Full wwPDB EM Validation Report (i)

Aug 26, 2026 – 04:47 pm BST

PDB ID	:	9SE4 / pdb_00009se4
EMDB ID	:	EMD-54801
Title	:	E. coli cytochrome bd-I monomer
Authors	:	van der Velden, T.T.; Kayastha, K.; Bruenle, S.; Jeuken, L.J.C.
Deposited on	:	2025-08-15
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

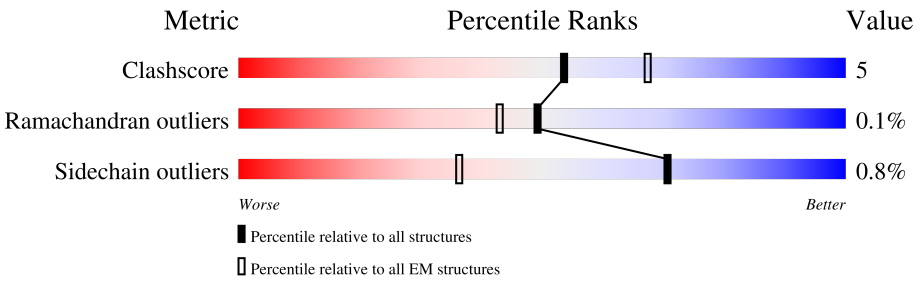
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

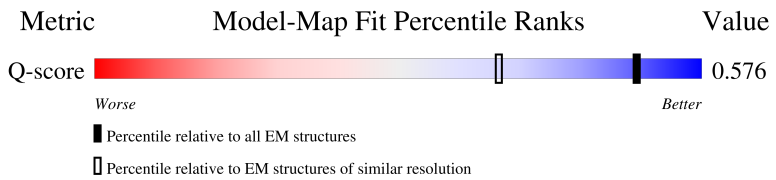
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	522	79% 8% 12%
2	B	379	88% 12%
3	H	29	79% 17%
4	X	37	76% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	A1JN4	A	601	X	-	-	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14633 atoms, of which 7284 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 Cytochrome bd-I ubiquinol oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	457	7175	2387	3565	583	617	23	0	0

- Molecule 2 is a protein called Cytochrome bd-I ubiquinol oxidase subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	379	6010	1986	3014	483	505	22	0	0

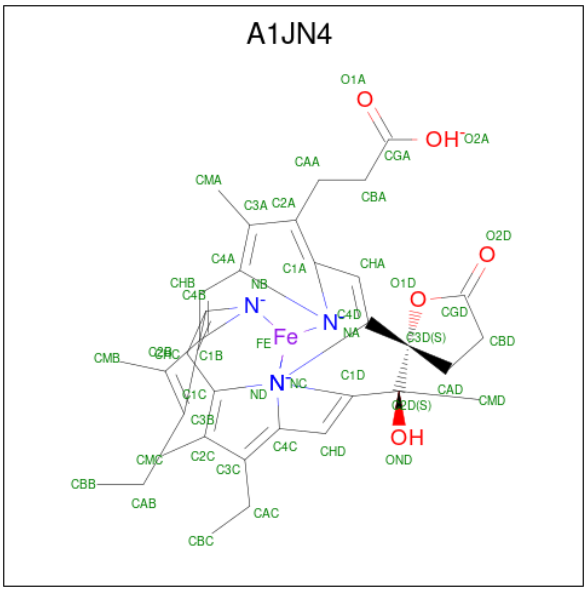
- Molecule 3 is a protein called Cytochrome bd-I ubiquinol oxidase CydH (Uncharacterized protein YnhF).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	H	29	432	139	222	32	38	1	0	0

- Molecule 4 is a protein called Cytochrome bd-I ubiquinol oxidase subunit X.

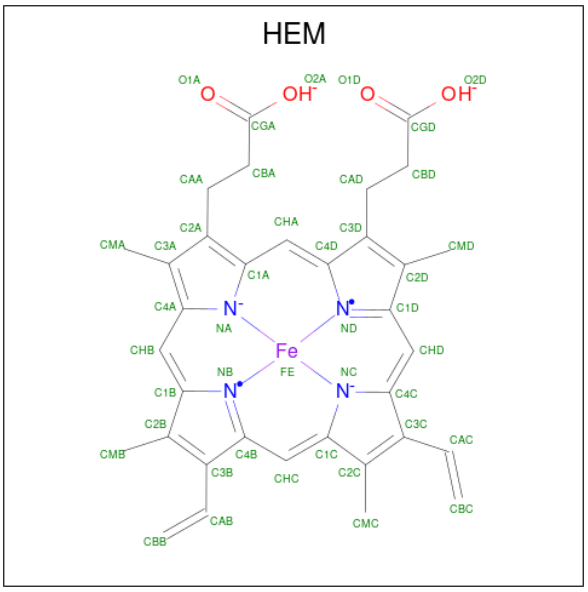
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	X	29	412	155	184	33	38	2	0	0

- Molecule 5 is TRANS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: A1JN4) (formula: $C_{34}H_{36}FeN_4O_5$).



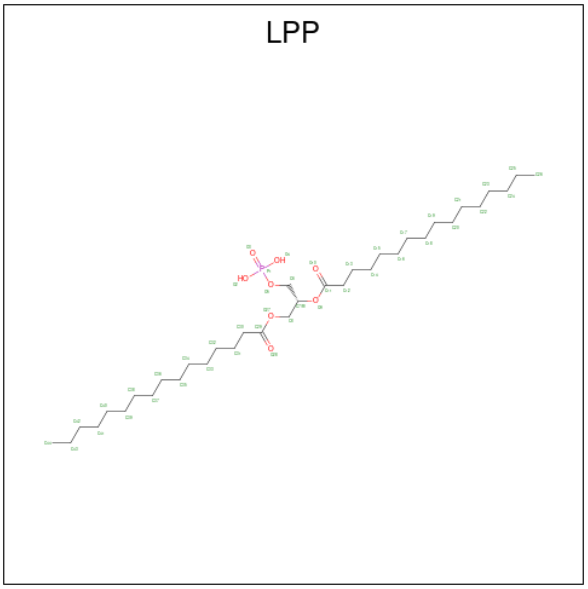
Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
5	A	1	75	34	1	31	4	5	0

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



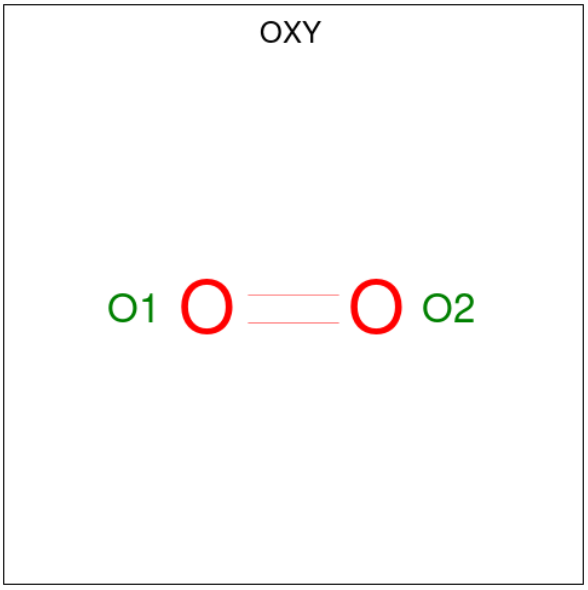
Mol	Chain	Residues	Atoms						AltConf
			Total	C	Fe	H	N	O	
6	A	1	73	34	1	30	4	4	0
			Total	C	Fe	H	N	O	
6	A	1	73	34	1	30	4	4	0

- Molecule 7 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$).



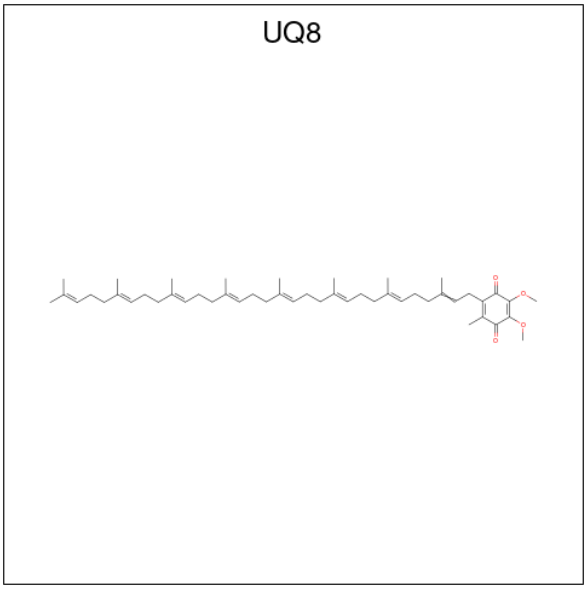
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	H	O	P	0
			111	35	67	8	1	
7	B	1	Total	C	H	O	P	0
			111	35	67	8	1	

- Molecule 8 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms		AltConf
			Total	O	
8	A	1	2	2	0

- Molecule 9 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
9	B	1	127	49	74	4	0

- Molecule 10 is water.

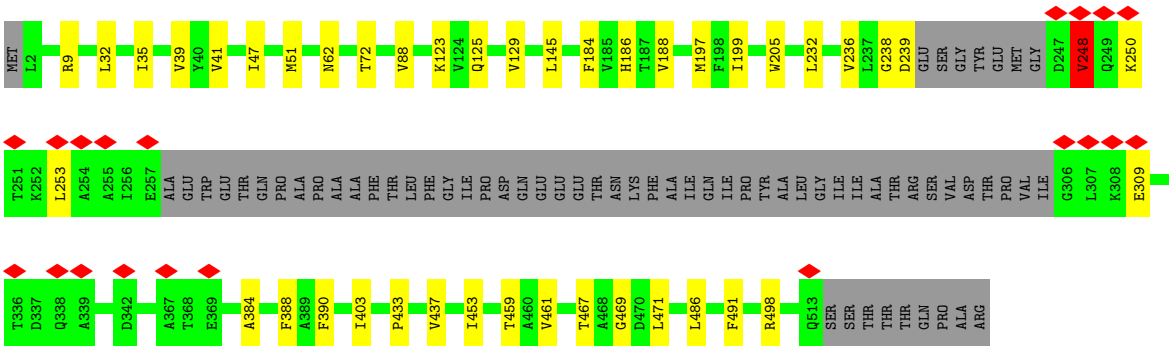
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
10	A	15	15	15	0
			Total	O	
10	B	17	17	17	0

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.

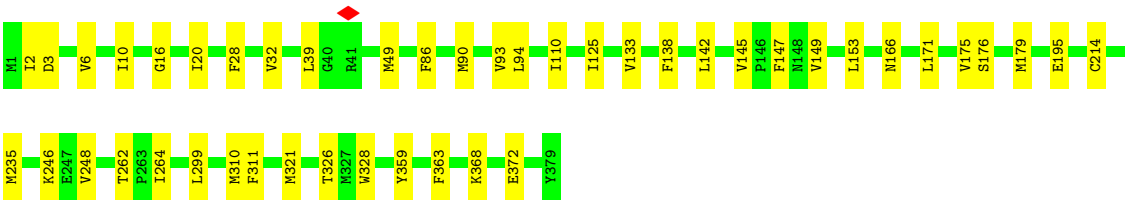
• Molecule 1: Cytochrome bd-I ubiquinol oxidase subunit 1

Chain A: 79% 8% 12%



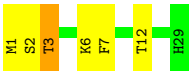
• Molecule 2: Cytochrome bd-I ubiquinol oxidase subunit 2

Chain B: 88% 12%



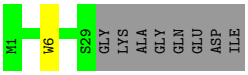
• Molecule 3: Cytochrome bd-I ubiquinol oxidase CydH (Uncharacterized protein YnhF)

Chain H: 79% 17%



• Molecule 4: Cytochrome bd-I ubiquinol oxidase subunit X

Chain X: 76% 22%


M1
W6
S29
GLY
LYS
ALA
GLY
GLN
GLU
ASP
ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	399575	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.555	Depositor
Minimum map value	-0.356	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0619	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A1JN4, HEM, LPP, OXY, UQ8

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	0.17	0/3702	0.33	2/5012 (0.0%)
2	B	0.16	0/3083	0.32	0/4212
3	H	0.83	2/211 (0.9%)	0.49	0/286
4	X	0.13	0/235	0.20	0/321
All	All	0.21	2/7231 (0.0%)	0.33	2/9831 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	SER	CA-C	-5.73	1.45	1.53
3	H	3	THR	N-CA	-5.29	1.39	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	390	PHE	CA-C-N	6.61	129.03	120.44
1	A	390	PHE	C-N-CA	6.61	129.03	120.44

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	3610	3565	3656	30	0
2	B	2996	3014	3025	32	0
3	H	210	222	238	4	0
4	X	228	184	227	1	0
5	A	44	31	0	0	0
6	A	86	60	60	11	0
7	A	44	67	67	4	0
7	B	44	67	67	5	0
8	A	2	0	0	0	0
9	B	53	74	74	9	0
10	A	15	0	0	0	0
10	B	17	0	0	0	0
All	All	7349	7284	7414	76	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 5.

All (76) 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)
6:A:602:HEM:HMC2	6:A:602:HEM:HBC2	1.61	0.83
2:B:16:GLY:HA3	9:B:402:UQ8:H45B	1.69	0.74
1:A:188:VAL:HG11	4:X:6:TRP:HE1	1.53	0.73
3:H:1:MET:HG2	3:H:6:LYS:HG3	1.72	0.70
6:A:603:HEM:HMC1	6:A:603:HEM:HBC2	1.78	0.66
3:H:1:MET:HG2	3:H:6:LYS:CG	2.28	0.64
1:A:309:GLU:H	1:A:309:GLU:CD	2.08	0.61
7:A:604:LPP:H263	7:A:604:LPP:H441	1.84	0.60
2:B:359:TYR:CE1	7:B:401:LPP:H342	2.37	0.59
2:B:326:THR:HG22	2:B:328:TRP:H	1.67	0.59
1:A:62:ASN:OD1	7:A:604:LPP:H261	2.02	0.59
1:A:491:PHE:HE2	2:B:110:ILE:HD11	1.68	0.59
2:B:179:MET:SD	2:B:299:LEU:HD23	2.43	0.59
2:B:359:TYR:CD1	7:B:401:LPP:H322	2.39	0.57
6:A:602:HEM:HMB1	6:A:602:HEM:HBB2	1.86	0.57
2:B:142:LEU:HD11	9:B:402:UQ8:C1M	2.36	0.56
2:B:235:MET:HE1	2:B:326:THR:HG21	1.88	0.56
1:A:232:LEU:O	1:A:236:VAL:HG22	2.06	0.55
9:B:402:UQ8:C1M	9:B:402:UQ8:C8	2.84	0.55
1:A:197:MET:HE1	1:A:403:ILE:HG21	1.89	0.55
1:A:186:HIS:HE1	1:A:238:GLY:HA2	1.72	0.54
1:A:186:HIS:CE1	1:A:238:GLY:HA2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:PHE:CZ	9:B:402:UQ8:H20B	2.42	0.54
2:B:175:VAL:HG22	2:B:214:CYS:HB3	1.89	0.54
1:A:467:THR:HG22	1:A:469:GLY:H	1.74	0.53
1:A:186:HIS:CE1	1:A:239:ASP:H	2.28	0.51
1:A:498:ARG:HG2	7:A:604:LPP:H122	1.93	0.51
1:A:145:LEU:HD13	1:A:184:PHE:HA	1.93	0.50
1:A:248:VAL:HG12	1:A:250:LYS:HE3	1.92	0.50
6:A:603:HEM:HHC	6:A:603:HEM:HBB2	1.94	0.49
2:B:138:PHE:CZ	9:B:402:UQ8:C20	2.95	0.49
1:A:72:THR:HA	2:B:94:LEU:HD21	1.95	0.49
9:B:402:UQ8:H4MA	9:B:402:UQ8:O3	2.12	0.49
1:A:32:LEU:HD13	1:A:199:ILE:HD12	1.95	0.49
6:A:602:HEM:HBB2	6:A:602:HEM:CMB	2.44	0.48
1:A:461:VAL:HG12	1:A:461:VAL:O	2.13	0.48
3:H:3:THR:HG23	3:H:7:PHE:CZ	2.48	0.48
1:A:35:ILE:O	1:A:39:VAL:HG23	2.14	0.47
2:B:149:VAL:HG13	2:B:153:LEU:HA	1.96	0.47
1:A:125:GLN:O	1:A:129:VAL:HG23	2.13	0.47
1:A:486:LEU:HD23	3:H:12:THR:HG23	1.96	0.47
2:B:248:VAL:HB	2:B:321:MET:O	2.14	0.47
2:B:28:PHE:O	2:B:32:VAL:HG23	2.14	0.47
1:A:437:VAL:HG12	6:A:602:HEM:HAC	1.97	0.46
2:B:145:VAL:HG23	2:B:147:PHE:HD1	1.79	0.46
2:B:171:LEU:O	2:B:175:VAL:HG23	2.15	0.46
6:A:602:HEM:HBA1	6:A:602:HEM:HHA	1.96	0.46
2:B:363:PHE:CE2	7:B:401:LPP:O9	2.69	0.45
1:A:205:TRP:CZ2	7:A:604:LPP:HC62	2.52	0.45
2:B:368:LYS:O	2:B:372:GLU:HG2	2.17	0.45
2:B:138:PHE:CD1	9:B:402:UQ8:H17	2.52	0.45
9:B:402:UQ8:C8	9:B:402:UQ8:H1MB	2.47	0.44
6:A:603:HEM:HBC2	6:A:603:HEM:CMC	2.44	0.44
2:B:142:LEU:HD11	9:B:402:UQ8:H1MB	2.00	0.44
2:B:93:VAL:HG23	2:B:133:VAL:HG11	1.99	0.44
1:A:384:ALA:O	1:A:388:PHE:HD2	2.01	0.44
6:A:603:HEM:HBB2	6:A:603:HEM:CHC	2.47	0.44
2:B:20:ILE:HG22	7:B:401:LPP:H442	1.99	0.43
2:B:2:ILE:HG22	2:B:3:ASP:N	2.32	0.43
2:B:262:THR:HG22	2:B:264:ILE:HG22	1.99	0.43
1:A:9:ARG:HD3	1:A:459:THR:HG21	2.00	0.43
1:A:47:ILE:O	1:A:51:MET:HG3	2.19	0.42
2:B:86:PHE:O	2:B:90:MET:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:602:HEM:HBC2	6:A:602:HEM:CMC	2.39	0.42
2:B:6:VAL:HG12	2:B:10:ILE:HD12	2.02	0.42
2:B:359:TYR:HD1	7:B:401:LPP:H322	1.81	0.42
1:A:248:VAL:HG12	1:A:250:LYS:NZ	2.35	0.41
1:A:88:VAL:HG11	1:A:453:ILE:HG13	2.03	0.41
2:B:310:MET:O	2:B:311:PHE:C	2.64	0.41
1:A:433:PRO:O	1:A:437:VAL:HG13	2.21	0.41
2:B:39:LEU:C	2:B:49:MET:HE1	2.46	0.41
2:B:195:GLU:OE2	2:B:195:GLU:O	2.39	0.41
1:A:239:ASP:HB3	6:A:602:HEM:C3A	2.56	0.41
2:B:176:SER:HA	2:B:179:MET:HE2	2.02	0.41
1:A:41:VAL:HG22	1:A:123:LYS:HG2	2.02	0.40
1:A:248:VAL:HG12	1:A:250:LYS:CE	2.51	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	451/522 (86%)	440 (98%)	10 (2%)	1 (0%)	43	63
2	B	377/379 (100%)	364 (97%)	13 (3%)	0	100	100
3	H	27/29 (93%)	27 (100%)	0	0	100	100
4	X	27/37 (73%)	27 (100%)	0	0	100	100
All	All	882/967 (91%)	858 (97%)	23 (3%)	1 (0%)	49	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	VAL

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	373/426 (88%)	370 (99%)	3 (1%)	73	88
2	B	313/313 (100%)	310 (99%)	3 (1%)	68	86
3	H	24/24 (100%)	24 (100%)	0	100	100
4	X	23/28 (82%)	23 (100%)	0	100	100
All	All	733/791 (93%)	727 (99%)	6 (1%)	70	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	VAL
1	A	253	LEU
1	A	471	LEU
2	B	125	ILE
2	B	166	ASN
2	B	246	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	76	GLN
1	A	80	ASN
1	A	86	HIS
1	A	186	HIS
2	B	143	GLN
2	B	160	ASN
2	B	374	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	HEM	A	603	1	50,50,50	1.48	6 (12%)	66,82,82	1.21	7 (10%)
9	UQ8	B	402	-	53,53,53	1.09	2 (3%)	64,67,67	1.60	16 (25%)
7	LPP	A	604	-	43,43,43	0.90	2 (4%)	47,48,48	1.41	7 (14%)
6	HEM	A	602	1	50,50,50	1.34	6 (12%)	66,82,82	1.26	8 (12%)
5	A1JN4	A	601	1	46,52,52	2.92	15 (32%)	62,89,89	4.87	38 (61%)
8	OXY	A	605	-	1,1,1	0.15	0	-		
7	LPP	B	401	-	43,43,43	0.95	3 (6%)	47,48,48	1.25	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEM	A	603	1	-	3/14/54/54	-
9	UQ8	B	402	-	-	14/51/75/75	0/1/1/1
7	LPP	A	604	-	-	15/45/45/45	-
6	HEM	A	602	1	-	4/14/54/54	-
5	A1JN4	A	601	1	2/2/12/12	4/9/89/89	0/1/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LPP	B	401	-	-	10/45/45/45	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	A1JN4	C3D-C2D	-11.96	1.25	1.55
9	B	402	UQ8	C6-C1	6.70	1.47	1.35
5	A	601	A1JN4	O1D-C3D	6.17	1.56	1.46
5	A	601	A1JN4	CBB-CAB	-5.83	1.25	1.51
5	A	601	A1JN4	CBC-CAC	-5.74	1.25	1.51
5	A	601	A1JN4	CBD-CGD	-4.32	1.41	1.50
7	B	401	LPP	O9-C11	4.31	1.46	1.34
5	A	601	A1JN4	O1D-CGD	-4.18	1.28	1.35
6	A	603	HEM	FE-NB	4.18	2.07	1.94
6	A	603	HEM	FE-ND	4.14	2.07	1.94
7	A	604	LPP	O27-C29	3.70	1.44	1.33
5	A	601	A1JN4	C1B-NB	-3.41	1.33	1.39
6	A	602	HEM	FE-NB	3.30	2.05	1.94
5	A	601	A1JN4	OND-C2D	3.24	1.49	1.42
5	A	601	A1JN4	CAD-C3D	3.13	1.59	1.53
6	A	602	HEM	FE-NC	3.01	2.05	1.95
7	A	604	LPP	O9-C11	2.99	1.42	1.34
6	A	603	HEM	FE-NA	2.95	2.05	1.95
5	A	601	A1JN4	C4C-NC	-2.91	1.34	1.39
6	A	603	HEM	CAC-C3C	2.89	1.55	1.47
6	A	602	HEM	CAB-C3B	2.87	1.55	1.47
7	B	401	LPP	O27-C29	2.75	1.41	1.33
6	A	603	HEM	FE-NC	2.74	2.04	1.95
6	A	602	HEM	CAC-C3C	2.71	1.54	1.47
9	B	402	UQ8	C4-C3	2.70	1.47	1.36
6	A	603	HEM	CAB-C3B	2.69	1.54	1.47
6	A	602	HEM	FE-ND	2.60	2.02	1.94
5	A	601	A1JN4	C2A-C3A	-2.52	1.32	1.38
6	A	602	HEM	FE-NA	2.46	2.03	1.95
5	A	601	A1JN4	CHA-C1A	-2.22	1.34	1.39
7	B	401	LPP	O9-C7	-2.21	1.41	1.46
5	A	601	A1JN4	CMC-C2C	2.19	1.55	1.50
5	A	601	A1JN4	C1A-NA	-2.16	1.35	1.39
5	A	601	A1JN4	C4D-ND	-2.10	1.34	1.37

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	A1JN4	O1D-C3D-C4D	-12.17	83.52	108.25
5	A	601	A1JN4	C3B-C4B-NB	-10.53	100.08	110.32
5	A	601	A1JN4	O1D-C3D-CAD	-10.06	84.10	103.01
5	A	601	A1JN4	CHD-C1D-ND	9.87	138.67	124.20
5	A	601	A1JN4	C4C-NC-C1C	9.38	114.53	105.35
5	A	601	A1JN4	C4B-NB-C1B	9.19	114.35	105.35
5	A	601	A1JN4	O1D-CGD-CBD	-9.14	100.97	110.19
5	A	601	A1JN4	OND-C2D-CMD	-8.20	94.49	109.59
5	A	601	A1JN4	CAC-C3C-C4C	-7.96	113.86	124.92
5	A	601	A1JN4	CHC-C4B-NB	7.79	132.86	124.44
5	A	601	A1JN4	C3C-C4C-NC	-7.02	102.30	110.15
5	A	601	A1JN4	C4B-C3B-C2B	6.71	115.88	107.13
5	A	601	A1JN4	C2A-C1A-NA	-6.58	102.80	110.15
5	A	601	A1JN4	C4A-NA-C1A	5.76	110.99	105.35
5	A	601	A1JN4	CAB-C3B-C4B	-5.76	115.61	124.68
5	A	601	A1JN4	CHB-C1B-NB	5.47	130.36	124.44
5	A	601	A1JN4	C1A-C2A-C3A	5.44	115.45	106.89
5	A	601	A1JN4	O1A-CGA-CBA	-5.11	106.66	123.08
5	A	601	A1JN4	CHD-C4C-NC	4.71	132.51	123.85
5	A	601	A1JN4	CHA-C4D-ND	-4.71	117.30	124.20
5	A	601	A1JN4	CAC-C3C-C2C	4.50	134.06	126.86
5	A	601	A1JN4	O2A-CGA-O1A	4.44	134.37	123.30
5	A	601	A1JN4	C2D-C1D-CHD	-4.11	117.50	124.28
5	A	601	A1JN4	C4A-C3A-C2A	-4.02	102.13	106.83
7	A	604	LPP	O9-C11-C12	3.91	119.93	111.50
7	B	401	LPP	O27-C29-C30	3.77	123.73	111.91
5	A	601	A1JN4	OND-C2D-C3D	-3.64	101.39	110.45
5	A	601	A1JN4	C3D-C4D-CHA	3.58	134.98	124.34
7	B	401	LPP	O27-C29-O28	-3.54	114.66	123.59
9	B	402	UQ8	C15-C14-C16	3.49	121.14	115.27
5	A	601	A1JN4	C4C-C3C-C2C	3.29	112.07	106.89
5	A	601	A1JN4	CBB-CAB-C3B	3.24	121.36	112.43
6	A	602	HEM	C4A-NA-C1A	3.23	108.51	105.35
5	A	601	A1JN4	CAA-CBA-CGA	-3.17	106.77	113.60
7	B	401	LPP	O9-C11-C12	3.15	118.30	111.50
9	B	402	UQ8	C22-C23-C24	-3.12	120.14	127.66
9	B	402	UQ8	C10-C9-C11	3.12	120.52	115.27
7	A	604	LPP	P1-O5-C6	3.10	126.83	118.30
5	A	601	A1JN4	C1B-C2B-C3B	-3.10	102.42	106.94
6	A	602	HEM	C4D-ND-C1D	3.06	108.23	105.07
9	B	402	UQ8	C27-C28-C29	-3.03	120.36	127.66
9	B	402	UQ8	C37-C38-C39	-2.98	120.48	127.66
5	A	601	A1JN4	CAA-C2A-C1A	-2.96	119.05	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	602	HEM	C4C-NC-C1C	2.94	108.23	105.35
6	A	603	HEM	C1B-NB-C4B	2.91	108.08	105.07
5	A	601	A1JN4	C1C-CHC-C4B	-2.90	115.77	124.74
9	B	402	UQ8	C32-C33-C34	-2.89	120.71	127.66
5	A	601	A1JN4	CHC-C1C-NC	2.87	129.12	123.85
5	A	601	A1JN4	C2C-C1C-NC	-2.78	105.85	110.08
5	A	601	A1JN4	CBA-CAA-C2A	-2.76	104.97	112.63
9	B	402	UQ8	C6-C1-C2	2.74	121.35	119.18
5	A	601	A1JN4	CAD-CBD-CGD	-2.72	100.36	104.56
6	A	602	HEM	C1B-NB-C4B	2.71	107.87	105.07
6	A	603	HEM	C4D-ND-C1D	2.71	107.87	105.07
9	B	402	UQ8	C12-C13-C14	-2.68	121.20	127.66
6	A	603	HEM	C4A-NA-C1A	2.67	107.97	105.35
9	B	402	UQ8	C40-C39-C41	2.62	119.67	115.27
9	B	402	UQ8	C7-C8-C9	-2.55	122.55	126.79
7	A	604	LPP	O27-C29-C30	2.54	119.87	111.91
6	A	603	HEM	C3B-C2B-C1B	2.52	108.36	106.49
7	A	604	LPP	C18-C17-C16	-2.50	101.71	114.42
9	B	402	UQ8	C25-C24-C26	2.50	119.48	115.27
6	A	603	HEM	C4C-NC-C1C	2.46	107.76	105.35
6	A	603	HEM	CAA-CBA-CGA	-2.41	108.41	113.60
9	B	402	UQ8	C35-C34-C36	2.34	119.21	115.27
6	A	602	HEM	C2A-C1A-NA	-2.32	107.55	110.15
9	B	402	UQ8	C7-C6-C5	2.25	121.18	118.48
7	A	604	LPP	O9-C11-O10	-2.24	118.28	123.70
9	B	402	UQ8	C1M-C1-C6	-2.23	120.76	124.40
5	A	601	A1JN4	CMA-C3A-C4A	2.22	128.75	125.37
7	A	604	LPP	C20-C19-C18	-2.19	103.29	114.42
6	A	602	HEM	C3D-C4D-ND	-2.19	107.73	110.17
5	A	601	A1JN4	CHA-C1A-C2A	2.18	130.12	125.36
7	A	604	LPP	C32-C31-C30	-2.17	105.38	113.19
9	B	402	UQ8	C11-C9-C8	-2.14	116.78	121.12
9	B	402	UQ8	C17-C18-C19	-2.14	122.51	127.66
6	A	602	HEM	C3B-C2B-C1B	2.12	108.06	106.49
6	A	603	HEM	C2A-C1A-NA	-2.06	107.84	110.15
6	A	602	HEM	CAD-CBD-CGD	-2.05	109.20	113.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	601	A1JN4	NB
5	A	601	A1JN4	ND

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	602	HEM	C1A-C2A-CAA-CBA
7	A	604	LPP	C6-O5-P1-O2
7	A	604	LPP	C6-O5-P1-O4
7	A	604	LPP	C12-C11-O9-C7
7	B	401	LPP	C6-O5-P1-O2
7	B	401	LPP	C6-O5-P1-O3
7	B	401	LPP	C6-O5-P1-O4
9	B	402	UQ8	C39-C41-C42-C43
5	A	601	A1JN4	C2C-C3C-CAC-CBC
5	A	601	A1JN4	C4C-C3C-CAC-CBC
7	A	604	LPP	O10-C11-O9-C7
9	B	402	UQ8	C12-C11-C9-C10
9	B	402	UQ8	C12-C11-C9-C8
7	A	604	LPP	C30-C29-O27-C8
7	A	604	LPP	O28-C29-O27-C8
7	A	604	LPP	C33-C34-C35-C36
7	B	401	LPP	C12-C13-C14-C15
7	A	604	LPP	C18-C19-C20-C21
7	B	401	LPP	C11-C12-C13-C14
7	A	604	LPP	C38-C39-C40-C41
7	B	401	LPP	C6-C7-C8-O27
9	B	402	UQ8	C1-C6-C7-C8
9	B	402	UQ8	C5-C6-C7-C8
7	A	604	LPP	C6-O5-P1-O3
7	A	604	LPP	C23-C24-C25-C26
7	B	401	LPP	O9-C7-C8-O27
6	A	602	HEM	C3A-C2A-CAA-CBA
7	A	604	LPP	C7-C6-O5-P1
7	B	401	LPP	C38-C39-C40-C41
7	A	604	LPP	O5-C6-C7-O9
9	B	402	UQ8	C40-C39-C41-C42
9	B	402	UQ8	C30-C29-C31-C32
7	B	401	LPP	C31-C32-C33-C34
6	A	603	HEM	C3D-CAD-CBD-CGD
9	B	402	UQ8	C28-C29-C31-C32
7	A	604	LPP	C6-C7-O9-C11
9	B	402	UQ8	C9-C11-C12-C13
6	A	602	HEM	CAD-CBD-CGD-O1D
9	B	402	UQ8	C29-C31-C32-C33
5	A	601	A1JN4	CAA-CBA-CGA-O1A
6	A	602	HEM	CAD-CBD-CGD-O2D
9	B	402	UQ8	C38-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
9	B	402	UQ8	C5-C4-O4-C4M
7	A	604	LPP	O5-C6-C7-C8
9	B	402	UQ8	C20-C19-C21-C22
6	A	603	HEM	CAA-CBA-CGA-O2A
6	A	603	HEM	CAA-CBA-CGA-O1A
9	B	402	UQ8	C36-C37-C38-C39
5	A	601	A1JN4	CAA-CBA-CGA-O2A
7	B	401	LPP	C20-C21-C22-C23

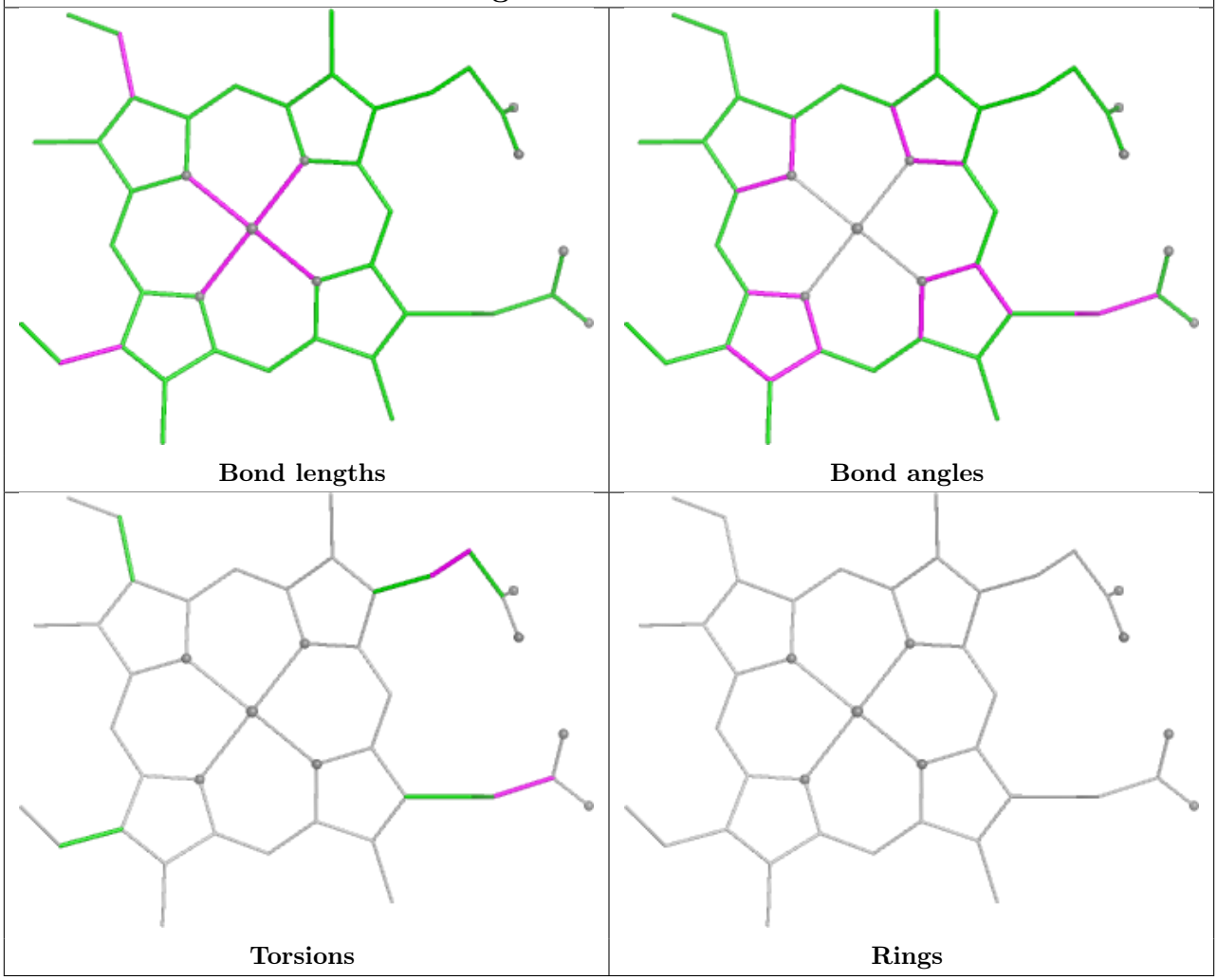
There are no ring outliers.

5 monomers are involved in 29 short contacts:

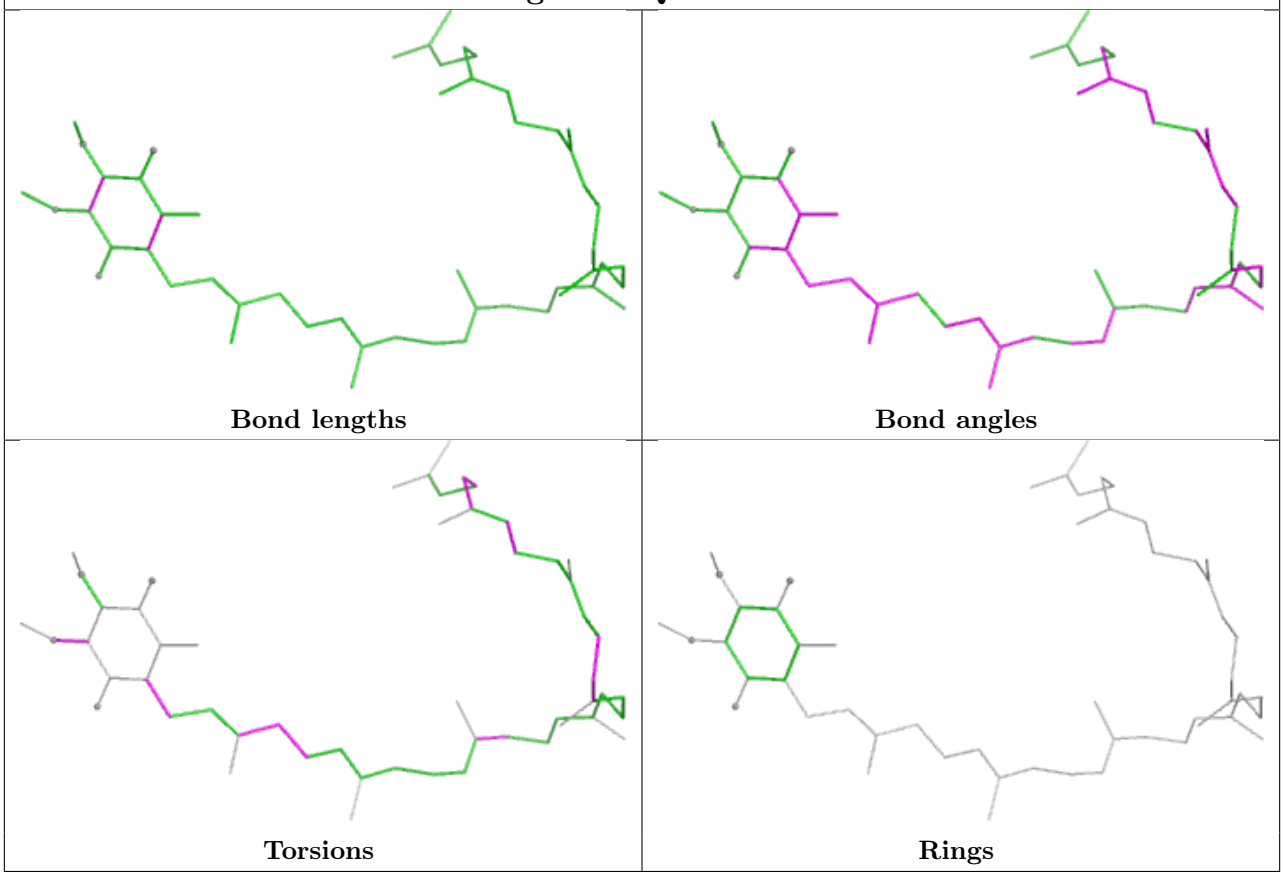
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	HEM	4	0
9	B	402	UQ8	9	0
7	A	604	LPP	4	0
6	A	602	HEM	7	0
7	B	401	LPP	5	0

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.

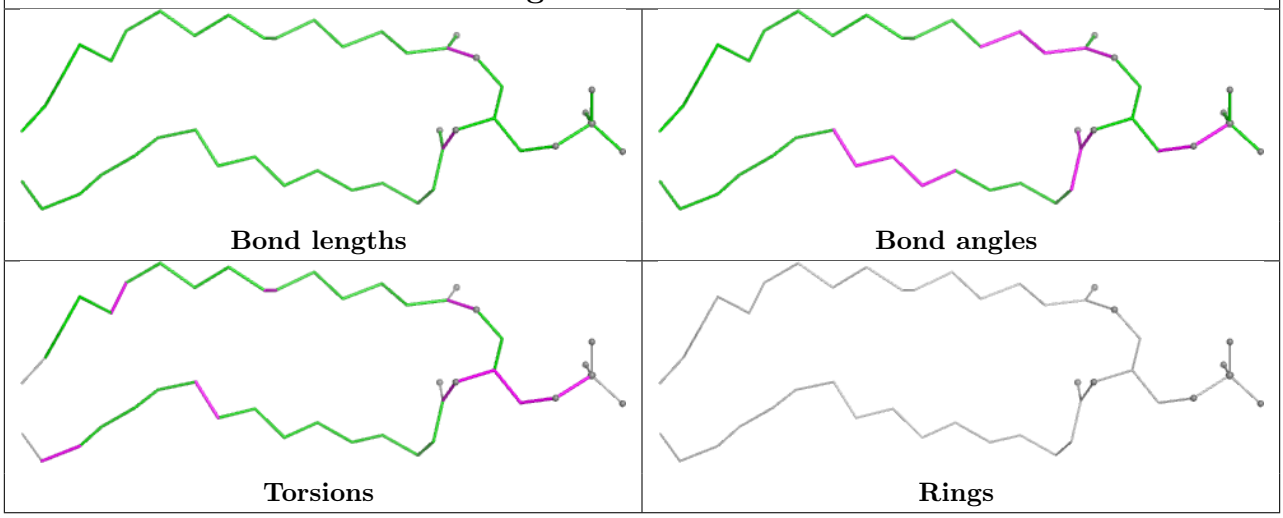
Ligand HEM A 603



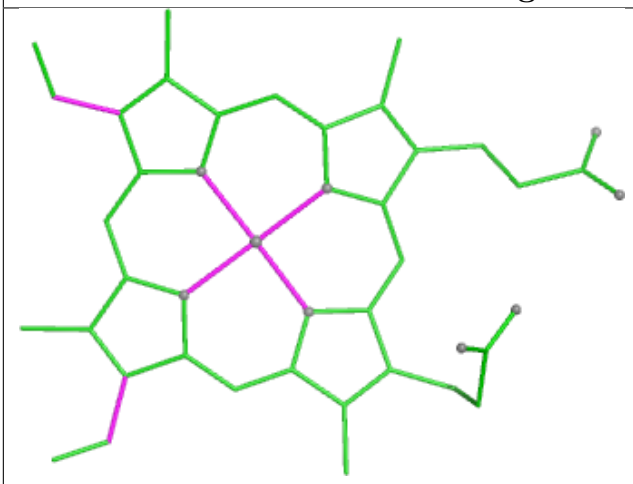
Ligand UQ8 B 402



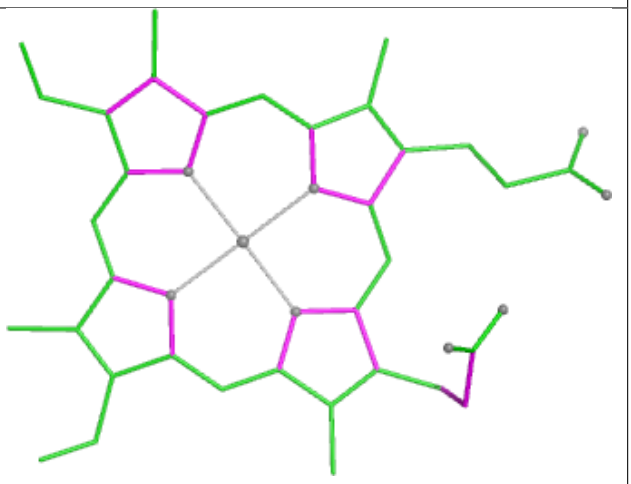
Ligand LPP A 604



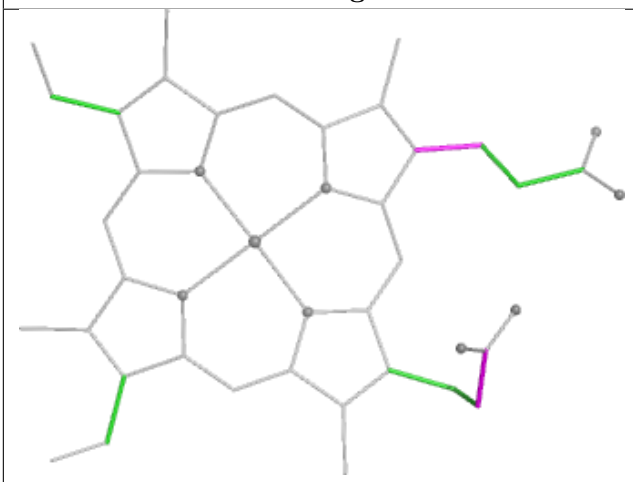
Ligand HEM A 602



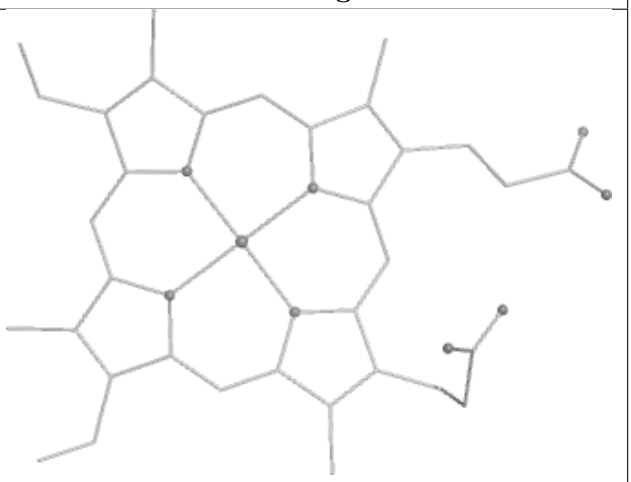
Bond lengths



Bond angles

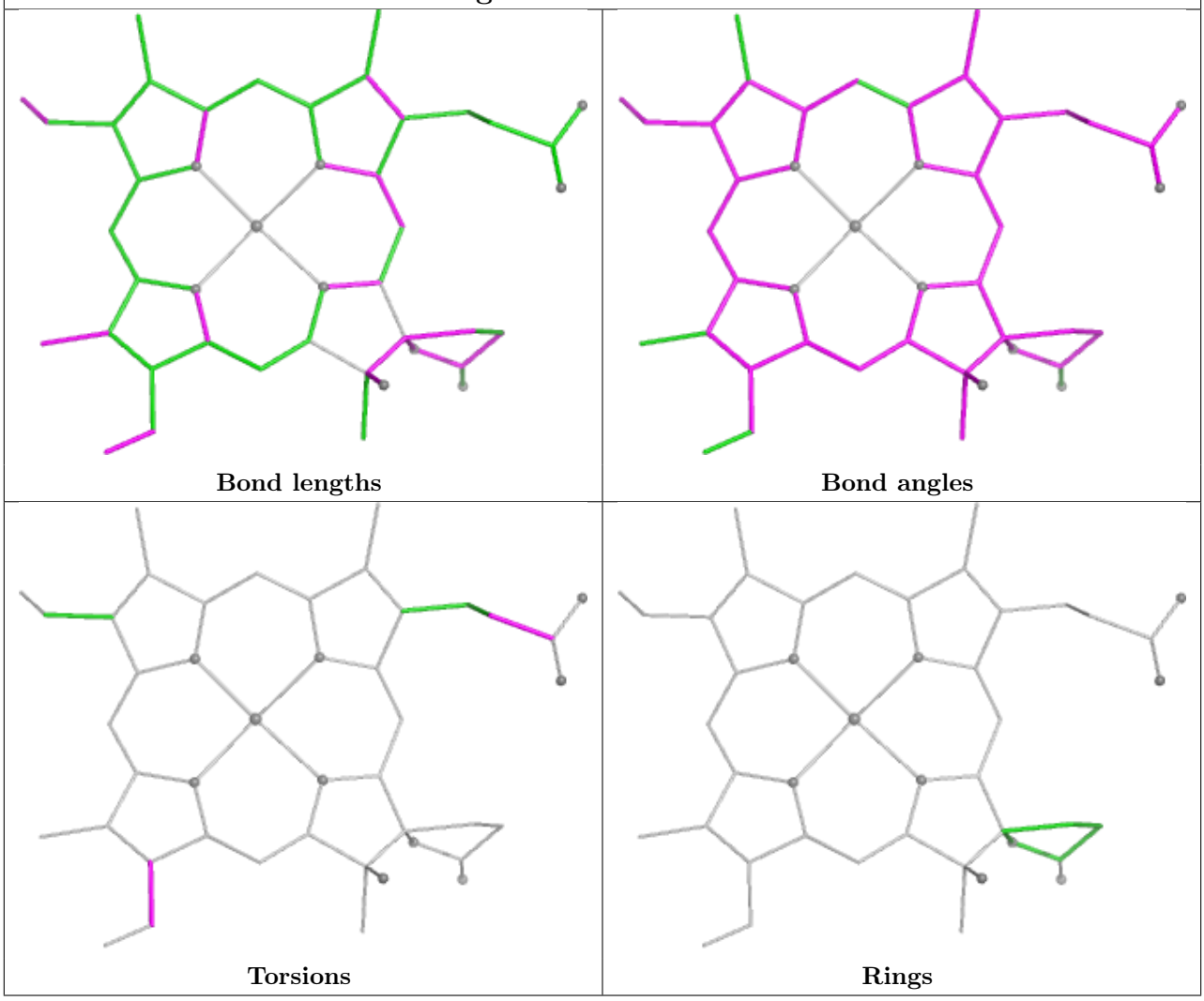


Torsions

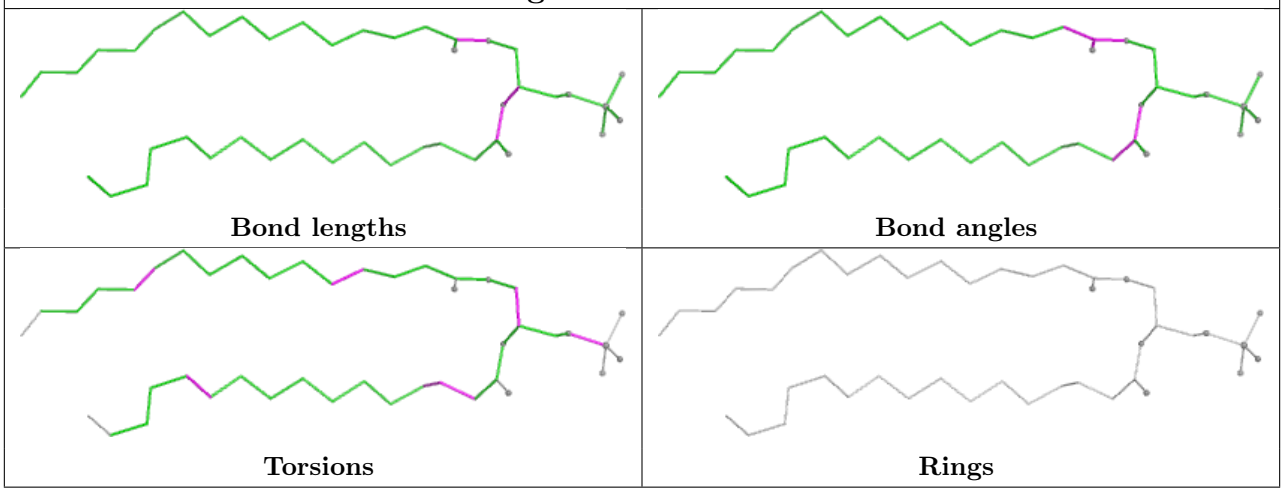


Rings

Ligand A1JN4 A 601



Ligand LPP B 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

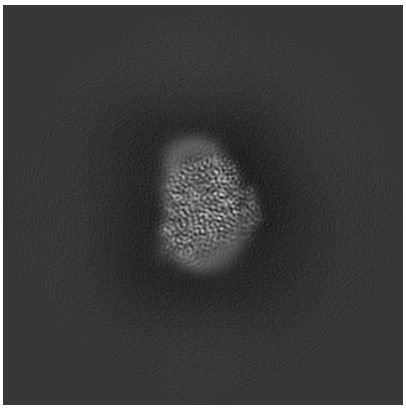
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-54801. These allow visual inspection of the internal detail of the map and identification of artifacts.

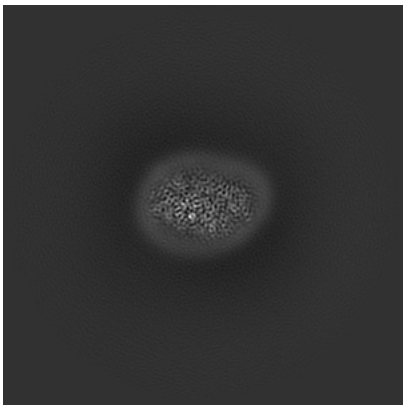
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

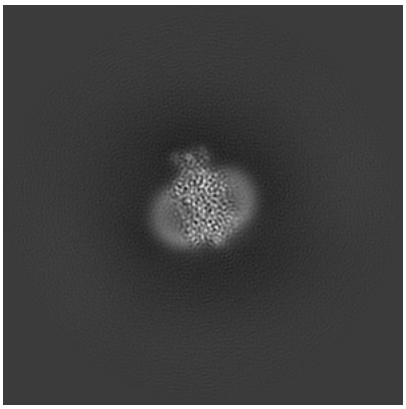
6.1.1 Primary map



X

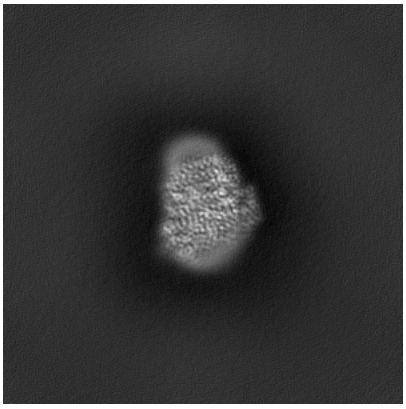


Y

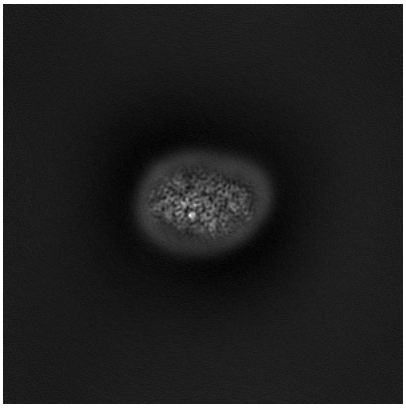


Z

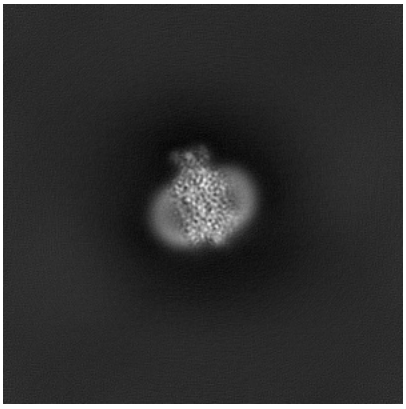
6.1.2 Raw map



X



Y

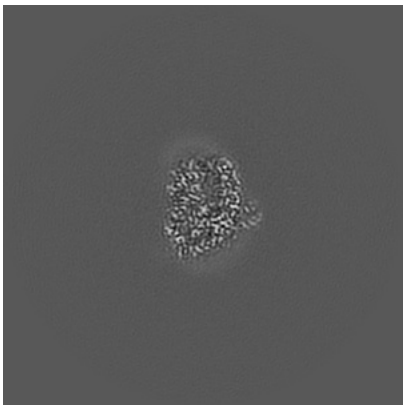


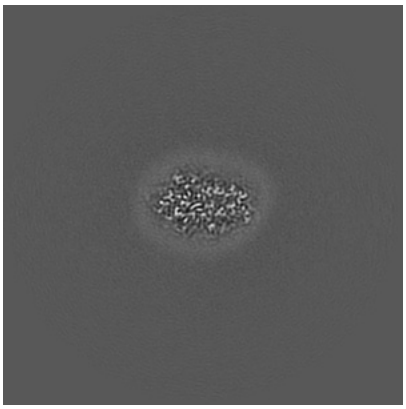
Z

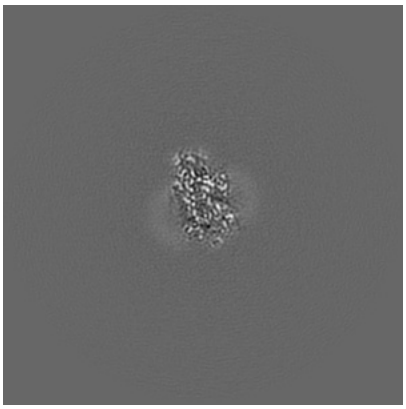
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

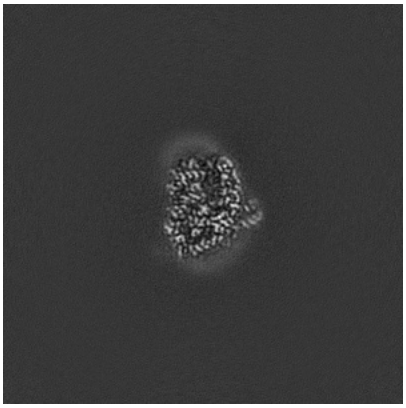
6.2.1 Primary map

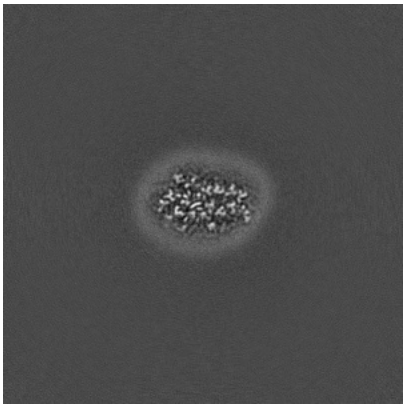

X Index: 180

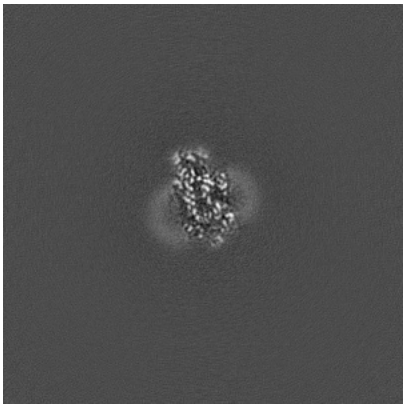

Y Index: 180


Z Index: 180

6.2.2 Raw map


X Index: 180

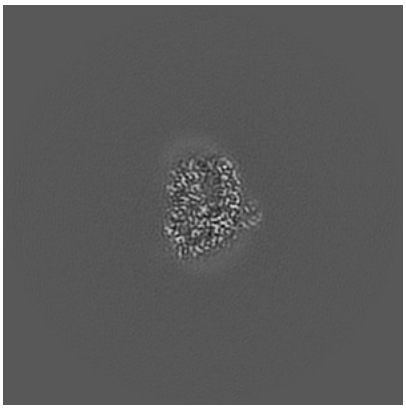

Y Index: 180

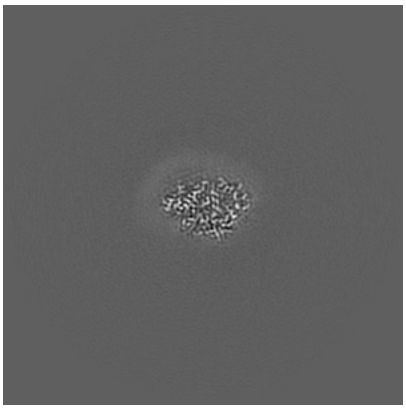

Z Index: 180

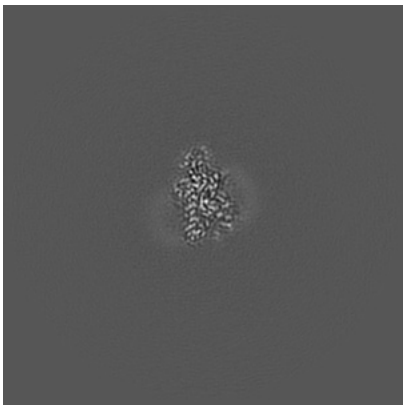
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

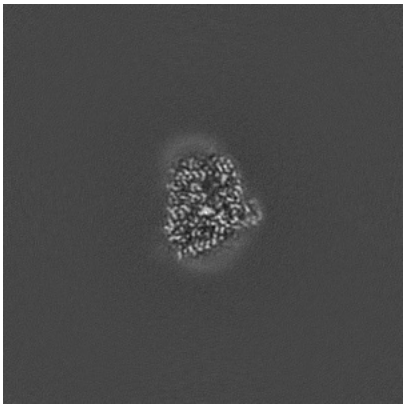
6.3.1 Primary map

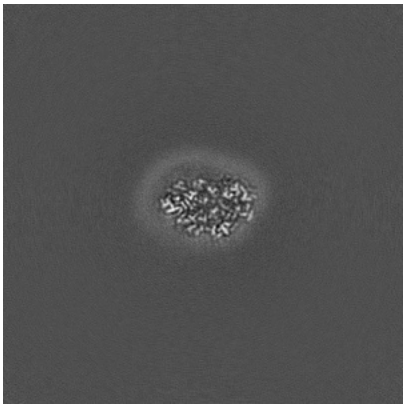

X Index: 180

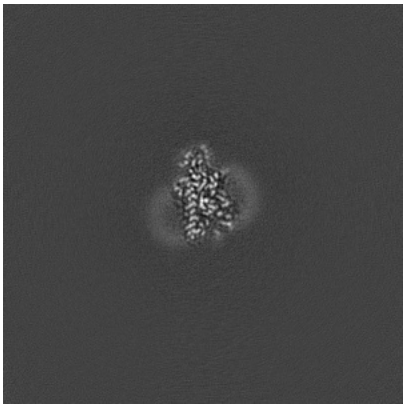

Y Index: 196


Z Index: 171

6.3.2 Raw map


X Index: 179

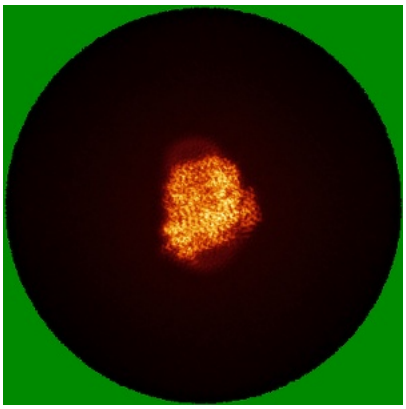

Y Index: 190

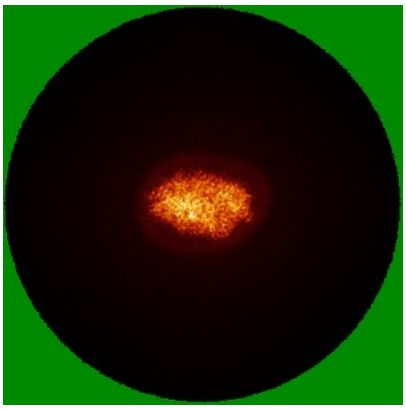

Z Index: 171

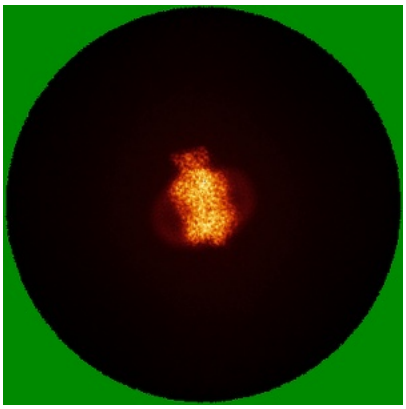
The images above show the largest variance slices of the map in three orthogonal directions.

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

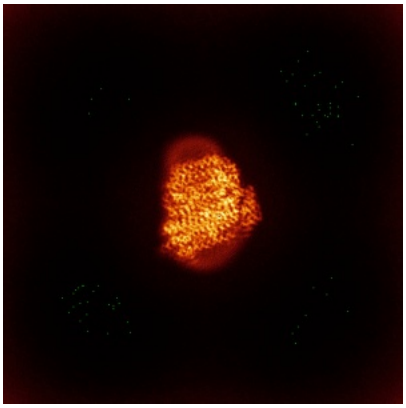
6.4.1 Primary map

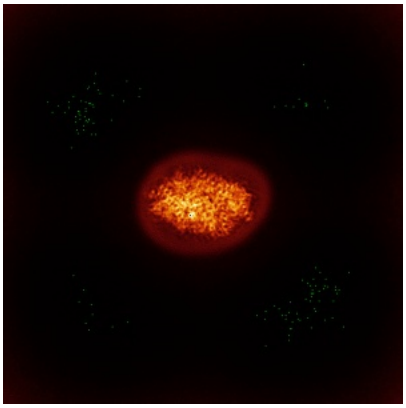

X

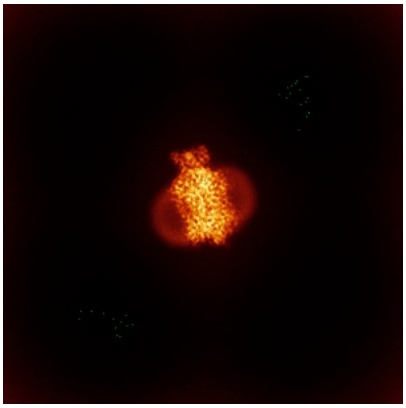

Y


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 0.0619. 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.

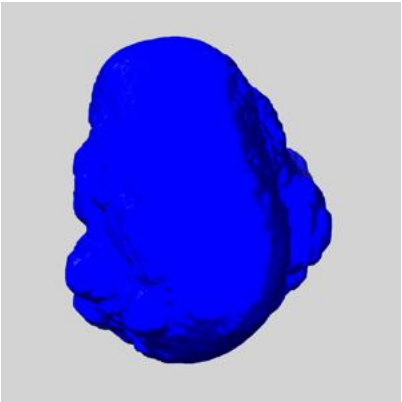
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

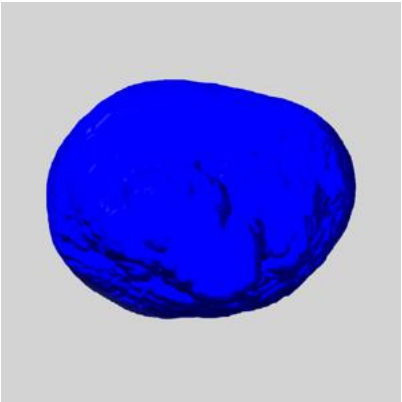
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

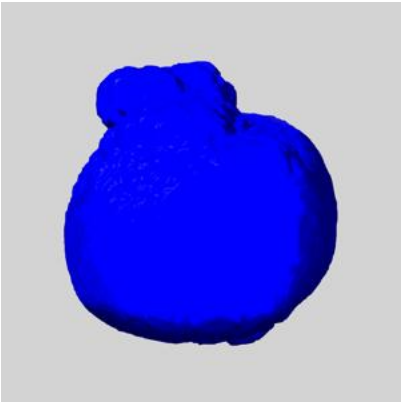
6.6.1 emd_54801_msk_1.map (i)



X



Y

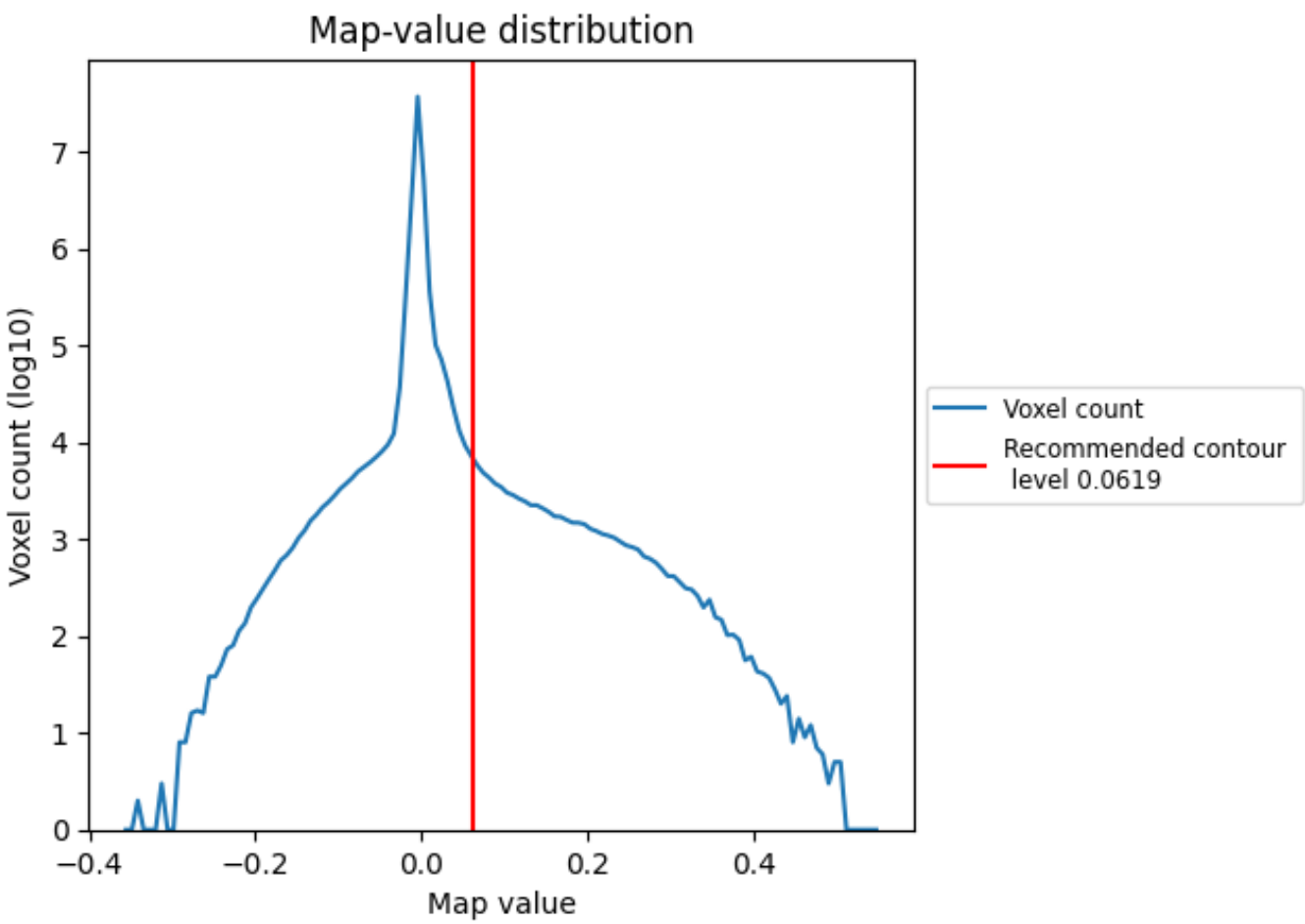


Z

7 Map analysis (i)

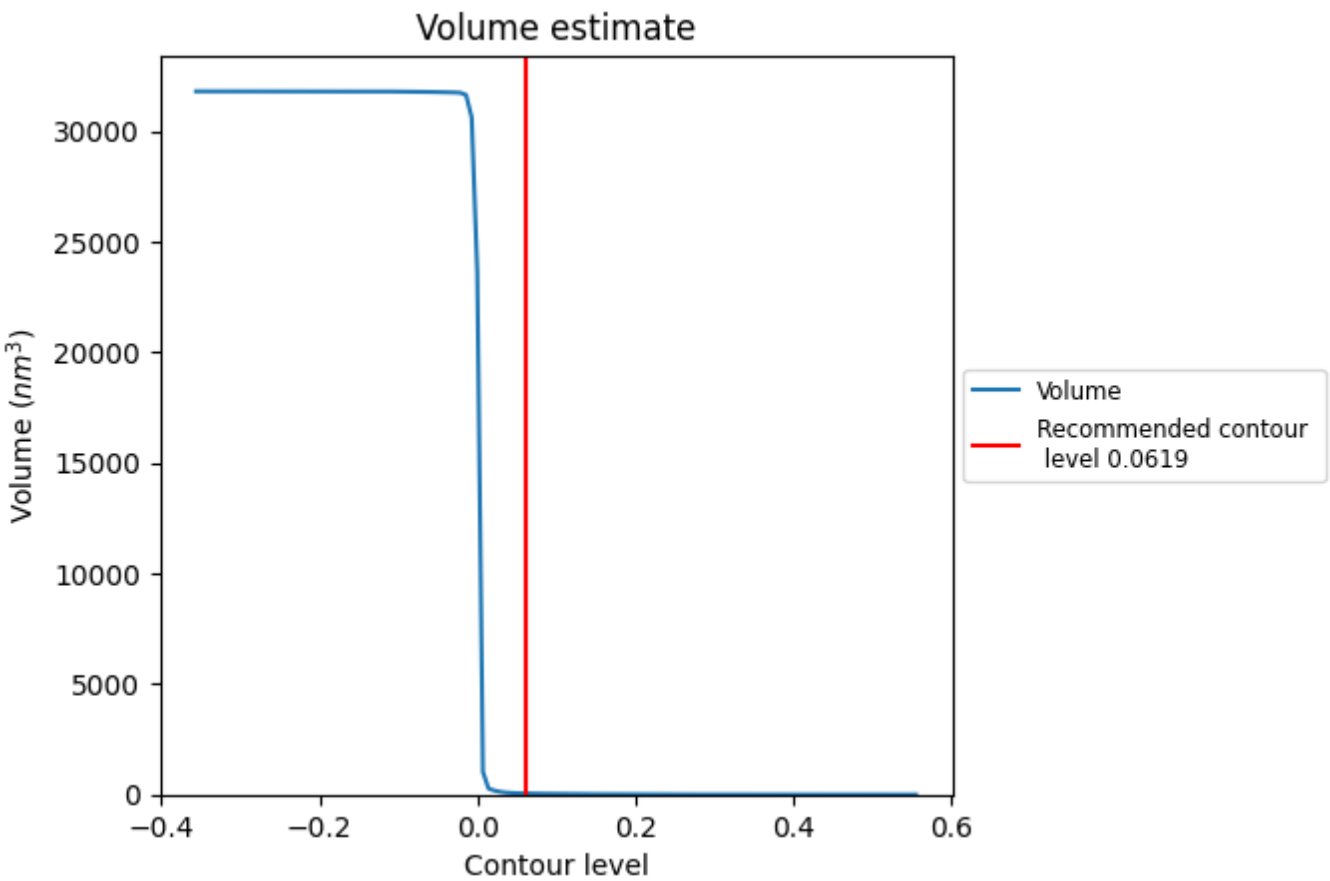
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

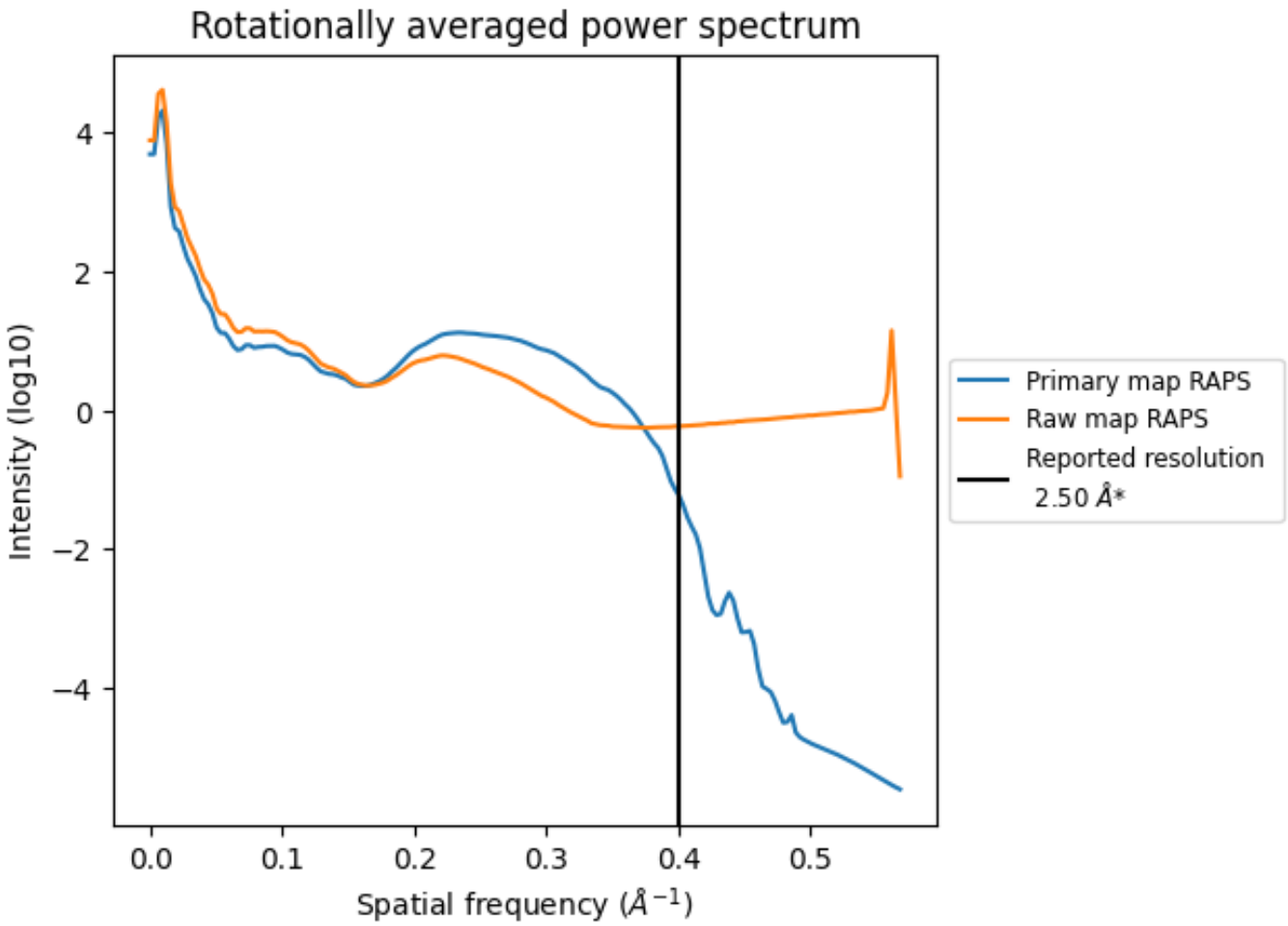
7.2 Volume estimate (i)



The volume at the recommended contour level is 48 nm^3; this corresponds to an approximate mass of 44 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)

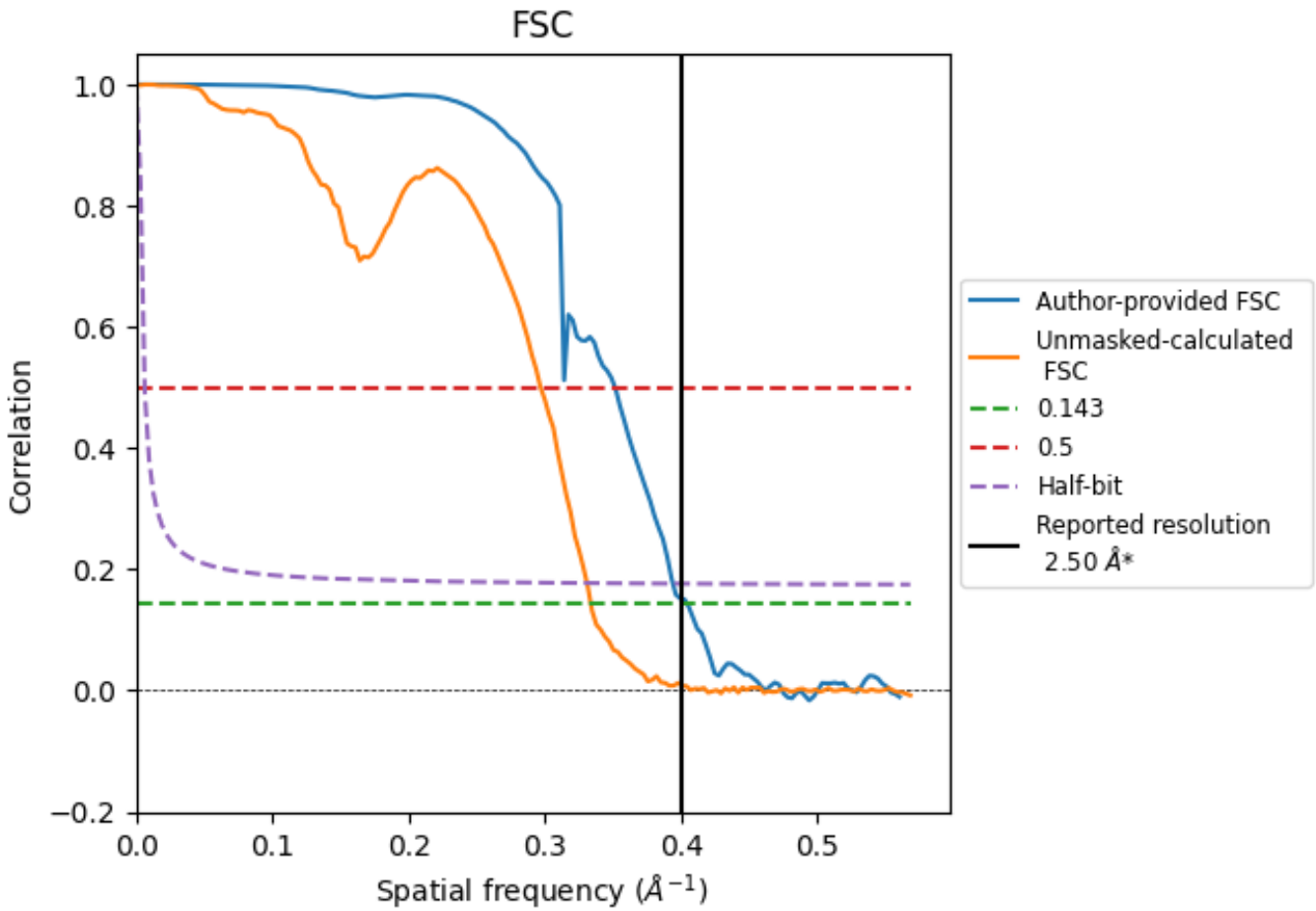


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates (i)

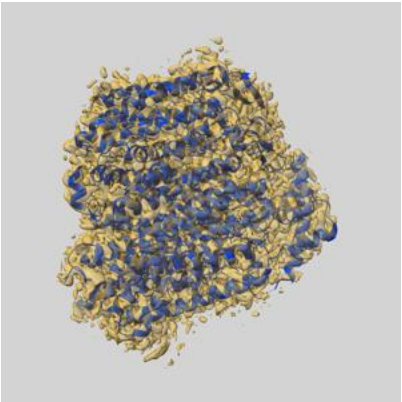
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.47	2.85	2.54
Unmasked-calculated*	3.00	3.37	3.02

*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 3.00 differs from the reported value 2.5 by more than 10 %

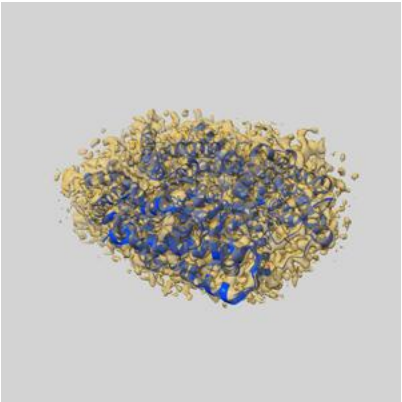
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-54801 and PDB model 9SE4. Per-residue inclusion information can be found in section 3 on page 8.

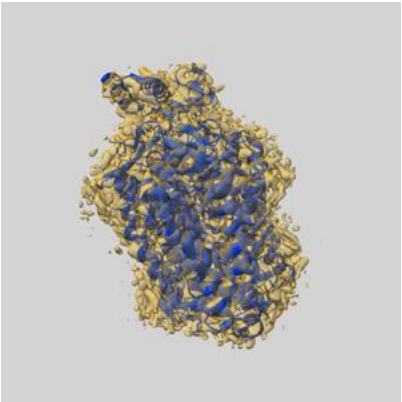
9.1 Map-model overlay (i)



X



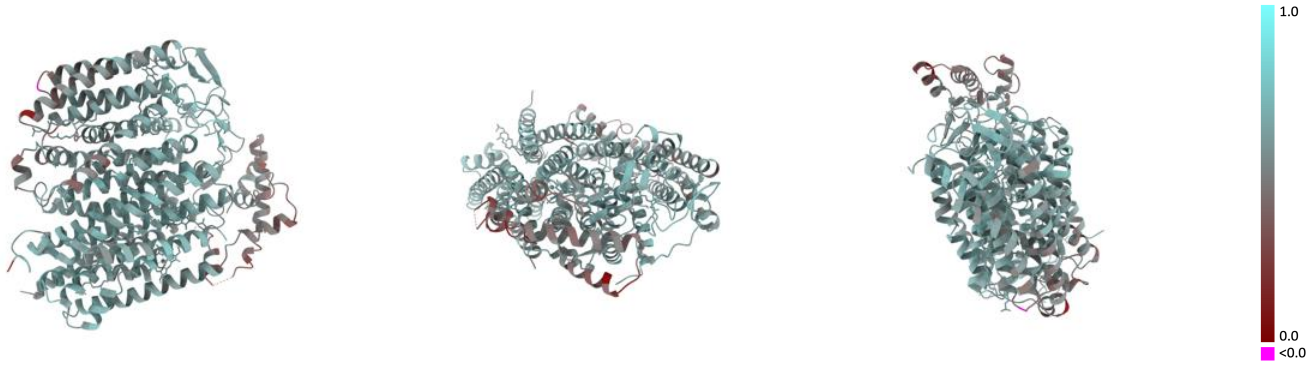
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0619 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.

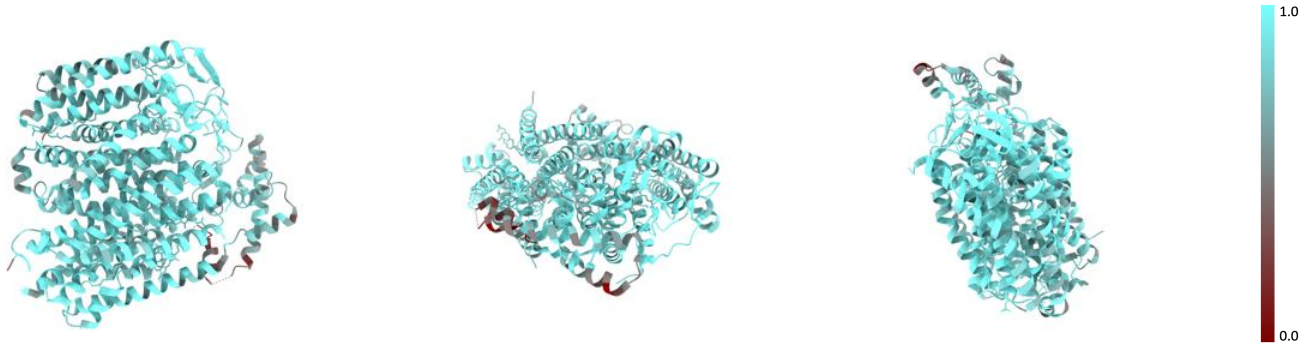
9.2 Q-score mapped to coordinate model (i)



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.

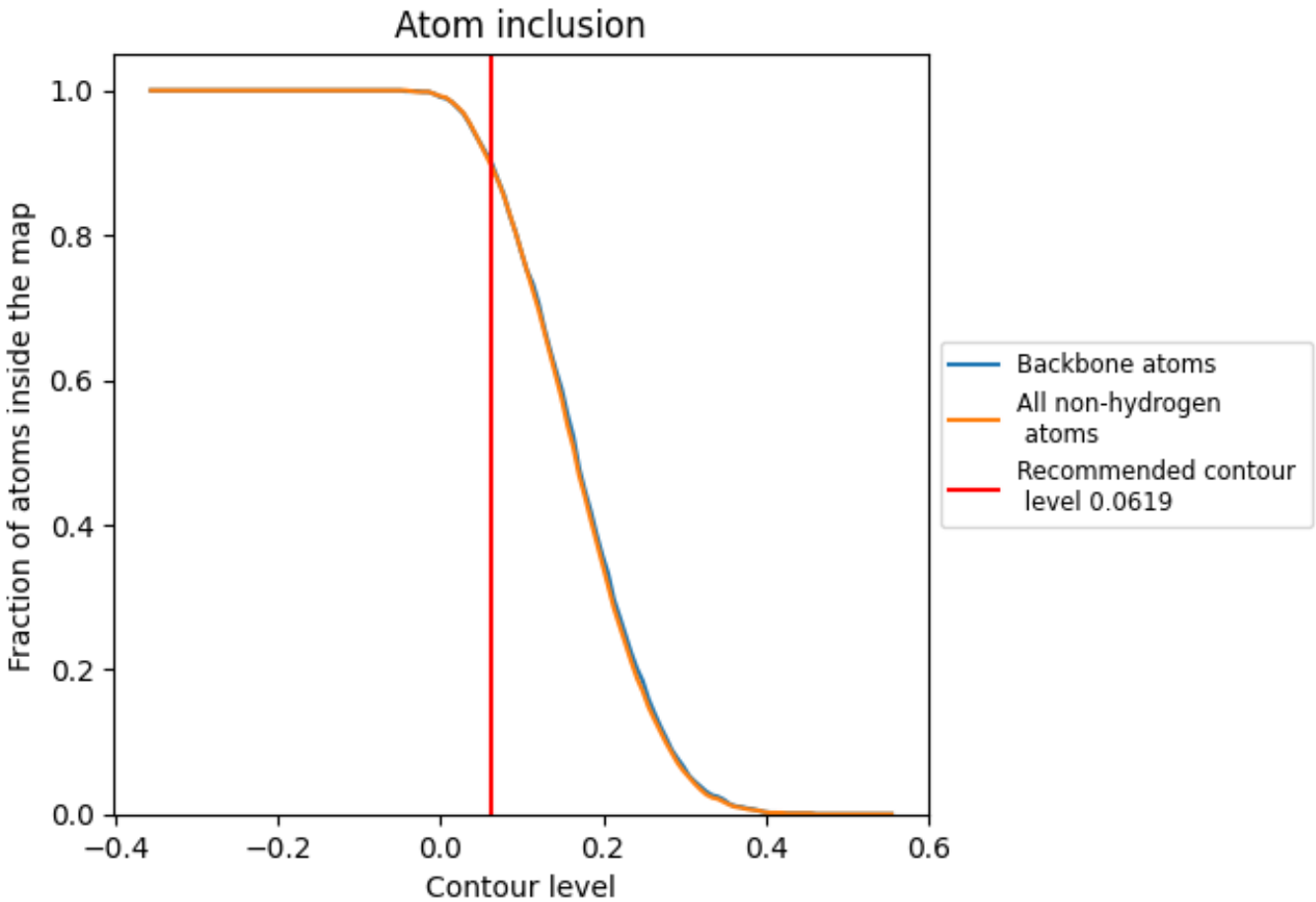
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0619).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (0.0619) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8970	0.5760
A	0.8910	0.5750
B	0.9160	0.5760
H	0.8520	0.5780
X	0.8360	0.5760