Full wwPDB EM Validation Report ⓘ

Feb 3, 2024 – 12:54 PM EST

PDB ID	:	8T57
EMDB ID	:	EMD-41044
Title	:	Structure of mechanically activated ion channel OSCA2.3 in peptidiscs
Authors	:	Jojoa-Cruz, S.; Burendei, B.; Lee, W.H.; Ward, A.B.
Deposited on	:	2023-06-12
Resolution	:	2.70 Å(reported)
Based on initial model	:	.

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:

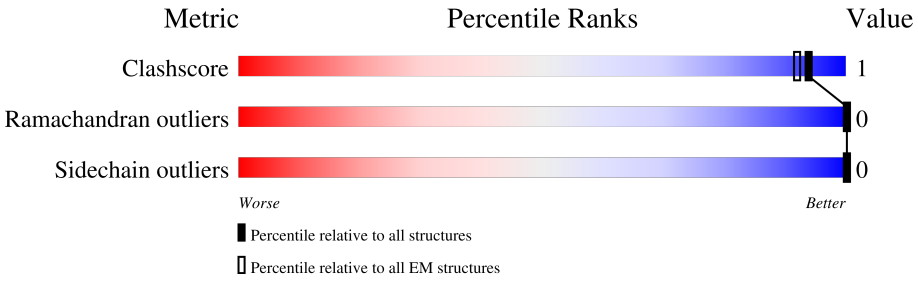
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	713	65% 5% 29%
1	B	713	65% 5% 29%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8466 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.

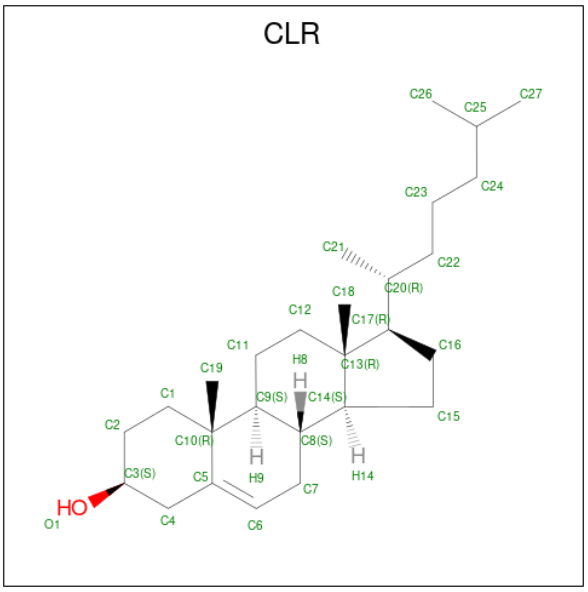
- Molecule 1 is a protein called CSC1-like protein HYP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	504	Total	C	N	O	S	0	0
			4033	2694	635	691	13		
1	B	504	Total	C	N	O	S	0	0
			4033	2694	635	691	13		

There are 20 discrepancies between the modelled and reference sequences:

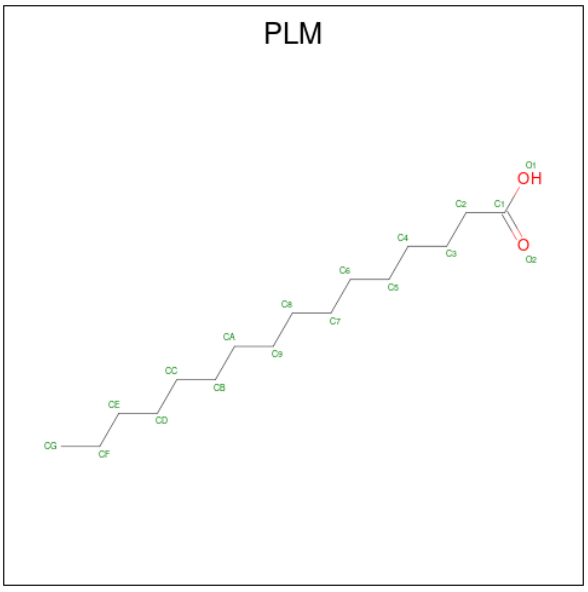
Chain	Residue	Modelled	Actual	Comment	Reference
A	704	GLY	-	expression tag	UNP Q8GUH7
A	705	THR	-	expression tag	UNP Q8GUH7
A	706	GLY	-	expression tag	UNP Q8GUH7
A	707	THR	-	expression tag	UNP Q8GUH7
A	708	LEU	-	expression tag	UNP Q8GUH7
A	709	GLU	-	expression tag	UNP Q8GUH7
A	710	VAL	-	expression tag	UNP Q8GUH7
A	711	LEU	-	expression tag	UNP Q8GUH7
A	712	PHE	-	expression tag	UNP Q8GUH7
A	713	GLN	-	expression tag	UNP Q8GUH7
B	704	GLY	-	expression tag	UNP Q8GUH7
B	705	THR	-	expression tag	UNP Q8GUH7
B	706	GLY	-	expression tag	UNP Q8GUH7
B	707	THR	-	expression tag	UNP Q8GUH7
B	708	LEU	-	expression tag	UNP Q8GUH7
B	709	GLU	-	expression tag	UNP Q8GUH7
B	710	VAL	-	expression tag	UNP Q8GUH7
B	711	LEU	-	expression tag	UNP Q8GUH7
B	712	PHE	-	expression tag	UNP Q8GUH7
B	713	GLN	-	expression tag	UNP Q8GUH7

- Molecule 2 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



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

- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



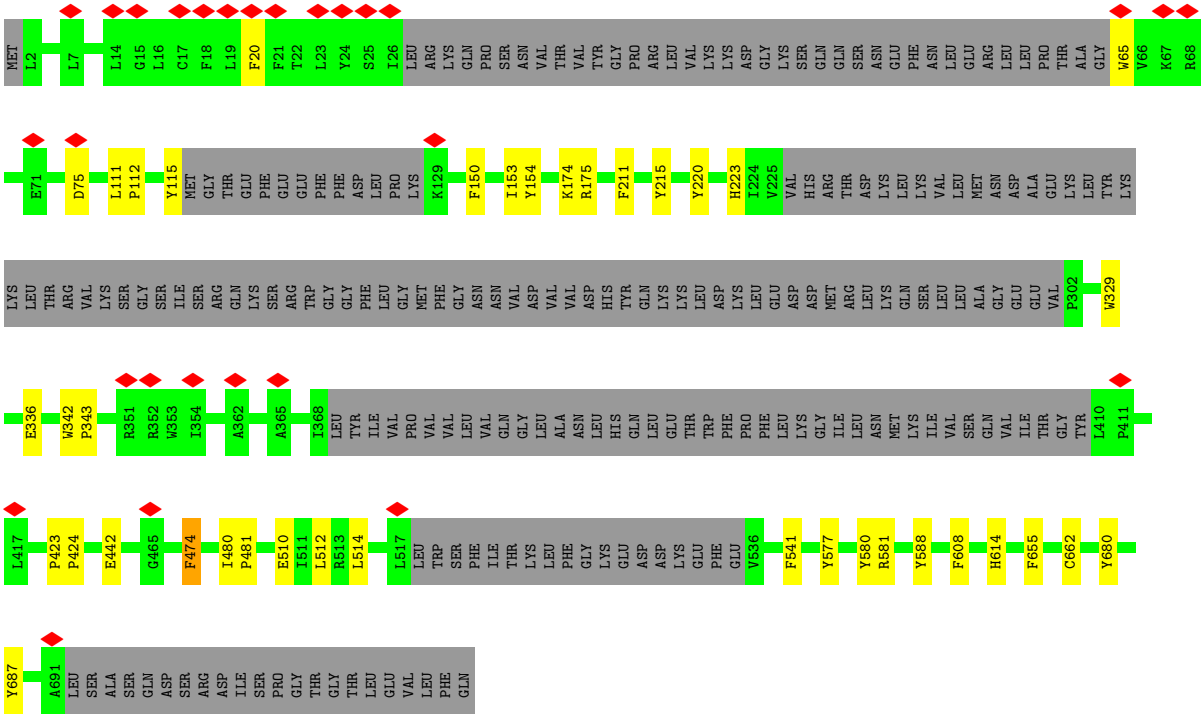
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total 18	C 16	O 2	0
3	A	1	Total 18	C 16	O 2	0
3	A	1	Total 18	C 16	O 2	0
3	A	1	Total 18	C 16	O 2	0
3	A	1	Total 18	C 16	O 2	0
3	A	1	Total 18	C 16	O 2	0
3	A	1	Total 18	C 16	O 2	0
3	A	1	Total 18	C 16	O 2	0
3	B	1	Total 18	C 16	O 2	0
3	B	1	Total 18	C 16	O 2	0
3	B	1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

3 Residue-property plots (i)

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

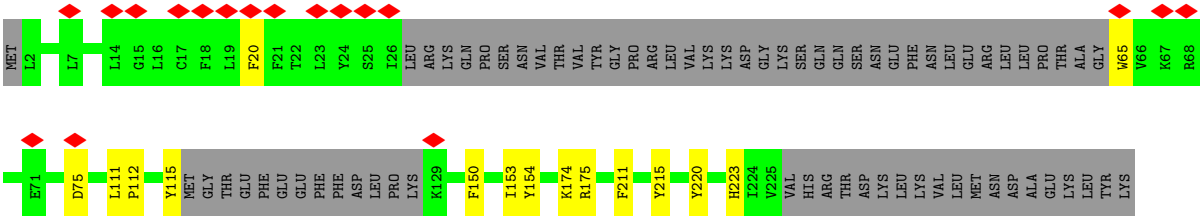
- Molecule 1: CSC1-like protein HYP1

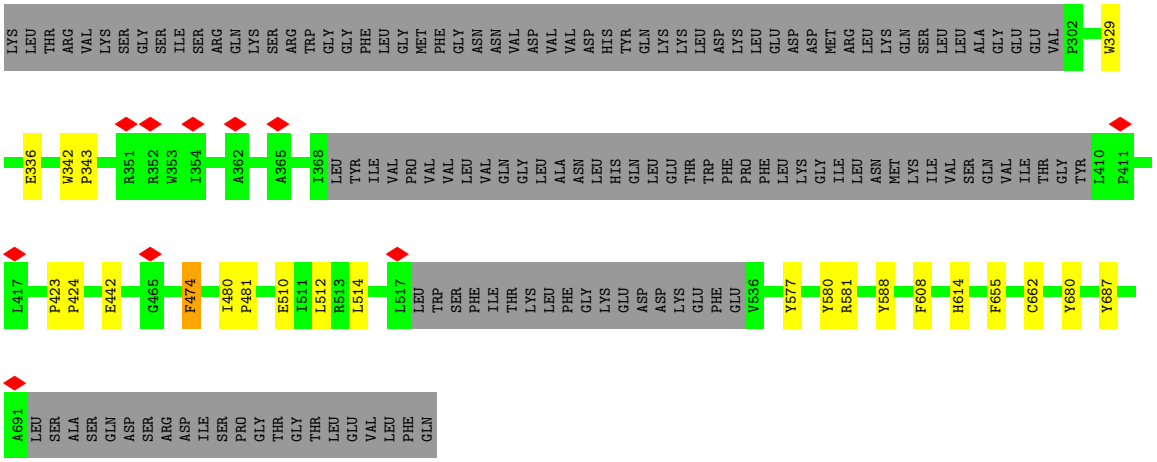
Chain A:



- Molecule 1: CSC1-like protein HYP1

Chain B:




LYS LEU THR ARG VAL LYS SER GLY SER ILE SER ARG GLN LYS SER ARG TRP GLY GLY PHE LEU GLY MET PHE GLY ASN ASN VAL ASP VAL VAL ASP HIS TYR GLN LYS LYS LEU ASP LYS LEU GLU ASP ASP MET ARG LEU LYS GLN SER LEU LEU ALA GLY GLU GLU VAL
P302
W329
E336
W342
P343
R351
R352
W353
I364
A362
A365
I368
LEU TYR ILE VAL PRO VAL VAL LEU VAL GLN GLY LEU ALA ASN ASN LEU HIS GLN LEU GLU GLU THR TRP PHE PRO PHE LEU LYS GLY ILE LEU ASN MET LYS ILE VAL SER GLN VAL ILE THR GLY TYR
L410
P411
L417
P423
P424
E442
G465
F474
I480
P481
E510
Y511
L512
R513
L514
L517
LEU TRP SER PHE ILE THR LYS LEU PHE GLY LYS GLU ASP ASP LYS GLU PHE GLU
V536
Y577
Y580
R581
Y588
F608
H614
F655
C662
Y680
Y687
A691
LEU SER ALA SER GLN ASP SER ARG ASP ILE SER PRO GLY THR GLY THR LEU GLU VAL LEU PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	180640	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.162	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0184	Depositor
Map size (Å)	206.0, 206.0, 206.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.35	31/4148 (0.7%)	0.90	11/5658 (0.2%)
1	B	1.35	31/4148 (0.7%)	0.90	11/5658 (0.2%)
All	All	1.35	62/8296 (0.7%)	0.90	22/11316 (0.2%)

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	510	GLU	CG-CD	-9.09	1.38	1.51
1	B	510	GLU	CG-CD	-9.08	1.38	1.51
1	B	154	TYR	CG-CD1	-8.37	1.28	1.39
1	A	154	TYR	CG-CD1	-8.37	1.28	1.39
1	A	154	TYR	CD1-CE1	-8.17	1.27	1.39
1	B	154	TYR	CD1-CE1	-8.17	1.27	1.39
1	A	662	CYS	CB-SG	-7.81	1.69	1.82
1	B	662	CYS	CB-SG	-7.81	1.69	1.82
1	A	115	TYR	CG-CD1	7.65	1.49	1.39
1	B	115	TYR	CG-CD1	7.60	1.49	1.39
1	A	65	TRP	CD2-CE3	6.98	1.50	1.40
1	B	65	TRP	CD2-CE3	6.94	1.50	1.40
1	B	115	TYR	CE1-CZ	6.83	1.47	1.38
1	A	115	TYR	CE1-CZ	6.82	1.47	1.38
1	A	115	TYR	CE2-CZ	6.74	1.47	1.38
1	B	115	TYR	CE2-CZ	6.69	1.47	1.38
1	A	115	TYR	CG-CD2	6.64	1.47	1.39
1	B	115	TYR	CG-CD2	6.64	1.47	1.39
1	B	65	TRP	CZ2-CH2	6.48	1.49	1.37
1	A	65	TRP	CZ2-CH2	6.47	1.49	1.37
1	B	211	PHE	CB-CG	-6.26	1.40	1.51
1	A	211	PHE	CB-CG	-6.22	1.40	1.51
1	B	510	GLU	CD-OE2	-6.22	1.18	1.25
1	A	510	GLU	CD-OE2	-6.18	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	TRP	CB-CG	-6.09	1.39	1.50
1	B	329	TRP	CB-CG	-6.08	1.39	1.50
1	A	329	TRP	CZ3-CH2	-5.84	1.30	1.40
1	B	329	TRP	CZ3-CH2	-5.81	1.30	1.40
1	B	510	GLU	CD-OE1	-5.74	1.19	1.25
1	A	510	GLU	CD-OE1	-5.73	1.19	1.25
1	B	336	GLU	CG-CD	-5.67	1.43	1.51
1	A	336	GLU	CG-CD	-5.66	1.43	1.51
1	B	336	GLU	CD-OE2	-5.66	1.19	1.25
1	A	336	GLU	CD-OE2	-5.64	1.19	1.25
1	A	223	HIS	CB-CG	-5.49	1.40	1.50
1	B	223	HIS	CB-CG	-5.45	1.40	1.50
1	A	215	TYR	CG-CD2	-5.45	1.32	1.39
1	B	215	TYR	CG-CD2	-5.42	1.32	1.39
1	B	65	TRP	CE3-CZ3	5.38	1.47	1.38
1	A	687	TYR	CB-CG	-5.38	1.43	1.51
1	B	687	TYR	CB-CG	-5.36	1.43	1.51
1	A	474	PHE	CB-CG	-5.36	1.42	1.51
1	B	474	PHE	CB-CG	-5.36	1.42	1.51
1	A	65	TRP	CE3-CZ3	5.35	1.47	1.38
1	B	580	TYR	CB-CG	-5.33	1.43	1.51
1	A	580	TYR	CB-CG	-5.32	1.43	1.51
1	A	614	HIS	CB-CG	-5.30	1.40	1.50
1	B	614	HIS	CB-CG	-5.28	1.40	1.50
1	B	577	TYR	CE2-CZ	-5.25	1.31	1.38
1	B	329	TRP	CD2-CE2	-5.23	1.35	1.41
1	A	577	TYR	CE2-CZ	-5.22	1.31	1.38
1	A	329	TRP	CD2-CE2	-5.20	1.35	1.41
1	A	336	GLU	CB-CG	-5.13	1.42	1.52
1	B	336	GLU	CB-CG	-5.13	1.42	1.52
1	B	655	PHE	CB-CG	-5.13	1.42	1.51
1	A	655	PHE	CB-CG	-5.12	1.42	1.51
1	A	154	TYR	CE1-CZ	-5.05	1.31	1.38
1	B	154	TYR	CE1-CZ	-5.05	1.31	1.38
1	B	442	GLU	CD-OE1	-5.02	1.20	1.25
1	B	588	TYR	CD2-CE2	-5.02	1.31	1.39
1	A	442	GLU	CD-OE1	-5.01	1.20	1.25
1	A	541	PHE	CB-CG	-5.01	1.42	1.51

All (22) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	581	ARG	NE-CZ-NH2	-11.58	114.51	120.30
1	A	581	ARG	NE-CZ-NH2	-11.57	114.51	120.30
1	A	175	ARG	NE-CZ-NH2	-9.99	115.30	120.30
1	B	175	ARG	NE-CZ-NH2	-9.99	115.31	120.30
1	A	154	TYR	CB-CG-CD1	-9.55	115.27	121.00
1	B	154	TYR	CB-CG-CD1	-9.52	115.29	121.00
1	A	577	TYR	CB-CG-CD2	-7.32	116.61	121.00
1	B	577	TYR	CB-CG-CD2	-7.28	116.63	121.00
1	A	581	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	B	581	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	B	220	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	A	220	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	A	680	TYR	CB-CG-CD1	-6.09	117.35	121.00
1	B	680	TYR	CB-CG-CD1	-6.08	117.35	121.00
1	A	588	TYR	CB-CG-CD2	-6.02	117.39	121.00
1	B	588	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	B	175	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	175	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	154	TYR	CB-CG-CD2	5.25	124.15	121.00
1	B	154	TYR	CB-CG-CD2	5.23	124.14	121.00
1	A	608	PHE	CB-CG-CD1	5.07	124.35	120.80
1	B	608	PHE	CB-CG-CD1	5.05	124.33	120.80

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	4033	0	4110	10	0
1	B	4033	0	4110	10	0
2	A	56	0	92	0	0
2	B	56	0	92	0	0
3	A	144	0	248	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	144	0	248	1	0
All	All	8466	0	8900	20	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 1.

All (20) 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:20:PHE:CZ	1:B:514:LEU:HD11	2.37	0.59
1:A:20:PHE:CZ	1:A:514:LEU:HD11	2.37	0.59
1:A:75:ASP:OD1	1:A:174:LYS:NZ	2.39	0.56
1:B:75:ASP:OD1	1:B:174:LYS:NZ	2.39	0.56
1:B:20:PHE:CE2	1:B:514:LEU:HD11	2.43	0.54
1:A:20:PHE:CE2	1:A:514:LEU:HD11	2.43	0.54
1:A:423:PRO:HB2	1:A:424:PRO:HD3	1.92	0.52
1:B:423:PRO:HB2	1:B:424:PRO:HD3	1.92	0.51
1:A:480:ILE:N	1:A:481:PRO:CD	2.81	0.44
1:B:480:ILE:N	1:B:481:PRO:CD	2.81	0.44
1:B:111:LEU:N	1:B:112:PRO:HD2	2.33	0.43
1:A:111:LEU:N	1:A:112:PRO:HD2	2.33	0.42
1:B:20:PHE:HE2	1:B:512:LEU:HD12	1.84	0.42
1:B:150:PHE:O	1:B:153:ILE:HG22	2.20	0.42
1:A:20:PHE:HE2	1:A:512:LEU:HD12	1.84	0.42
1:A:150:PHE:O	1:A:153:ILE:HG22	2.20	0.42
1:B:342:TRP:N	1:B:343:PRO:CD	2.83	0.42
1:A:342:TRP:N	1:A:343:PRO:CD	2.83	0.41
1:A:474:PHE:HB2	3:A:804:PLM:HG3	2.02	0.41
1:B:474:PHE:HB2	3:B:804:PLM:HG3	2.02	0.41

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	492/713 (69%)	488 (99%)	4 (1%)	0	100	100
1	B	492/713 (69%)	488 (99%)	4 (1%)	0	100	100
All	All	984/1426 (69%)	976 (99%)	8 (1%)	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	452/640 (71%)	452 (100%)	0	100	100
1	B	452/640 (71%)	452 (100%)	0	100	100
All	All	904/1280 (71%)	904 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

20 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	$\#\|Z\| > 2$
3	PLM	A	806	-	17,17,17	0.83	0	17,17,17	0.52	0
3	PLM	B	809	-	17,17,17	0.83	1 (5%)	17,17,17	0.65	0
3	PLM	A	805	-	17,17,17	0.86	1 (5%)	17,17,17	0.66	0
3	PLM	B	805	-	17,17,17	0.86	1 (5%)	17,17,17	0.66	0
3	PLM	A	809	-	17,17,17	0.83	1 (5%)	17,17,17	0.65	0
2	CLR	B	801	-	31,31,31	3.90	21 (67%)	48,48,48	2.31	17 (35%)
3	PLM	A	803	-	17,17,17	0.78	0	17,17,17	0.65	0
3	PLM	B	807	-	17,17,17	0.82	1 (5%)	17,17,17	0.75	0
3	PLM	B	808	-	17,17,17	0.79	0	17,17,17	0.61	0
3	PLM	B	803	-	17,17,17	0.78	0	17,17,17	0.65	0
3	PLM	A	808	-	17,17,17	0.78	0	17,17,17	0.61	0
3	PLM	B	810	-	17,17,17	0.82	1 (5%)	17,17,17	0.67	0
3	PLM	A	807	-	17,17,17	0.82	1 (5%)	17,17,17	0.76	0
2	CLR	B	802	-	31,31,31	4.07	21 (67%)	48,48,48	2.38	19 (39%)
2	CLR	A	801	-	31,31,31	3.90	21 (67%)	48,48,48	2.31	17 (35%)
3	PLM	A	810	-	17,17,17	0.82	1 (5%)	17,17,17	0.68	0
3	PLM	B	806	-	17,17,17	0.83	0	17,17,17	0.52	0
2	CLR	A	802	-	31,31,31	4.06	21 (67%)	48,48,48	2.39	19 (39%)
3	PLM	A	804	-	17,17,17	0.78	0	17,17,17	0.72	0
3	PLM	B	804	-	17,17,17	0.78	0	17,17,17	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLM	A	806	-	-	9/15/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLM	B	809	-	-	6/15/15/15	-
3	PLM	A	805	-	-	2/15/15/15	-
3	PLM	B	805	-	-	2/15/15/15	-
3	PLM	A	809	-	-	6/15/15/15	-
2	CLR	B	801	-	-	6/10/68/68	0/4/4/4
3	PLM	A	803	-	-	4/15/15/15	-
3	PLM	B	807	-	-	3/15/15/15	-
3	PLM	B	808	-	-	6/15/15/15	-
3	PLM	B	803	-	-	4/15/15/15	-
3	PLM	A	808	-	-	6/15/15/15	-
3	PLM	B	810	-	-	7/15/15/15	-
3	PLM	A	807	-	-	3/15/15/15	-
2	CLR	B	802	-	-	7/10/68/68	0/4/4/4
2	CLR	A	801	-	-	6/10/68/68	0/4/4/4
3	PLM	A	810	-	-	7/15/15/15	-
3	PLM	B	806	-	-	9/15/15/15	-
2	CLR	A	802	-	-	7/10/68/68	0/4/4/4
3	PLM	A	804	-	-	6/15/15/15	-
3	PLM	B	804	-	-	6/15/15/15	-

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	CLR	C10-C9	9.49	1.72	1.56
2	A	802	CLR	C10-C9	9.49	1.72	1.56
2	A	801	CLR	C10-C9	8.85	1.70	1.56
2	B	801	CLR	C10-C9	8.82	1.70	1.56
2	B	802	CLR	C4-C5	6.81	1.66	1.51
2	A	802	CLR	C4-C5	6.77	1.66	1.51
2	B	801	CLR	C4-C5	6.69	1.66	1.51
2	A	801	CLR	C4-C5	6.68	1.66	1.51
2	B	802	CLR	C8-C14	6.55	1.66	1.53
2	B	802	CLR	C4-C3	6.53	1.63	1.52
2	A	802	CLR	C8-C14	6.51	1.66	1.53
2	A	802	CLR	C4-C3	6.49	1.63	1.52
2	A	801	CLR	C8-C14	6.48	1.66	1.53
2	B	801	CLR	C8-C14	6.45	1.65	1.53
2	B	801	CLR	C4-C3	5.95	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	CLR	C4-C3	5.94	1.62	1.52
2	B	802	CLR	C13-C17	5.84	1.66	1.55
2	A	802	CLR	C13-C17	5.83	1.66	1.55
2	B	801	CLR	C13-C17	5.67	1.65	1.55
2	A	801	CLR	C13-C17	5.67	1.65	1.55
2	A	802	CLR	C11-C9	5.56	1.63	1.53
2	B	802	CLR	C11-C9	5.55	1.63	1.53
2	B	801	CLR	C7-C6	5.43	1.61	1.50
2	B	801	CLR	C20-C17	5.43	1.63	1.54
2	A	801	CLR	C7-C6	5.42	1.61	1.50
2	A	801	CLR	C20-C17	5.42	1.63	1.54
2	B	802	CLR	C8-C9	5.36	1.63	1.53
2	A	802	CLR	C8-C9	5.33	1.63	1.53
2	B	802	CLR	C20-C17	5.29	1.63	1.54
2	A	802	CLR	C20-C17	5.27	1.63	1.54
2	A	802	CLR	C7-C6	5.06	1.61	1.50
2	B	802	CLR	C7-C6	5.05	1.61	1.50
2	B	802	CLR	C1-C10	5.04	1.63	1.54
2	A	802	CLR	C1-C10	5.02	1.63	1.54
2	A	801	CLR	C8-C9	4.91	1.63	1.53
2	B	801	CLR	C8-C9	4.91	1.63	1.53
2	A	801	CLR	C1-C10	4.90	1.63	1.54
2	B	801	CLR	C1-C10	4.90	1.63	1.54
2	B	801	CLR	C11-C9	4.82	1.61	1.53
2	A	801	CLR	C11-C9	4.81	1.61	1.53
2	A	802	CLR	C10-C5	4.20	1.61	1.52
2	B	802	CLR	C10-C5	4.16	1.61	1.52
2	A	802	CLR	C12-C11	4.06	1.62	1.53
2	B	802	CLR	C12-C11	4.04	1.62	1.53
2	B	801	CLR	C10-C5	4.02	1.60	1.52
2	A	801	CLR	C10-C5	4.00	1.60	1.52
2	B	801	CLR	C12-C11	3.76	1.61	1.53
2	A	801	CLR	C12-C11	3.75	1.61	1.53
2	A	801	CLR	C7-C8	3.54	1.59	1.53
2	B	801	CLR	C7-C8	3.54	1.59	1.53
2	A	802	CLR	C7-C8	3.48	1.59	1.53
2	B	802	CLR	C7-C8	3.47	1.59	1.53
2	A	801	CLR	C18-C13	3.10	1.59	1.54
2	B	801	CLR	C18-C13	3.09	1.59	1.54
2	A	802	CLR	C18-C13	3.04	1.59	1.54
2	B	802	CLR	C18-C13	3.04	1.59	1.54
2	B	802	CLR	C22-C20	2.97	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	CLR	C22-C20	2.96	1.62	1.54
2	B	802	CLR	C1-C2	2.88	1.59	1.53
2	A	802	CLR	C1-C2	2.86	1.59	1.53
2	A	801	CLR	C1-C2	2.55	1.58	1.53
2	B	801	CLR	C1-C2	2.52	1.58	1.53
2	B	802	CLR	C12-C13	2.50	1.58	1.54
2	A	802	CLR	C12-C13	2.48	1.58	1.54
2	A	801	CLR	C22-C20	2.45	1.60	1.54
2	B	801	CLR	C22-C20	2.45	1.60	1.54
2	A	801	CLR	C12-C13	2.43	1.58	1.54
2	A	801	CLR	C6-C5	2.43	1.38	1.33
2	B	801	CLR	C6-C5	2.42	1.38	1.33
2	B	801	CLR	C12-C13	2.41	1.58	1.54
2	A	802	CLR	C15-C14	2.28	1.59	1.54
2	B	801	CLR	C15-C14	2.26	1.59	1.54
2	B	802	CLR	C15-C14	2.25	1.59	1.54
2	A	801	CLR	C15-C14	2.24	1.59	1.54
2	B	801	CLR	C19-C10	2.23	1.58	1.54
2	A	802	CLR	C6-C5	2.23	1.37	1.33
2	A	801	CLR	C19-C10	2.22	1.58	1.54
3	B	807	PLM	C2-C1	2.21	1.55	1.50
2	B	802	CLR	C6-C5	2.21	1.37	1.33
3	A	807	PLM	C2-C1	2.21	1.55	1.50
3	A	805	PLM	C2-C1	2.19	1.55	1.50
3	B	805	PLM	C2-C1	2.19	1.55	1.50
2	B	801	CLR	C13-C14	2.18	1.59	1.55
2	B	802	CLR	C13-C14	2.18	1.59	1.55
2	A	802	CLR	C19-C10	2.17	1.58	1.54
2	A	801	CLR	C13-C14	2.16	1.59	1.55
3	A	810	PLM	C2-C1	2.15	1.55	1.50
2	A	802	CLR	C13-C14	2.15	1.59	1.55
2	B	802	CLR	C19-C10	2.14	1.58	1.54
3	B	810	PLM	C2-C1	2.13	1.55	1.50
3	A	809	PLM	C2-C1	2.13	1.55	1.50
3	B	809	PLM	C2-C1	2.12	1.55	1.50

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	802	CLR	C3-C4-C5	7.00	123.90	112.03
2	B	802	CLR	C3-C4-C5	6.99	123.88	112.03
2	A	801	CLR	C7-C8-C14	5.48	118.84	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	CLR	C7-C8-C14	5.45	118.81	110.91
2	B	801	CLR	C4-C5-C6	5.15	128.02	120.61
2	A	801	CLR	C4-C5-C6	5.12	127.99	120.61
2	A	802	CLR	C7-C8-C14	4.92	118.04	110.91
2	B	802	CLR	C7-C8-C14	4.91	118.03	110.91
2	B	801	CLR	C4-C5-C10	-4.86	109.96	116.42
2	A	801	CLR	C4-C5-C10	-4.85	109.97	116.42
2	B	801	CLR	C3-C4-C5	4.60	119.82	112.03
2	A	801	CLR	C3-C4-C5	4.59	119.82	112.03
2	A	801	CLR	C12-C11-C9	4.19	120.37	113.11
2	B	801	CLR	C12-C11-C9	4.18	120.36	113.11
2	A	802	CLR	C4-C5-C6	4.09	126.51	120.61
2	B	802	CLR	C4-C5-C6	4.09	126.50	120.61
2	B	802	CLR	C4-C5-C10	-4.04	111.05	116.42
2	A	802	CLR	C4-C5-C10	-4.03	111.06	116.42
2	A	802	CLR	C22-C20-C17	4.00	118.55	110.28
2	B	802	CLR	C22-C20-C17	3.99	118.53	110.28
2	B	801	CLR	C22-C20-C17	3.64	117.81	110.28
2	A	801	CLR	C22-C20-C17	3.63	117.79	110.28
2	B	802	CLR	C12-C11-C9	3.59	119.34	113.11
2	A	802	CLR	C12-C11-C9	3.59	119.34	113.11
2	A	802	CLR	C14-C8-C9	3.53	113.82	109.09
2	B	801	CLR	C16-C17-C20	3.52	117.59	112.15
2	B	802	CLR	C14-C8-C9	3.51	113.79	109.09
2	A	801	CLR	C16-C17-C20	3.51	117.58	112.15
2	B	801	CLR	C18-C13-C12	-3.51	105.05	110.59
2	A	801	CLR	C18-C13-C12	-3.51	105.05	110.59
2	A	802	CLR	C18-C13-C12	-3.41	105.21	110.59
2	B	802	CLR	C18-C13-C12	-3.39	105.23	110.59
2	A	802	CLR	C1-C10-C9	3.38	113.44	108.73
2	B	802	CLR	C1-C10-C9	3.34	113.39	108.73
2	A	802	CLR	C16-C17-C20	3.21	117.12	112.15
2	B	802	CLR	C16-C17-C20	3.21	117.11	112.15
2	B	801	CLR	C17-C13-C14	3.17	103.83	100.07
2	A	801	CLR	C17-C13-C14	3.16	103.81	100.07
2	A	802	CLR	C19-C10-C9	-3.04	108.05	111.68
2	B	802	CLR	C19-C10-C9	-3.04	108.05	111.68
2	A	801	CLR	C1-C10-C5	2.94	114.14	108.75
2	B	801	CLR	C1-C10-C5	2.94	114.14	108.75
2	B	801	CLR	C2-C1-C10	2.92	119.06	112.74
2	A	801	CLR	C2-C1-C10	2.91	119.05	112.74
2	B	802	CLR	C11-C9-C10	2.90	116.90	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	802	CLR	C1-C2-C3	2.89	114.18	110.47
2	A	802	CLR	C1-C2-C3	2.88	114.17	110.47
2	A	802	CLR	C11-C9-C10	2.88	116.87	113.08
2	B	801	CLR	C14-C8-C9	2.79	112.83	109.09
2	A	801	CLR	C14-C8-C9	2.77	112.80	109.09
2	A	801	CLR	C11-C9-C10	2.66	116.58	113.08
2	B	801	CLR	C11-C9-C10	2.65	116.57	113.08
2	B	802	CLR	C19-C10-C1	-2.63	105.27	109.43
2	A	802	CLR	C19-C10-C1	-2.63	105.28	109.43
2	A	802	CLR	C15-C14-C8	2.62	123.39	119.08
2	B	801	CLR	C15-C14-C8	2.60	123.37	119.08
2	A	801	CLR	C15-C14-C8	2.59	123.34	119.08
2	B	802	CLR	C15-C14-C8	2.59	123.34	119.08
2	B	801	CLR	C19-C10-C5	-2.55	104.21	108.34
2	A	801	CLR	C19-C10-C5	-2.55	104.22	108.34
2	A	802	CLR	C2-C3-C4	2.45	113.66	110.31
2	B	802	CLR	C2-C3-C4	2.43	113.64	110.31
2	A	802	CLR	C2-C1-C10	2.35	117.82	112.74
2	A	801	CLR	C19-C10-C1	-2.32	105.76	109.43
2	B	802	CLR	C2-C1-C10	2.32	117.78	112.74
2	B	801	CLR	C19-C10-C1	-2.32	105.77	109.43
2	B	802	CLR	C16-C17-C13	-2.22	101.17	103.84
2	A	802	CLR	C16-C17-C13	-2.21	101.18	103.84
2	A	801	CLR	C1-C2-C3	2.20	113.29	110.47
2	B	801	CLR	C1-C2-C3	2.20	113.28	110.47
2	A	802	CLR	C16-C15-C14	2.01	109.12	105.13
2	B	802	CLR	C16-C15-C14	2.00	109.10	105.13

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	CLR	C13-C17-C20-C21
2	A	801	CLR	C16-C17-C20-C21
2	B	801	CLR	C13-C17-C20-C21
2	B	801	CLR	C16-C17-C20-C21
2	A	802	CLR	C16-C17-C20-C21
2	B	802	CLR	C16-C17-C20-C21
2	A	802	CLR	C13-C17-C20-C21
2	B	802	CLR	C13-C17-C20-C21
2	A	801	CLR	C13-C17-C20-C22
2	B	801	CLR	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
2	A	801	CLR	C16-C17-C20-C22
2	B	801	CLR	C16-C17-C20-C22
2	A	802	CLR	C13-C17-C20-C22
2	B	802	CLR	C13-C17-C20-C22
2	A	802	CLR	C17-C20-C22-C23
2	B	802	CLR	C17-C20-C22-C23
2	A	801	CLR	C20-C22-C23-C24
2	B	801	CLR	C20-C22-C23-C24
2	A	802	CLR	C16-C17-C20-C22
2	B	802	CLR	C16-C17-C20-C22
2	A	801	CLR	C22-C23-C24-C25
2	B	801	CLR	C22-C23-C24-C25
3	A	806	PLM	CB-CC-CD-CE
3	B	806	PLM	CB-CC-CD-CE
3	A	803	PLM	C6-C7-C8-C9
3	A	810	PLM	C6-C7-C8-C9
3	B	803	PLM	C6-C7-C8-C9
3	B	810	PLM	C6-C7-C8-C9
2	A	802	CLR	C22-C23-C24-C25
2	B	802	CLR	C22-C23-C24-C25
3	A	804	PLM	CC-CD-CE-CF
3	B	804	PLM	CC-CD-CE-CF
3	A	808	PLM	C2-C3-C4-C5
3	B	808	PLM	C2-C3-C4-C5
3	B	809	PLM	C2-C3-C4-C5
3	A	809	PLM	C2-C3-C4-C5
3	A	808	PLM	C7-C8-C9-CA
3	B	808	PLM	C7-C8-C9-CA
3	B	809	PLM	CA-CB-CC-CD
3	A	809	PLM	CA-CB-CC-CD
3	A	804	PLM	C6-C7-C8-C9
3	B	804	PLM	C6-C7-C8-C9
3	A	809	PLM	C8-C9-CA-CB
3	B	809	PLM	C8-C9-CA-CB
3	A	804	PLM	C4-C5-C6-C7
3	A	807	PLM	CD-CE-CF-CG
3	B	804	PLM	C4-C5-C6-C7
3	B	807	PLM	CD-CE-CF-CG
3	B	810	PLM	C5-C6-C7-C8
3	A	810	PLM	C5-C6-C7-C8
3	A	806	PLM	CC-CD-CE-CF
3	B	806	PLM	CC-CD-CE-CF

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Mol	Chain	Res	Type	Atoms
3	A	808	PLM	CC-CD-CE-CF
3	B	808	PLM	CC-CD-CE-CF
3	A	809	PLM	C4-C5-C6-C7
3	B	809	PLM	C4-C5-C6-C7
3	A	806	PLM	CA-CB-CC-CD
3	B	806	PLM	CA-CB-CC-CD
3	A	810	PLM	O1-C1-C2-C3
3	B	810	PLM	O1-C1-C2-C3
3	A	805	PLM	O2-C1-C2-C3
3	B	805	PLM	O2-C1-C2-C3
3	A	804	PLM	O1-C1-C2-C3
3	B	804	PLM	O1-C1-C2-C3
3	A	806	PLM	C2-C3-C4-C5
3	B	806	PLM	C2-C3-C4-C5
3	A	810	PLM	O2-C1-C2-C3
3	B	810	PLM	O2-C1-C2-C3
3	A	806	PLM	C7-C8-C9-CA
3	B	806	PLM	C7-C8-C9-CA
3	A	804	PLM	O2-C1-C2-C3
3	B	804	PLM	O2-C1-C2-C3
3	A	804	PLM	C2-C3-C4-C5
3	B	804	PLM	C2-C3-C4-C5
2	A	802	CLR	C20-C22-C23-C24
3	A	803	PLM	O2-C1-C2-C3
3	B	803	PLM	O2-C1-C2-C3
2	B	802	CLR	C20-C22-C23-C24
3	A	805	PLM	O1-C1-C2-C3
3	B	805	PLM	O1-C1-C2-C3
3	A	807	PLM	O1-C1-C2-C3
3	B	807	PLM	O1-C1-C2-C3
3	A	803	PLM	O1-C1-C2-C3
3	A	806	PLM	O2-C1-C2-C3
3	B	803	PLM	O1-C1-C2-C3
3	B	806	PLM	O2-C1-C2-C3
3	B	806	PLM	O1-C1-C2-C3
3	A	806	PLM	O1-C1-C2-C3
3	B	806	PLM	C9-CA-CB-CC
3	A	806	PLM	C9-CA-CB-CC
3	A	807	PLM	O2-C1-C2-C3
3	A	808	PLM	O1-C1-C2-C3
3	B	807	PLM	O2-C1-C2-C3
3	B	808	PLM	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	810	PLM	CD-CE-CF-CG
3	B	810	PLM	CD-CE-CF-CG
3	A	803	PLM	C7-C8-C9-CA
3	A	806	PLM	C5-C6-C7-C8
3	B	806	PLM	C5-C6-C7-C8
3	B	803	PLM	C7-C8-C9-CA
3	A	808	PLM	O2-C1-C2-C3
3	B	808	PLM	O2-C1-C2-C3
3	A	809	PLM	O1-C1-C2-C3
3	B	809	PLM	O1-C1-C2-C3
3	A	809	PLM	O2-C1-C2-C3
3	B	809	PLM	O2-C1-C2-C3
3	B	810	PLM	CB-CC-CD-CE
3	A	810	PLM	CB-CC-CD-CE
3	A	808	PLM	C5-C6-C7-C8
3	B	808	PLM	C5-C6-C7-C8
3	B	810	PLM	C7-C8-C9-CA
3	A	810	PLM	C7-C8-C9-CA

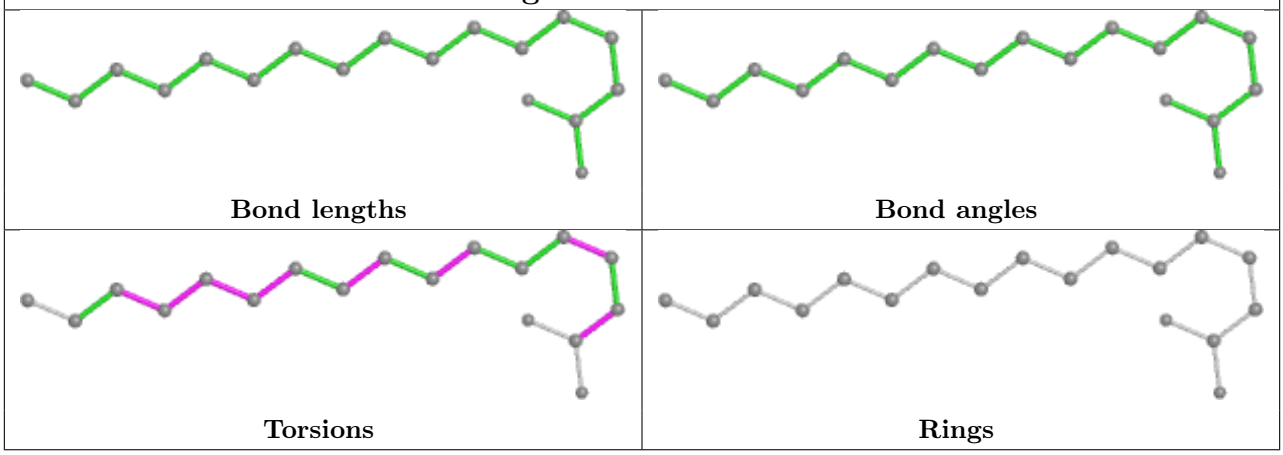
There are no ring outliers.

2 monomers are involved in 2 short contacts:

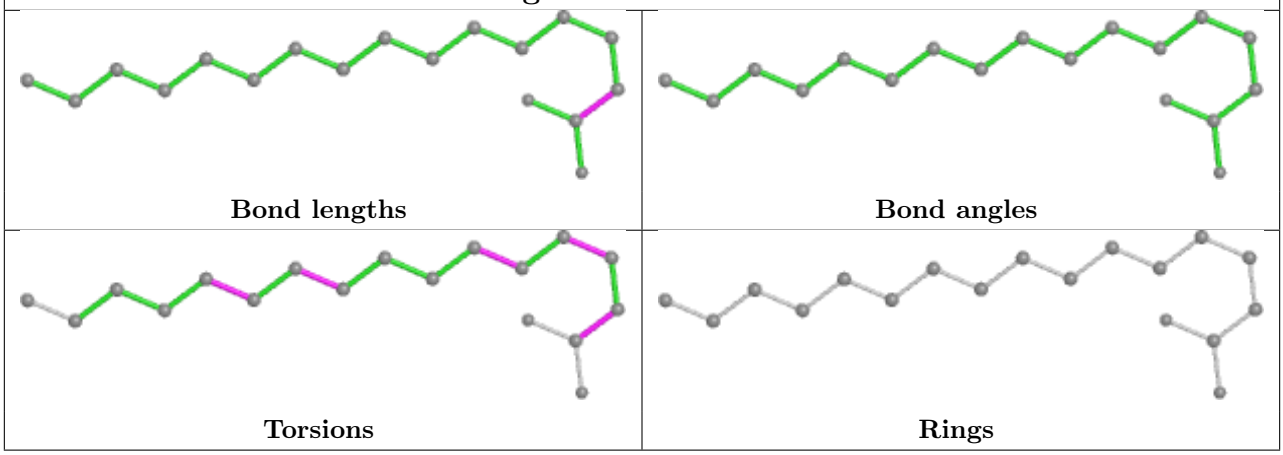
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	PLM	1	0
3	B	804	PLM	1	0

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.

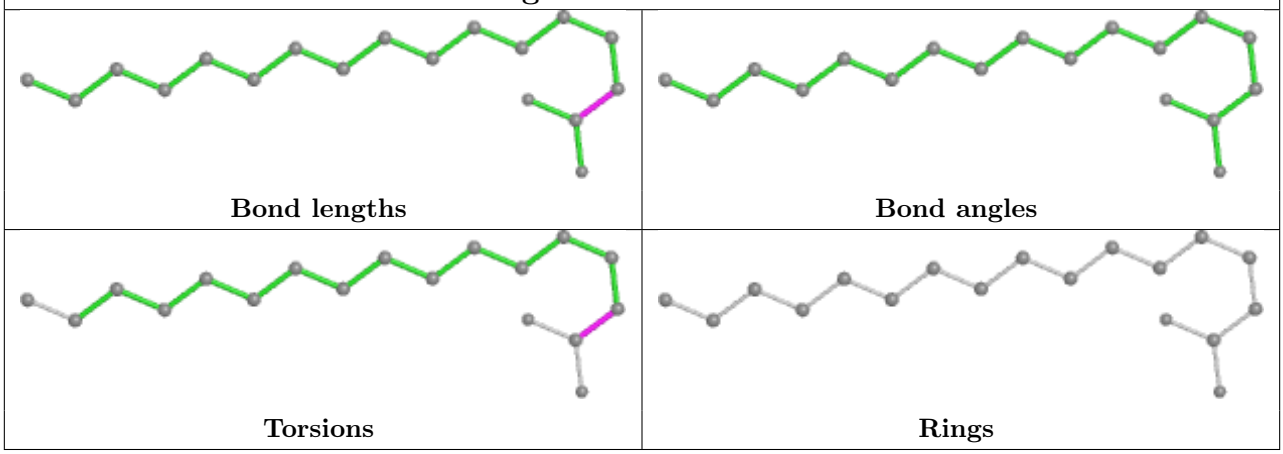
Ligand PLM A 806



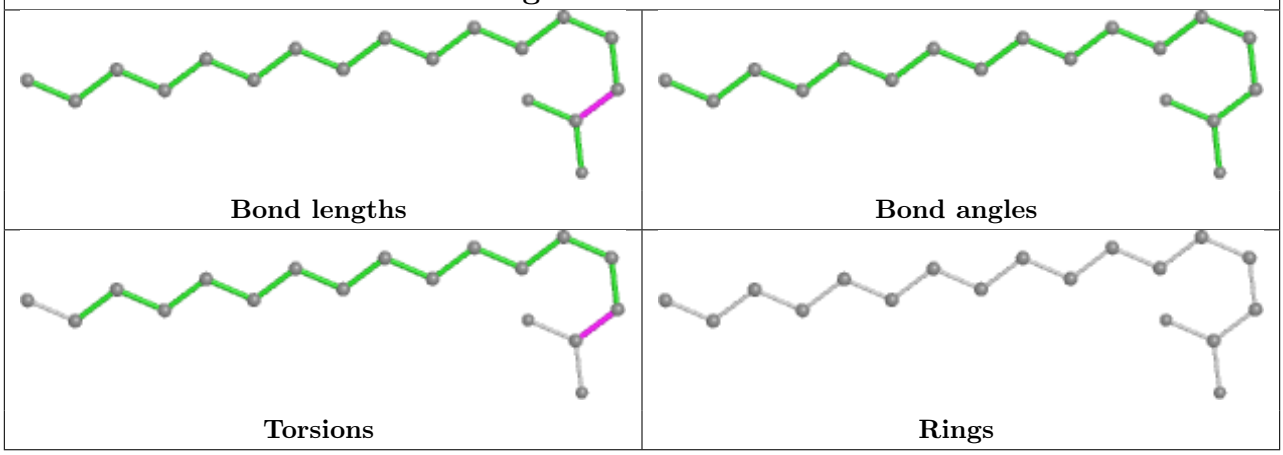
Ligand PLM B 809



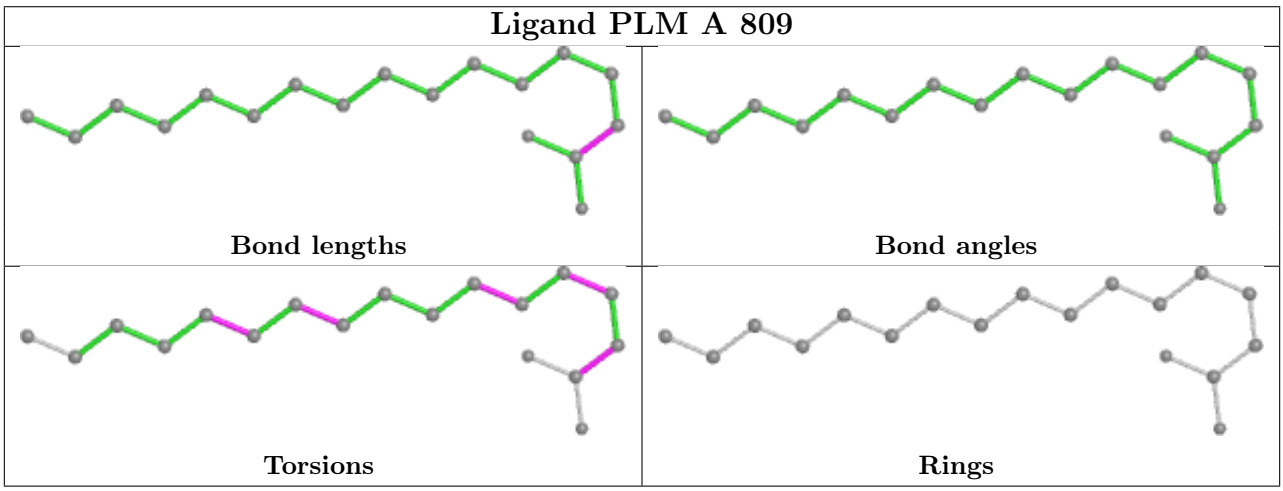
Ligand PLM A 805



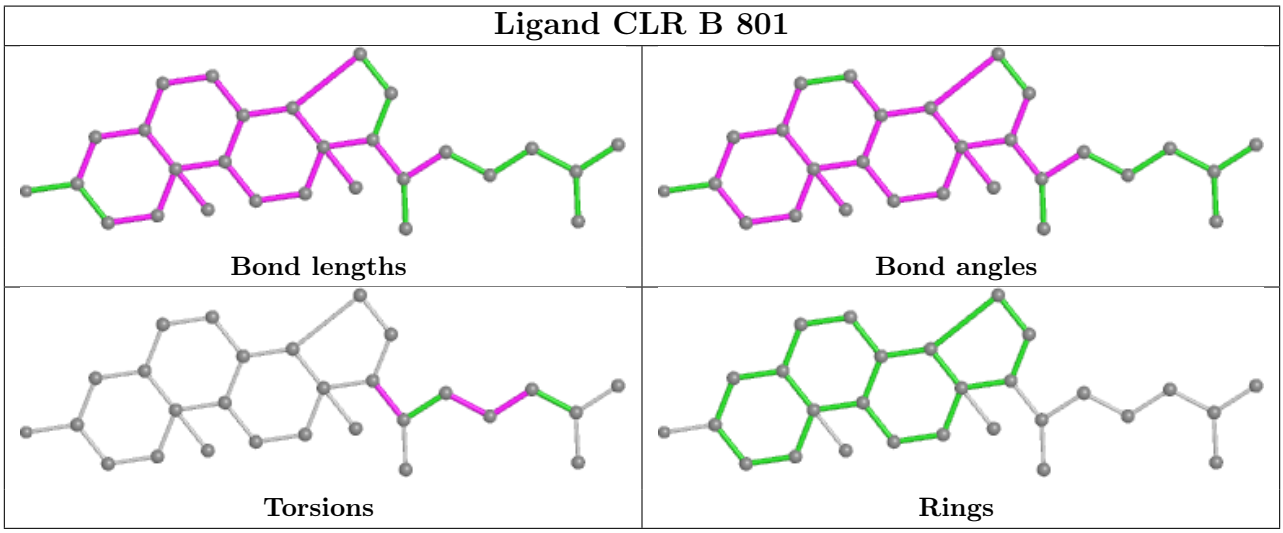
Ligand PLM B 805



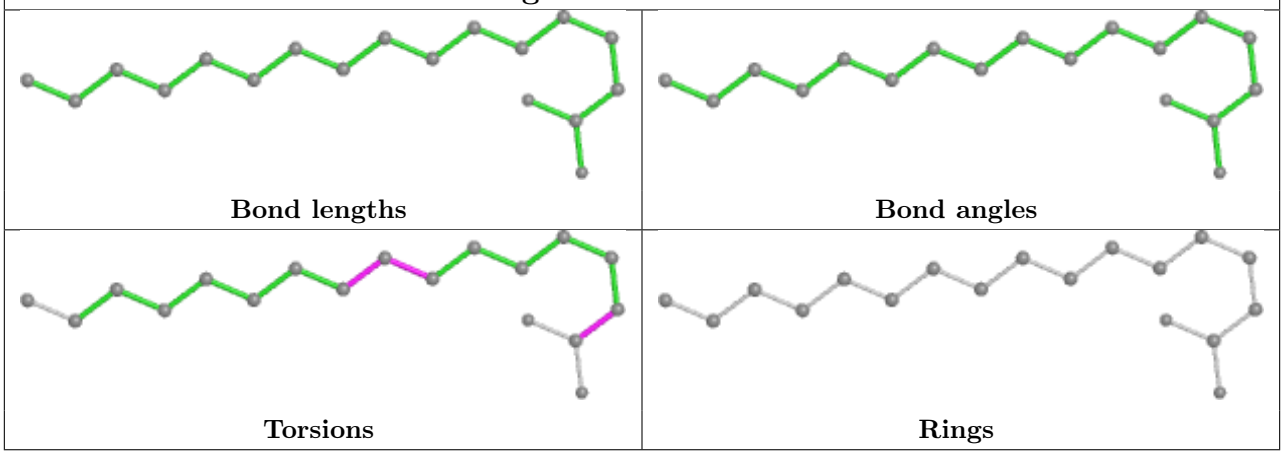
Ligand PLM A 809



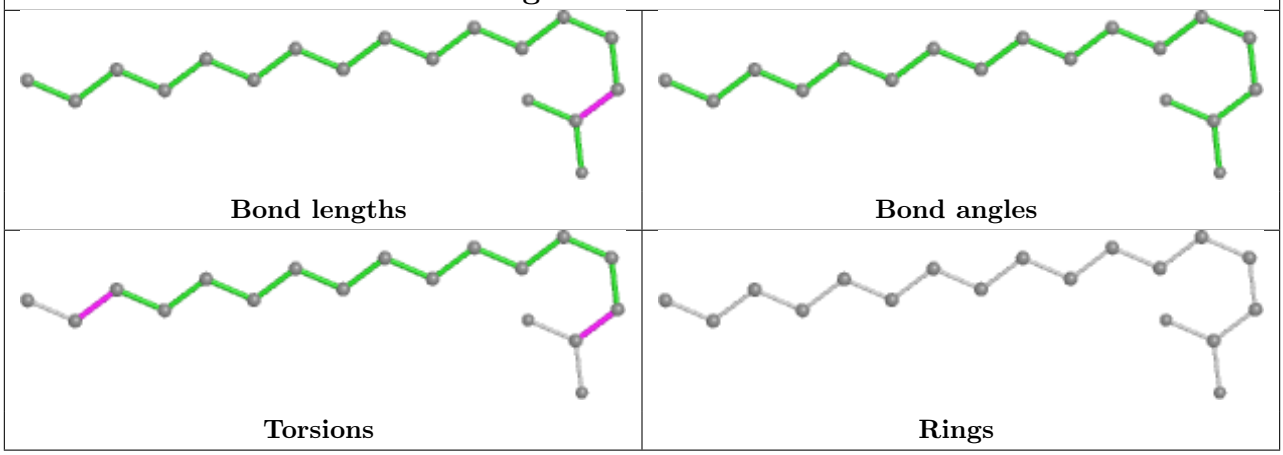
Ligand CLR B 801



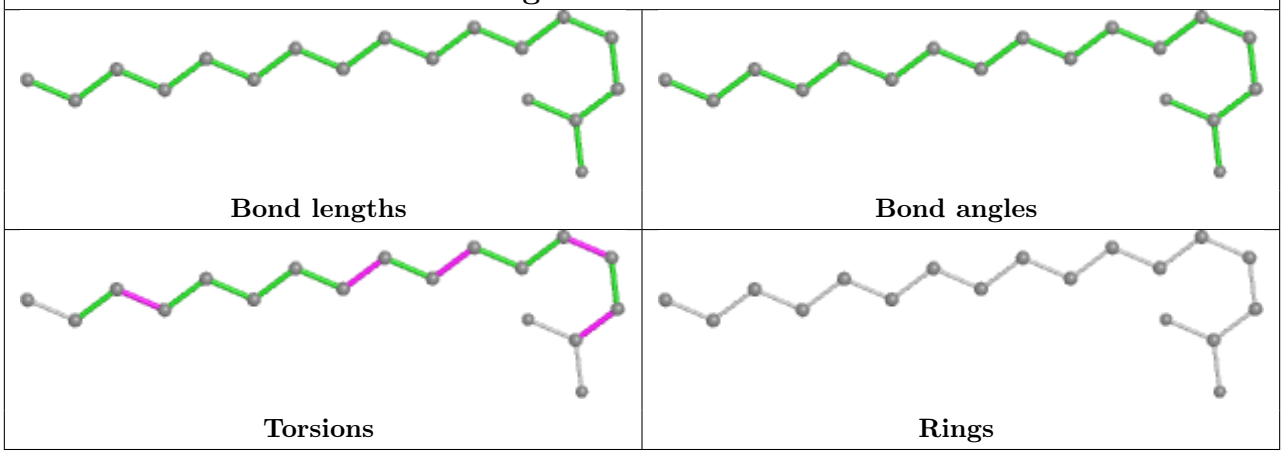
Ligand PLM A 803



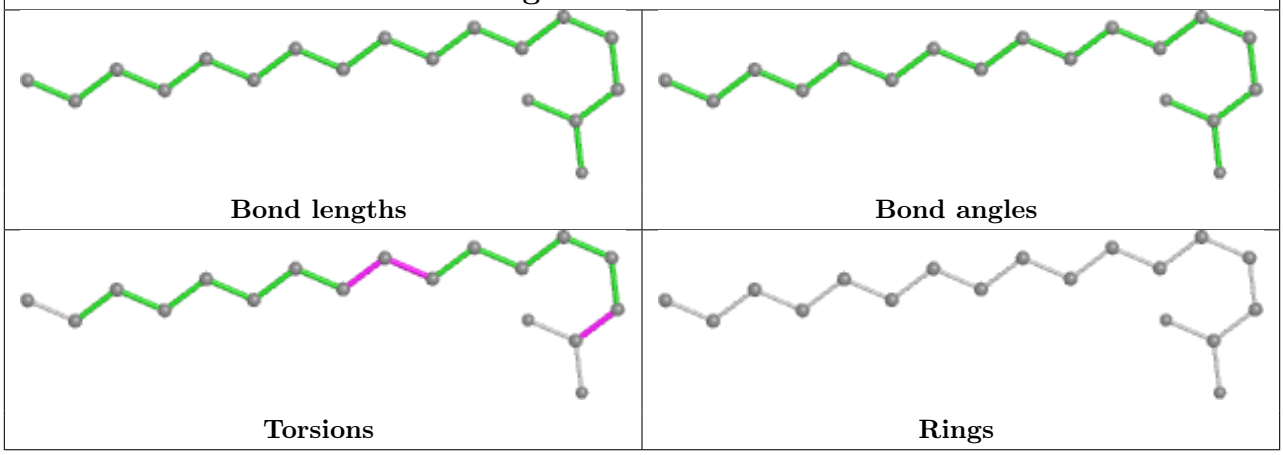
Ligand PLM B 807



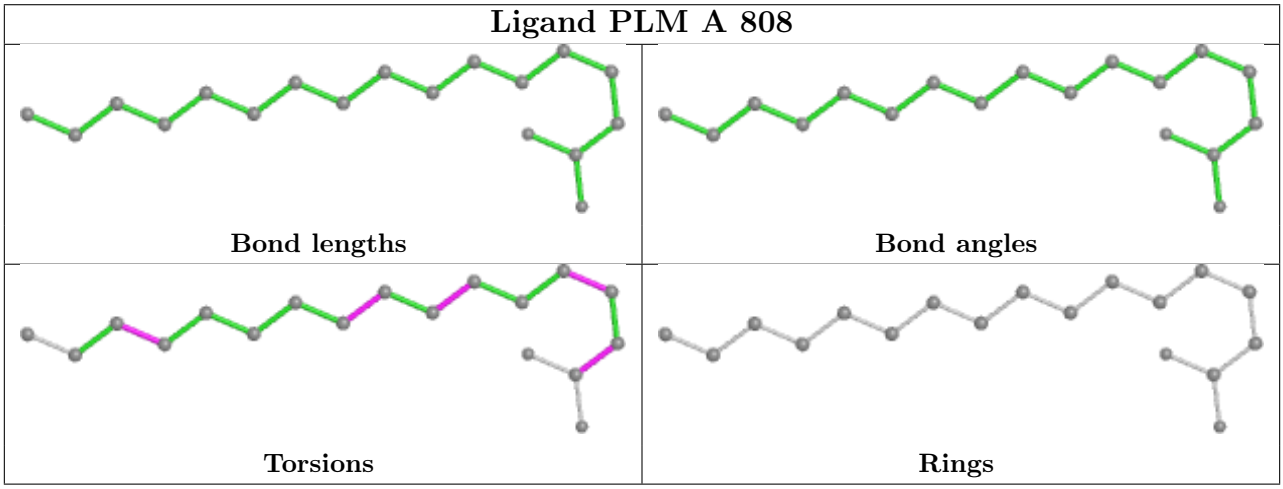
Ligand PLM B 808



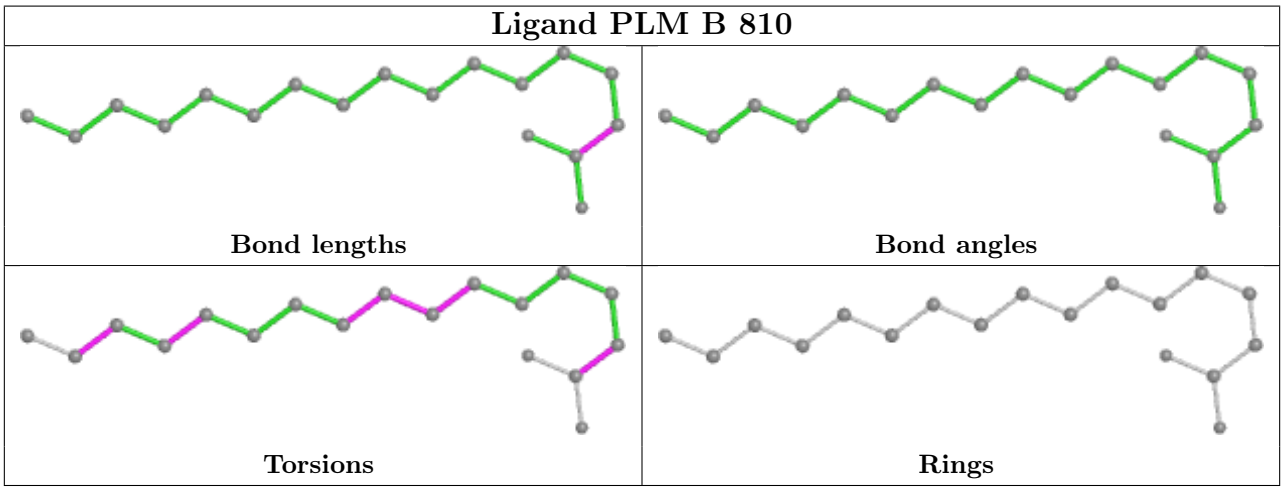
Ligand PLM B 803



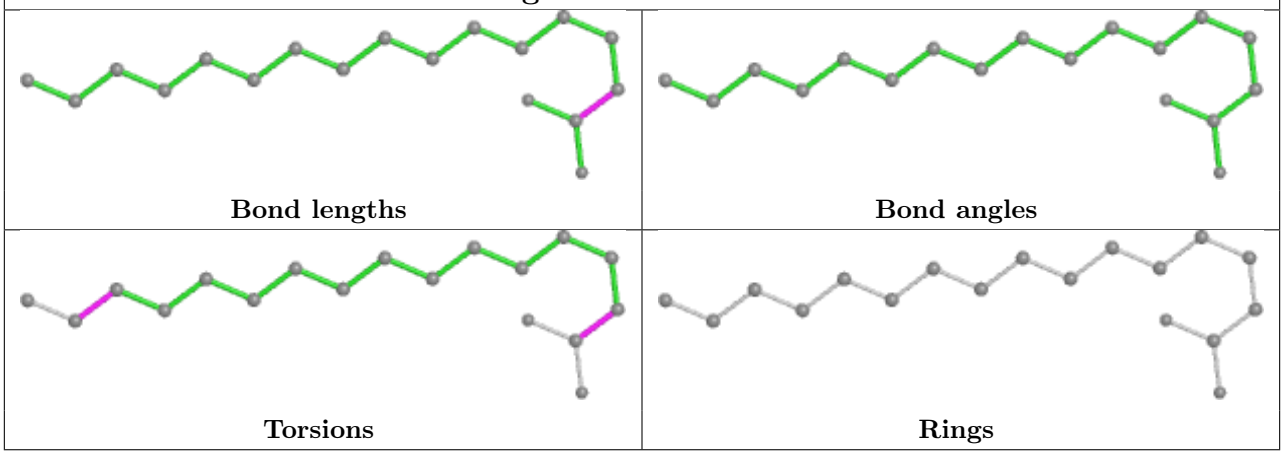
Ligand PLM A 808



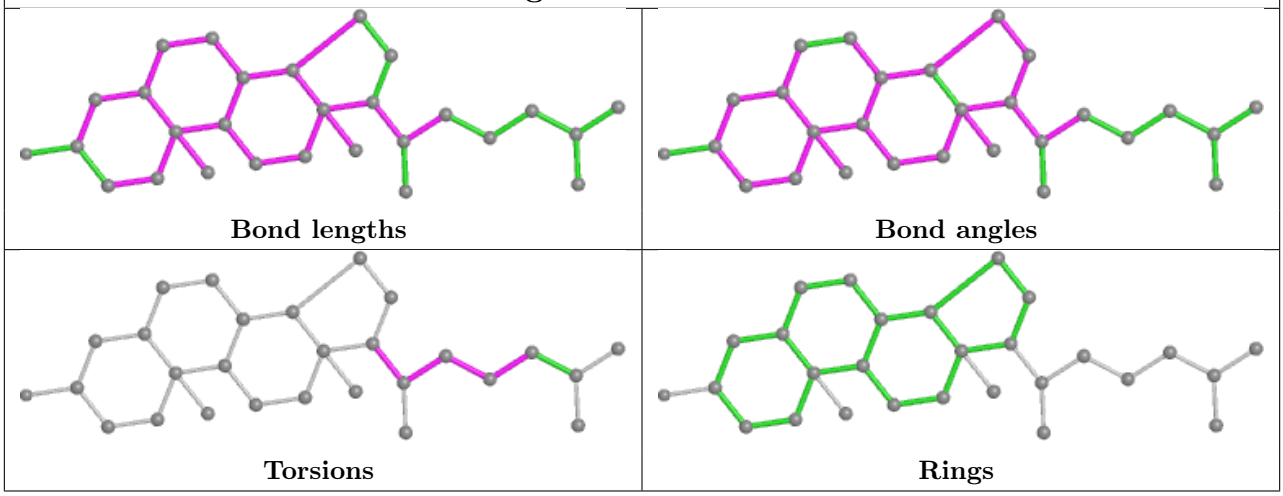
Ligand PLM B 810



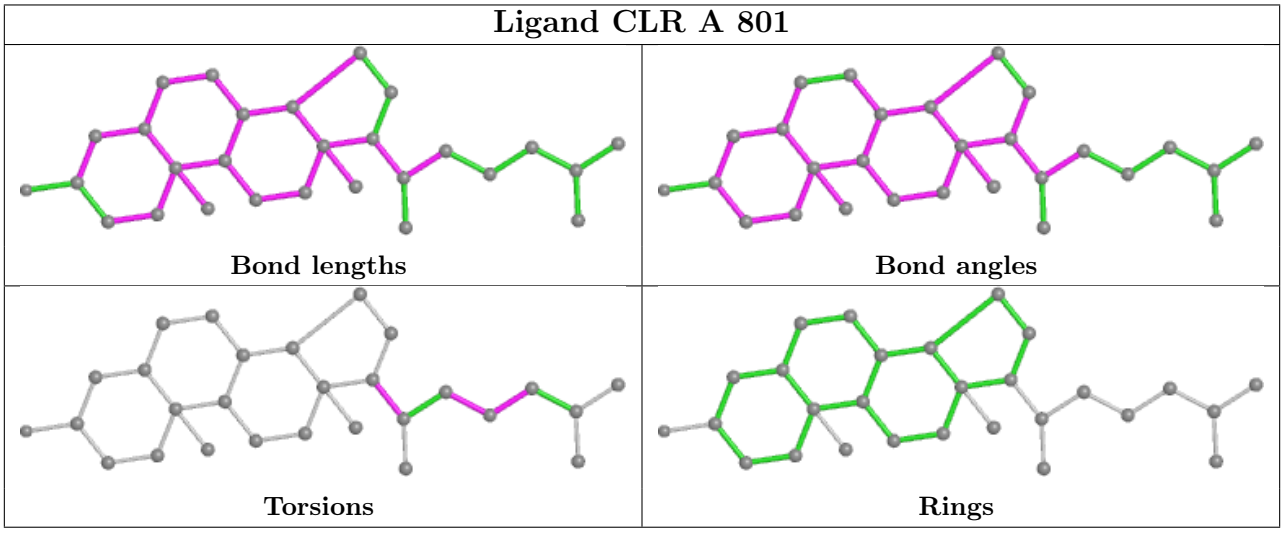
Ligand PLM A 807



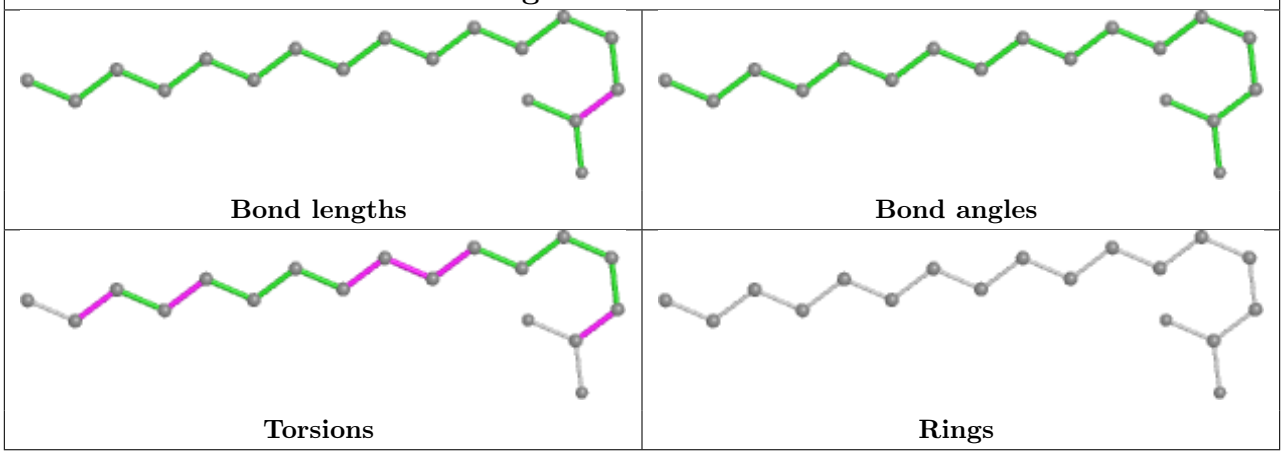
Ligand CLR B 802



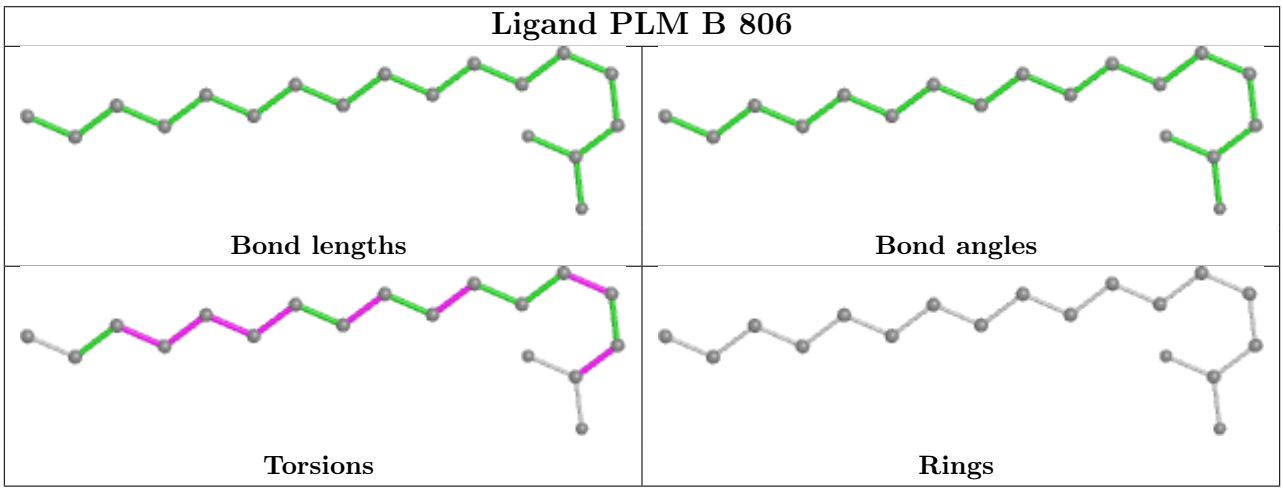
Ligand CLR A 801



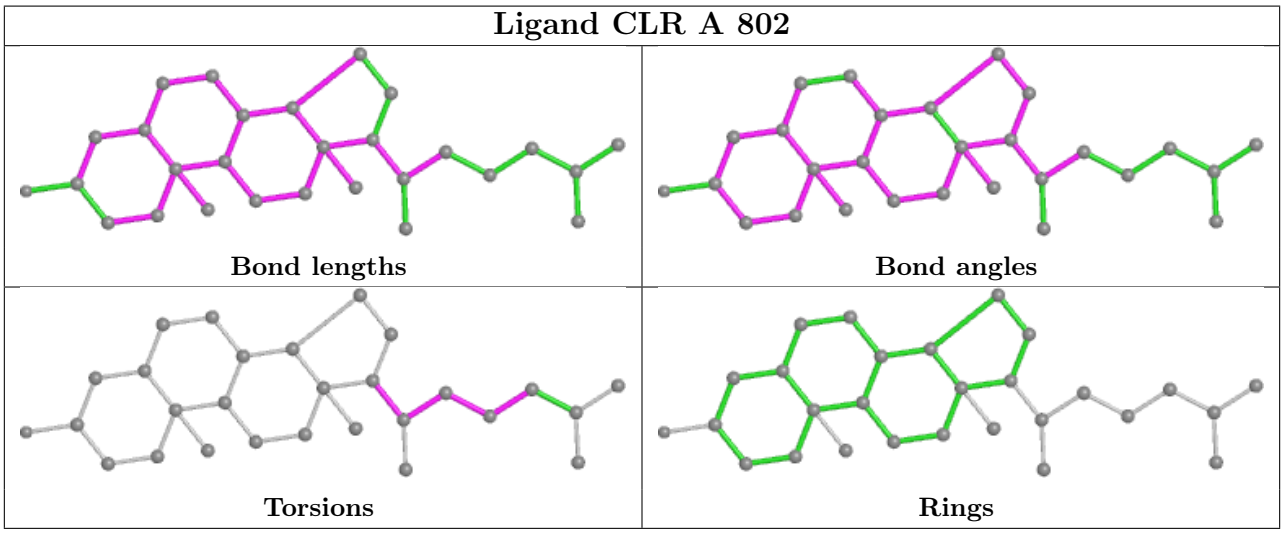
Ligand PLM A 810

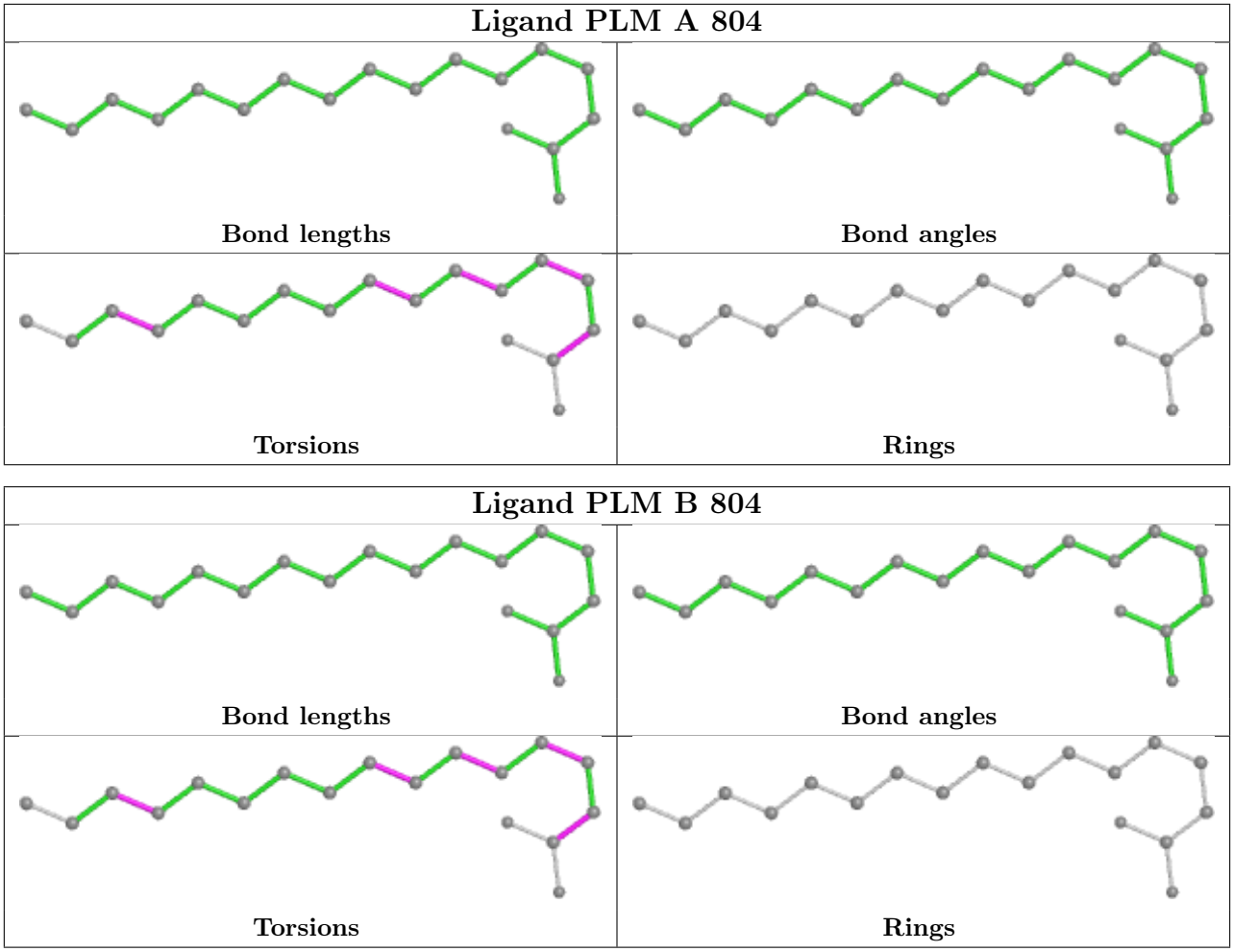


Ligand PLM B 806



Ligand CLR A 802





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

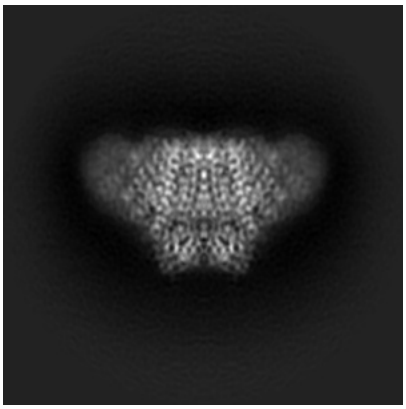
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41044. These allow visual inspection of the internal detail of the map and identification of artifacts.

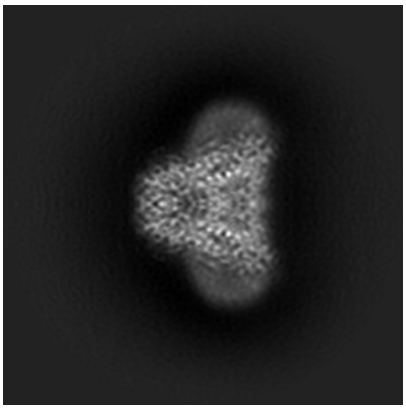
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

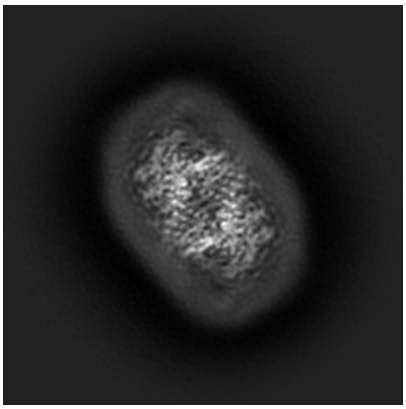
6.1.1 Primary map



X

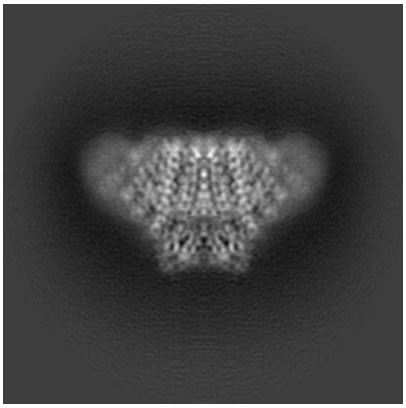


Y

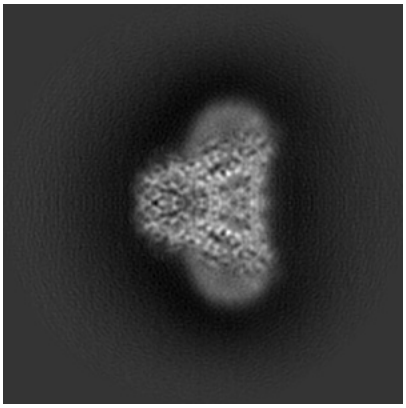


Z

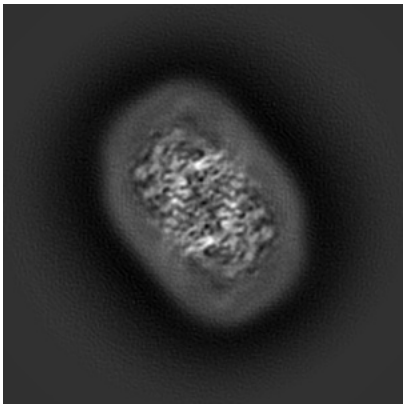
6.1.2 Raw map



X



Y



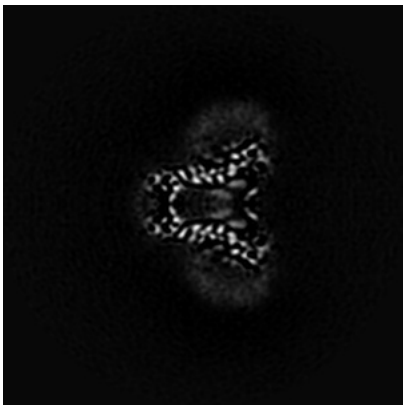
Z

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

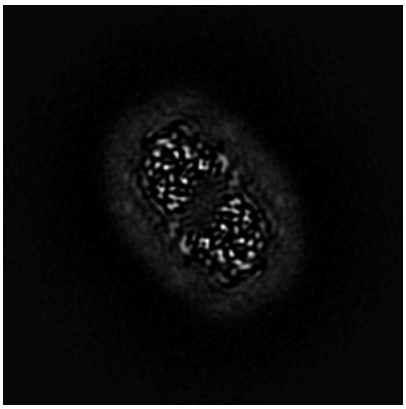
6.2 Central slices (i)

6.2.1 Primary map

X Index: 100

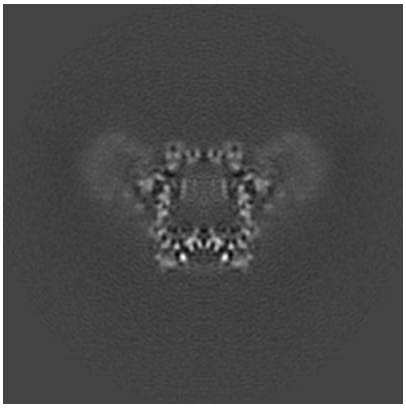


Y Index: 100

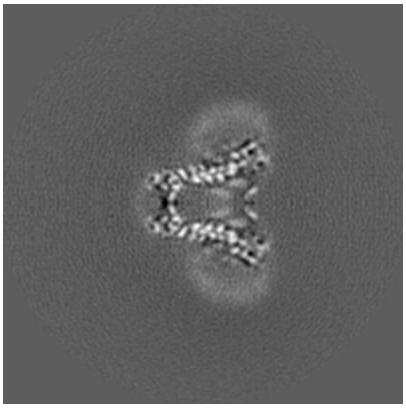


Z Index: 100

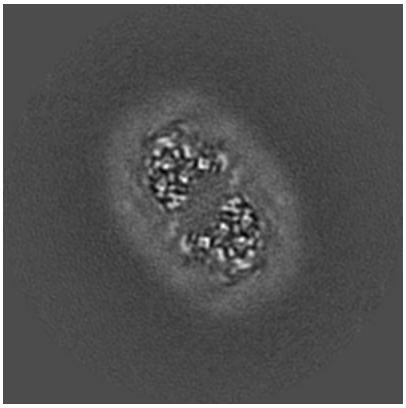
6.2.2 Raw map



X Index: 100



Y Index: 100

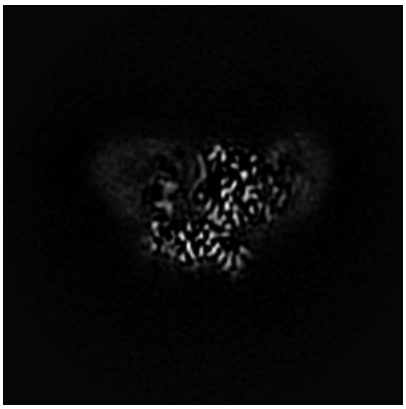


Z Index: 100

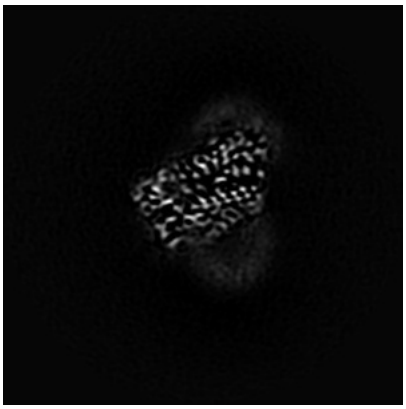
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

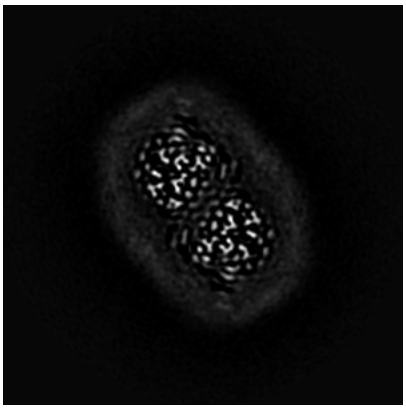
6.3.1 Primary map



X Index: 90

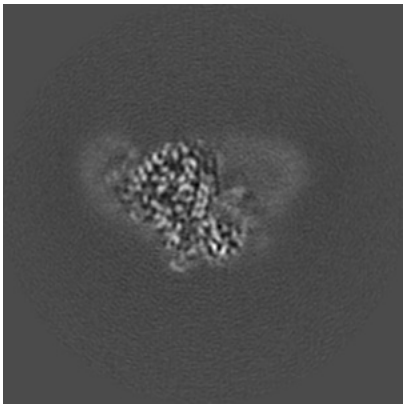


Y Index: 82

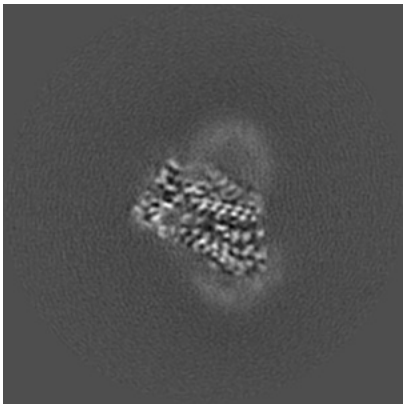


Z Index: 108

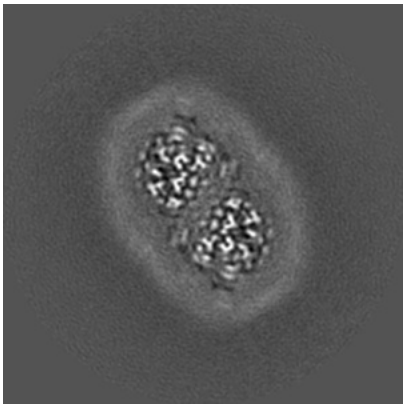
6.3.2 Raw map



X Index: 114



Y Index: 118

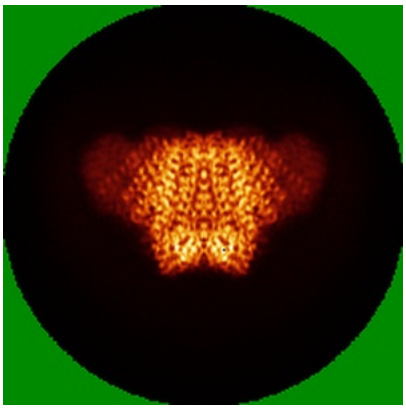


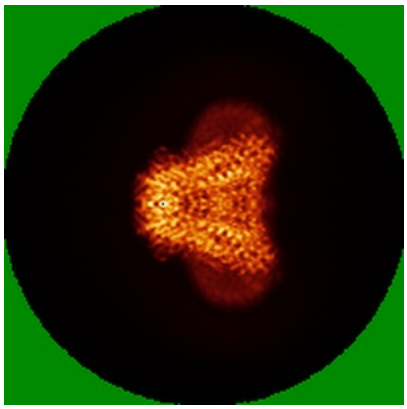
Z Index: 108

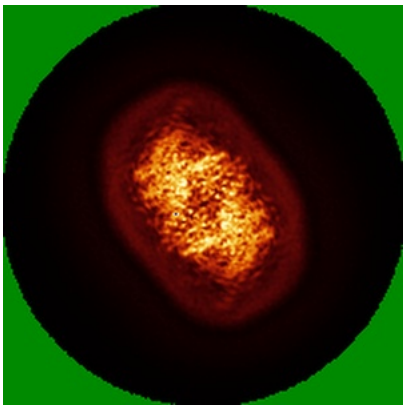
The images above show the largest variance slices of the map in three orthogonal directions.

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

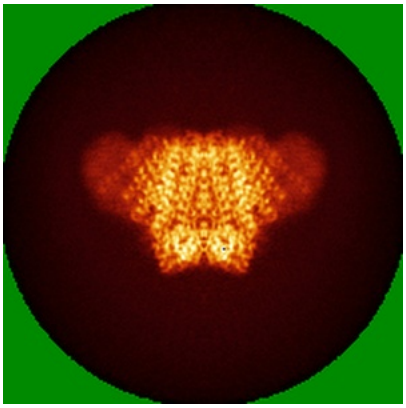
6.4.1 Primary map

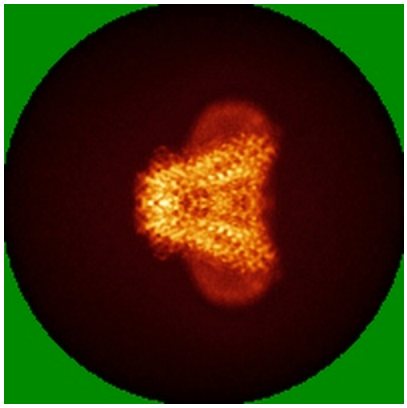

X

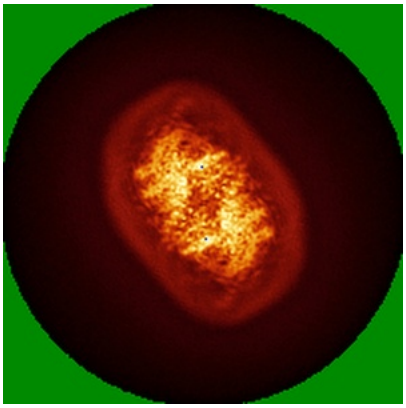

Y


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 0.0184. 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.

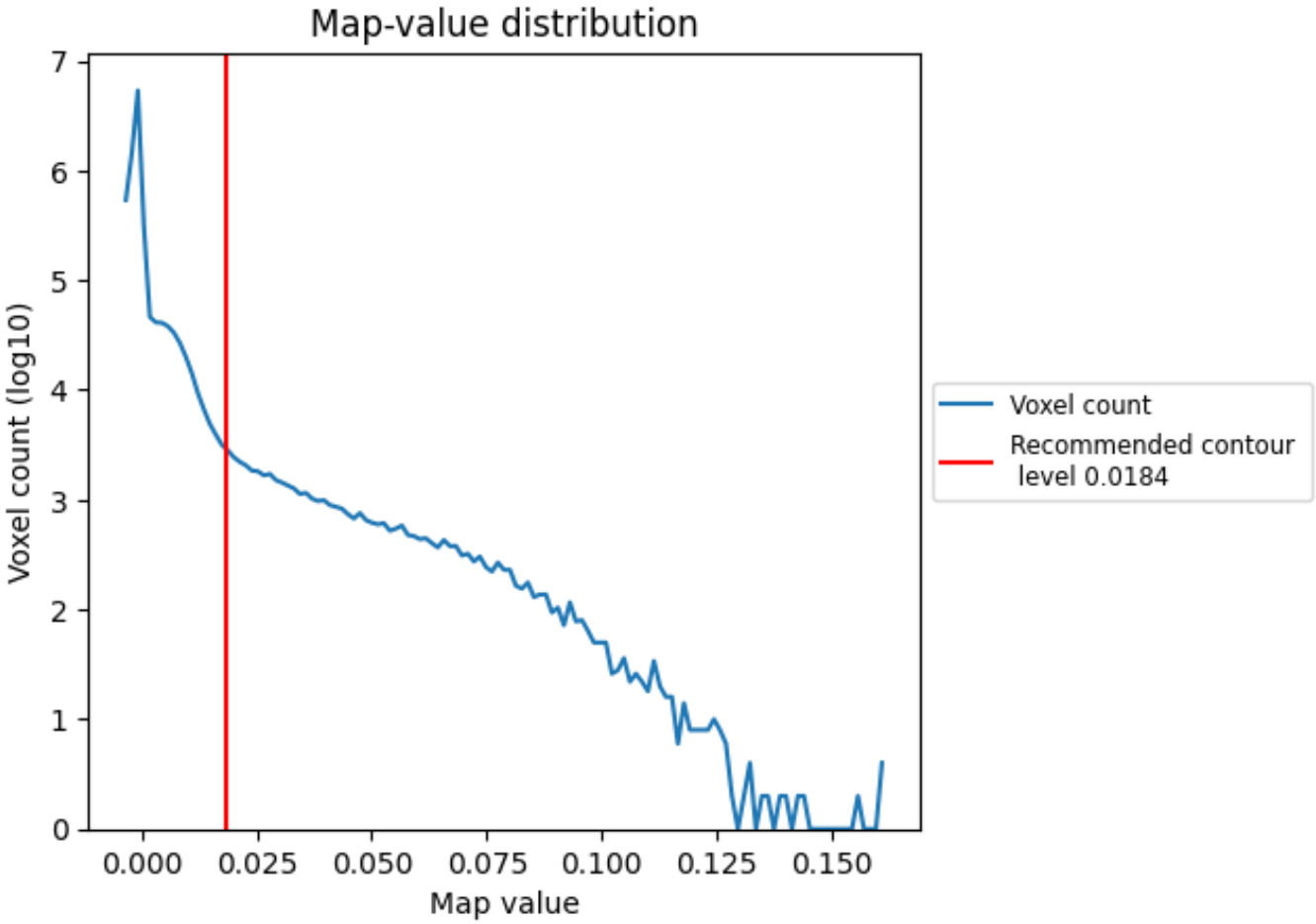
6.6 Mask visualisation (i)

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

7 Map analysis

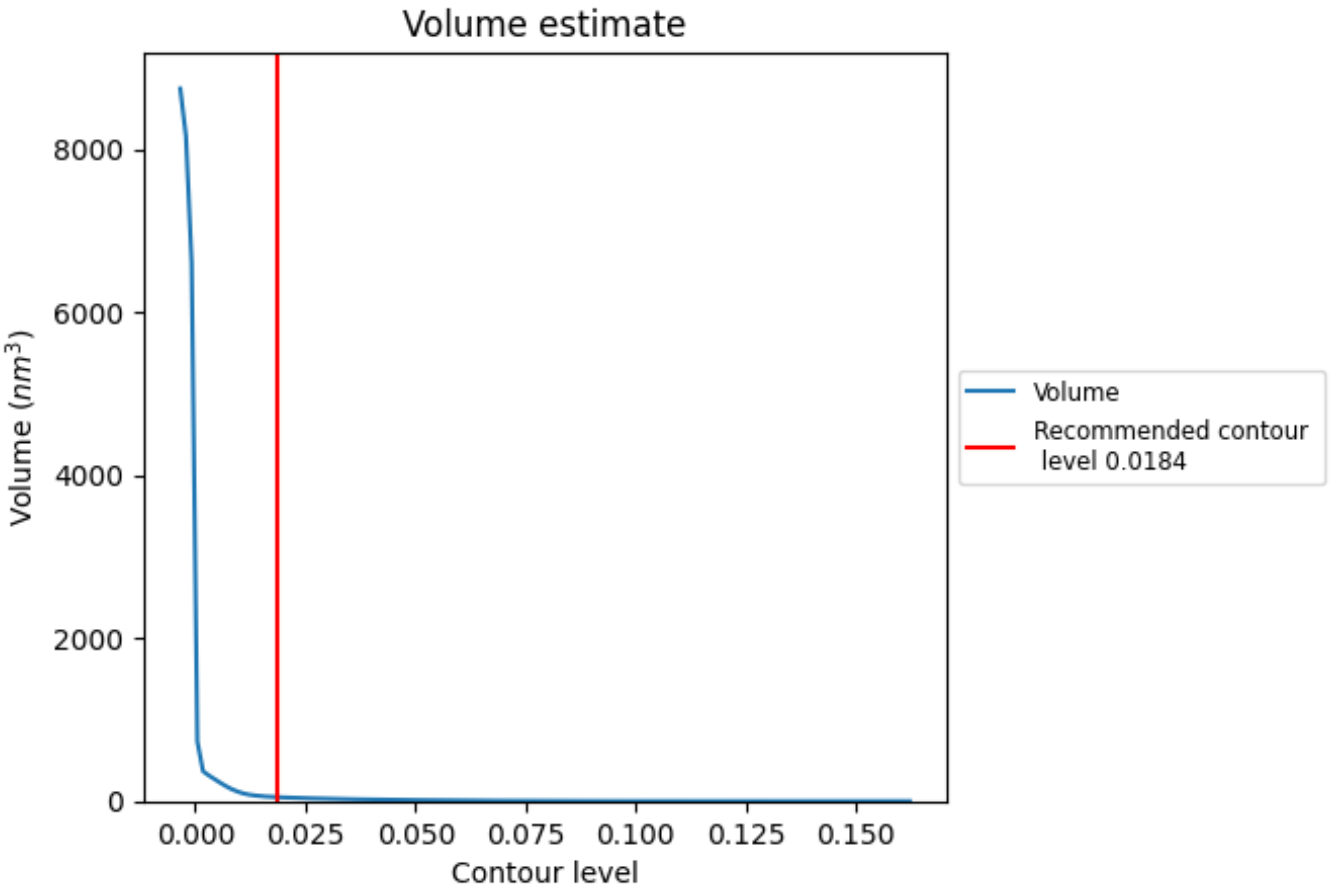
This section contains the results of statistical analysis of the map.

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.

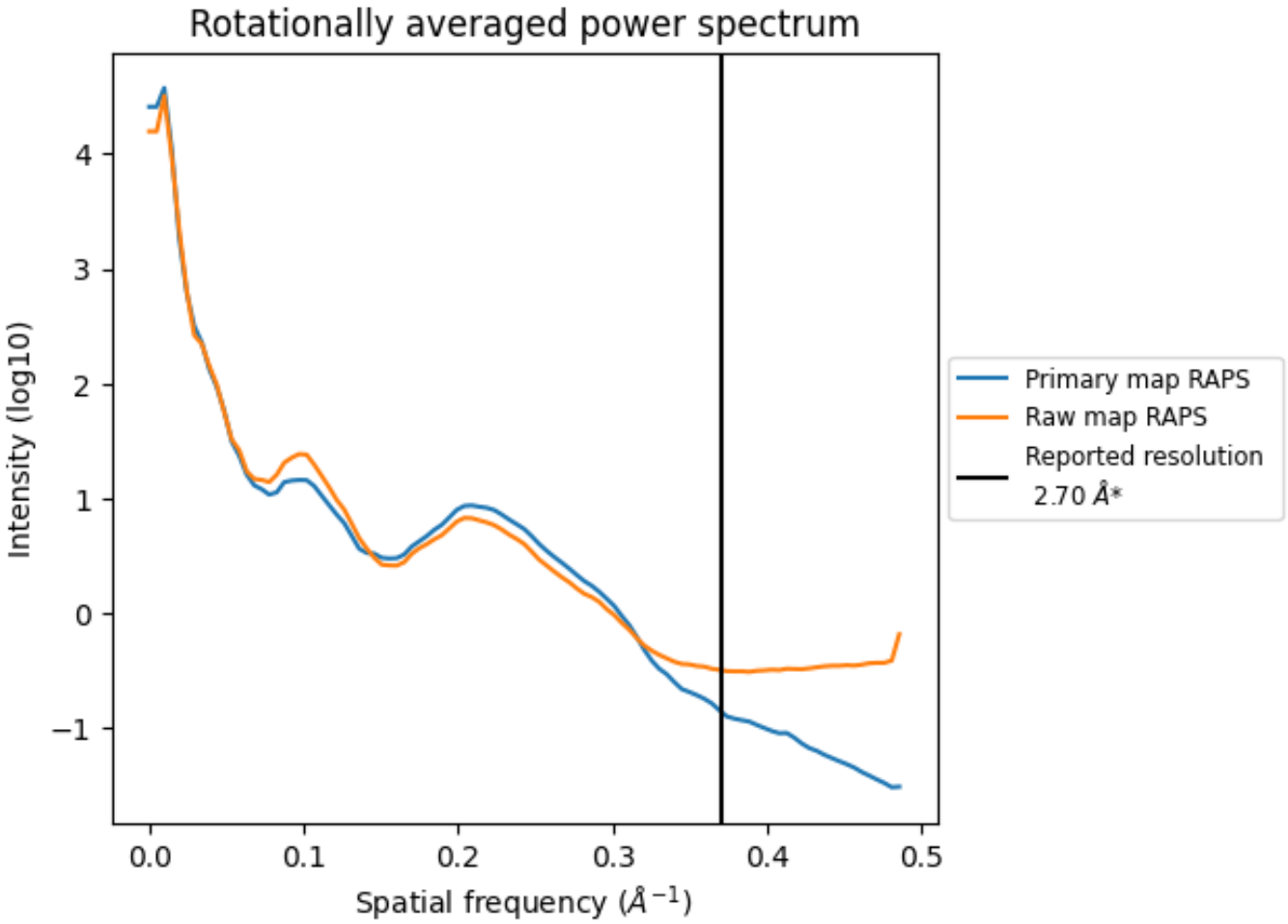
7.2 Volume estimate



The volume at the recommended contour level is 50 nm^3; this corresponds to an approximate mass of 45 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)

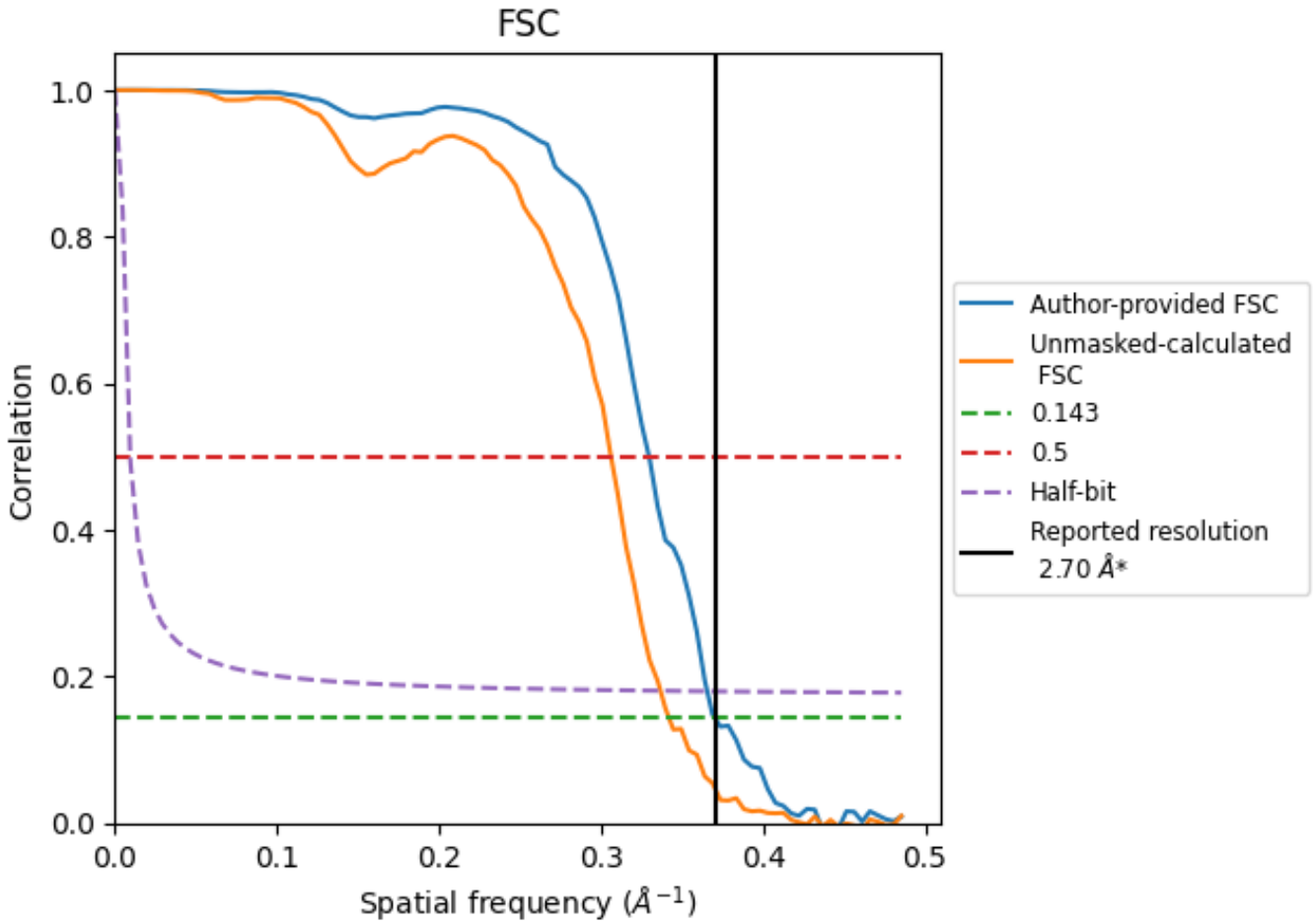


*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

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)

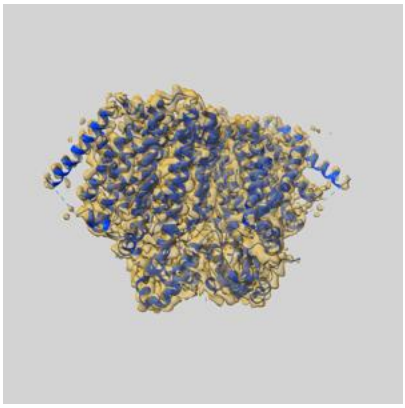
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.03	2.74
Unmasked-calculated*	2.92	3.27	2.97

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

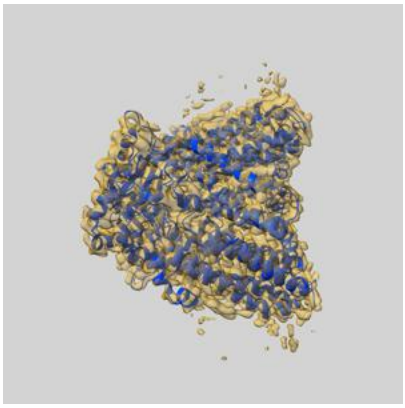
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41044 and PDB model 8T57. Per-residue inclusion information can be found in section 3 on page 6.

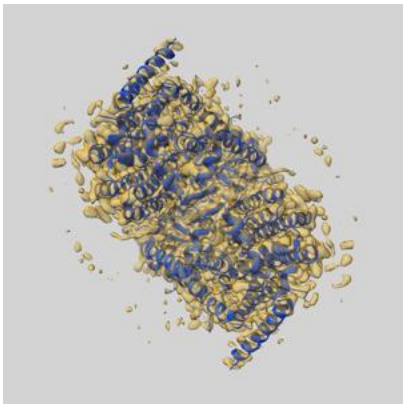
9.1 Map-model overlay



X



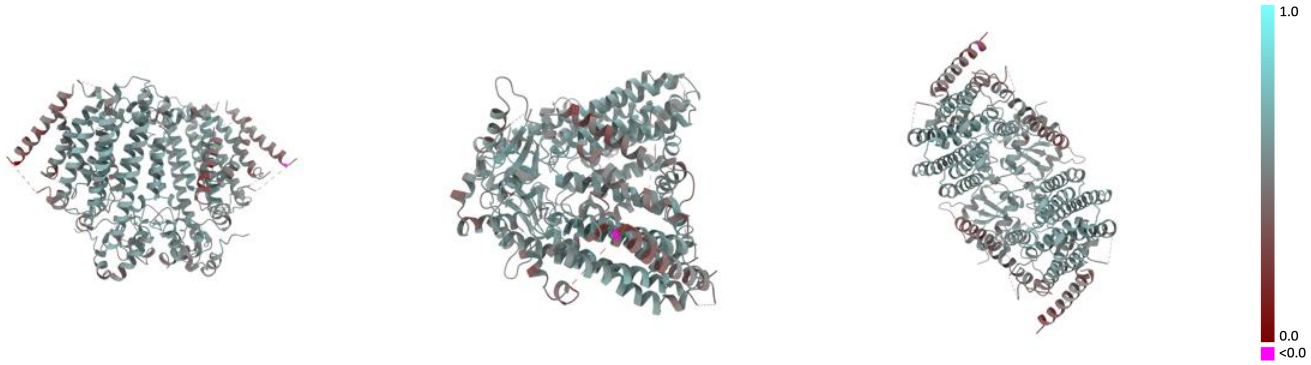
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0184 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.

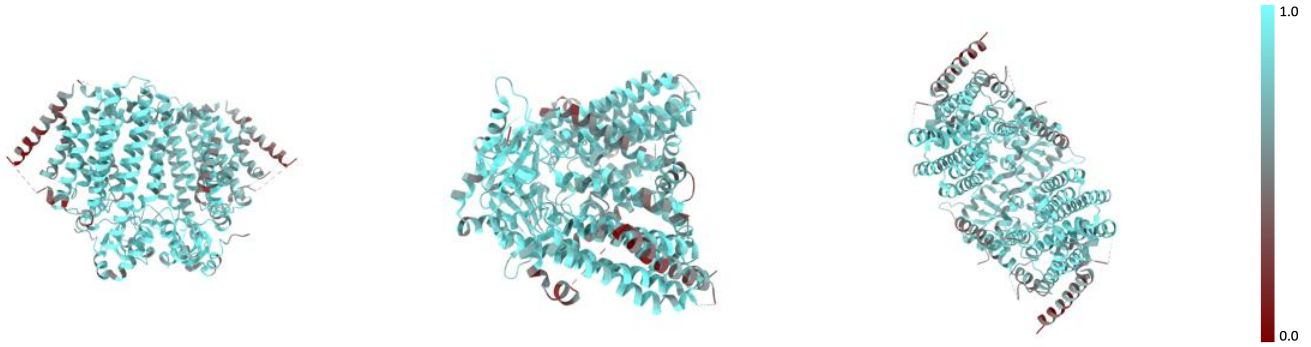
9.2 Q-score mapped to coordinate model (i)



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.

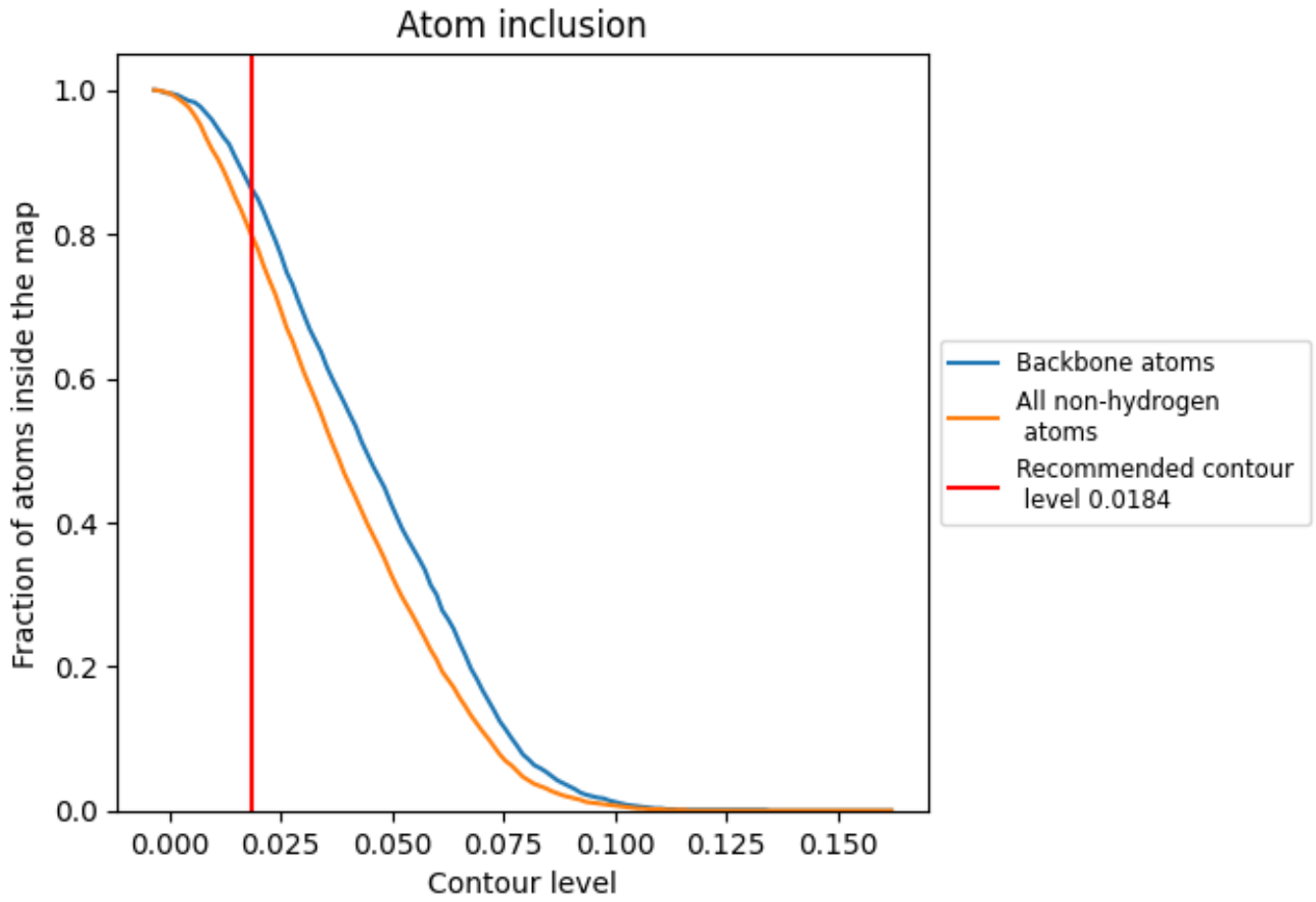
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0184).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.0184) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.5300
A	0.7990	0.5300
B	0.8000	0.5300