Full wwPDB EM Validation Report ⓘ

Sep 3, 2024 – 03:07 PM EDT

PDB ID	:	9B4E
EMDB ID	:	EMD-44178
Title	:	Structure of wild type human PSS1
Authors	:	Long, T.; Li, X.
Deposited on	:	2024-03-20
Resolution	:	2.70 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:

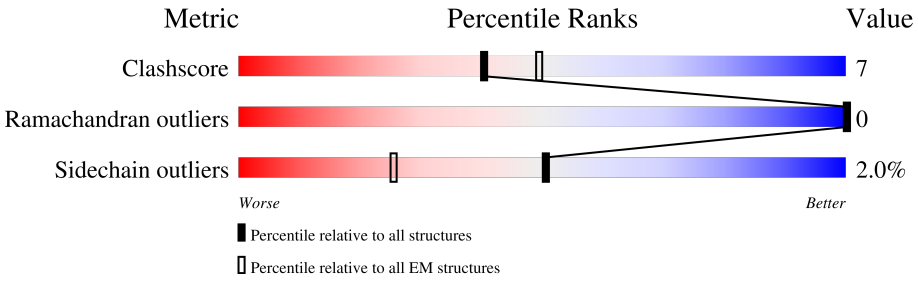
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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 <=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	409	5% 80% 14% 5%
1	B	409	5% 80% 14% 5%

2 Entry composition

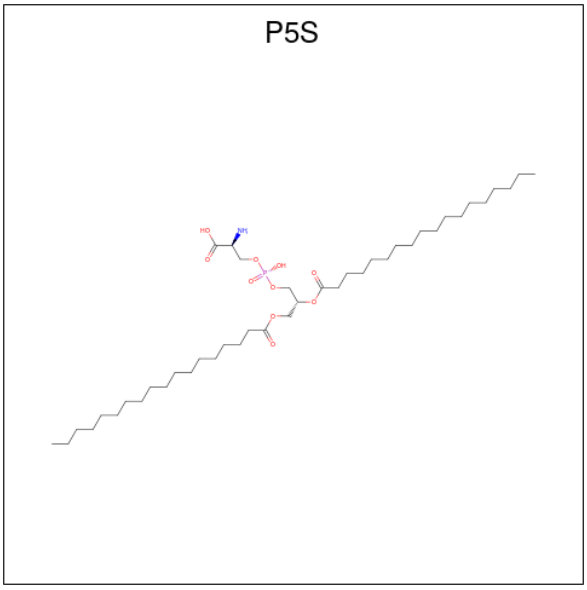
There are 7 unique types of molecules in this entry. The entry contains 6968 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphatidylserine synthase 1.

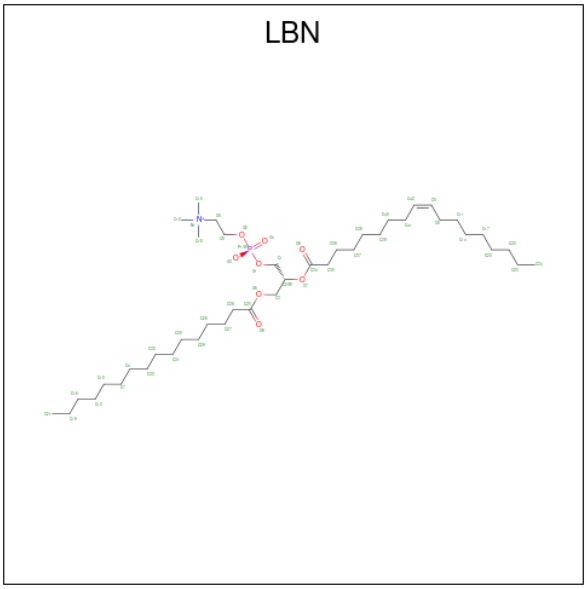
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	389	Total	C	N	O	S	0	0
			3241	2181	515	524	21		
1	B	389	Total	C	N	O	S	0	0
			3241	2181	515	524	21		

- Molecule 2 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: $C_{42}H_{82}NO_{10}P$).



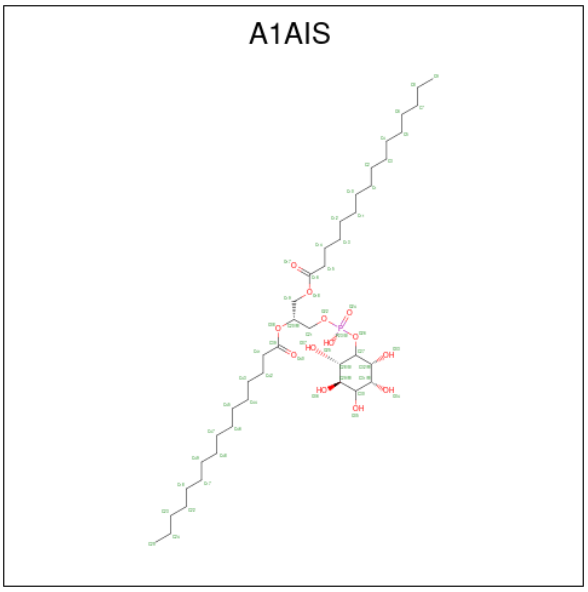
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			43	31	1	10	1	
2	A	1	Total	C	N	O	P	0
			31	19	1	10	1	
2	B	1	Total	C	N	O	P	0
			43	31	1	10	1	
2	B	1	Total	C	N	O	P	0
			31	19	1	10	1	

- Molecule 3 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (three-letter code: LBN) (formula: $C_{42}H_{82}NO_8P$).



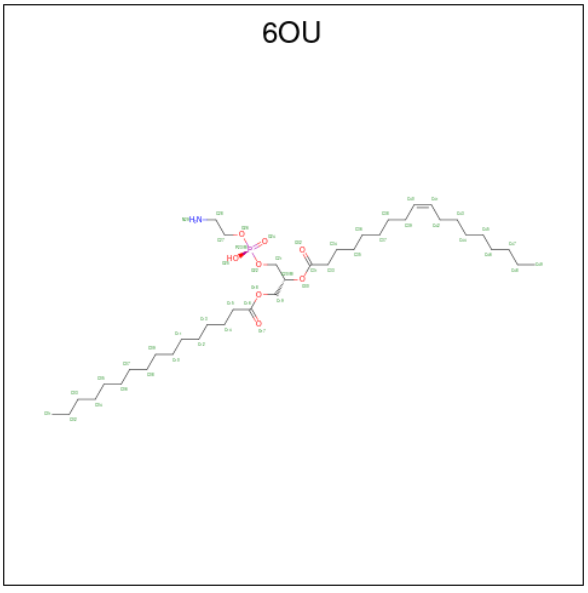
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
3	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	B	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	B	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 4 is (2R)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propane-1,2-diyl dihexadecanoate (three-letter code: A1AIS) (formula: $C_{41}H_{79}O_{13}P$).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			40	26	13	1	
4	B	1	Total	C	O	P	0
			40	26	13	1	

- Molecule 5 is [(2 {R})-1-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-3-hexadecanoyloxy-propan-2-yl] ({Z})-octadec-9-enoate (three-letter code: 6OU) (formula: $C_{39}H_{76}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			32	22	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	

- Molecule 7 is water.

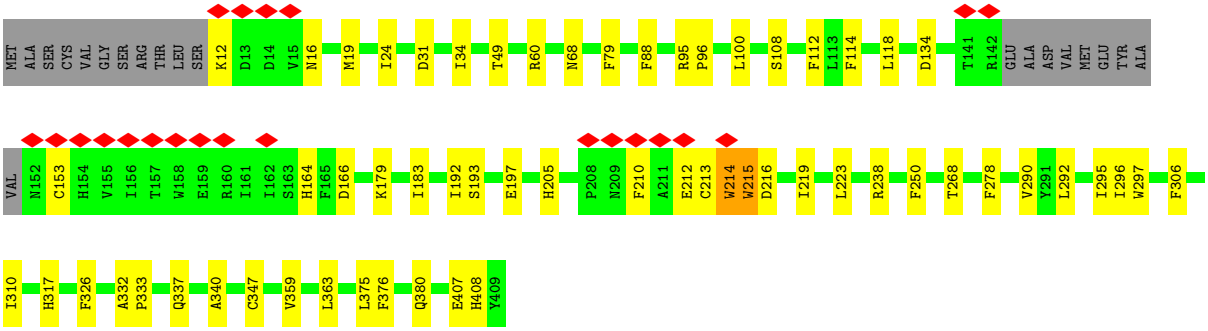
Mol	Chain	Residues	Atoms		AltConf
7	A	8	Total	O	0
			8	8	
7	B	8	Total	O	0
			8	8	

3 Residue-property plots (i)

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

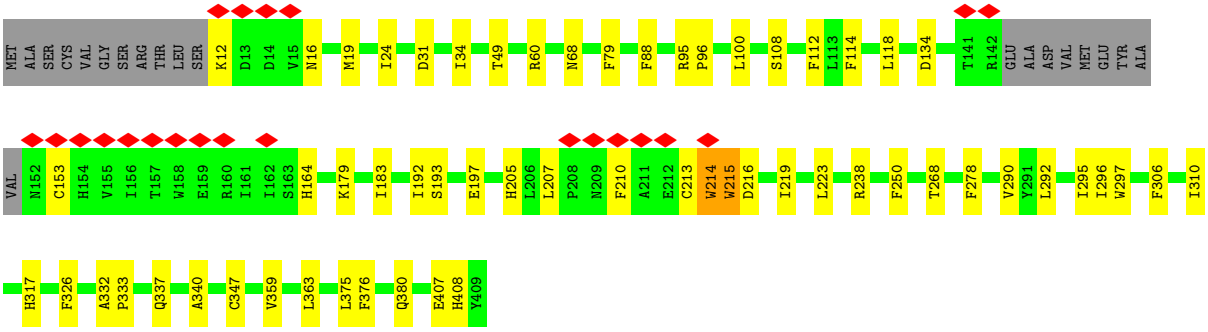
• Molecule 1: Phosphatidylserine synthase 1

Chain A:



• Molecule 1: Phosphatidylserine synthase 1

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	384020	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.077	Depositor
Minimum map value	-2.974	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.087	Depositor
Recommended contour level	0.477	Depositor
Map size (Å)	250.29, 250.29, 250.29	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8343, 0.8343, 0.8343	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P5S, CA, 6OU, LBN, A1AIS

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	0.32	0/3356	0.43	0/4572
1	B	0.32	0/3356	0.43	0/4572
All	All	0.32	0/6712	0.43	0/9144

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3241	0	3169	46	0
1	B	3241	0	3169	45	0
2	A	74	0	80	2	0
2	B	74	0	80	2	0
3	A	88	0	0	0	0
3	B	88	0	0	0	0
4	A	40	0	0	0	0
4	B	40	0	0	0	0
5	A	32	0	0	0	0
5	B	32	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	A	8	0	0	0	0
7	B	8	0	0	0	0
All	All	6968	0	6498	91	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 7.

All (91) 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:24:ILE:CD1	1:B:340:ALA:HB1	1.94	0.98
1:A:24:ILE:CD1	1:A:340:ALA:HB1	1.94	0.96
1:B:114:PHE:CE2	1:B:118:LEU:HD11	2.09	0.88
1:A:114:PHE:CE2	1:A:118:LEU:HD11	2.09	0.87
1:A:24:ILE:HD13	1:A:340:ALA:CB	2.05	0.85
1:A:24:ILE:HD13	1:A:340:ALA:HB1	1.58	0.85
1:B:24:ILE:HD13	1:B:340:ALA:CB	2.05	0.85
1:B:24:ILE:HD13	1:B:340:ALA:HB1	1.58	0.84
1:A:24:ILE:HD11	1:A:340:ALA:HB1	1.61	0.81
1:B:24:ILE:HD11	1:B:340:ALA:HB1	1.61	0.80
1:B:24:ILE:HD12	1:B:347:CYS:SG	2.30	0.71
1:A:24:ILE:HD12	1:A:347:CYS:SG	2.30	0.71
1:A:24:ILE:CD1	1:A:340:ALA:CB	2.68	0.66
1:B:24:ILE:CD1	1:B:340:ALA:CB	2.68	0.65
1:A:213:CYS:SG	1:A:214:TRP:N	2.71	0.64
1:B:213:CYS:SG	1:B:214:TRP:N	2.71	0.64
1:A:34:ILE:HD11	1:A:250:PHE:HB3	1.82	0.62
1:B:34:ILE:HD11	1:B:250:PHE:HB3	1.82	0.62
1:B:24:ILE:HD13	1:B:340:ALA:HB3	1.82	0.61
1:A:215:TRP:HD1	1:A:216:ASP:N	1.98	0.60
1:A:24:ILE:HD13	1:A:340:ALA:HB3	1.82	0.60
1:B:215:TRP:HD1	1:B:216:ASP:N	1.98	0.60
1:A:60:ARG:NH2	1:A:68:ASN:OD1	2.34	0.59
1:B:16:ASN:HA	1:B:19:MET:HG2	1.84	0.58
1:A:16:ASN:HA	1:A:19:MET:HG2	1.84	0.58
1:A:95:ARG:HG2	1:A:268:THR:O	2.05	0.57
1:B:95:ARG:HG2	1:B:268:THR:O	2.05	0.57
1:B:60:ARG:NH2	1:B:68:ASN:OD1	2.34	0.56
1:A:114:PHE:O	1:A:118:LEU:HG	2.07	0.55
1:B:114:PHE:O	1:B:118:LEU:HG	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:PRO:HG2	1:B:100:LEU:HD12	1.89	0.54
1:A:96:PRO:HG2	1:A:100:LEU:HD12	1.89	0.53
1:A:108:SER:HA	1:A:326:PHE:HZ	1.74	0.53
1:B:108:SER:HA	1:B:326:PHE:HZ	1.74	0.52
1:A:359:VAL:O	1:A:363:LEU:HG	2.11	0.51
1:B:359:VAL:O	1:B:363:LEU:HG	2.11	0.51
1:B:96:PRO:HD3	2:B:602:P5S:H40A	1.93	0.51
1:B:193:SER:O	1:B:197:GLU:HG2	2.11	0.50
1:A:193:SER:O	1:A:197:GLU:HG2	2.11	0.50
1:A:24:ILE:HG22	1:A:337:GLN:HG2	1.95	0.49
1:B:24:ILE:HG22	1:B:337:GLN:HG2	1.95	0.49
1:A:96:PRO:HD3	2:A:501:P5S:H40A	1.93	0.49
1:A:205:HIS:CE1	1:A:214:TRP:HE1	2.32	0.47
1:B:215:TRP:CD1	1:B:216:ASP:N	2.82	0.47
1:A:31:ASP:O	2:A:502:P5S:N	2.41	0.47
1:B:205:HIS:CE1	1:B:214:TRP:HE1	2.32	0.47
1:A:215:TRP:CD1	1:A:216:ASP:N	2.82	0.47
1:B:376:PHE:HD1	1:B:380:GLN:HB3	1.80	0.47
1:A:407:GLU:HG3	1:A:408:HIS:ND1	2.30	0.46
1:A:376:PHE:HD1	1:A:380:GLN:HB3	1.80	0.46
1:A:24:ILE:CG2	1:A:337:GLN:HG2	2.46	0.46
1:B:24:ILE:CG2	1:B:337:GLN:HG2	2.46	0.46
1:B:407:GLU:HG3	1:B:408:HIS:ND1	2.30	0.46
1:A:192:ILE:HG13	1:A:297:TRP:CE3	2.51	0.46
1:B:219:ILE:HG23	1:B:223:LEU:HD12	1.98	0.46
1:B:292:LEU:O	1:B:296:ILE:HG12	2.16	0.45
1:A:292:LEU:O	1:A:296:ILE:HG12	2.16	0.45
1:A:24:ILE:HG22	1:A:24:ILE:O	2.15	0.45
1:B:12:LYS:HA	1:B:12:LYS:HE2	1.99	0.45
1:B:24:ILE:HG22	1:B:24:ILE:O	2.16	0.45
1:A:12:LYS:HE2	1:A:12:LYS:HA	1.99	0.45
1:A:219:ILE:HG23	1:A:223:LEU:HD12	1.98	0.45
1:A:278:PHE:CE1	1:A:290:VAL:HG11	2.53	0.44
1:B:192:ILE:HG13	1:B:297:TRP:CE3	2.51	0.44
1:A:134:ASP:OD2	1:A:317:HIS:NE2	2.49	0.44
1:A:166:ASP:OD1	1:A:166:ASP:N	2.47	0.44
1:B:31:ASP:O	2:B:603:P5S:N	2.41	0.44
1:B:112:PHE:CE1	1:B:363:LEU:HD11	2.53	0.43
1:A:306:PHE:O	1:A:310:ILE:HG12	2.18	0.43
1:B:306:PHE:O	1:B:310:ILE:HG12	2.18	0.43
1:A:112:PHE:CE1	1:A:363:LEU:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:PHE:CE1	1:B:290:VAL:HG11	2.53	0.43
1:B:332:ALA:HB3	1:B:333:PRO:HD3	2.01	0.43
1:A:332:ALA:HB3	1:A:333:PRO:HD3	2.01	0.43
1:A:213:CYS:HB3	1:A:215:TRP:CD1	2.54	0.42
1:A:49:THR:HG23	1:A:79:PHE:CE1	2.54	0.42
1:B:213:CYS:HB3	1:B:215:TRP:CD1	2.54	0.42
1:A:179:LYS:O	1:A:183:ILE:HG12	2.20	0.42
1:B:179:LYS:O	1:B:183:ILE:HG12	2.20	0.42
1:B:278:PHE:HE1	1:B:290:VAL:HG11	1.84	0.42
1:A:278:PHE:HE1	1:A:290:VAL:HG11	1.84	0.41
1:B:112:PHE:HE1	1:B:363:LEU:HD11	1.86	0.41
1:B:49:THR:HG23	1:B:79:PHE:CE1	2.54	0.41
1:B:295:ILE:HD13	1:B:295:ILE:HA	1.92	0.41
1:A:375:LEU:HD23	1:A:375:LEU:HA	1.89	0.41
1:B:134:ASP:OD2	1:B:317:HIS:NE2	2.49	0.41
1:A:112:PHE:HE1	1:A:363:LEU:HD11	1.86	0.41
1:B:375:LEU:HD23	1:B:375:LEU:HA	1.89	0.41
1:B:207:LEU:HD11	1:B:376:PHE:CE1	2.56	0.41
1:A:295:ILE:HD13	1:A:295:ILE:HA	1.93	0.40
1:A:212:GLU:O	1:A:213:CYS:HB2	2.22	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	385/409 (94%)	370 (96%)	15 (4%)	0	100	100
1	B	385/409 (94%)	370 (96%)	15 (4%)	0	100	100
All	All	770/818 (94%)	740 (96%)	30 (4%)	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	342/367 (93%)	335 (98%)	7 (2%)	50 78
1	B	342/367 (93%)	335 (98%)	7 (2%)	50 78
All	All	684/734 (93%)	670 (98%)	14 (2%)	50 78

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	PHE
1	A	153	CYS
1	A	164	HIS
1	A	210	PHE
1	A	214	TRP
1	A	215	TRP
1	A	238	ARG
1	B	88	PHE
1	B	153	CYS
1	B	164	HIS
1	B	210	PHE
1	B	214	TRP
1	B	215	TRP
1	B	238	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	205	HIS
1	A	314	GLN
1	B	28	GLN
1	B	205	HIS
1	B	314	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)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	6OU	B	606	-	31,31,48	1.23	4 (12%)	34,36,53	1.05	2 (5%)
4	A1AIS	A	504	-	40,40,55	1.06	4 (10%)	49,52,67	1.28	5 (10%)
2	P5S	A	501	-	41,42,53	1.20	3 (7%)	43,49,60	1.01	2 (4%)
3	LBN	A	503	-	51,51,51	1.09	5 (9%)	57,59,59	0.88	2 (3%)
3	LBN	B	601	-	35,35,51	1.31	5 (14%)	41,43,59	1.10	2 (4%)
2	P5S	B	602	-	41,42,53	1.20	3 (7%)	43,49,60	1.01	2 (4%)
4	A1AIS	B	605	-	40,40,55	1.05	4 (10%)	49,52,67	1.28	5 (10%)
5	6OU	A	505	-	31,31,48	1.23	4 (12%)	34,36,53	1.05	2 (5%)
3	LBN	B	604	-	51,51,51	1.09	5 (9%)	57,59,59	0.88	2 (3%)
2	P5S	A	502	-	29,30,53	1.34	3 (10%)	31,37,60	1.13	2 (6%)
2	P5S	B	603	-	29,30,53	1.34	3 (10%)	31,37,60	1.13	2 (6%)
3	LBN	A	507	-	35,35,51	1.31	4 (11%)	41,43,59	1.10	2 (4%)

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
5	6OU	B	606	-	-	21/35/35/52	-
4	A1AIS	A	504	-	-	17/35/59/74	0/1/1/1
2	P5S	A	501	-	-	21/48/48/59	-
3	LBN	A	503	-	-	22/55/55/55	-
3	LBN	B	601	-	-	25/39/39/55	-
2	P5S	B	602	-	-	21/48/48/59	-
4	A1AIS	B	605	-	-	17/35/59/74	0/1/1/1
5	6OU	A	505	-	-	21/35/35/52	-
3	LBN	B	604	-	-	22/55/55/55	-
2	P5S	A	502	-	-	21/36/36/59	-
2	P5S	B	603	-	-	21/36/36/59	-
3	LBN	A	507	-	-	25/39/39/55	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	P5S	O19-C17	3.31	1.43	1.33
2	B	602	P5S	O19-C17	3.31	1.43	1.33
2	A	502	P5S	O19-C17	3.21	1.42	1.33
2	B	603	P5S	O19-C17	3.21	1.42	1.33
3	A	503	LBN	O7-C34	3.14	1.43	1.34
3	B	604	LBN	O7-C34	3.13	1.43	1.34
5	A	505	6OU	O18-C16	3.09	1.42	1.33
5	B	606	6OU	O18-C16	3.08	1.42	1.33
3	B	601	LBN	O7-C34	3.08	1.43	1.34
3	A	507	LBN	O7-C34	3.07	1.42	1.34
2	A	501	P5S	O37-C38	3.04	1.42	1.34
2	B	602	P5S	O37-C38	3.04	1.42	1.34
2	B	603	P5S	O37-C38	3.04	1.42	1.34
2	A	502	P5S	O37-C38	3.02	1.42	1.34
4	A	504	A1AIS	O38-C20	-2.86	1.39	1.46
4	B	605	A1AIS	O38-C20	-2.85	1.39	1.46
3	B	601	LBN	O5-C25	2.66	1.41	1.33
3	A	507	LBN	O5-C25	2.65	1.41	1.33
5	A	505	6OU	O30-C20	-2.54	1.40	1.46
5	B	606	6OU	O30-C20	-2.53	1.40	1.46
5	A	505	6OU	O30-C31	2.50	1.41	1.34
5	B	606	6OU	O30-C31	2.48	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	LBN	O5-C25	2.48	1.40	1.33
3	B	604	LBN	O5-C25	2.48	1.40	1.33
2	B	603	P5S	O37-C2	-2.36	1.41	1.46
2	A	502	P5S	O37-C2	-2.34	1.41	1.46
4	A	504	A1AIS	O18-C19	-2.33	1.40	1.45
3	B	601	LBN	C6-N1	-2.32	1.44	1.51
3	A	507	LBN	C6-N1	-2.32	1.44	1.51
4	B	605	A1AIS	O18-C19	-2.31	1.40	1.45
2	A	501	P5S	O37-C2	-2.31	1.41	1.46
2	B	602	P5S	O37-C2	-2.31	1.41	1.46
3	B	604	LBN	O5-C3	-2.15	1.40	1.45
3	A	503	LBN	O5-C3	-2.15	1.40	1.45
4	B	605	A1AIS	O18-C16	2.13	1.39	1.33
3	A	507	LBN	O5-C3	-2.13	1.40	1.45
5	A	505	6OU	P23-O22	2.12	1.67	1.59
4	A	504	A1AIS	O18-C16	2.12	1.39	1.33
5	B	606	6OU	P23-O22	2.12	1.67	1.59
3	B	604	LBN	O7-C2	-2.11	1.41	1.46
3	A	503	LBN	O7-C2	-2.10	1.41	1.46
3	B	601	LBN	O5-C3	-2.09	1.40	1.45
3	A	503	LBN	C18-N1	-2.02	1.44	1.50
4	A	504	A1AIS	P23-O26	2.01	1.65	1.59
3	B	604	LBN	C18-N1	-2.01	1.44	1.50
4	B	605	A1AIS	P23-O26	2.01	1.65	1.59
3	B	601	LBN	O7-C2	-2.01	1.41	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	504	A1AIS	O38-C39-C41	4.47	121.14	111.48
4	B	605	A1AIS	O38-C39-C41	4.45	121.11	111.48
3	A	507	LBN	O7-C34-C35	4.17	120.50	111.48
3	B	601	LBN	O7-C34-C35	4.16	120.49	111.48
5	B	606	6OU	O30-C31-C33	3.93	119.98	111.48
2	A	501	P5S	O37-C38-C39	3.92	119.96	111.48
5	A	505	6OU	O30-C31-C33	3.92	119.96	111.48
2	B	602	P5S	O37-C38-C39	3.90	119.92	111.48
3	A	503	LBN	O7-C34-C35	3.63	119.33	111.48
3	B	604	LBN	O7-C34-C35	3.62	119.31	111.48
2	A	502	P5S	O37-C38-C39	3.41	118.86	111.48
2	B	603	P5S	O37-C38-C39	3.40	118.83	111.48
4	B	605	A1AIS	C31-C32-C27	3.32	117.21	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	504	A1AIS	C31-C32-C27	3.31	117.20	109.68
4	A	504	A1AIS	C32-C31-C30	3.30	116.62	110.83
4	B	605	A1AIS	C32-C31-C30	3.30	116.62	110.83
2	A	502	P5S	O19-C17-C20	2.99	120.95	111.83
2	B	603	P5S	O19-C17-C20	2.99	120.95	111.83
3	A	503	LBN	O5-C25-C26	2.87	120.58	111.83
2	A	501	P5S	O19-C17-C20	2.86	120.57	111.83
3	B	604	LBN	O5-C25-C26	2.86	120.56	111.83
2	B	602	P5S	O19-C17-C20	2.86	120.54	111.83
5	A	505	6OU	O18-C16-C15	2.81	120.42	111.83
5	B	606	6OU	O18-C16-C15	2.80	120.37	111.83
4	A	504	A1AIS	O18-C16-C15	2.76	120.25	111.83
4	B	605	A1AIS	O18-C16-C15	2.74	120.20	111.83
3	A	507	LBN	O5-C25-C26	2.68	120.00	111.83
3	B	601	LBN	O5-C25-C26	2.68	120.00	111.83
4	B	605	A1AIS	C20-O38-C39	-2.24	112.44	117.80
4	A	504	A1AIS	C20-O38-C39	-2.23	112.46	117.80

There are no chirality outliers.

All (254) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	P5S	CB-OG-P12-O16
2	A	501	P5S	C3-O16-P12-OG
2	A	501	P5S	C3-O16-P12-O13
2	A	501	P5S	C39-C38-O37-C2
2	A	502	P5S	C-CA-CB-OG
2	A	502	P5S	N-CA-CB-OG
2	A	502	P5S	CB-OG-P12-O15
2	A	502	P5S	C3-O16-P12-OG
2	A	502	P5S	C3-O16-P12-O13
2	A	502	P5S	C3-O16-P12-O15
2	B	602	P5S	CB-OG-P12-O16
2	B	602	P5S	C3-O16-P12-OG
2	B	602	P5S	C3-O16-P12-O13
2	B	602	P5S	C39-C38-O37-C2
2	B	603	P5S	C-CA-CB-OG
2	B	603	P5S	N-CA-CB-OG
2	B	603	P5S	CB-OG-P12-O15
2	B	603	P5S	C3-O16-P12-OG
2	B	603	P5S	C3-O16-P12-O13
2	B	603	P5S	C3-O16-P12-O15

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Mol	Chain	Res	Type	Atoms
3	A	507	LBN	C1-O1-P1-O2
3	A	507	LBN	C1-O1-P1-O3
3	A	507	LBN	C1-O1-P1-O4
3	B	601	LBN	C1-O1-P1-O2
3	B	601	LBN	C1-O1-P1-O3
3	B	601	LBN	C1-O1-P1-O4
5	A	505	6OU	C21-O22-P23-O24
5	A	505	6OU	C21-O22-P23-O25
5	A	505	6OU	C21-O22-P23-O26
5	A	505	6OU	O26-C27-C28-N29
5	A	505	6OU	C33-C31-O30-C20
5	B	606	6OU	C21-O22-P23-O24
5	B	606	6OU	C21-O22-P23-O25
5	B	606	6OU	C21-O22-P23-O26
5	B	606	6OU	O26-C27-C28-N29
5	B	606	6OU	C33-C31-O30-C20
3	A	507	LBN	O6-C25-O5-C3
3	B	601	LBN	O6-C25-O5-C3
2	A	501	P5S	O47-C38-O37-C2
2	B	602	P5S	O47-C38-O37-C2
5	A	505	6OU	O32-C31-O30-C20
5	B	606	6OU	O32-C31-O30-C20
3	A	507	LBN	C26-C25-O5-C3
3	B	601	LBN	C26-C25-O5-C3
4	A	504	A1AIS	O40-C39-O38-C20
3	A	507	LBN	C35-C34-O7-C2
3	B	601	LBN	C35-C34-O7-C2
4	A	504	A1AIS	C41-C39-O38-C20
4	B	605	A1AIS	C41-C39-O38-C20
4	B	605	A1AIS	O40-C39-O38-C20
2	A	501	P5S	C20-C17-O19-C1
2	B	602	P5S	C20-C17-O19-C1
4	A	504	A1AIS	C11-C12-C13-C14
4	A	504	A1AIS	C44-C45-C46-C47
4	B	605	A1AIS	C11-C12-C13-C14
4	B	605	A1AIS	C44-C45-C46-C47
5	A	505	6OU	C13-C14-C15-C16
5	B	606	6OU	C13-C14-C15-C16
3	A	503	LBN	C35-C34-O7-C2
3	B	604	LBN	C35-C34-O7-C2
4	A	504	A1AIS	C39-C41-C42-C43
3	A	507	LBN	O8-C34-O7-C2

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Mol	Chain	Res	Type	Atoms
3	B	601	LBN	O8-C34-O7-C2
4	B	605	A1AIS	C39-C41-C42-C43
2	A	501	P5S	O18-C17-O19-C1
2	B	602	P5S	O18-C17-O19-C1
2	A	501	P5S	C17-C20-C21-C22
2	A	502	P5S	C17-C20-C21-C22
2	A	502	P5S	C38-C39-C40-C41
2	B	602	P5S	C17-C20-C21-C22
2	B	603	P5S	C17-C20-C21-C22
2	B	603	P5S	C38-C39-C40-C41
3	A	503	LBN	C25-C26-C27-C28
3	A	507	LBN	C34-C35-C36-C37
3	B	601	LBN	C34-C35-C36-C37
3	B	604	LBN	C25-C26-C27-C28
5	A	505	6OU	C31-C33-C34-C35
5	B	606	6OU	C31-C33-C34-C35
3	A	503	LBN	O8-C34-O7-C2
3	B	604	LBN	O8-C34-O7-C2
2	A	502	P5S	C20-C17-O19-C1
2	B	603	P5S	C20-C17-O19-C1
2	A	502	P5S	C39-C38-O37-C2
2	B	603	P5S	C39-C38-O37-C2
4	A	504	A1AIS	C15-C16-O18-C19
4	B	605	A1AIS	C15-C16-O18-C19
2	A	501	P5S	C26-C27-C28-C29
2	B	602	P5S	C26-C27-C28-C29
5	A	505	6OU	C11-C12-C13-C14
5	B	606	6OU	C11-C12-C13-C14
2	A	502	P5S	O47-C38-O37-C2
2	B	603	P5S	O47-C38-O37-C2
3	A	507	LBN	C30-C31-C32-C33
3	B	601	LBN	C30-C31-C32-C33
3	B	601	LBN	C26-C27-C28-C29
3	A	507	LBN	C26-C27-C28-C29
3	A	503	LBN	C27-C28-C29-C30
3	B	604	LBN	C27-C28-C29-C30
2	A	501	P5S	C23-C24-C25-C26
2	B	602	P5S	C23-C24-C25-C26
2	A	502	P5S	O18-C17-O19-C1
2	B	603	P5S	O18-C17-O19-C1
3	A	507	LBN	C28-C29-C30-C31
3	B	601	LBN	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
3	A	503	LBN	C26-C25-O5-C3
3	B	604	LBN	C26-C25-O5-C3
3	A	507	LBN	C25-C26-C27-C28
3	B	601	LBN	C25-C26-C27-C28
2	A	502	P5S	C20-C21-C22-C23
2	B	603	P5S	C20-C21-C22-C23
3	A	503	LBN	C30-C31-C32-C33
3	B	604	LBN	C30-C31-C32-C33
3	A	507	LBN	C32-C33-C4-C7
3	B	601	LBN	C32-C33-C4-C7
2	A	501	P5S	C40-C41-C42-C43
2	B	602	P5S	C40-C41-C42-C43
4	A	504	A1AIS	O17-C16-O18-C19
4	B	605	A1AIS	O17-C16-O18-C19
3	A	503	LBN	C9-C6-N1-C12
3	B	604	LBN	C9-C6-N1-C12
3	A	503	LBN	C35-C36-C37-C38
3	B	604	LBN	C35-C36-C37-C38
2	A	501	P5S	C28-C29-C30-C31
2	B	602	P5S	C28-C29-C30-C31
3	A	503	LBN	O6-C25-O5-C3
3	B	604	LBN	O6-C25-O5-C3
3	B	604	LBN	C10-C13-C16-C19
4	B	605	A1AIS	C42-C43-C44-C45
3	A	503	LBN	C10-C13-C16-C19
4	A	504	A1AIS	C42-C43-C44-C45
5	A	505	6OU	C09-C10-C11-C12
5	B	606	6OU	C09-C10-C11-C12
5	A	505	6OU	C15-C16-O18-C19
5	B	606	6OU	C15-C16-O18-C19
5	A	505	6OU	C19-C20-C21-O22
5	B	606	6OU	C19-C20-C21-O22
2	A	502	P5S	O19-C1-C2-C3
2	B	603	P5S	O19-C1-C2-C3
4	A	504	A1AIS	O18-C19-C20-C21
4	B	605	A1AIS	O18-C19-C20-C21
5	A	505	6OU	C33-C34-C35-C36
5	B	606	6OU	C33-C34-C35-C36
5	A	505	6OU	O17-C16-O18-C19
5	B	606	6OU	O17-C16-O18-C19
3	A	503	LBN	C14-C11-C8-C5
3	B	604	LBN	C14-C11-C8-C5

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Mol	Chain	Res	Type	Atoms
3	B	601	LBN	C27-C28-C29-C30
3	A	507	LBN	C27-C28-C29-C30
5	A	505	6OU	C35-C36-C37-C38
5	B	606	6OU	C35-C36-C37-C38
2	A	501	P5S	C22-C23-C24-C25
2	B	602	P5S	C22-C23-C24-C25
3	A	503	LBN	C26-C27-C28-C29
3	B	604	LBN	C26-C27-C28-C29
5	A	505	6OU	C37-C38-C39-C40
5	B	606	6OU	C37-C38-C39-C40
3	A	503	LBN	C9-C6-N1-C18
3	B	604	LBN	C9-C6-N1-C18
5	A	505	6OU	O18-C19-C20-C21
5	B	606	6OU	O18-C19-C20-C21
4	A	504	A1AIS	C41-C42-C43-C44
4	B	605	A1AIS	C41-C42-C43-C44
3	A	507	LBN	C2-C1-O1-P1
3	B	601	LBN	C2-C1-O1-P1
2	A	501	P5S	O19-C1-C2-O37
2	A	502	P5S	O19-C1-C2-O37
2	B	602	P5S	O19-C1-C2-O37
2	B	603	P5S	O19-C1-C2-O37
4	A	504	A1AIS	O18-C19-C20-O38
4	B	605	A1AIS	O18-C19-C20-O38
2	A	502	P5S	C39-C40-C41-C42
2	B	603	P5S	C39-C40-C41-C42
2	A	502	P5S	C1-C2-C3-O16
2	B	603	P5S	C1-C2-C3-O16
2	A	501	P5S	C20-C21-C22-C23
2	B	602	P5S	C20-C21-C22-C23
4	A	504	A1AIS	O38-C20-C21-O22
4	B	605	A1AIS	O38-C20-C21-O22
2	A	501	P5S	O19-C1-C2-C3
2	B	602	P5S	O19-C1-C2-C3
3	A	503	LBN	O7-C2-C3-O5
3	B	604	LBN	O7-C2-C3-O5
5	A	505	6OU	O18-C19-C20-O30
5	B	606	6OU	O18-C19-C20-O30
2	A	501	P5S	N-CA-CB-OG
2	B	602	P5S	N-CA-CB-OG
3	A	507	LBN	N1-C6-C9-O2
3	B	601	LBN	N1-C6-C9-O2

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Mol	Chain	Res	Type	Atoms
3	A	503	LBN	C9-C6-N1-C15
3	B	604	LBN	C9-C6-N1-C15
3	A	507	LBN	O1-C1-C2-C3
3	B	601	LBN	O1-C1-C2-C3
2	A	502	P5S	O37-C2-C3-O16
2	B	603	P5S	O37-C2-C3-O16
3	A	507	LBN	O1-C1-C2-O7
3	B	601	LBN	O1-C1-C2-O7
5	A	505	6OU	O30-C20-C21-O22
5	B	606	6OU	O30-C20-C21-O22
3	A	507	LBN	C29-C30-C31-C32
3	B	601	LBN	C29-C30-C31-C32
3	A	503	LBN	C1-C2-C3-O5
3	B	604	LBN	C1-C2-C3-O5
2	A	501	P5S	CB-OG-P12-O13
2	A	502	P5S	CB-OG-P12-O16
2	B	602	P5S	CB-OG-P12-O13
2	B	603	P5S	CB-OG-P12-O16
3	A	503	LBN	C1-O1-P1-O4
3	B	604	LBN	C1-O1-P1-O4
4	A	504	A1AIS	C21-O22-P23-O25
4	A	504	A1AIS	C21-O22-P23-O26
4	B	605	A1AIS	C21-O22-P23-O25
4	B	605	A1AIS	C21-O22-P23-O26
5	A	505	6OU	C27-O26-P23-O24
5	B	606	6OU	C27-O26-P23-O24
3	A	503	LBN	C2-C1-O1-P1
3	B	604	LBN	C2-C1-O1-P1
2	B	603	P5S	C21-C22-C23-C24
2	A	502	P5S	C21-C22-C23-C24
5	A	505	6OU	C19-C20-O30-C31
5	B	606	6OU	C19-C20-O30-C31
4	A	504	A1AIS	C19-C20-C21-O22
4	B	605	A1AIS	C19-C20-C21-O22
4	A	504	A1AIS	C20-C21-O22-P23
4	B	605	A1AIS	C20-C21-O22-P23
2	B	602	P5S	C30-C31-C32-C33
2	A	501	P5S	C30-C31-C32-C33
3	A	503	LBN	C42-C5-C8-C11
3	B	604	LBN	C42-C5-C8-C11
3	A	507	LBN	C1-C2-O7-C34
3	A	507	LBN	C3-C2-O7-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	601	LBN	C1-C2-O7-C34
3	B	601	LBN	C3-C2-O7-C34
3	A	503	LBN	C20-C22-C23-C24
3	B	604	LBN	C20-C22-C23-C24
3	A	503	LBN	C40-C41-C42-C5
3	B	604	LBN	C40-C41-C42-C5
3	A	507	LBN	C35-C36-C37-C38
3	B	601	LBN	C35-C36-C37-C38
3	A	507	LBN	O5-C25-C26-C27
3	B	601	LBN	O5-C25-C26-C27
3	B	604	LBN	C33-C4-C7-C10
3	A	503	LBN	C33-C4-C7-C10
3	A	507	LBN	C13-C10-C7-C4
3	B	601	LBN	C13-C10-C7-C4
2	A	501	P5S	C24-C25-C26-C27
2	B	602	P5S	C24-C25-C26-C27
4	A	504	A1AIS	C10-C11-C12-C13
4	B	605	A1AIS	C10-C11-C12-C13
2	B	603	P5S	O37-C38-C39-C40
3	B	601	LBN	O6-C25-C26-C27
3	A	507	LBN	O6-C25-C26-C27
2	A	502	P5S	O37-C38-C39-C40
2	B	602	P5S	C44-C45-C46-C48
2	A	501	P5S	C44-C45-C46-C48

There are no ring outliers.

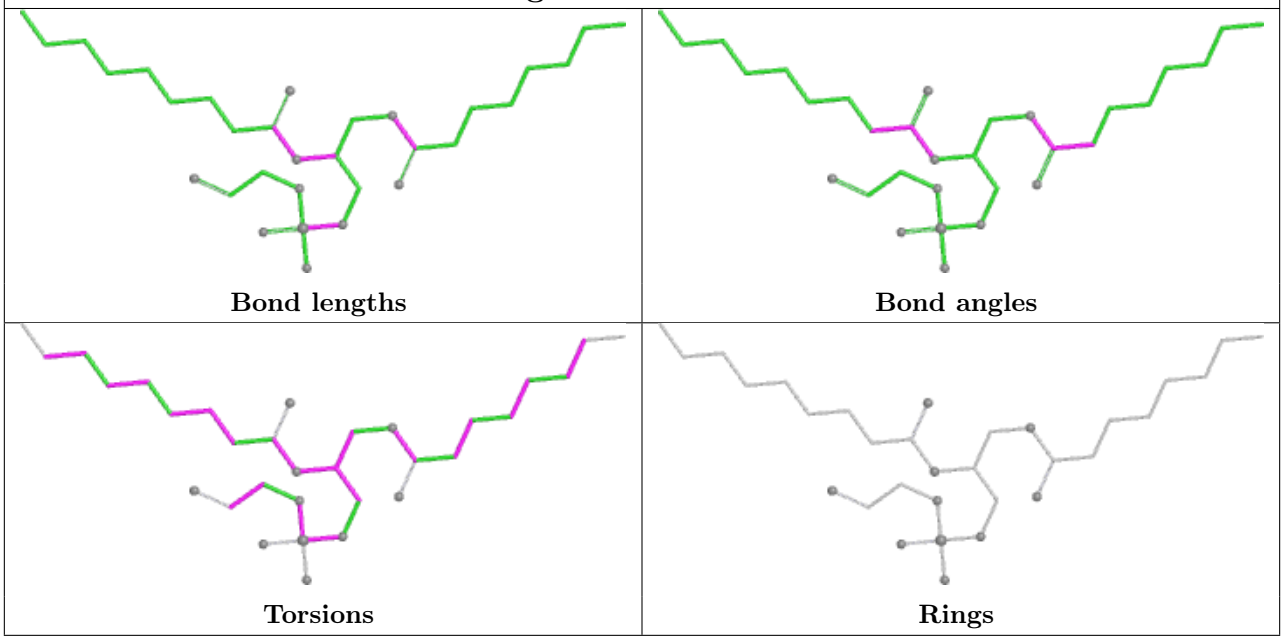
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	P5S	1	0
2	B	602	P5S	1	0
2	A	502	P5S	1	0
2	B	603	P5S	1	0

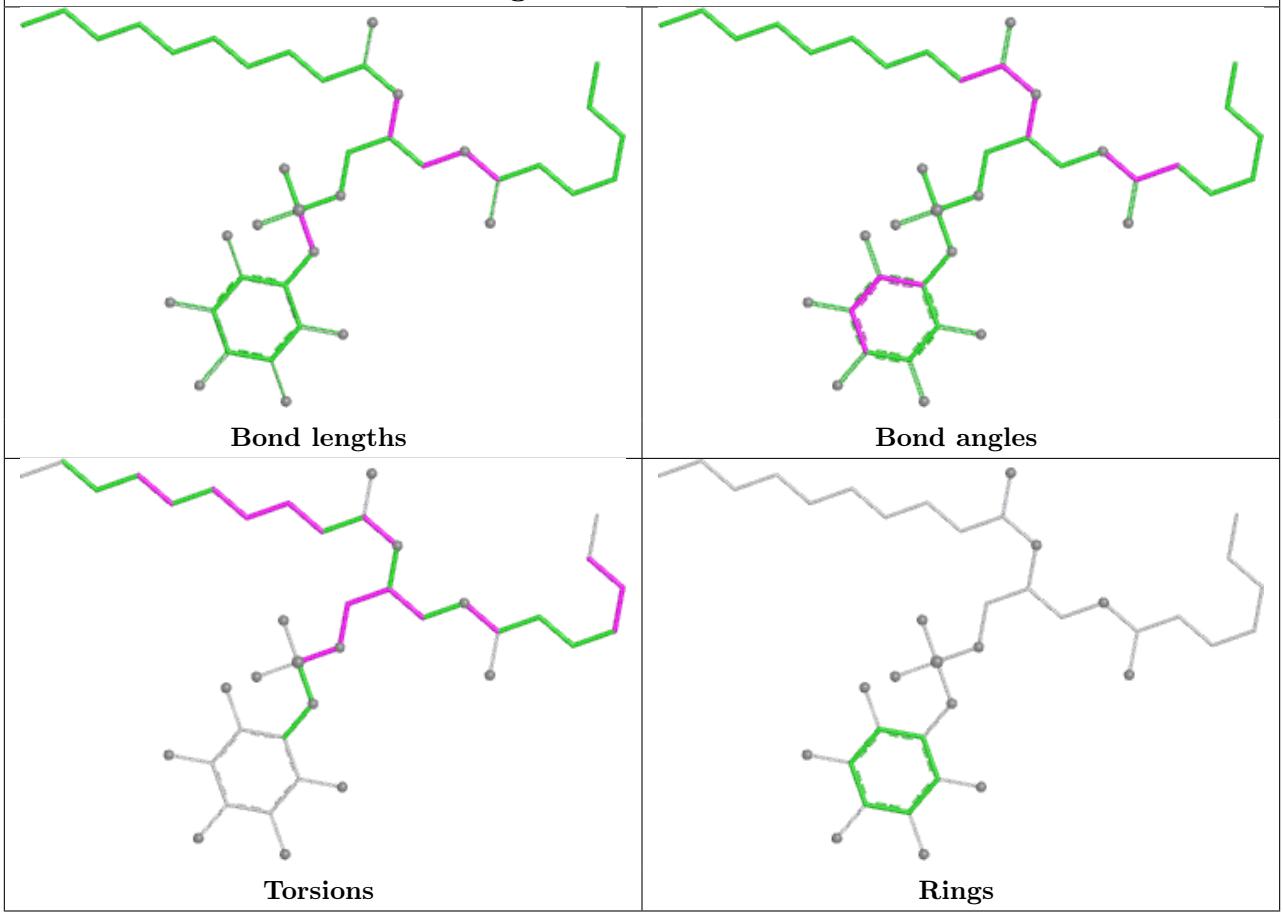
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

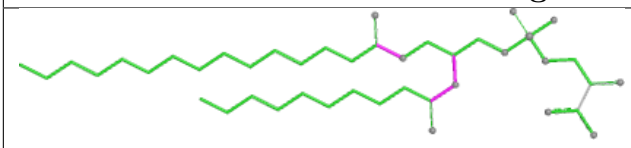
Ligand 6OU B 606



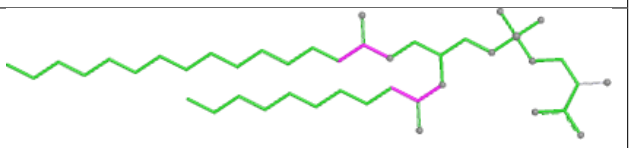
Ligand A1AIS A 504



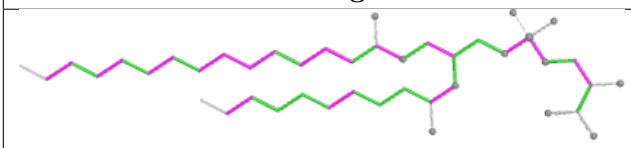
Ligand P5S A 501



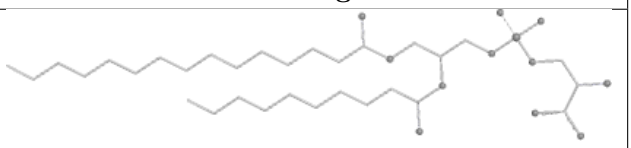
Bond lengths



Bond angles

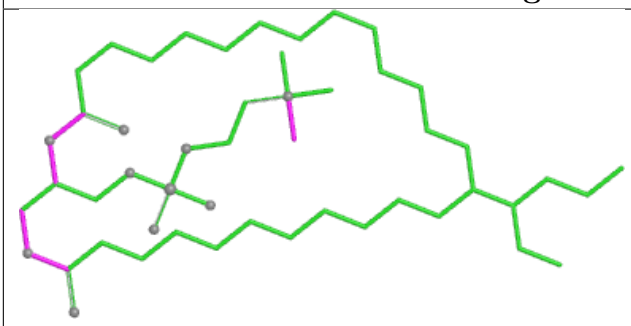


Torsions

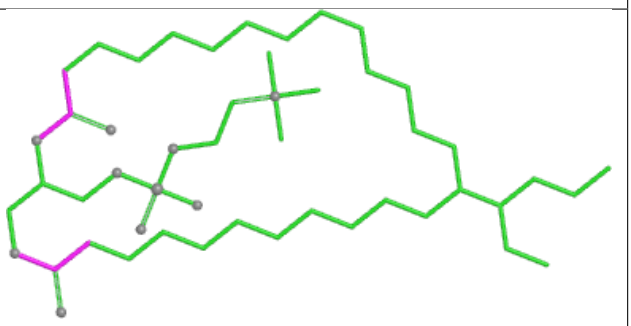


Rings

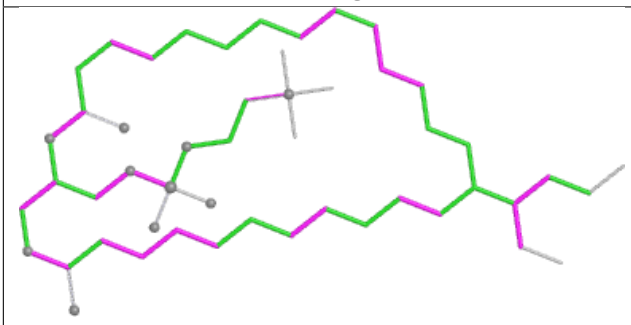
Ligand LBN A 503



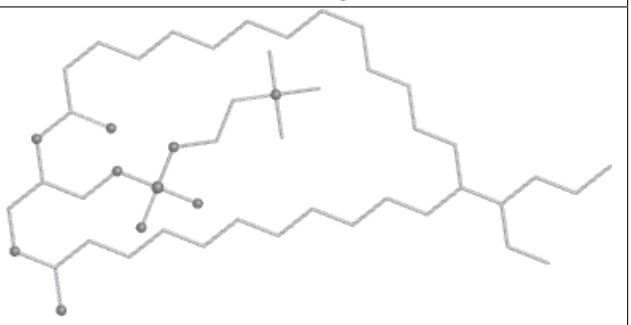
Bond lengths



Bond angles

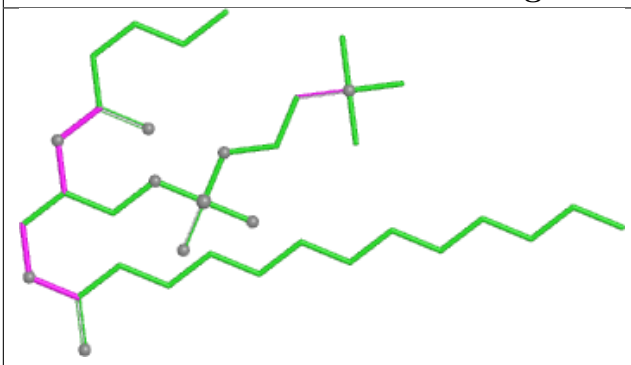


Torsions

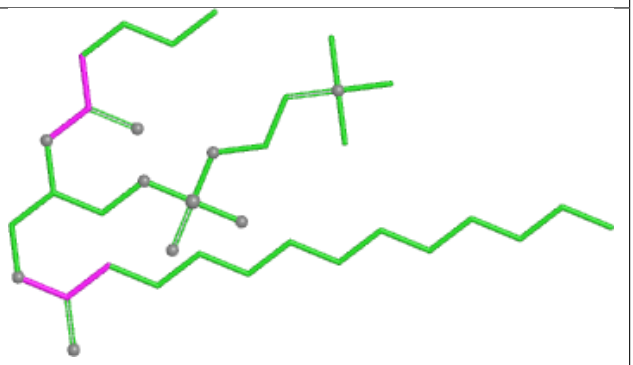


Rings

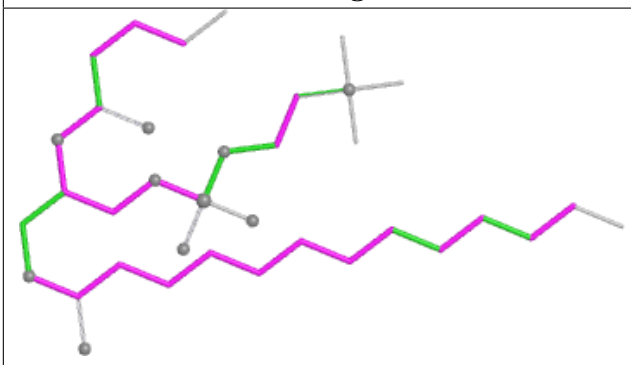
Ligand LBN B 601



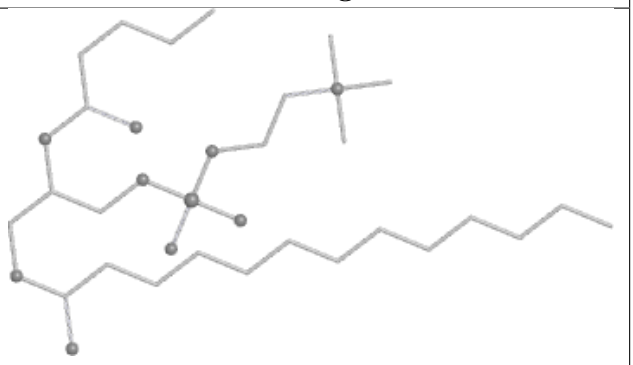
Bond lengths



Bond angles

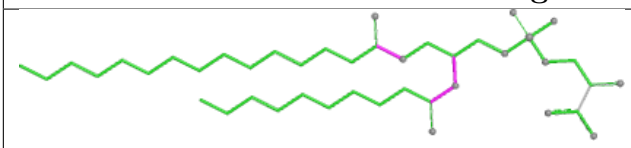


Torsions

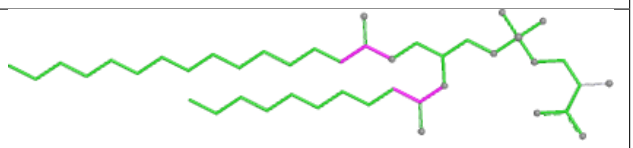


Rings

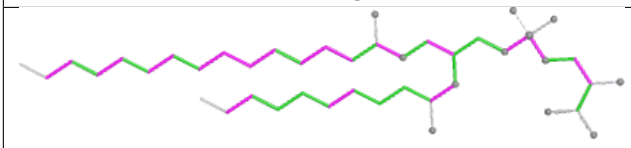
Ligand P5S B 602



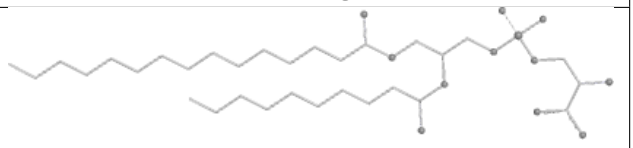
Bond lengths



Bond angles

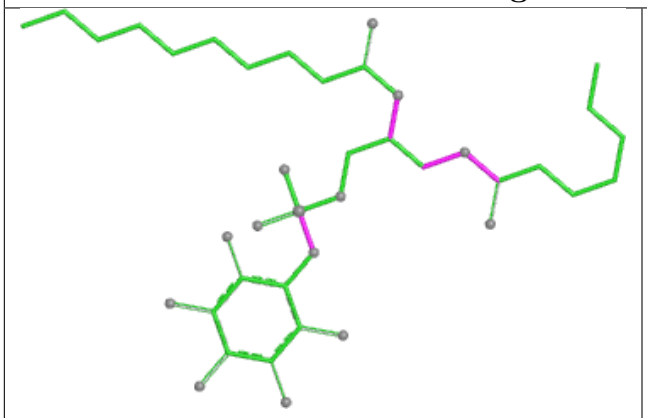


Torsions

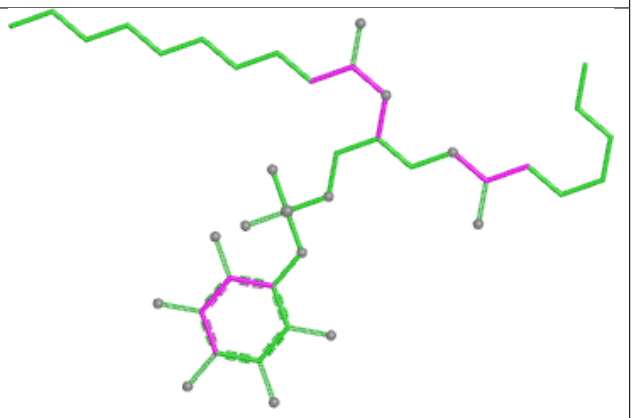


Rings

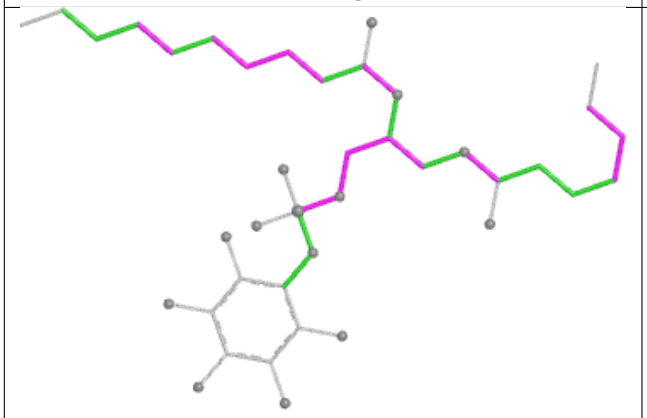
Ligand A1AIS B 605



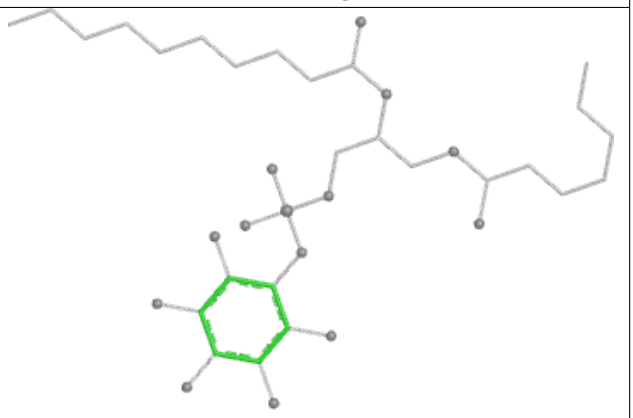
Bond lengths



Bond angles

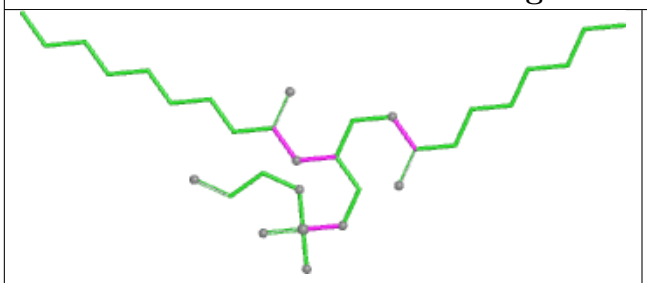


Torsions

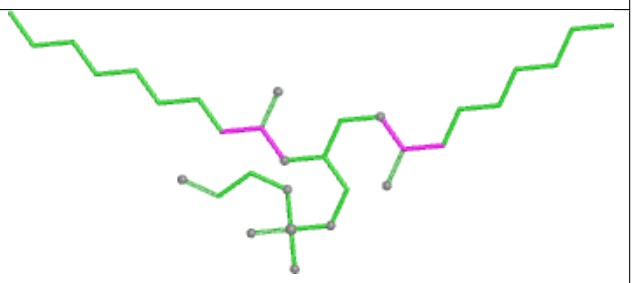


Rings

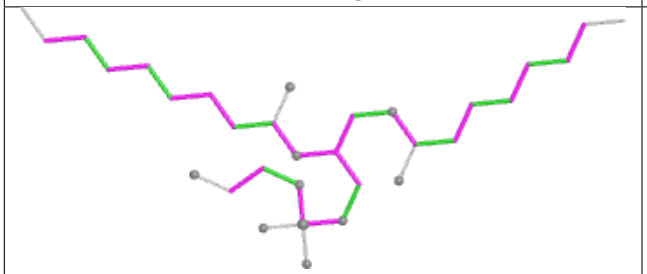
Ligand 6OU A 505



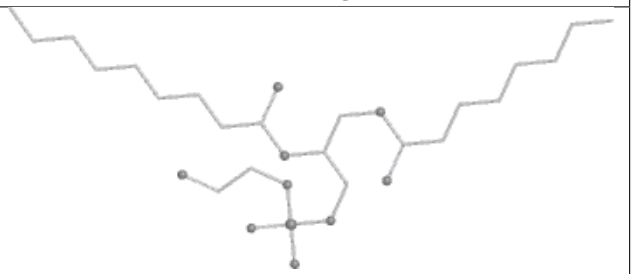
Bond lengths



Bond angles

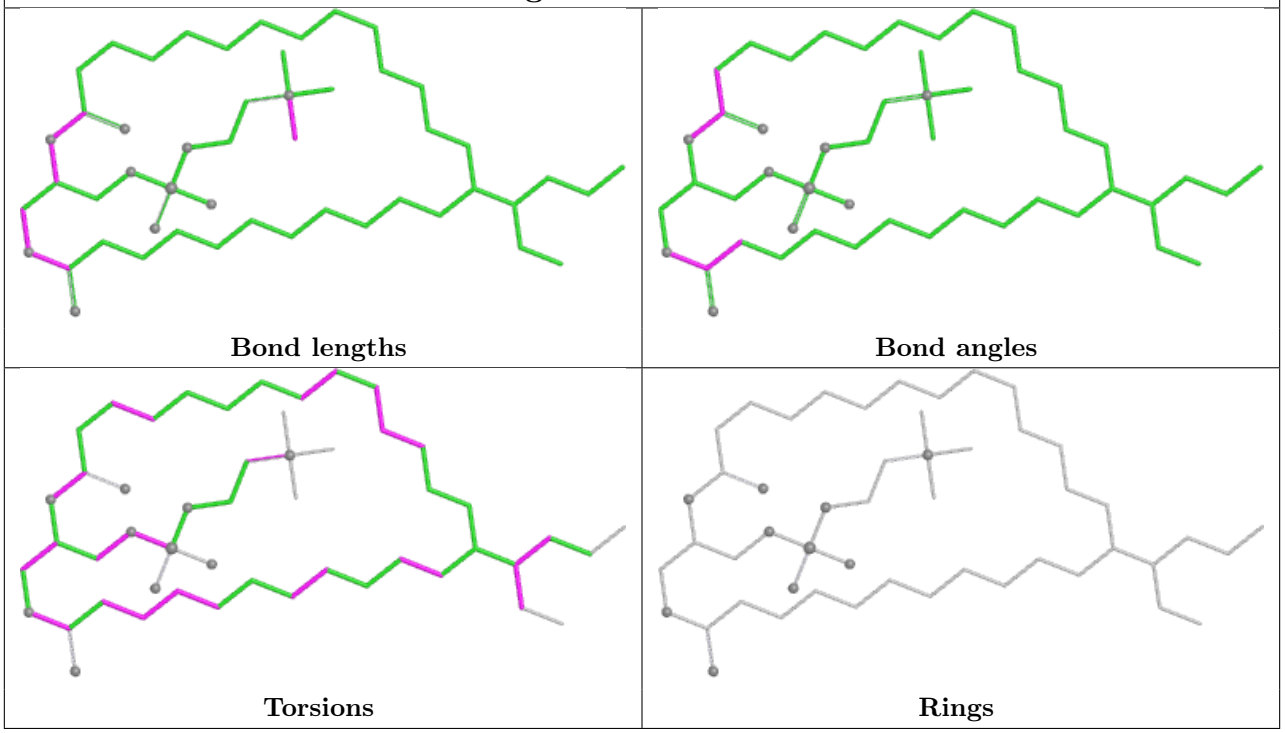


Torsions

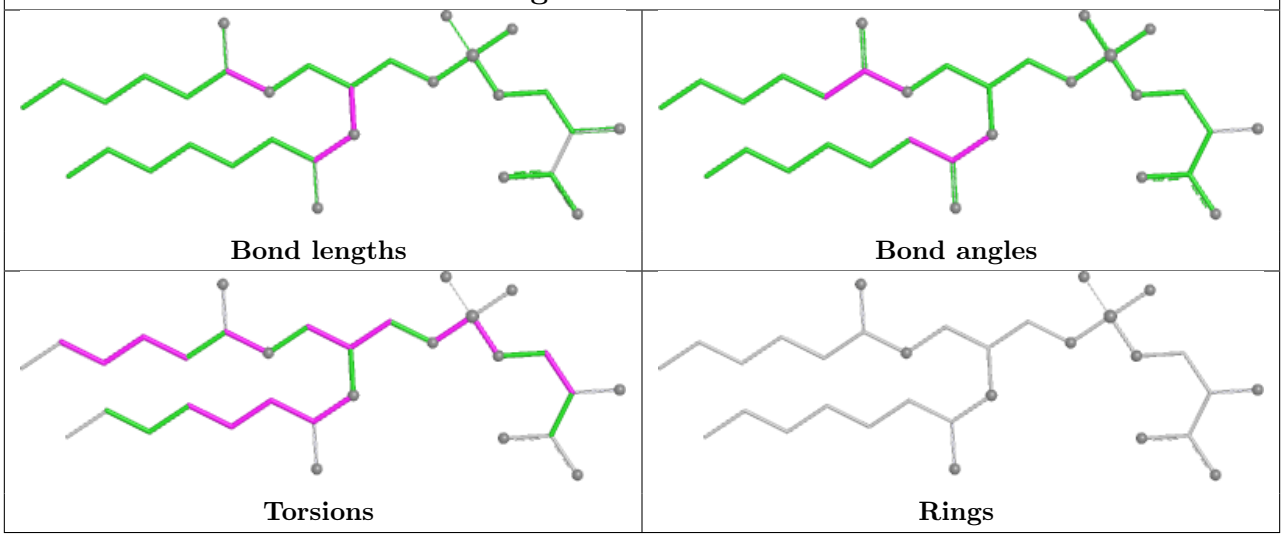


Rings

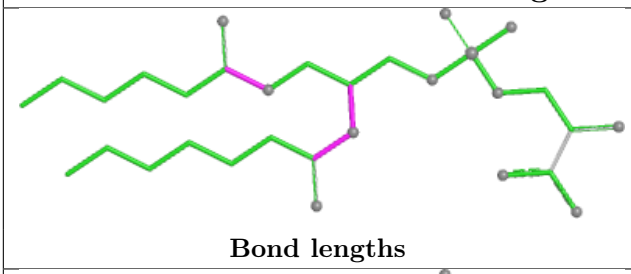
Ligand LBN B 604



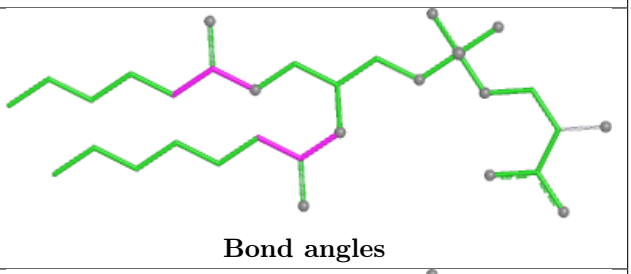
Ligand P5S A 502



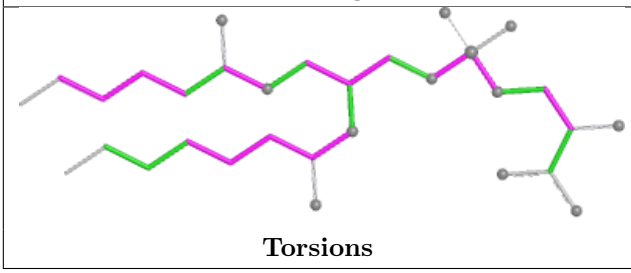
Ligand P5S B 603



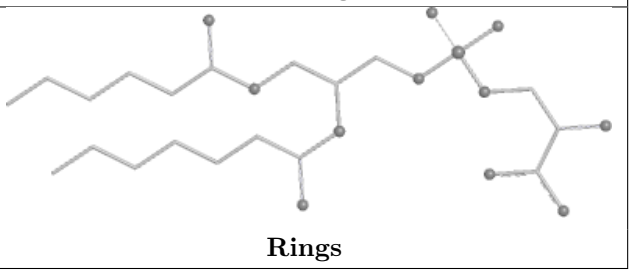
Bond lengths



Bond angles

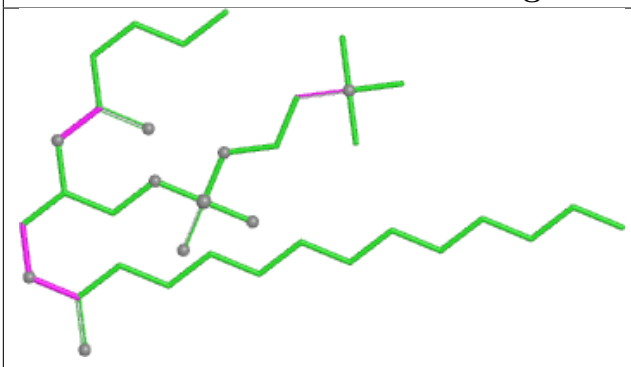


Torsions

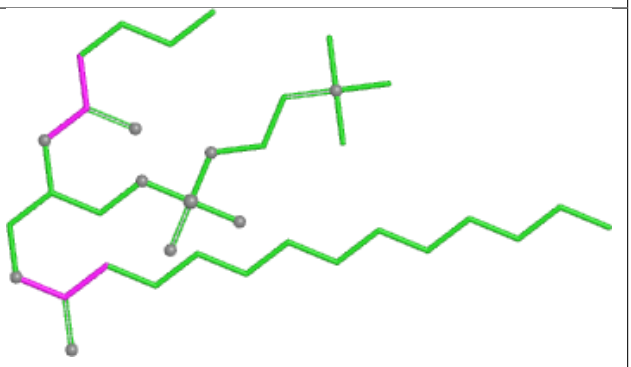


Rings

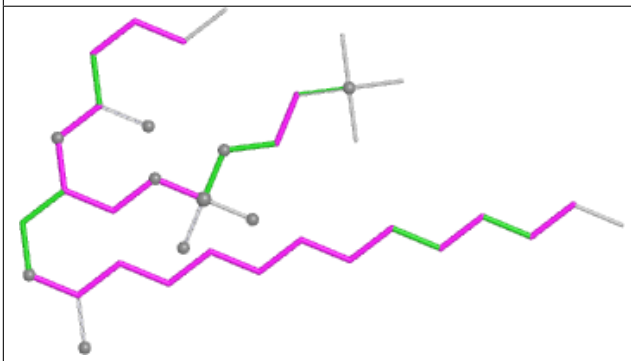
Ligand LBN A 507



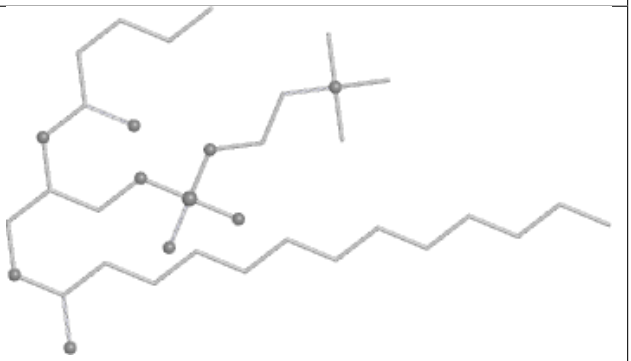
Bond lengths



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.

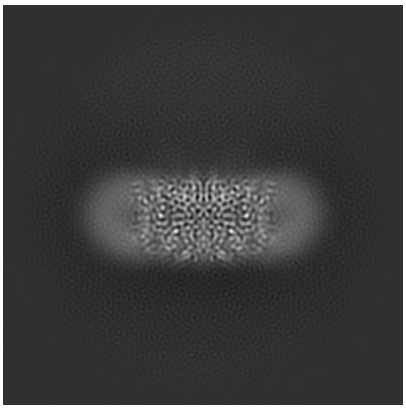
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44178. These allow visual inspection of the internal detail of the map and identification of artifacts.

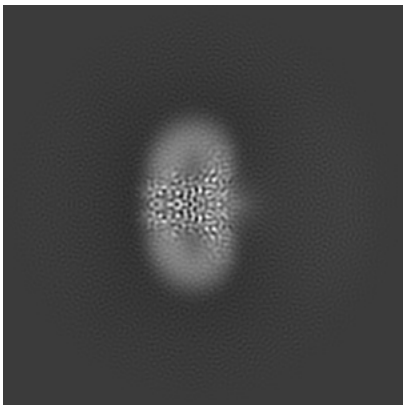
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

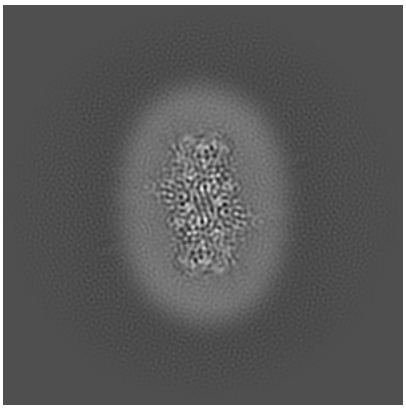
6.1.1 Primary map



X

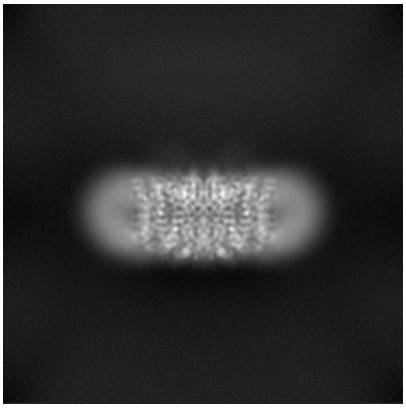


Y

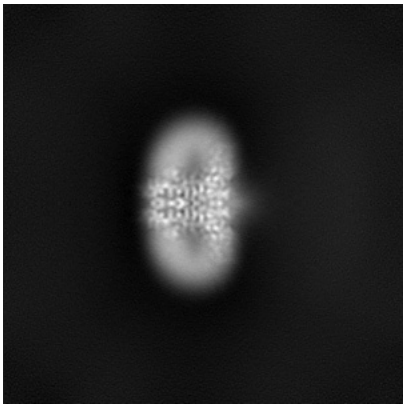


Z

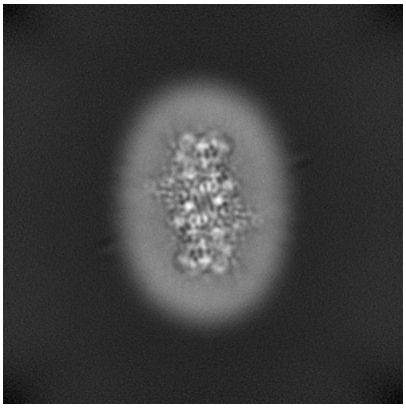
6.1.2 Raw map



X



Y

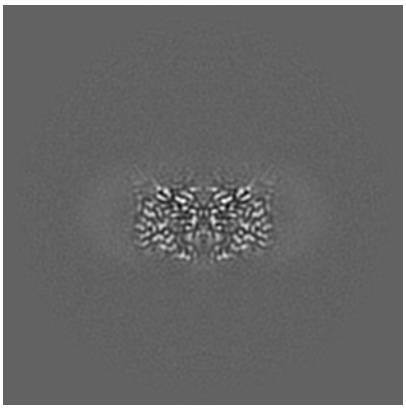


Z

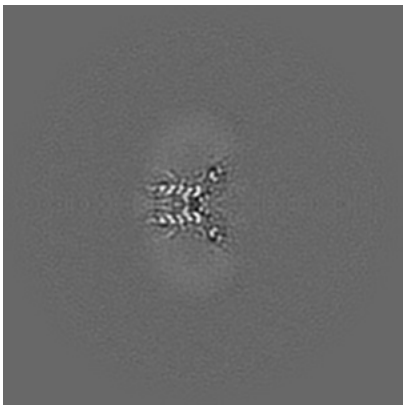
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

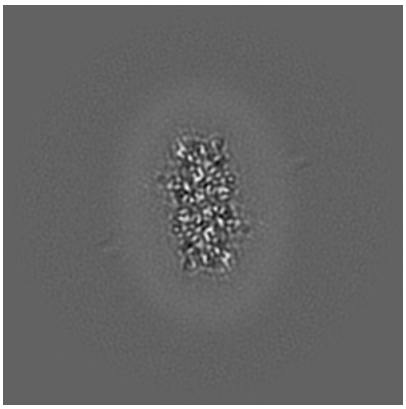
6.2.1 Primary map



X Index: 150

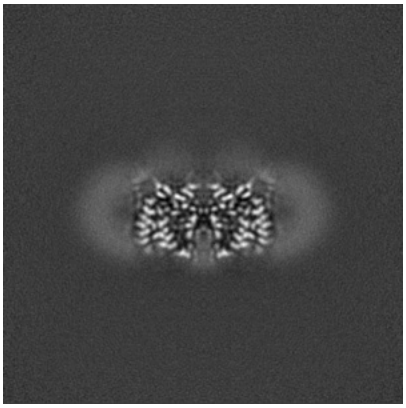


Y Index: 150

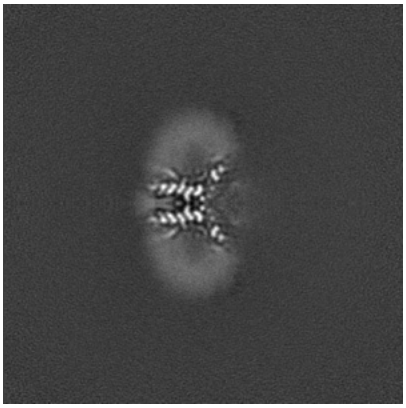


Z Index: 150

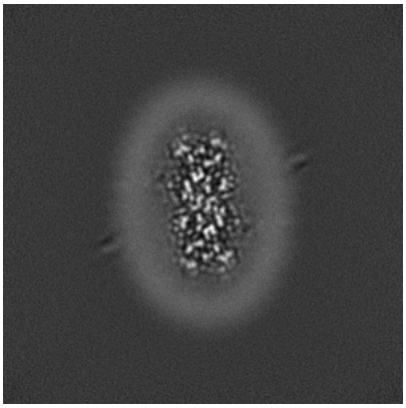
6.2.2 Raw map



X Index: 150



Y Index: 150

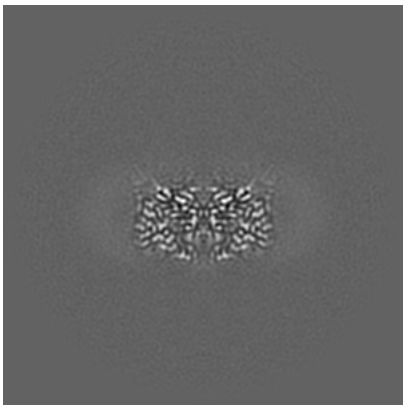


Z Index: 150

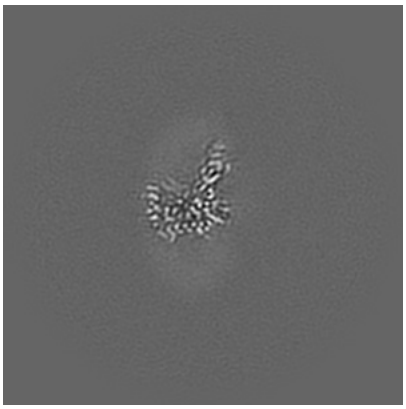
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

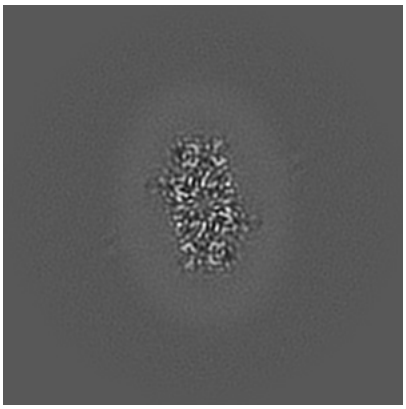
6.3.1 Primary map



X Index: 150

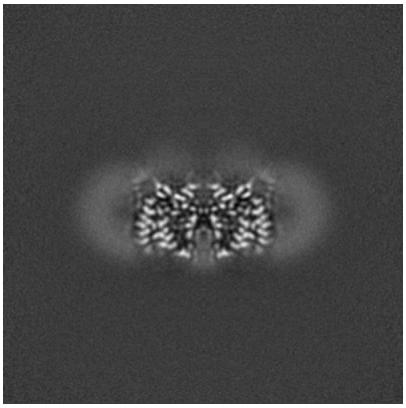


Y Index: 136

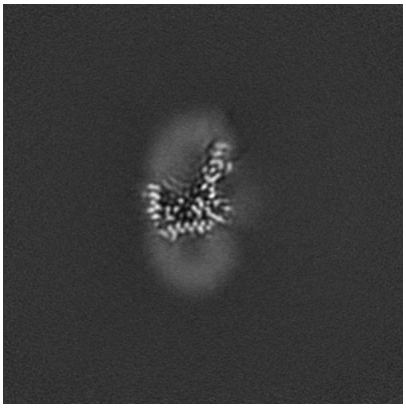


Z Index: 153

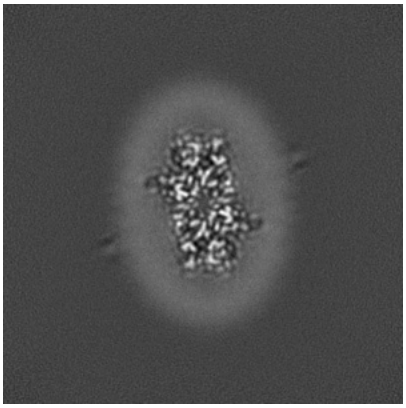
6.3.2 Raw map



X Index: 150



Y Index: 136

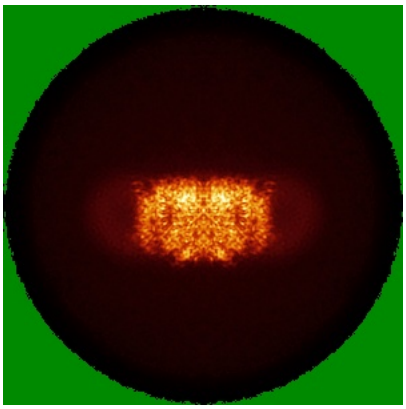


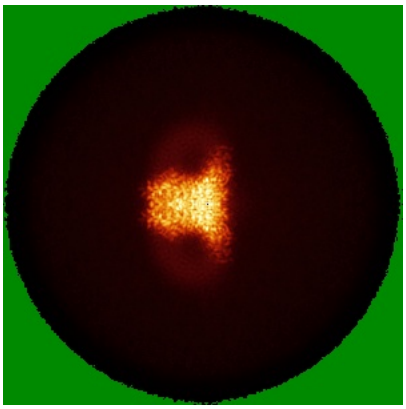
Z Index: 154

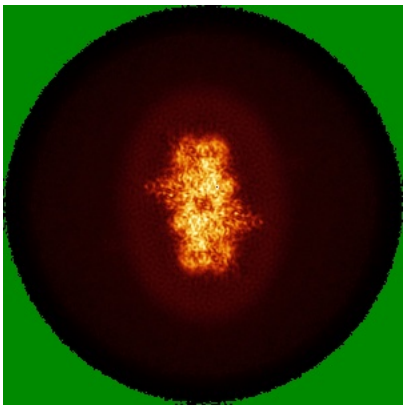
The images above show the largest variance slices of the map in three orthogonal directions.

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

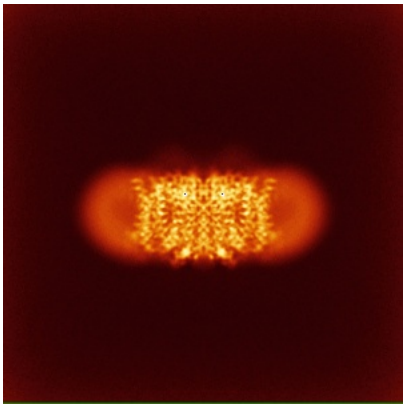
6.4.1 Primary map

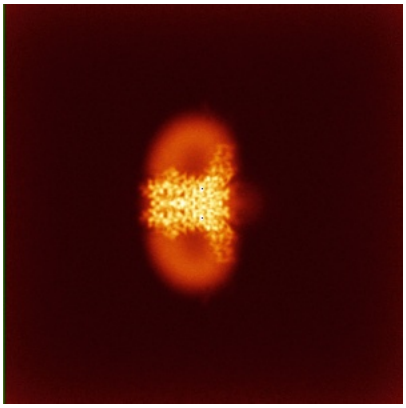

X

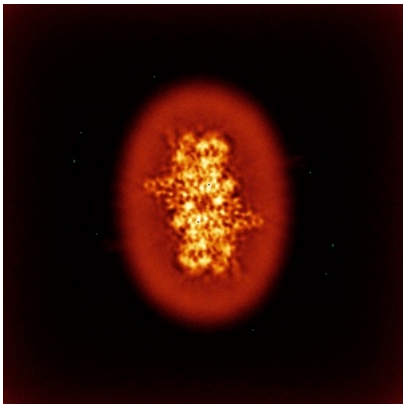

Y


Z

6.4.2 Raw map


X

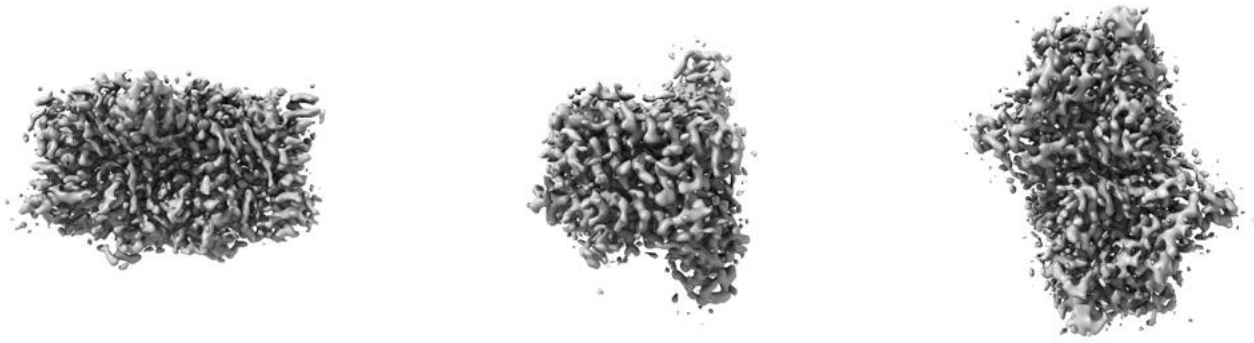

Y


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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.477. 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

X Y Z

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.

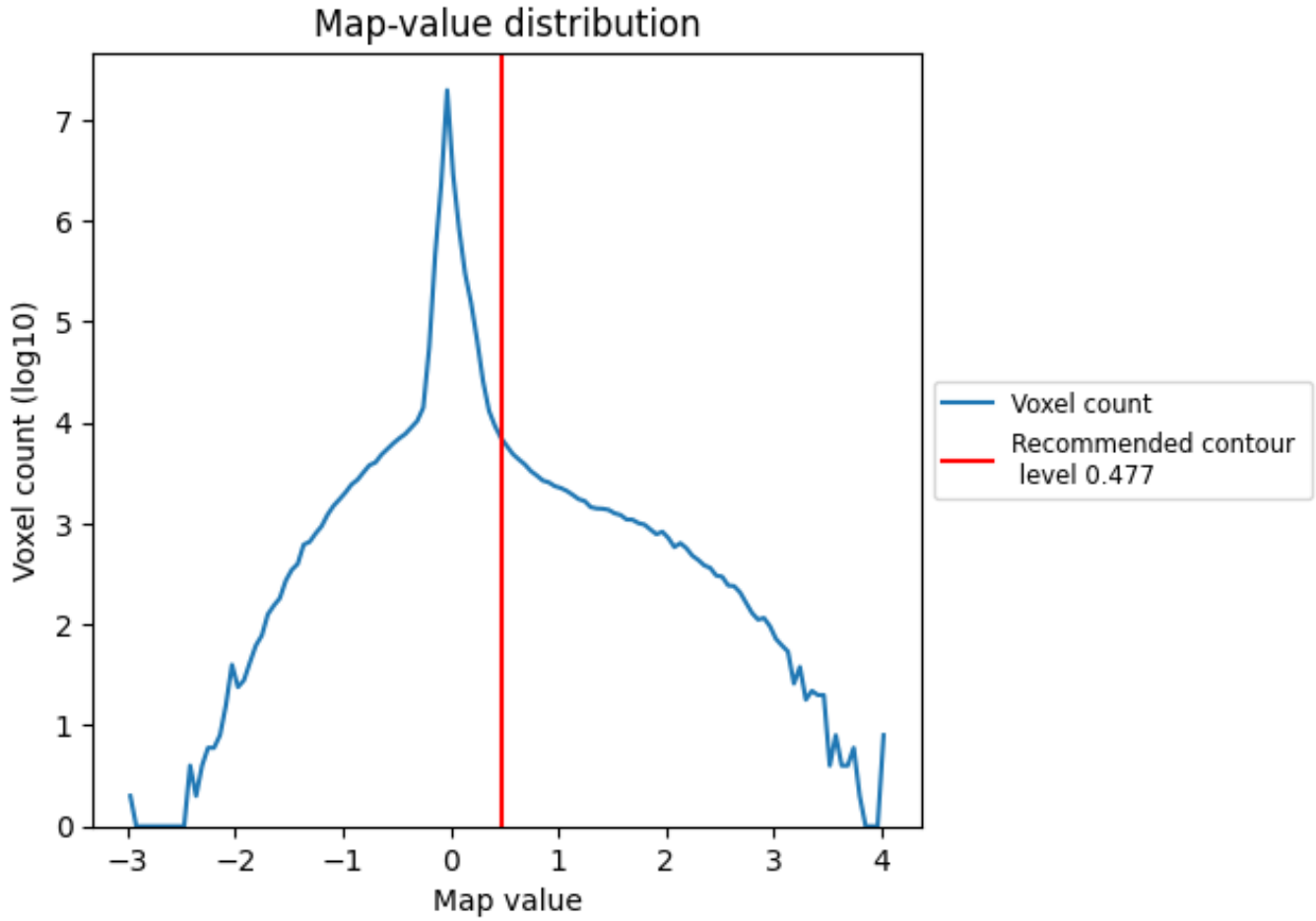
6.6 Mask visualisation (i)

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

7 Map analysis

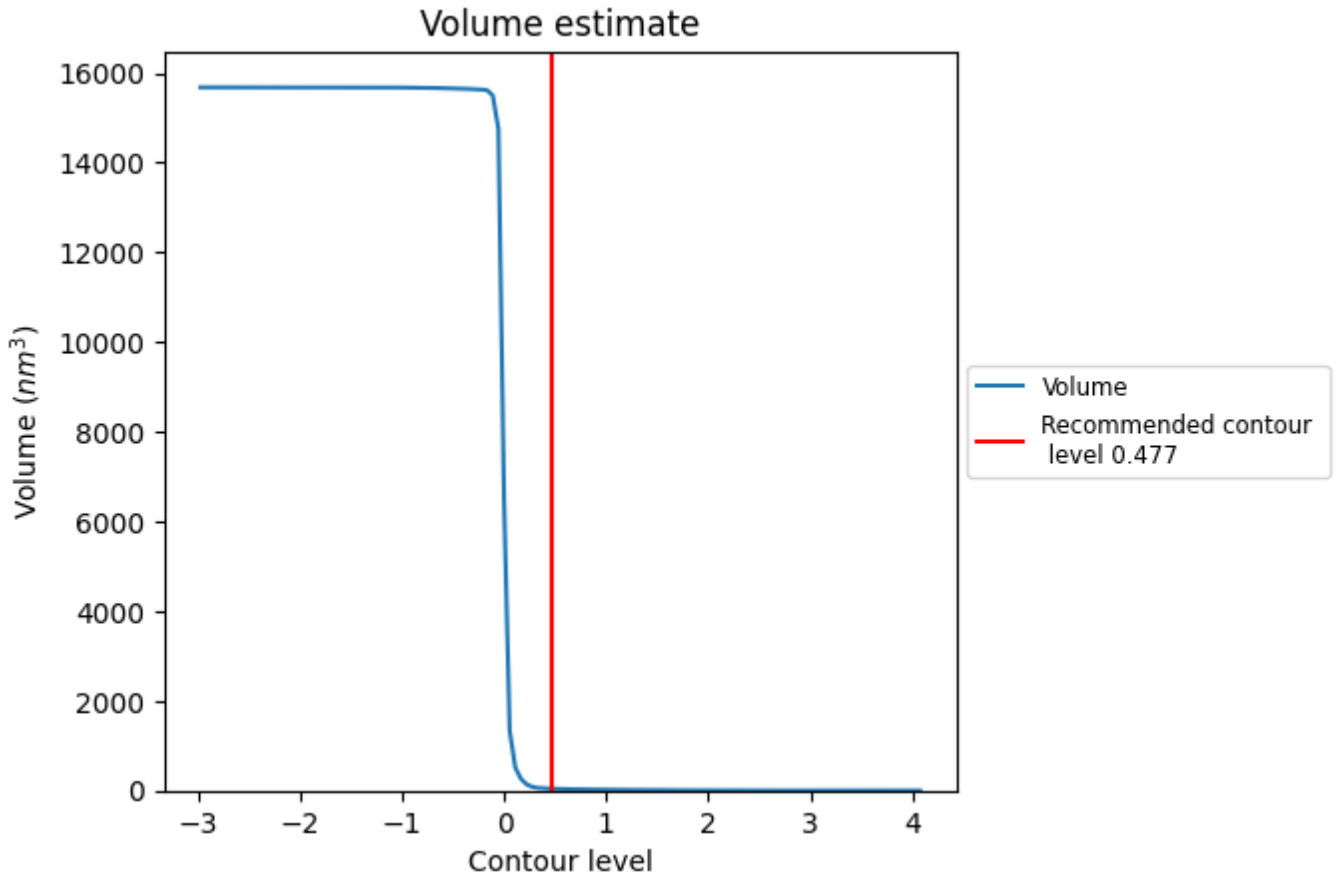
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

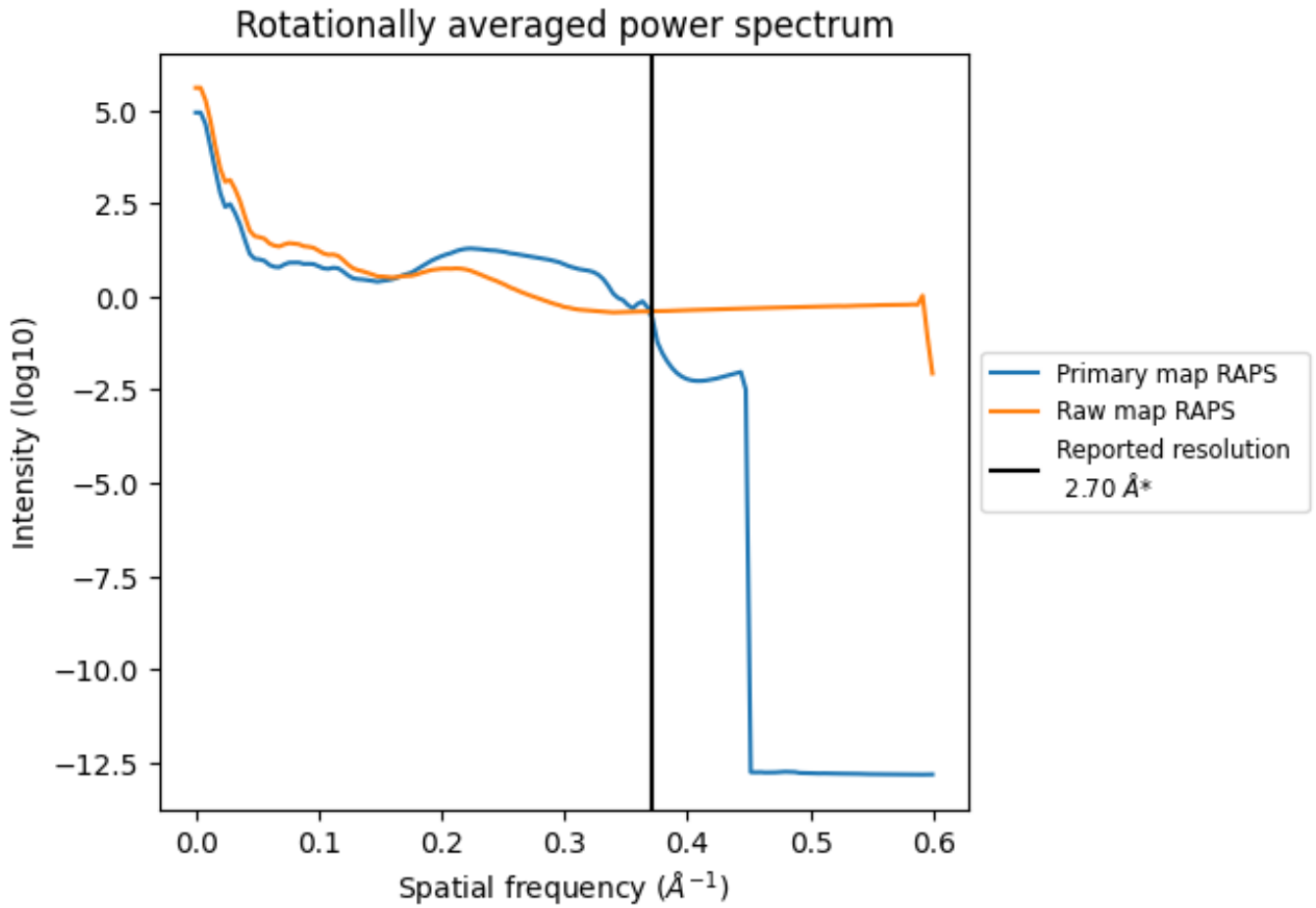
7.2 Volume estimate



The volume at the recommended contour level is 40 nm^3; this corresponds to an approximate mass of 37 kDa.

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

7.3 Rotationally averaged power spectrum (i)

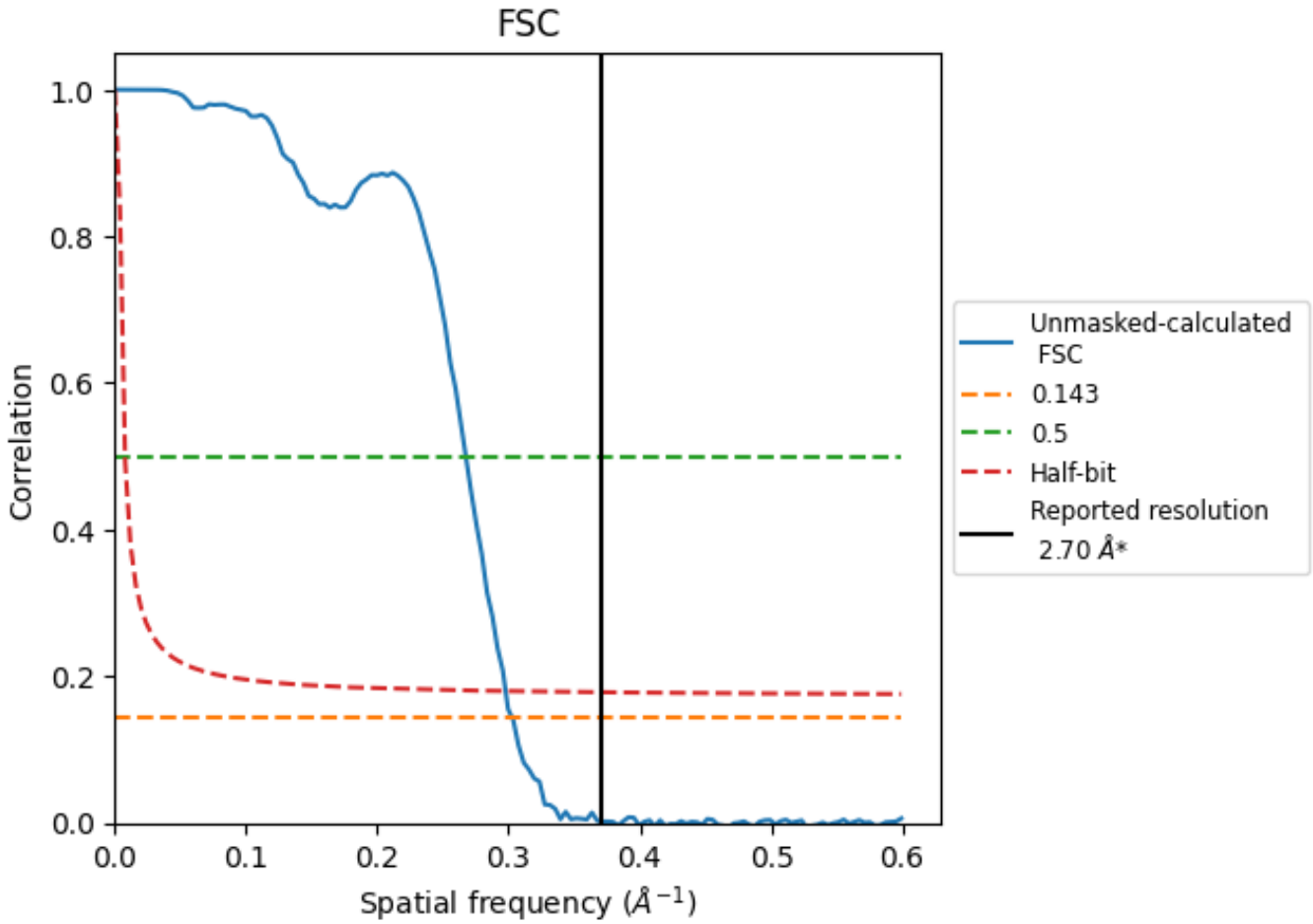


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation

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



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

8.2 Resolution estimates (i)

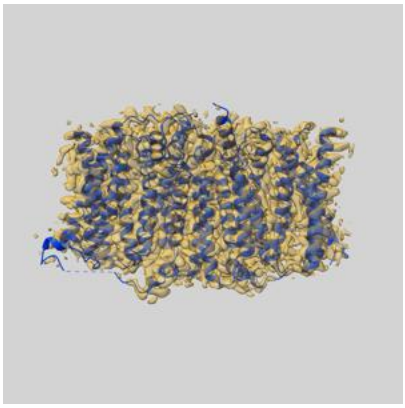
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.30	3.74	3.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.30 differs from the reported value 2.7 by more than 10 %

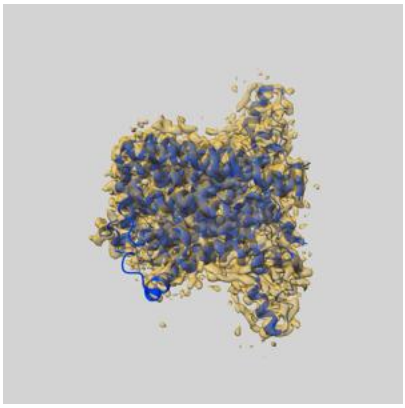
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44178 and PDB model 9B4E. Per-residue inclusion information can be found in section 3 on page 7.

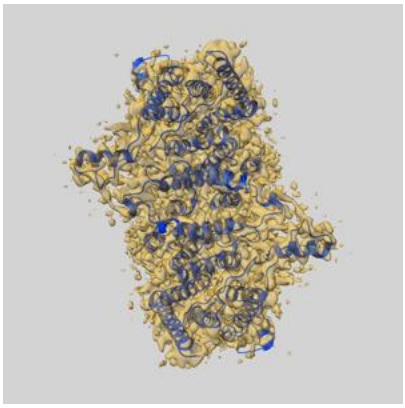
9.1 Map-model overlay



X



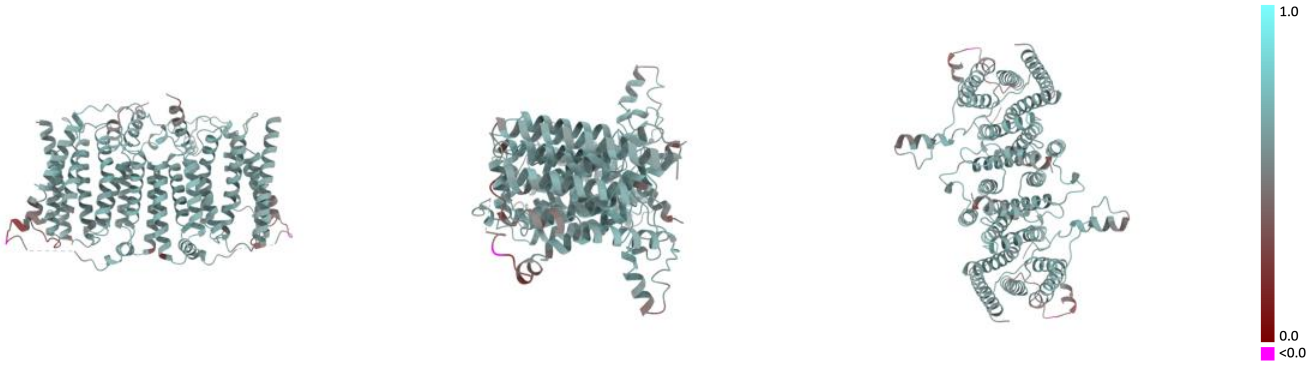
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.477 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

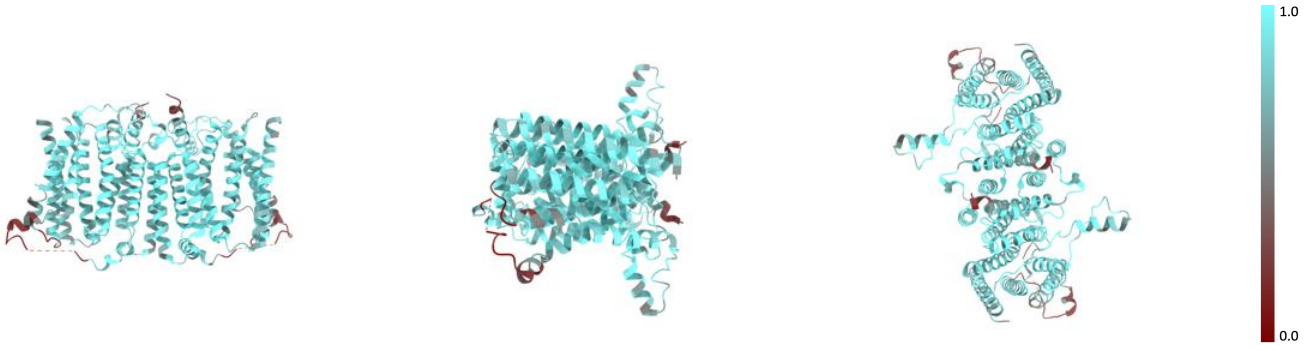
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

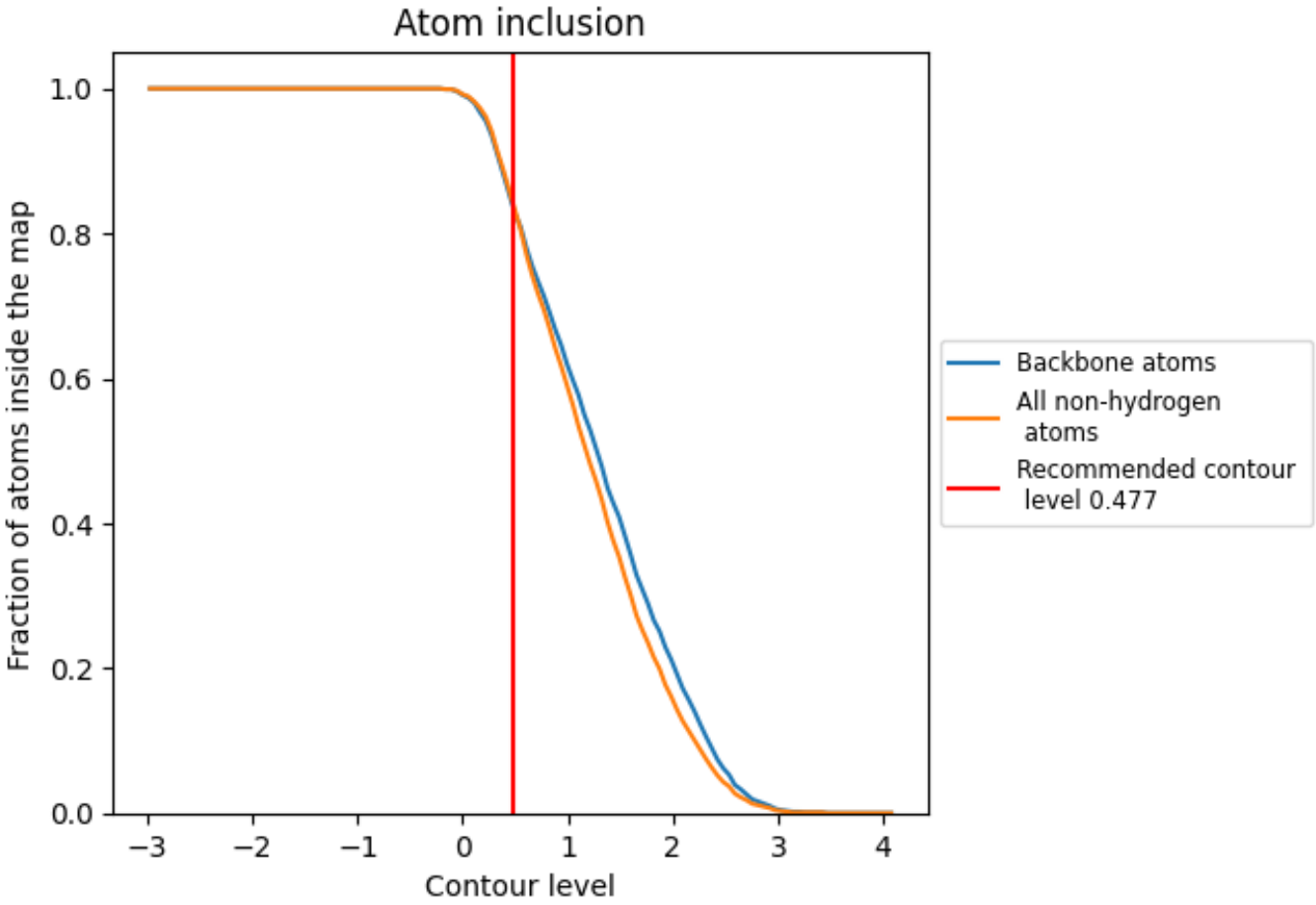
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.477).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.477) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8420	0.5900
A	0.8430	0.5900
B	0.8460	0.5890