D-C3E-C3F
6	A	906	P5S	C2-C3-O16-P12
6	B	902	P5S	O19-C1-C2-C3
6	B	908	P5S	O19-C1-C2-C3
6	B	908	P5S	C2-C3-O16-P12
5	B	907	PC1	C32-C33-C34-C35
6	A	906	P5S	O37-C2-C3-O16
3	B	909	3PE	C35-C36-C37-C38
5	A	905	PC1	C33-C34-C35-C36
6	A	906	P5S	O19-C1-C2-O37
6	B	902	P5S	O19-C1-C2-O37
6	A	909	P5S	CA-CB-OG-P12
6	B	902	P5S	CA-CB-OG-P12
6	A	909	P5S	O-C-CA-CB
6	B	908	P5S	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
6	A	906	P5S	C25-C26-C27-C28
3	A	907	3PE	C37-C38-C39-C3A
5	B	901	PC1	C25-C26-C27-C28
6	B	908	P5S	C48-C49-C50-C51
3	A	907	3PE	C22-C23-C24-C25
6	B	908	P5S	C24-C25-C26-C27
5	A	908	PC1	C1-O11-P-O13
3	A	907	3PE	C11-O13-P-O14
5	A	908	PC1	C11-O13-P-O14
5	B	901	PC1	C11-O13-P-O14
5	B	901	PC1	C1-O11-P-O12
5	B	907	PC1	C11-O13-P-O12
6	A	906	P5S	C3-O16-P12-O15
6	A	909	P5S	C3-O16-P12-O13
6	B	902	P5S	CB-OG-P12-O13
6	B	908	P5S	CB-OG-P12-O13
6	B	908	P5S	C1-C2-C3-O16
3	B	909	3PE	C3B-C3C-C3D-C3E
5	A	905	PC1	C3E-C3F-C3G-C3H
3	A	907	3PE	C3D-C3E-C3F-C3G
6	B	908	P5S	C25-C26-C27-C28
3	B	909	3PE	C25-C26-C27-C28
5	A	908	PC1	O13-C11-C12-N
5	B	901	PC1	O13-C11-C12-N
5	B	907	PC1	C2B-C2C-C2D-C2E
3	A	907	3PE	C3C-C3D-C3E-C3F
2	B	903	Y01	CAC-CBB-CBE-CBI
6	A	909	P5S	C30-C31-C32-C33
6	B	908	P5S	C23-C24-C25-C26
2	B	904	Y01	CAN-CAJ-CAO-CBB
3	B	905	3PE	C2C-C2D-C2E-C2F
6	A	909	P5S	C42-C43-C44-C45
2	B	903	Y01	CAO-CBB-CBE-CAP
6	A	906	P5S	C21-C22-C23-C24
3	B	909	3PE	C2D-C2E-C2F-C2G
5	B	901	PC1	C3-C2-O21-C21
6	A	906	P5S	C23-C24-C25-C26
6	B	902	P5S	O37-C2-C3-O16
6	B	902	P5S	C2-C1-O19-C17
5	A	905	PC1	C2B-C2C-C2D-C2E
2	B	903	Y01	CAM-CAY-OAW-CBC
6	A	909	P5S	C39-C38-O37-C2

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Mol	Chain	Res	Type	Atoms
6	A	906	P5S	C48-C49-C50-C51
3	B	905	3PE	C3F-C3G-C3H-C3I
3	A	903	3PE	C1-O11-P-O13
3	B	905	3PE	C11-O13-P-O11
3	A	907	3PE	C38-C39-C3A-C3B
6	B	902	P5S	C48-C49-C50-C51
6	A	906	P5S	C24-C25-C26-C27
6	A	909	P5S	C31-C32-C33-C34
5	B	907	PC1	C37-C38-C39-C3A
2	B	903	Y01	OAG-CAY-OAW-CBC
3	B	909	3PE	C3A-C3B-C3C-C3D
2	A	901	Y01	CAJ-CAO-CBB-CAC
2	A	901	Y01	CAM-CAL-CAX-OAH
5	A	908	PC1	C2F-C2G-C2H-C2I
2	B	904	Y01	CAM-CAL-CAX-OAH
2	B	903	Y01	CAM-CAL-CAX-OAF
2	A	901	Y01	CAM-CAL-CAX-OAF
6	A	909	P5S	O47-C38-O37-C2
5	B	901	PC1	C2D-C2E-C2F-C2G
6	A	909	P5S	C40-C41-C42-C43
6	A	906	P5S	OXT-C-CA-CB
5	B	901	PC1	C32-C33-C34-C35
6	B	902	P5S	C42-C43-C44-C45
2	A	902	Y01	CAJ-CAO-CBB-CAC
2	B	903	Y01	CAM-CAL-CAX-OAH
5	B	907	PC1	C33-C34-C35-C36
2	B	904	Y01	CAM-CAL-CAX-OAF
4	B	906	CLR	C22-C23-C24-C25
5	A	908	PC1	O21-C2-C3-O31
5	B	907	PC1	C38-C39-C3A-C3B
3	A	903	3PE	C2C-C2D-C2E-C2F
2	A	901	Y01	CAJ-CAN-CBA-CAB
2	A	902	Y01	CAJ-CAN-CBA-CAA
5	B	901	PC1	C2A-C2B-C2C-C2D
6	A	906	P5S	C3-C2-O37-C38
3	A	903	3PE	C38-C39-C3A-C3B
5	A	908	PC1	C28-C29-C2A-C2B
6	A	909	P5S	O19-C1-C2-C3
3	B	909	3PE	C22-C23-C24-C25
2	B	903	Y01	CAN-CAJ-CAO-CBB
3	A	907	3PE	O11-C1-C2-C3
6	A	906	P5S	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
6	A	909	P5S	C20-C21-C22-C23
6	A	906	P5S	O-C-CA-CB
6	A	909	P5S	N-CA-CB-OG
6	B	902	P5S	C40-C41-C42-C43
3	A	903	3PE	C34-C35-C36-C37
3	B	909	3PE	C29-C2A-C2B-C2C
5	A	908	PC1	C26-C27-C28-C29
5	B	907	PC1	C2C-C2D-C2E-C2F
3	A	903	3PE	C3F-C3G-C3H-C3I
3	B	905	3PE	C11-O13-P-O14
5	A	905	PC1	C11-O13-P-O12
5	A	908	PC1	C1-O11-P-O12
6	B	908	P5S	C3-O16-P12-O15
3	B	909	3PE	C36-C37-C38-C39
5	A	905	PC1	C36-C37-C38-C39
2	B	904	Y01	CAL-CAM-CAY-OAW
5	A	905	PC1	C12-C11-O13-P
5	B	901	PC1	C12-C11-O13-P
5	B	907	PC1	C12-C11-O13-P
6	B	908	P5S	C3-C2-O37-C38
3	A	907	3PE	C24-C25-C26-C27
5	B	901	PC1	O21-C21-C22-C23
2	A	902	Y01	CAL-CAM-CAY-OAW
3	B	909	3PE	O21-C21-C22-C23
5	A	908	PC1	O31-C31-C32-C33
3	A	907	3PE	C2A-C2B-C2C-C2D
3	A	907	3PE	C36-C37-C38-C39
5	A	908	PC1	O32-C31-C32-C33
5	A	908	PC1	C25-C26-C27-C28
3	B	909	3PE	O22-C21-C22-C23

There are no ring outliers.

15 monomers are involved in 61 short contacts:

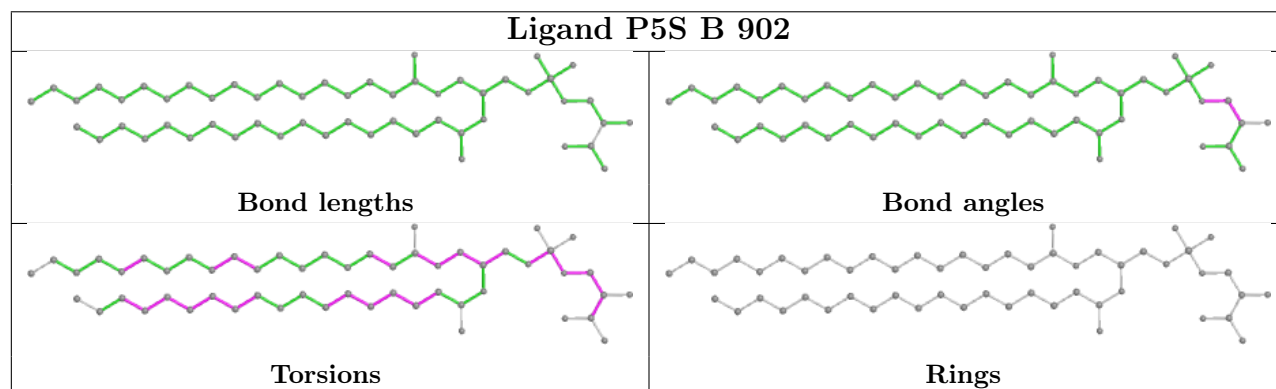
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	902	P5S	2	0
3	B	909	3PE	9	0
5	B	901	PC1	7	0
6	A	909	P5S	12	0
2	B	903	Y01	4	0
2	B	904	Y01	4	0
5	B	907	PC1	2	0

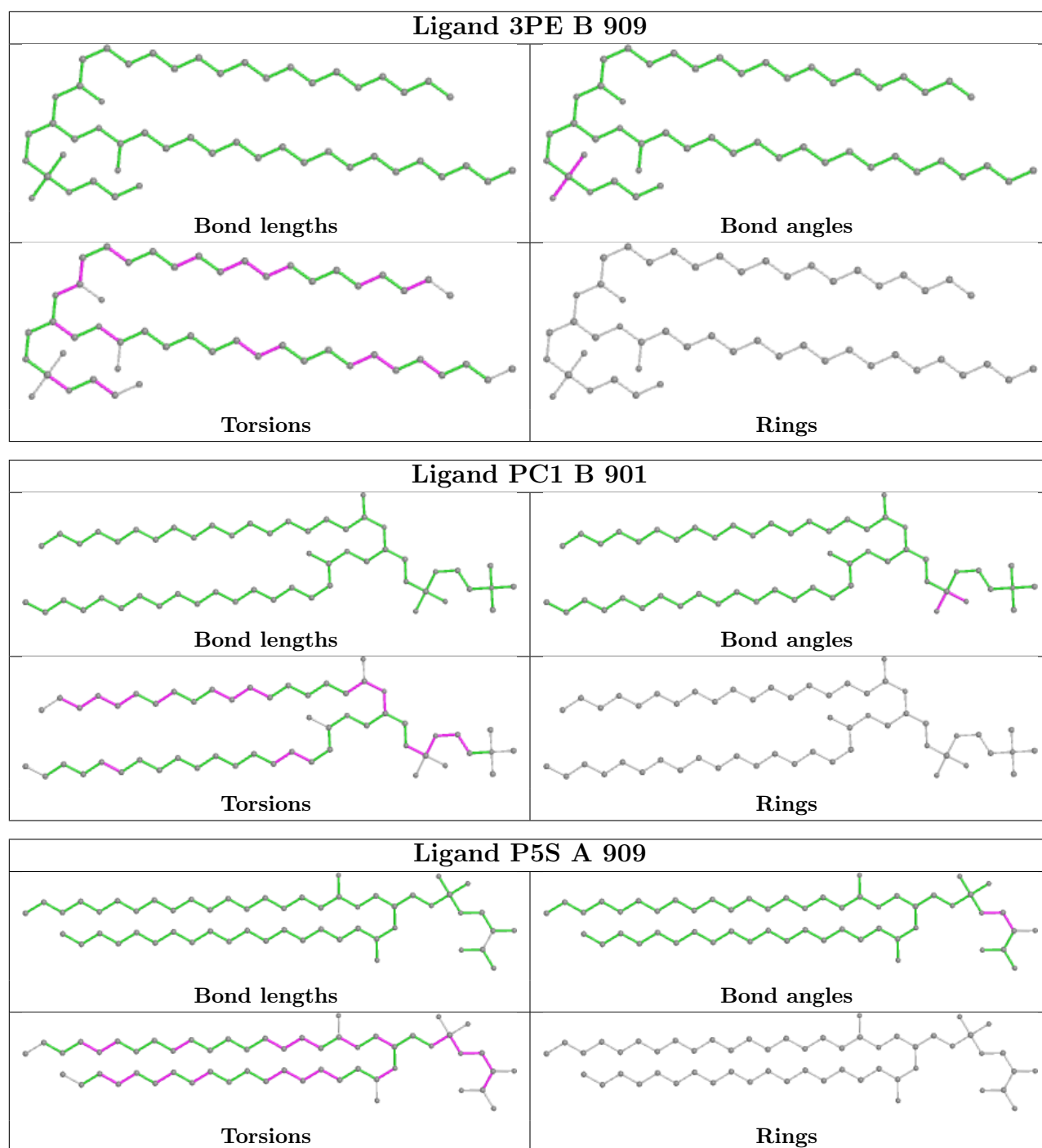
Continued on next page...

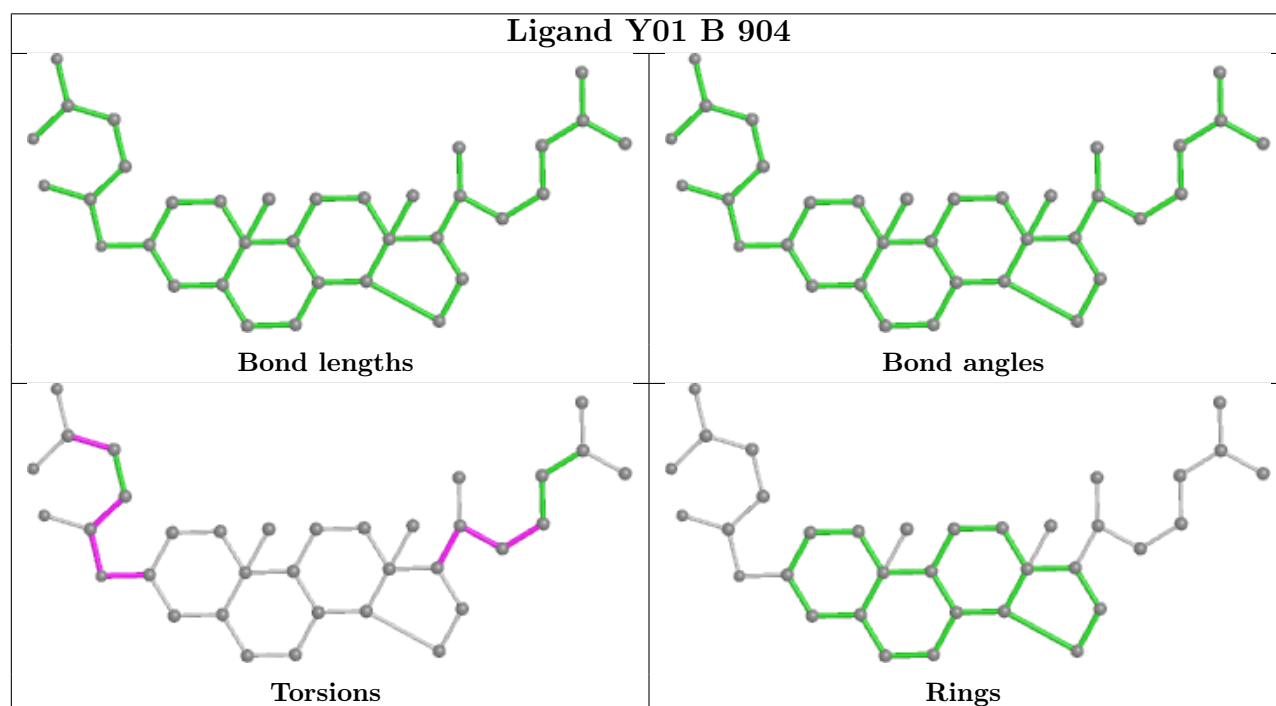
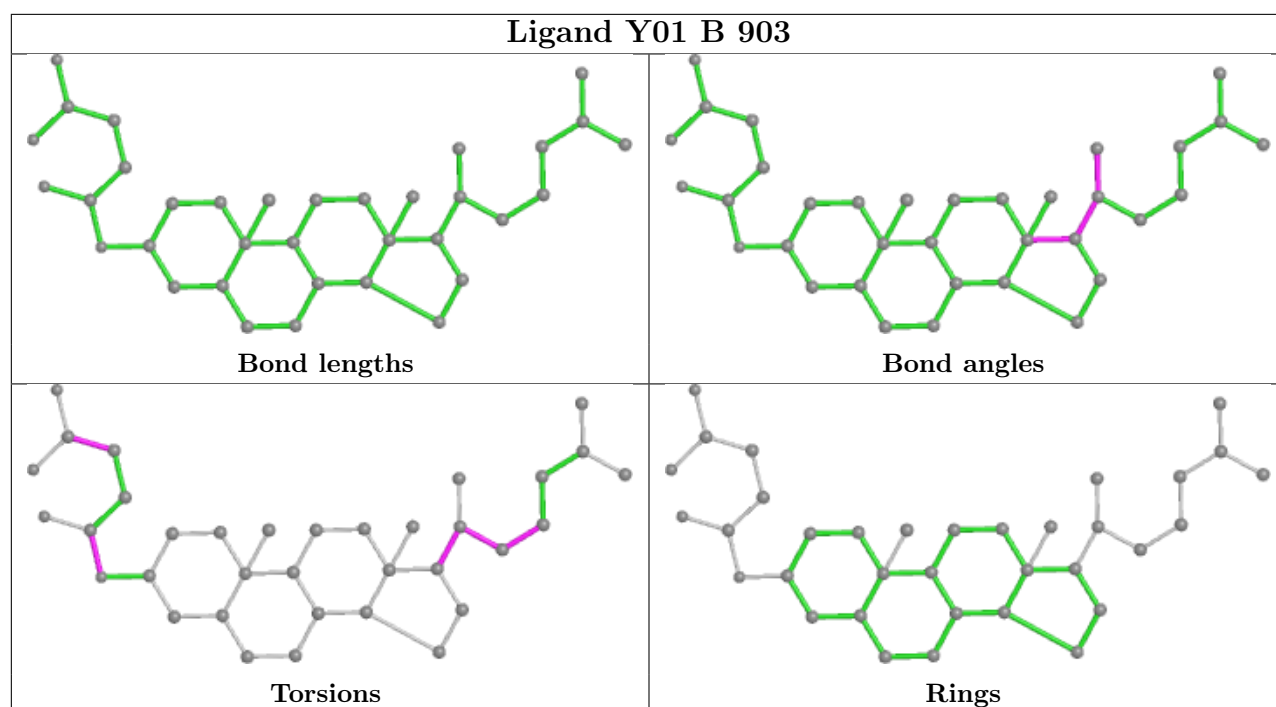
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	Y01	5	0
5	A	905	PC1	2	0
5	A	908	PC1	11	0
6	B	908	P5S	4	0
3	A	907	3PE	8	0
6	A	906	P5S	5	0
3	A	903	3PE	1	0
2	A	901	Y01	6	0

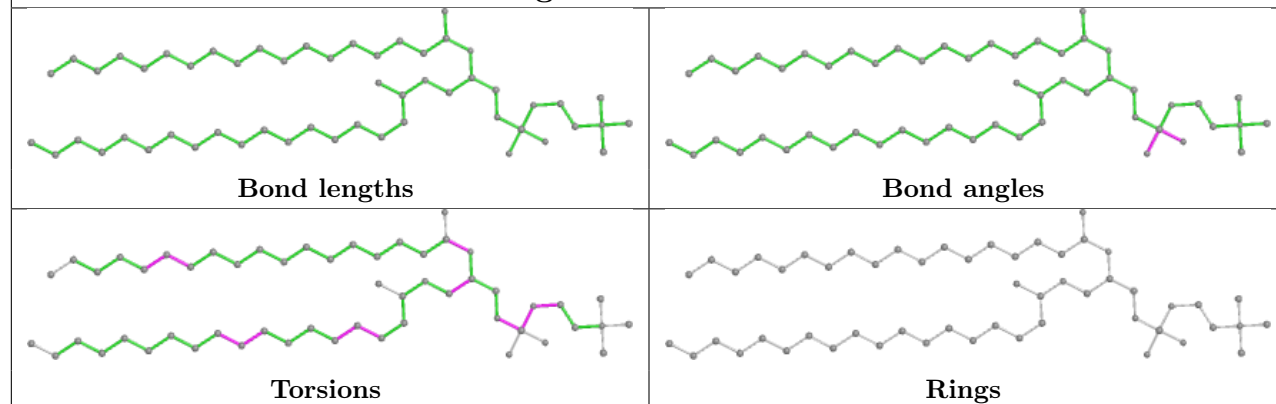
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



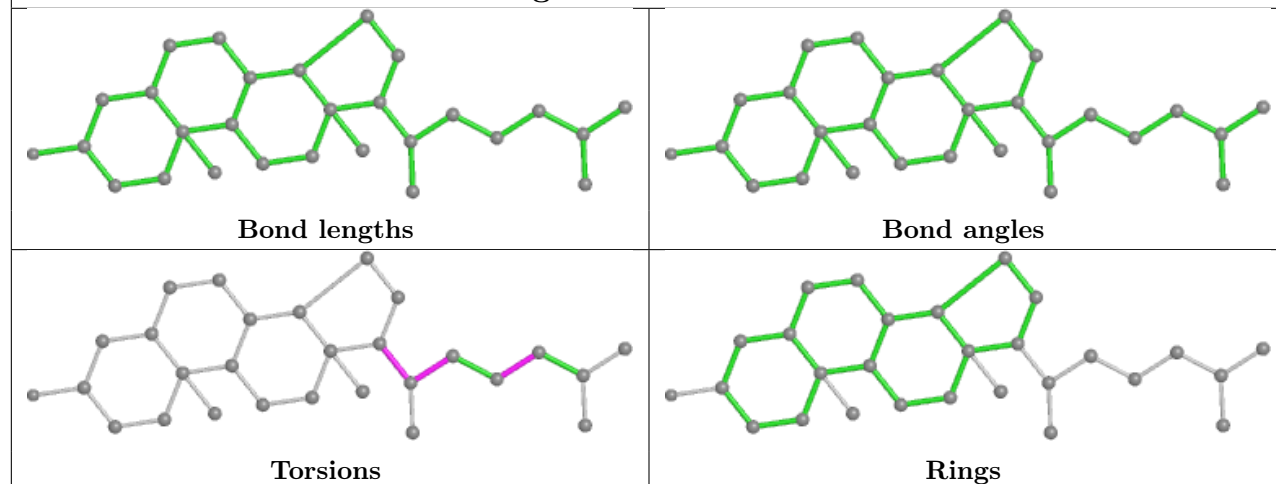




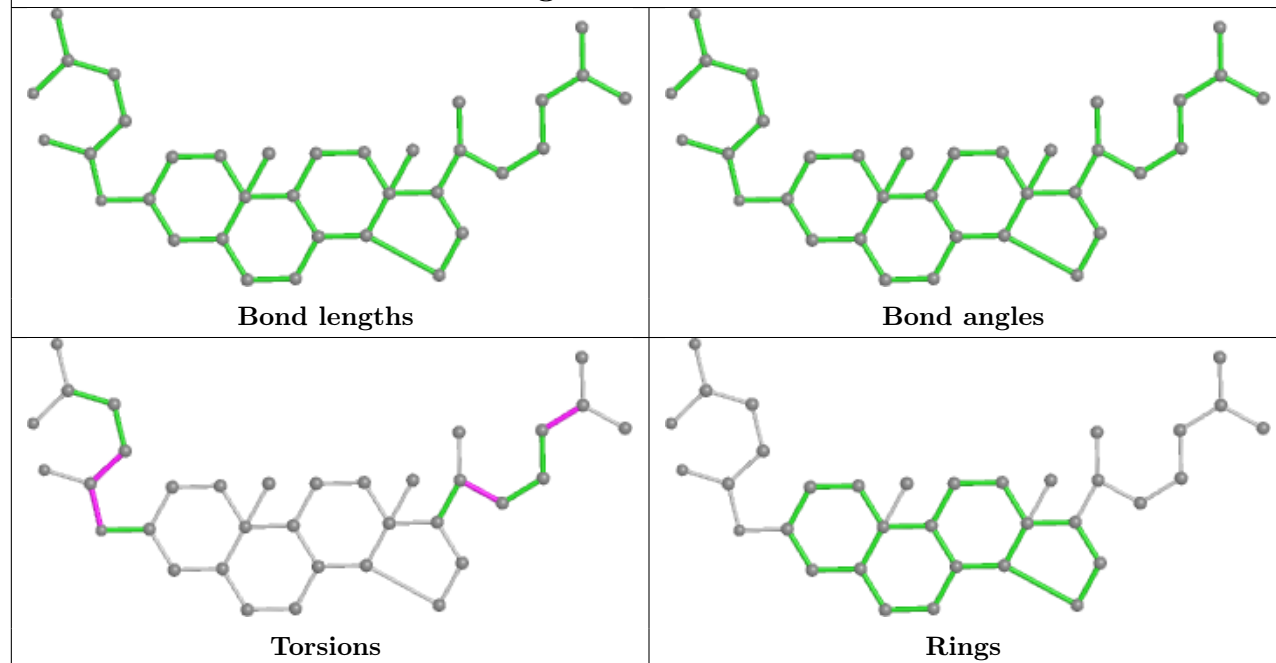
Ligand PC1 B 907



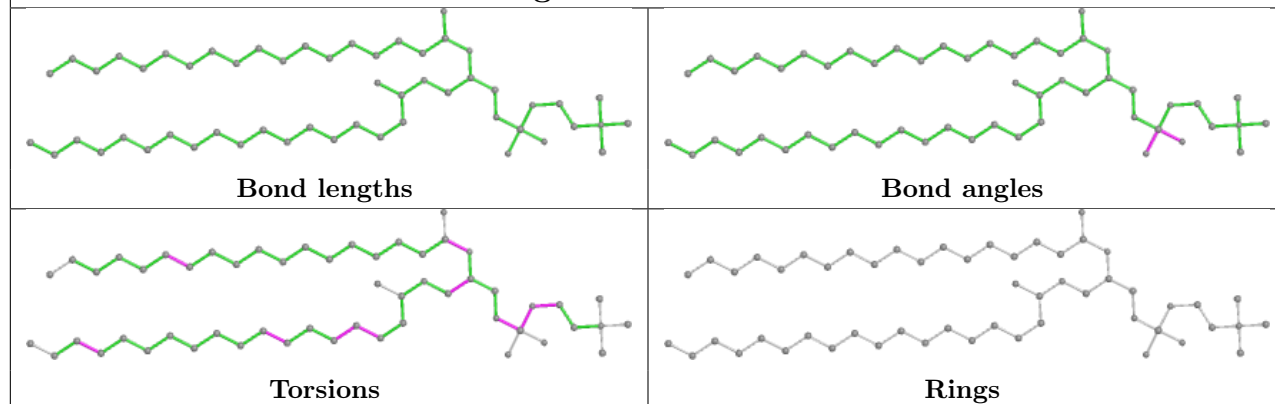
Ligand CLR B 906



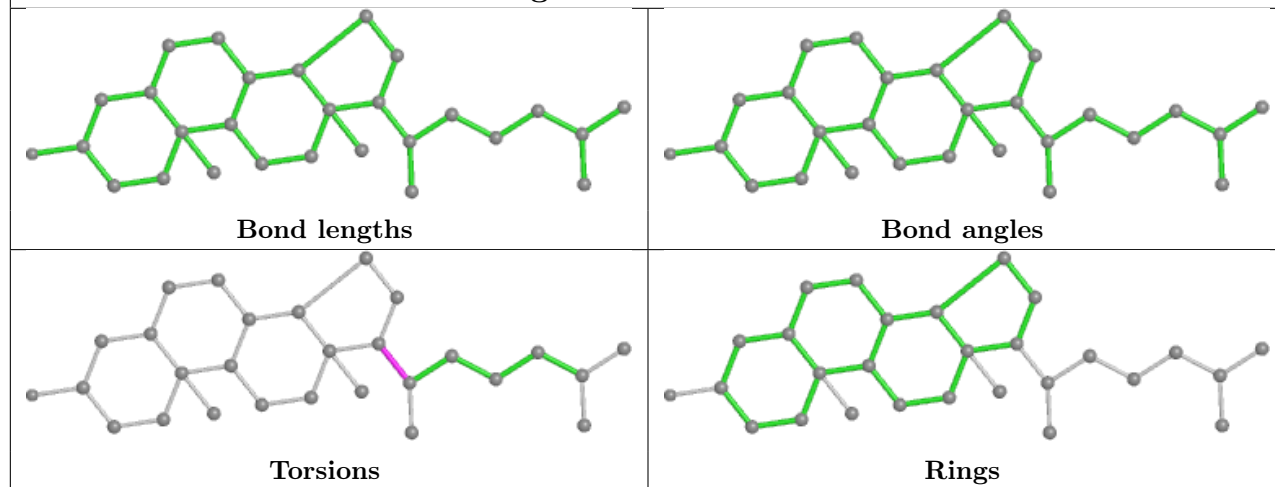
Ligand Y01 A 902



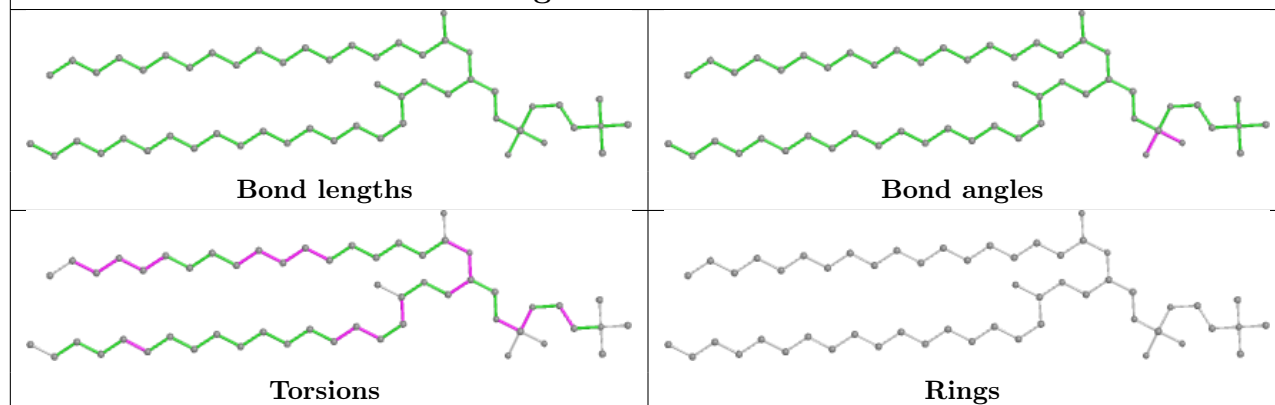
Ligand PC1 A 905

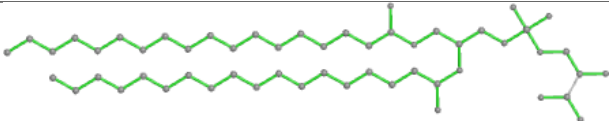
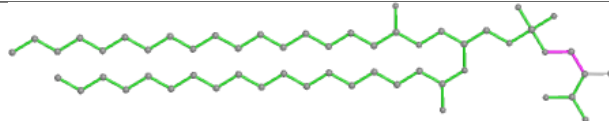
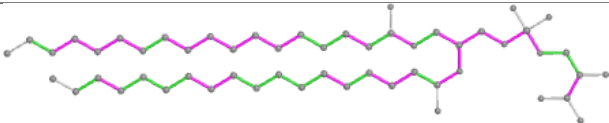
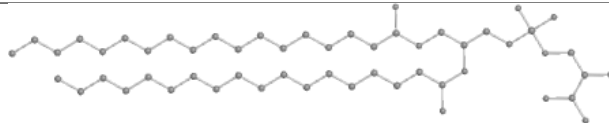


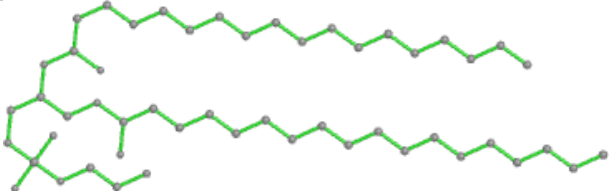
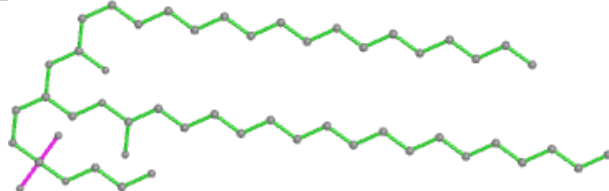
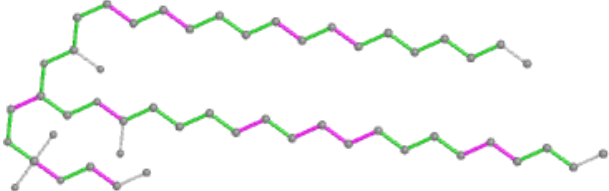
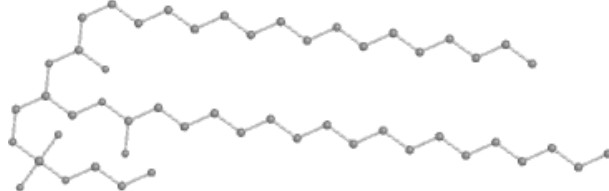
Ligand CLR A 904

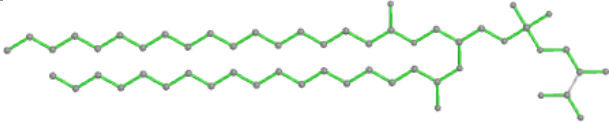
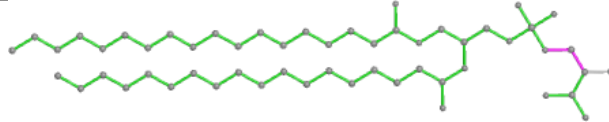
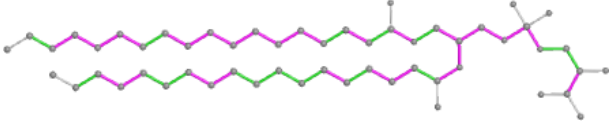



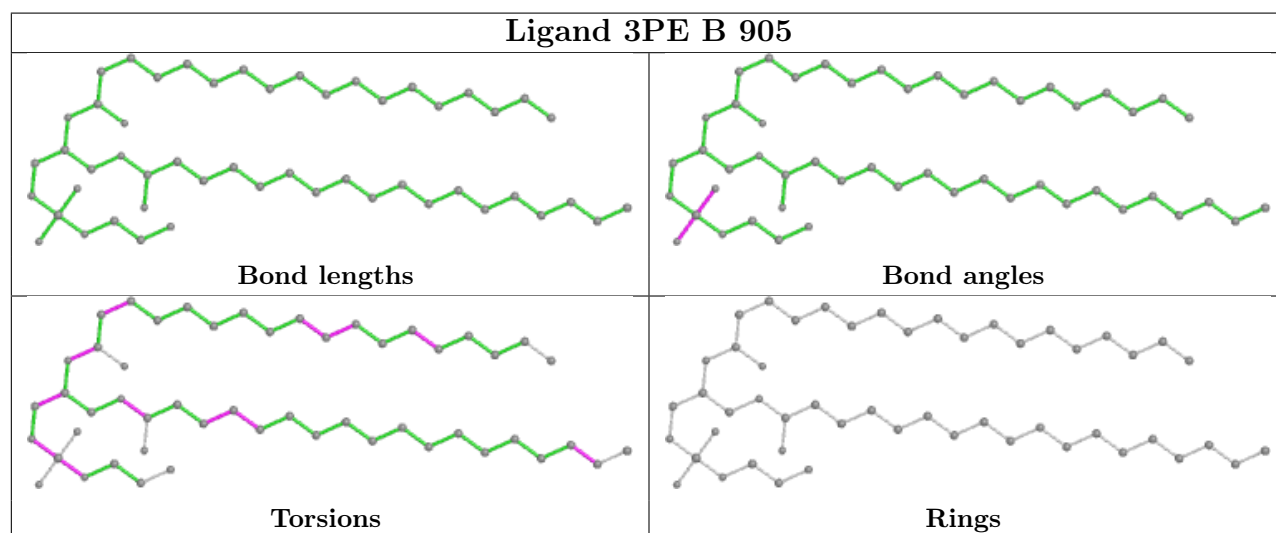
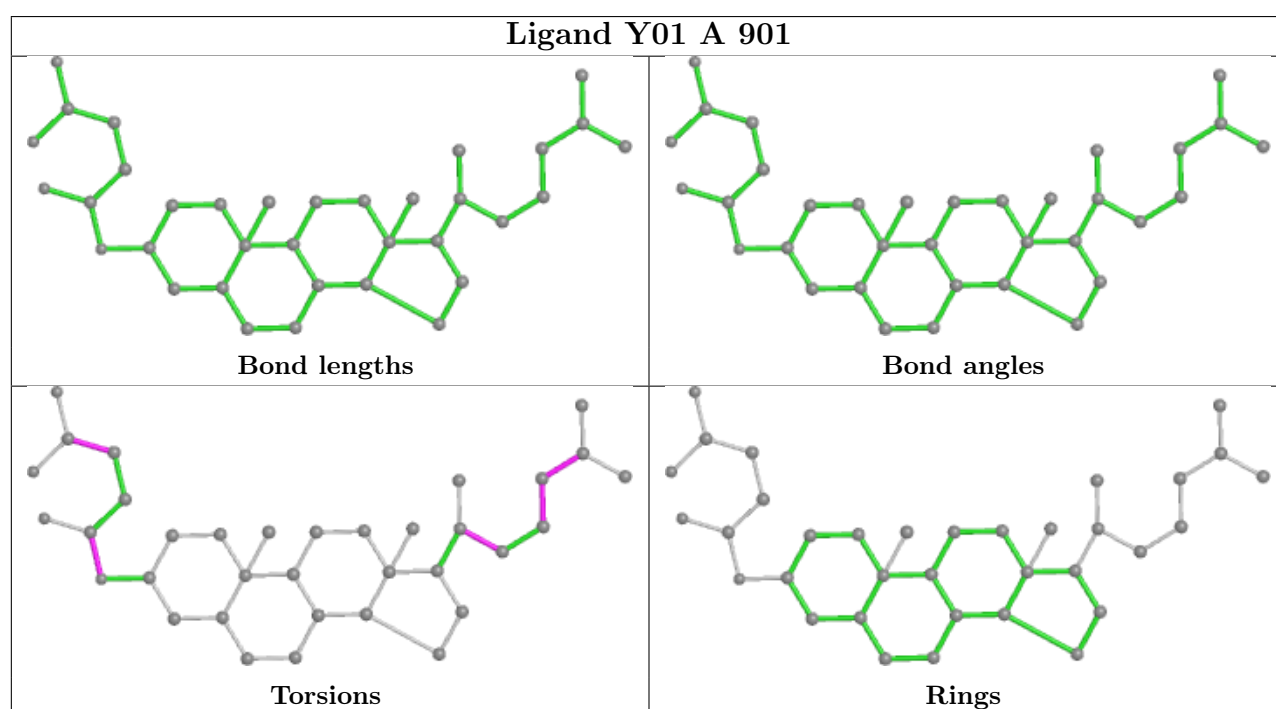
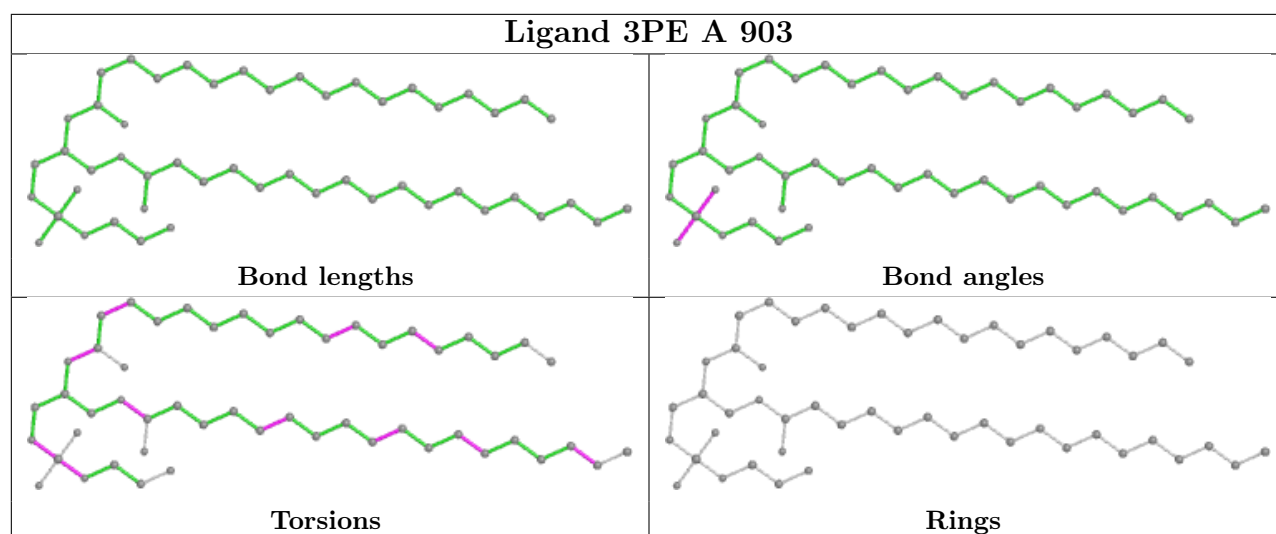
Ligand PC1 A 908



Ligand P5S B 908	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 3PE A 907	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand P5S A 906	
	
Bond lengths	Bond angles
	
Torsions	Rings



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.

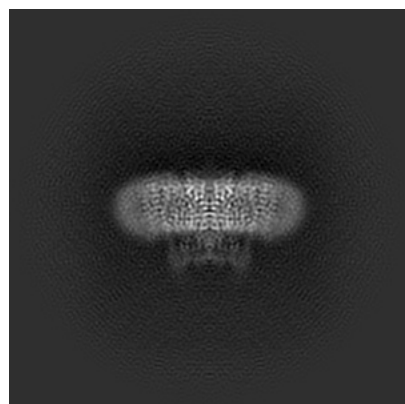
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61312. These allow visual inspection of the internal detail of the map and identification of artifacts.

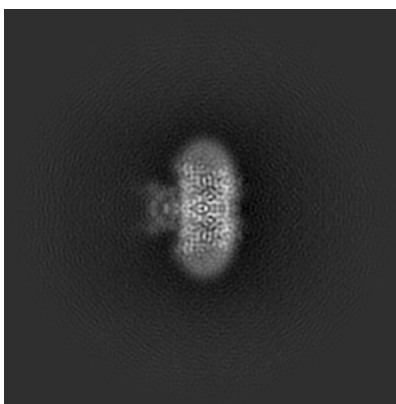
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

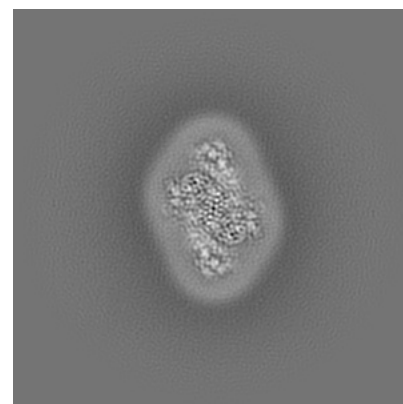
6.1.1 Primary map



X

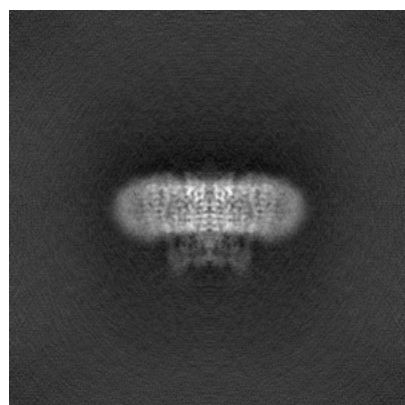


Y

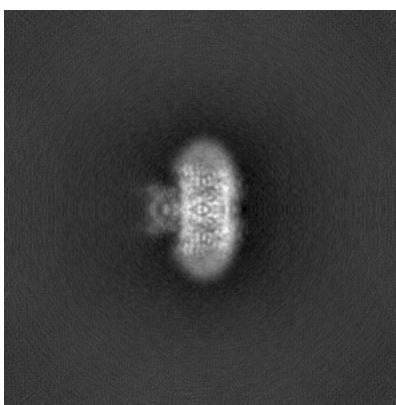


Z

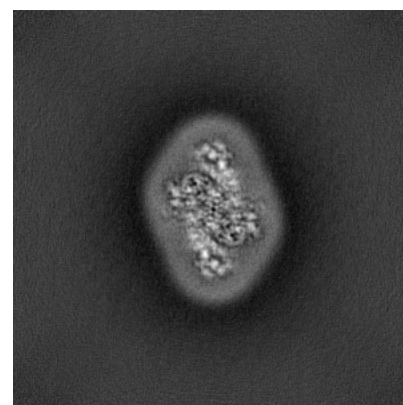
6.1.2 Raw map



X



Y

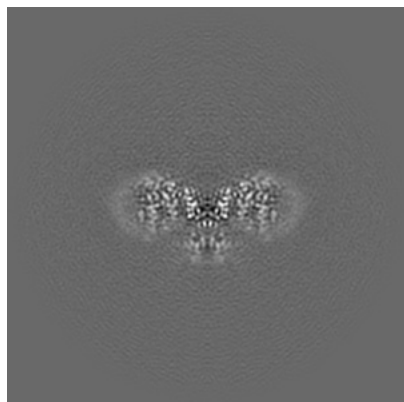


Z

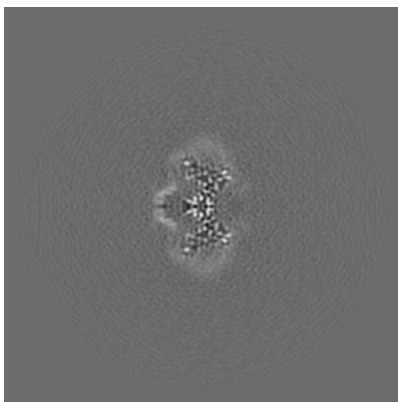
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

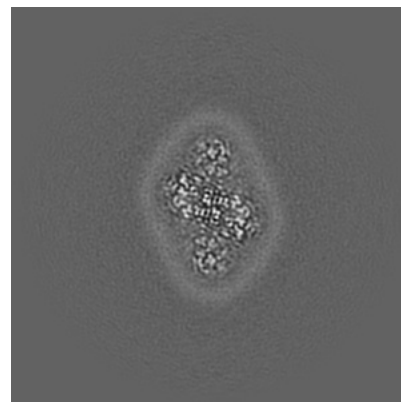
6.2.1 Primary map



X Index: 200

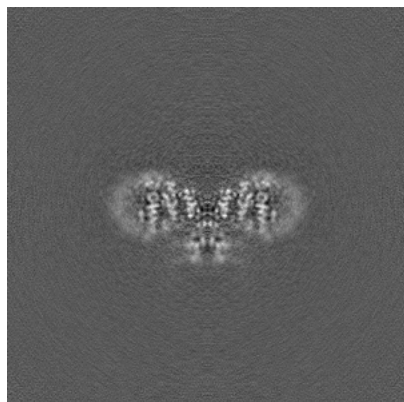


Y Index: 200

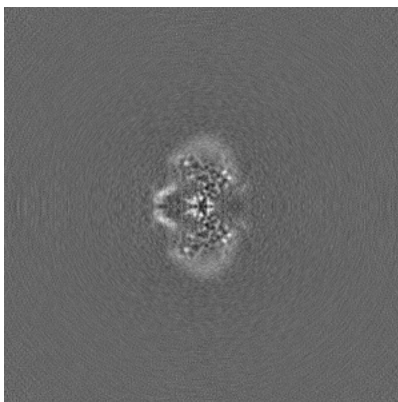


Z Index: 200

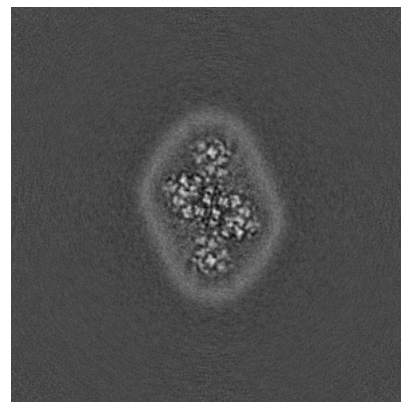
6.2.2 Raw map



X Index: 200



Y Index: 200

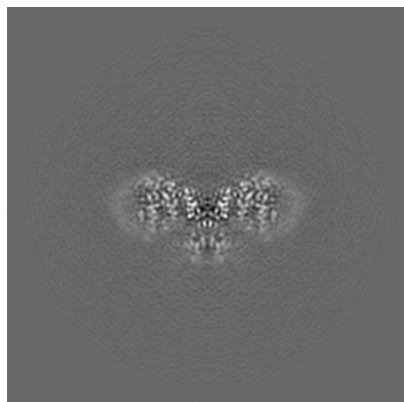


Z Index: 200

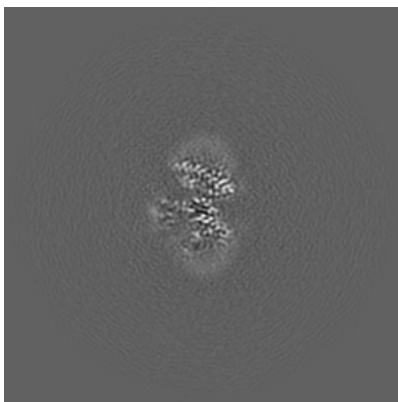
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

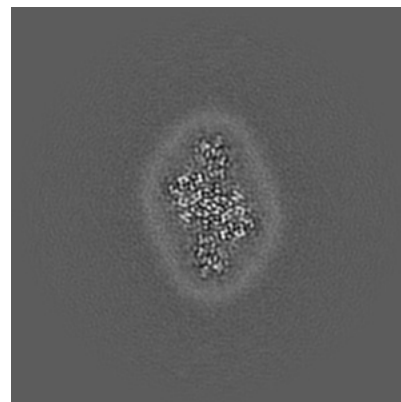
6.3.1 Primary map



X Index: 200

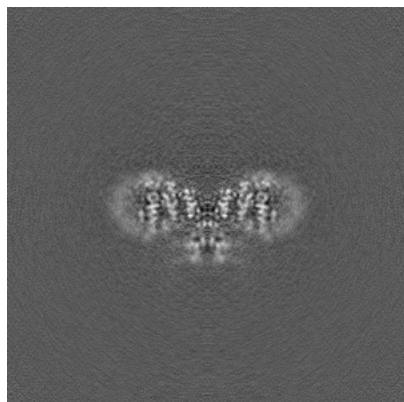


Y Index: 193

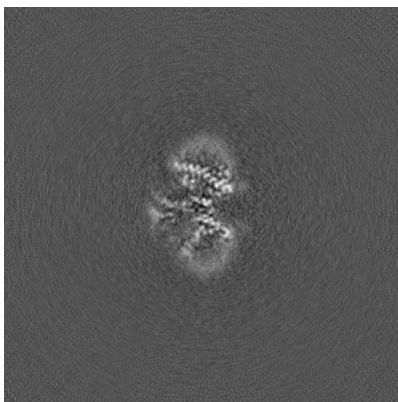


Z Index: 205

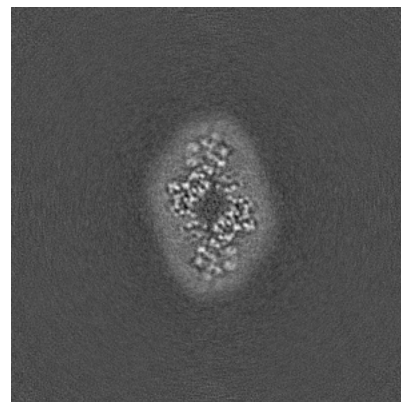
6.3.2 Raw map



X Index: 200



Y Index: 194

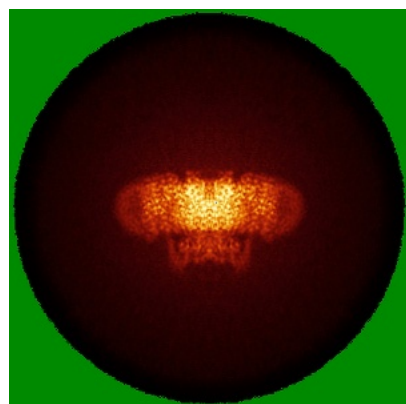


Z Index: 221

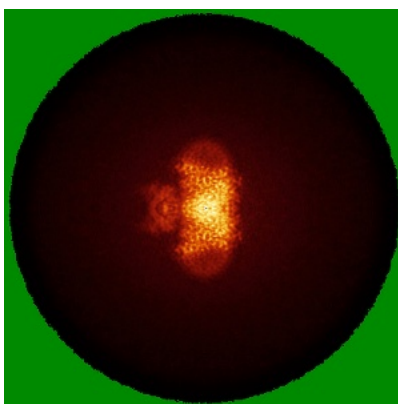
The images above show the largest variance slices of the map in three orthogonal directions.

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

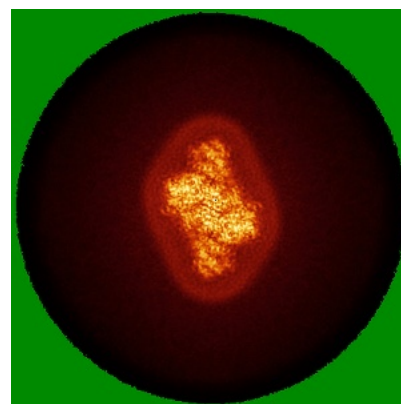
6.4.1 Primary map



X

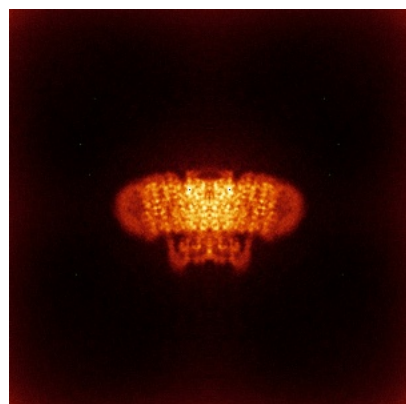


Y

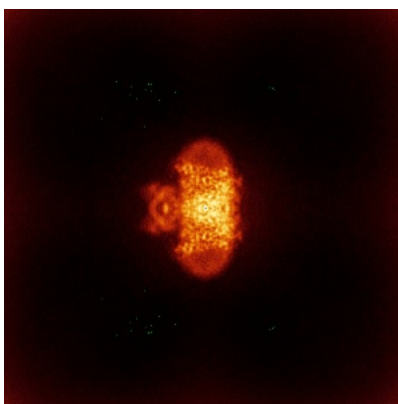


Z

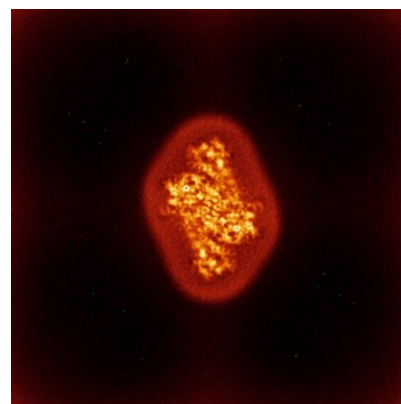
6.4.2 Raw map



X



Y

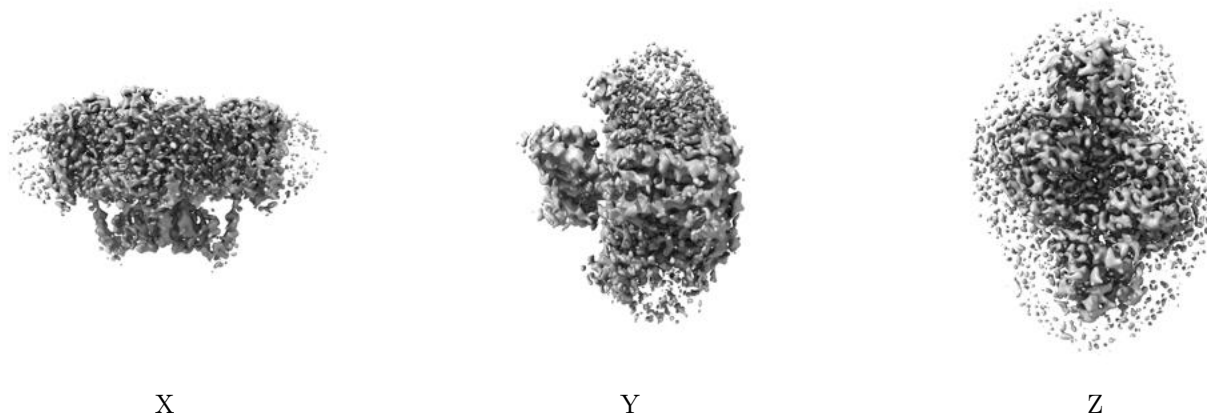


Z

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.

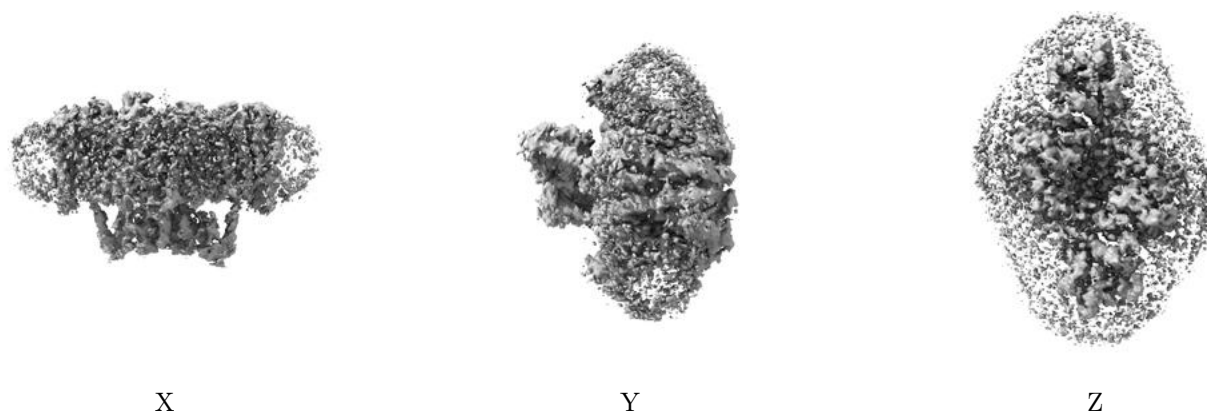
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.23. 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.

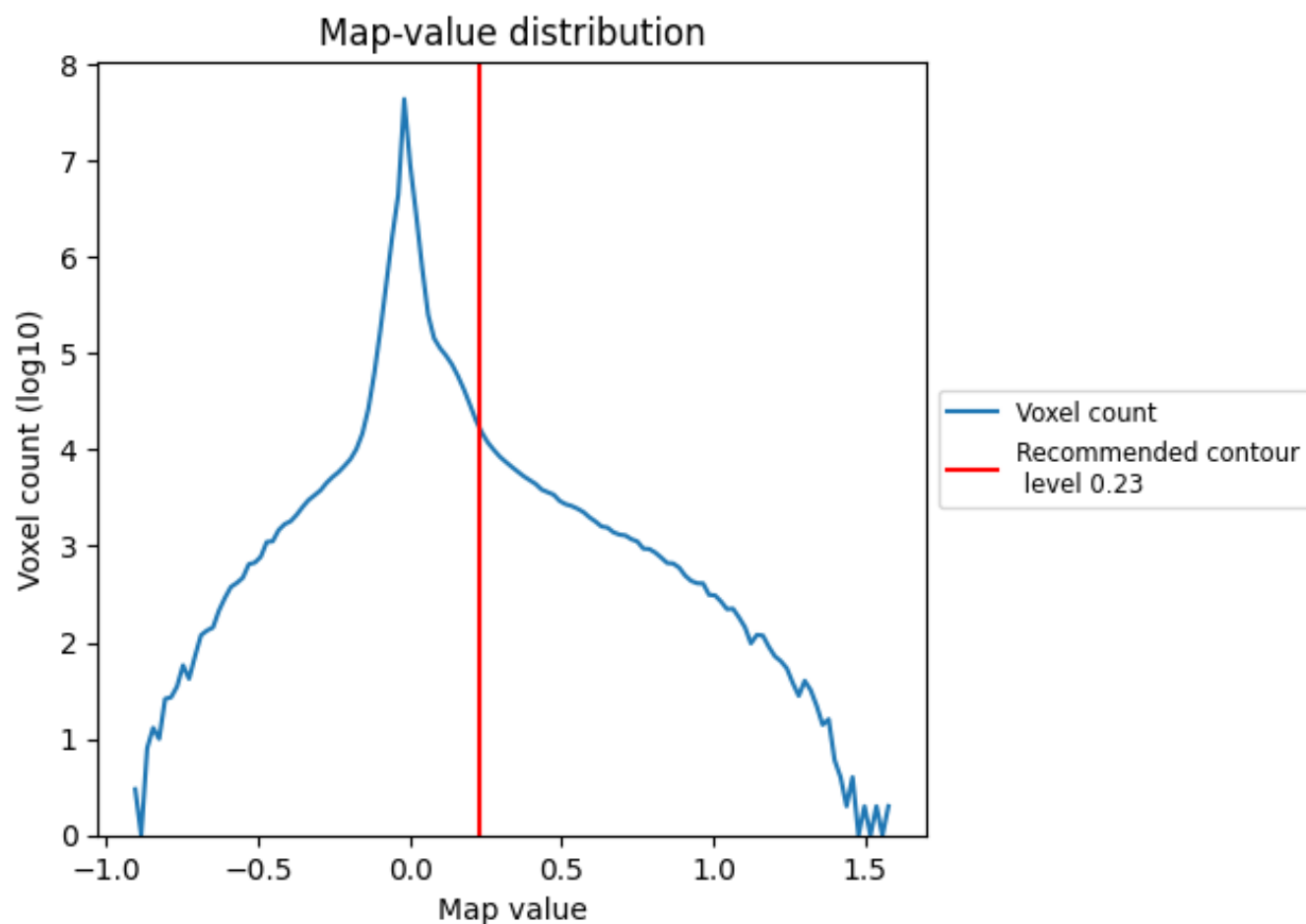
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

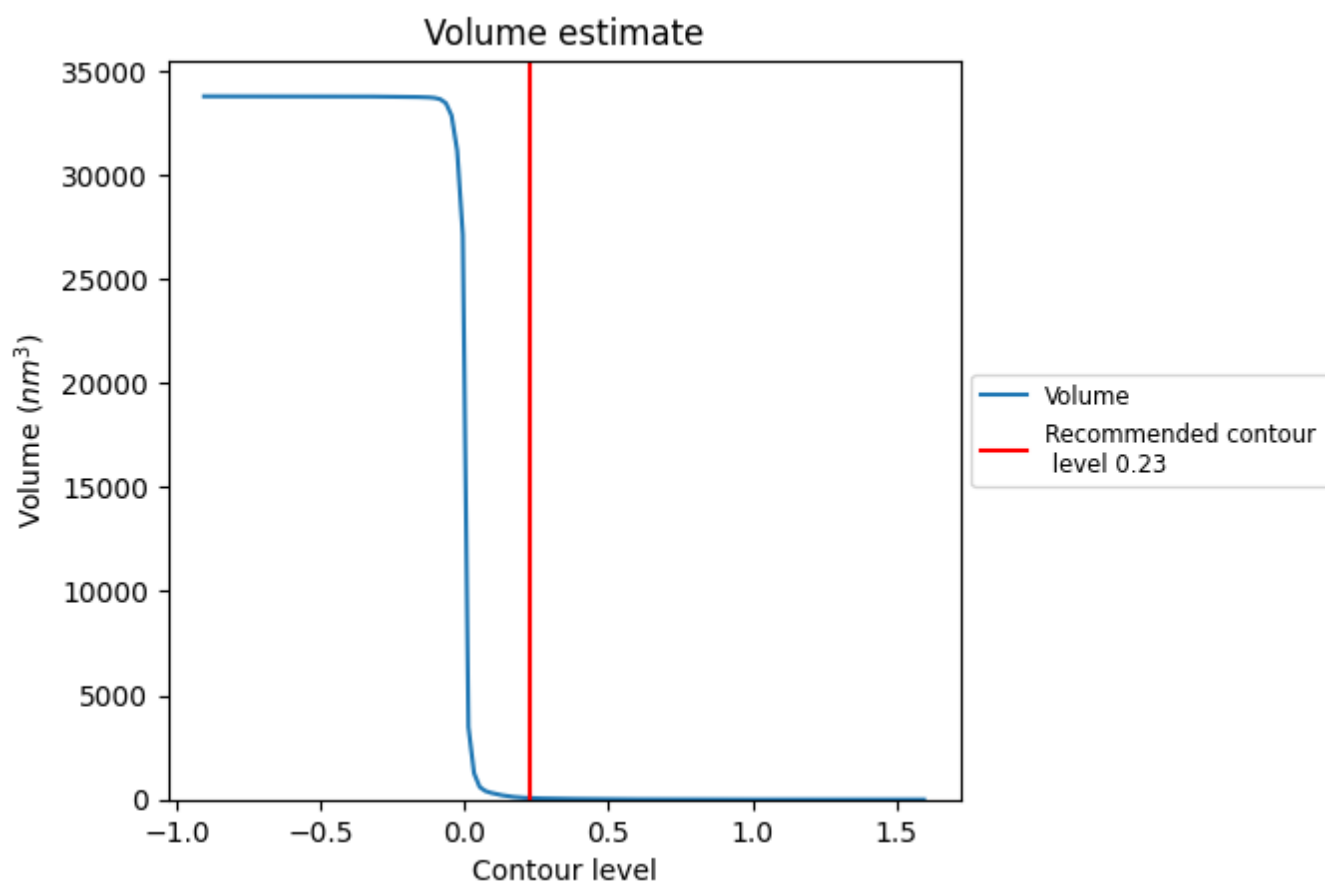
This section contains the results of statistical analysis of the map.

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.

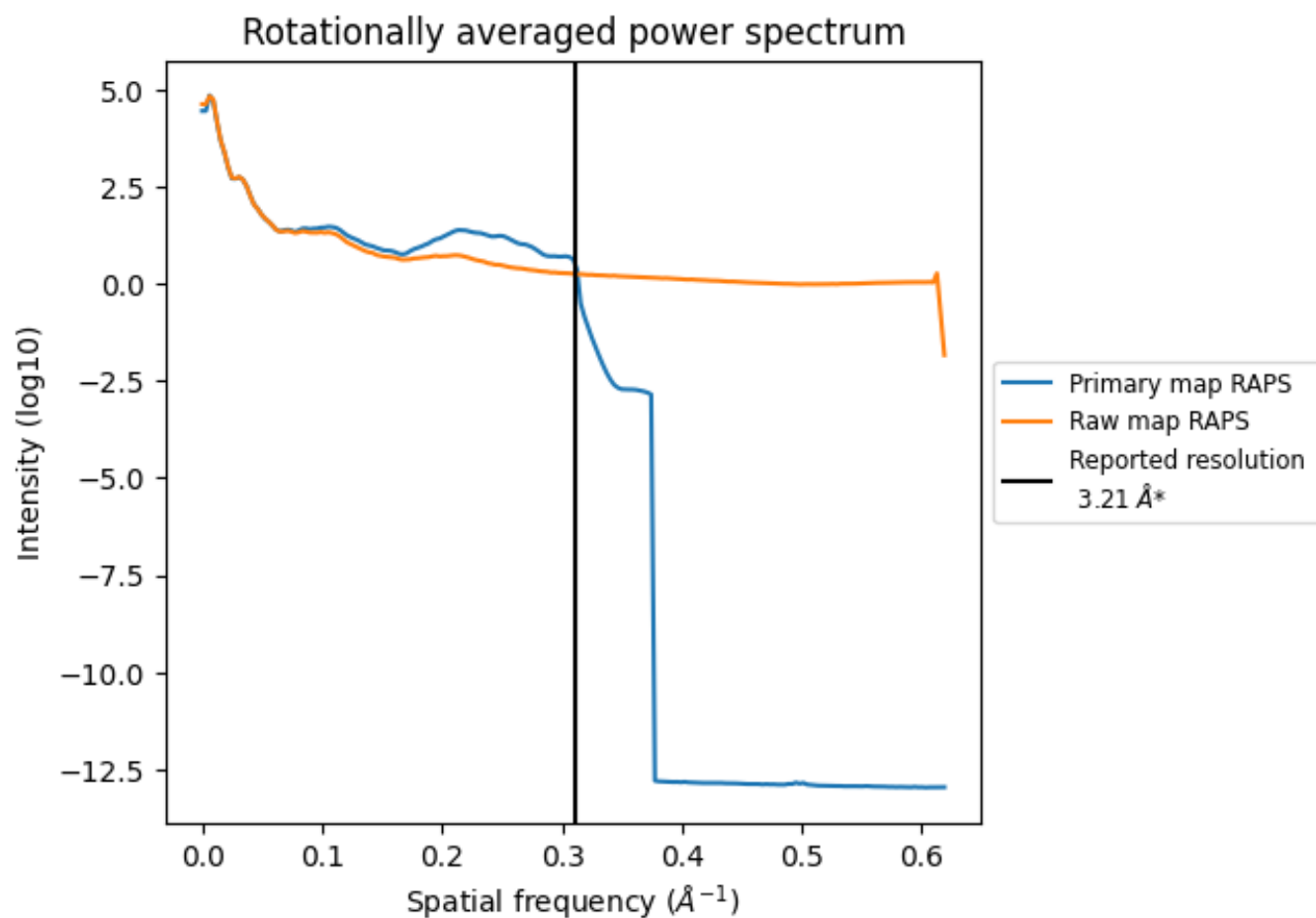
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 71 nm^3 ; this corresponds to an approximate mass of 64 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 ⓘ

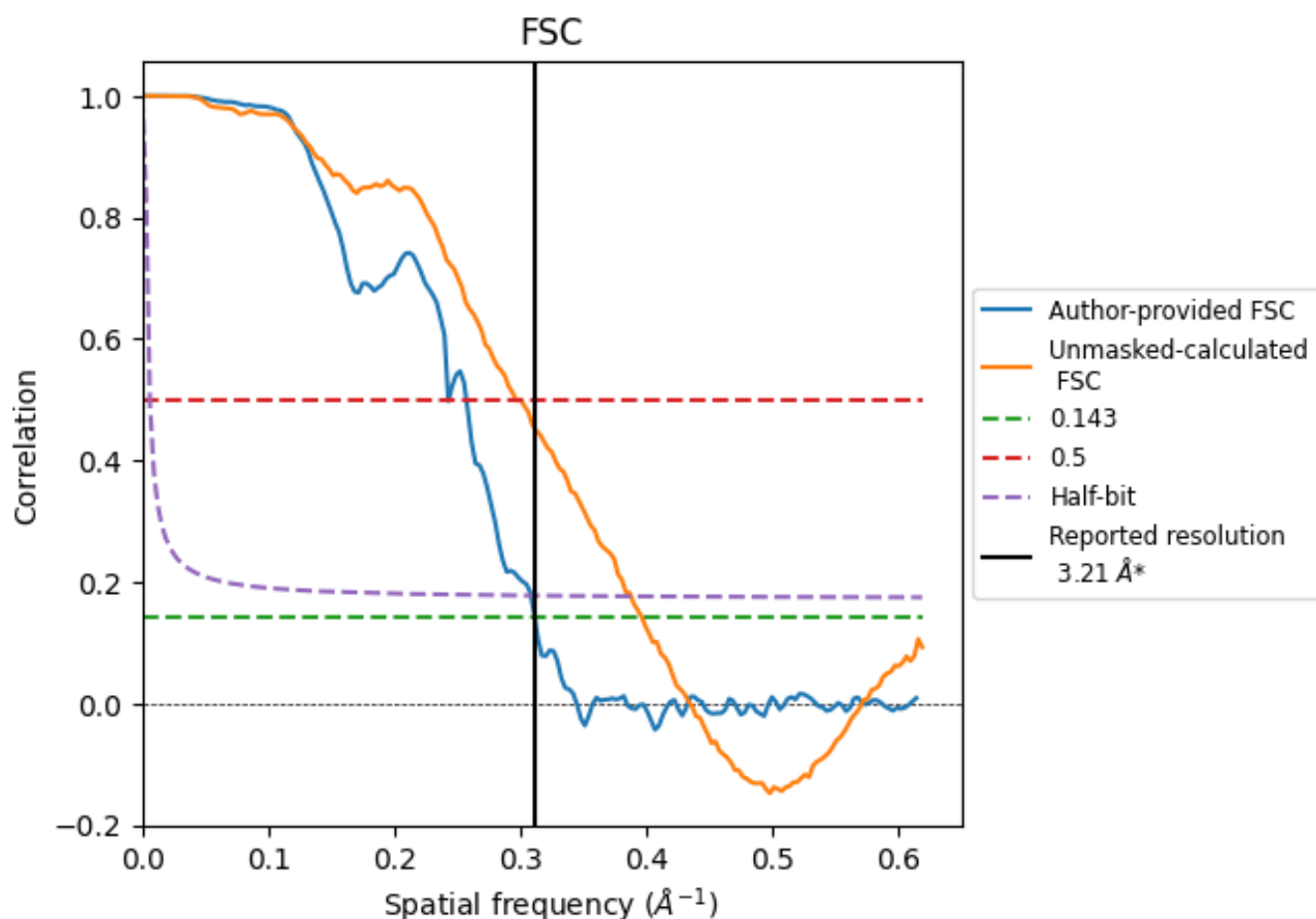


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

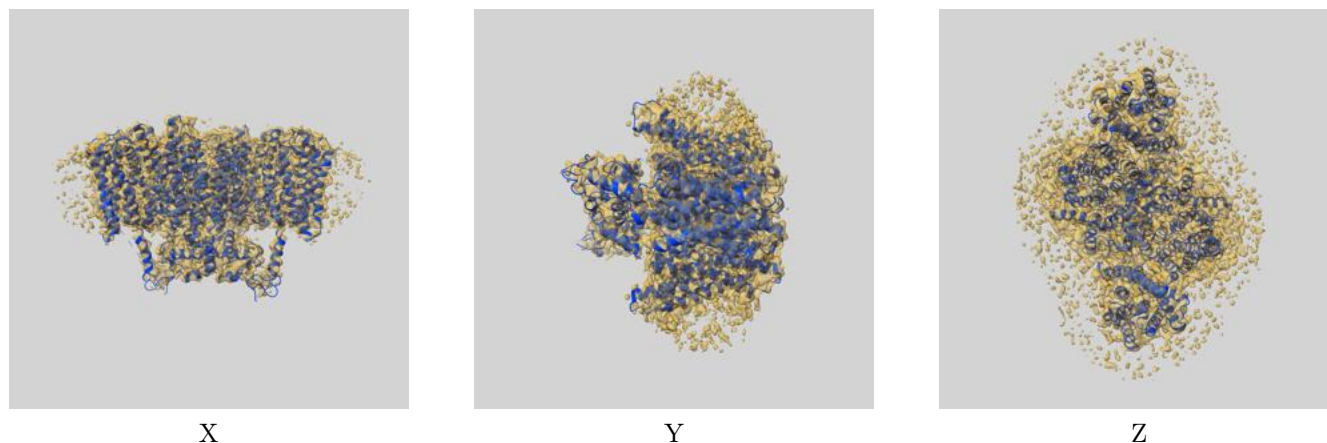
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	3.21	4.12	3.24
Unmasked-calculated*	2.52	3.37	2.58

*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 2.52 differs from the reported value 3.21 by more than 10 %

9 Map-model fit [i](#)

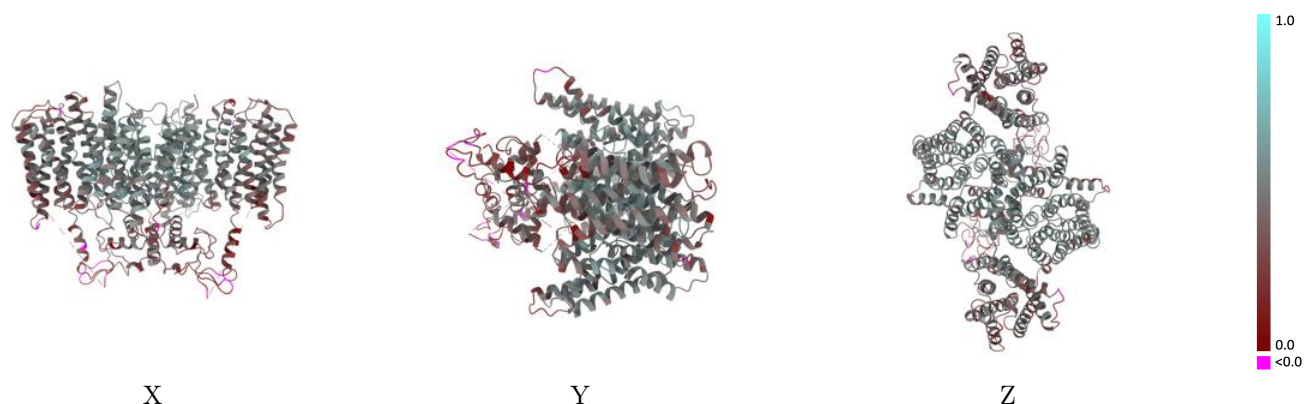
This section contains information regarding the fit between EMDB map EMD-61312 and PDB model 9JBF. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



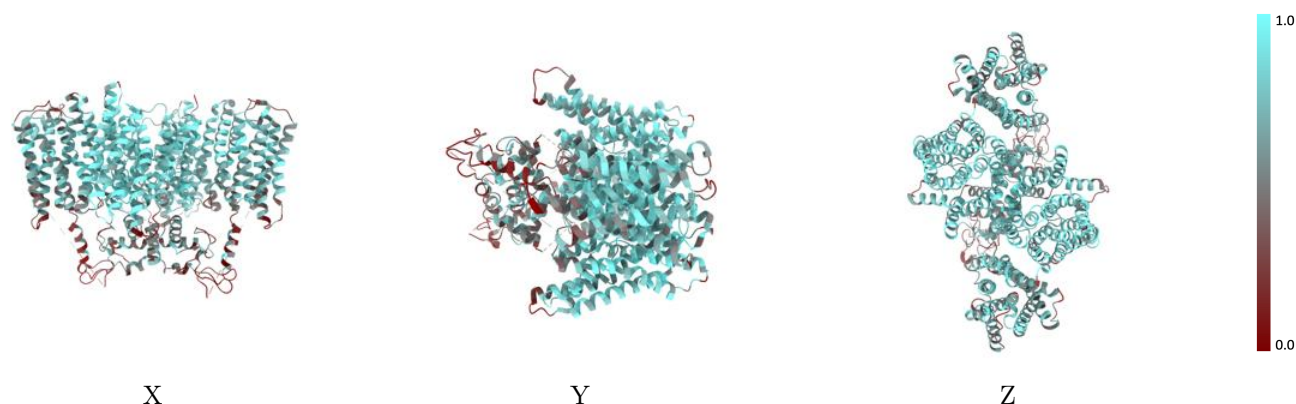
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



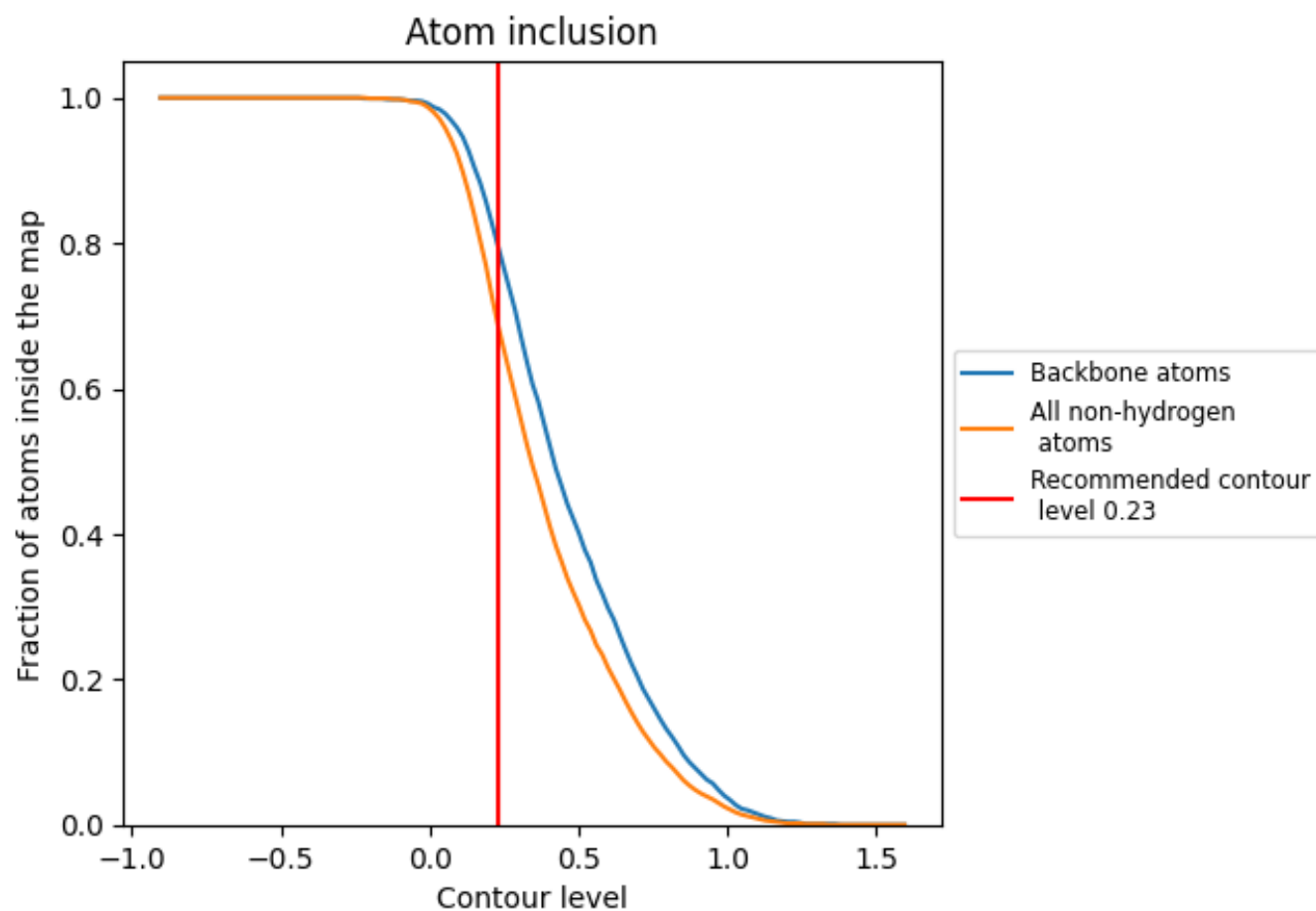
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.23).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 69% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6870	<div></div> 0.4310
A	<div></div> 0.6870	<div></div> 0.4320
B	<div></div> 0.6870	<div></div> 0.4300

