Full wwPDB EM Validation Report (i)

Aug 6, 2026 – 04:22 PM JST

PDB ID	:	8GO3 / pdb_00008go3
EMDB ID	:	EMD-34171
Title	:	Cryo-EM structure of Escherichia coli cytochrome bo3 in DDM detergent
Authors	:	Cao, H.Y.; Li, K.; Li, C.Y.
Deposited on	:	2022-08-24
Resolution	:	3.09 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:

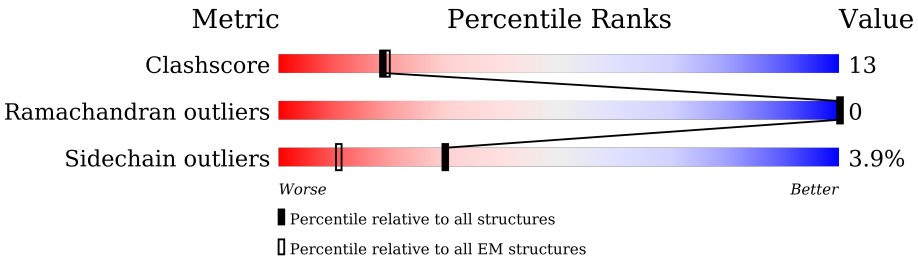
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

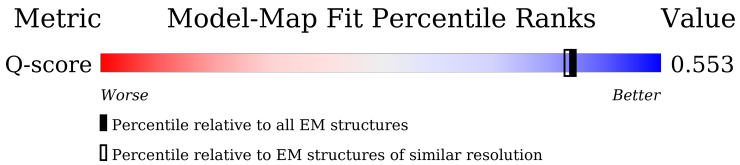
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.09 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	14003 (2.59 - 3.59)

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	663	70% 28% • •
2	B	315	63% 19% • 17%
3	C	204	71% 19% 10%
4	D	109	71% 18% • 9%

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
6	HEO	A	702	X	-	-	-
9	3PE	A	705	-	-	X	-
9	3PE	C	301	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 9739 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 Cytochrome bo(3) ubiquinol oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	658	5224	3504	826	857	37	0	0

- Molecule 2 is a protein called Cytochrome bo(3) ubiquinol oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	262	2047	1338	330	368	11	0	0

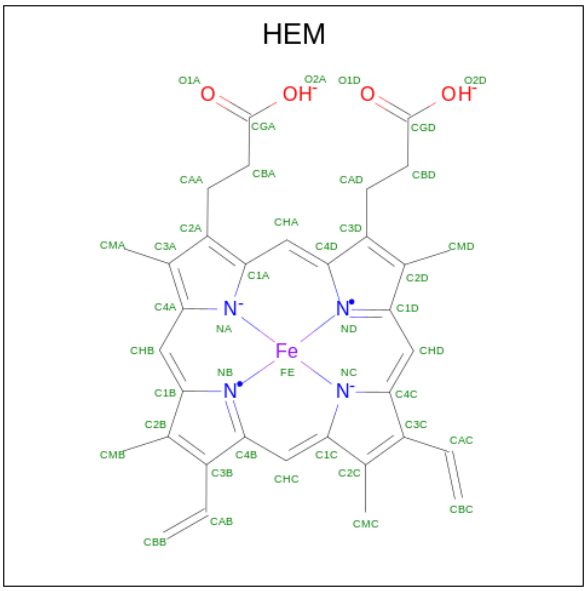
- Molecule 3 is a protein called ubiquinol oxidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	184	1441	965	226	237	13	0	0

- Molecule 4 is a protein called Cytochrome bo(3) ubiquinol oxidase subunit 4.

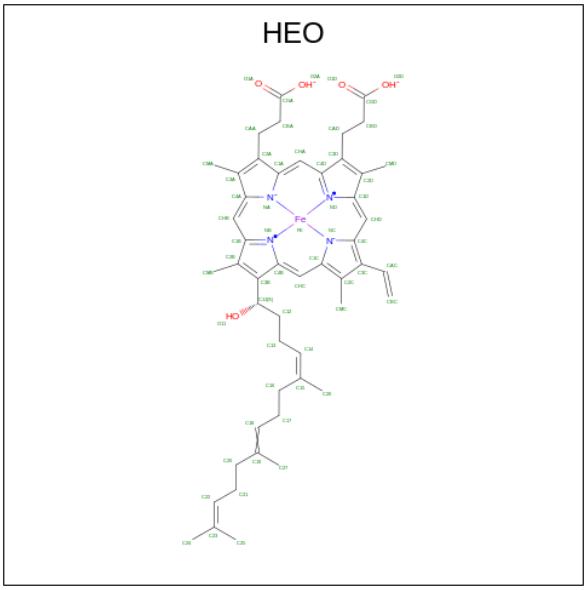
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	99	769	514	119	125	11	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
5	A	1	43	34	1	4	4	0

- Molecule 6 is HEME O (CCD ID: HEO) (formula: $C_{49}H_{58}FeN_4O_5$).

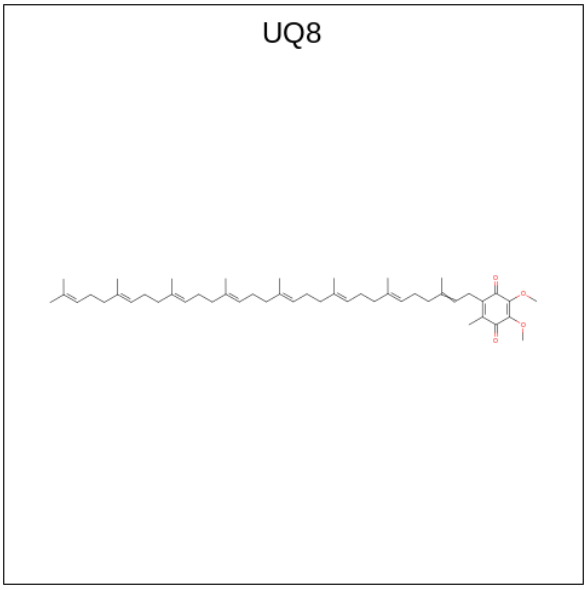


Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
6	A	1	59	49	1	4	5	0

- Molecule 7 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

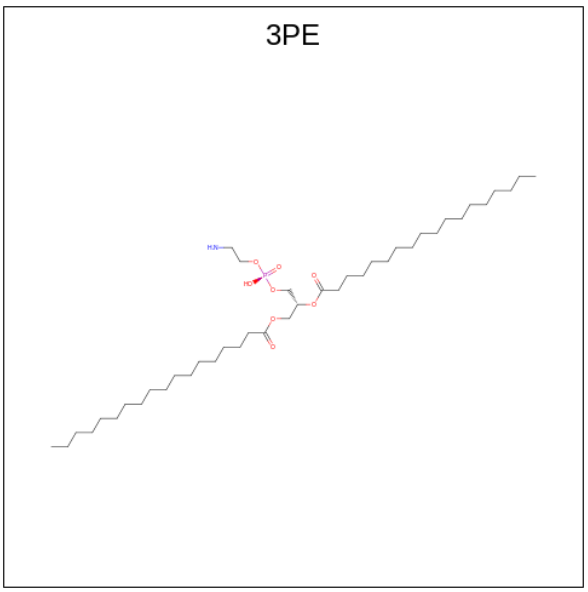
Mol	Chain	Residues	Atoms		AltConf
			Total	Cu	
7	A	1	1	1	0

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



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	A	1	53	49	4	0

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



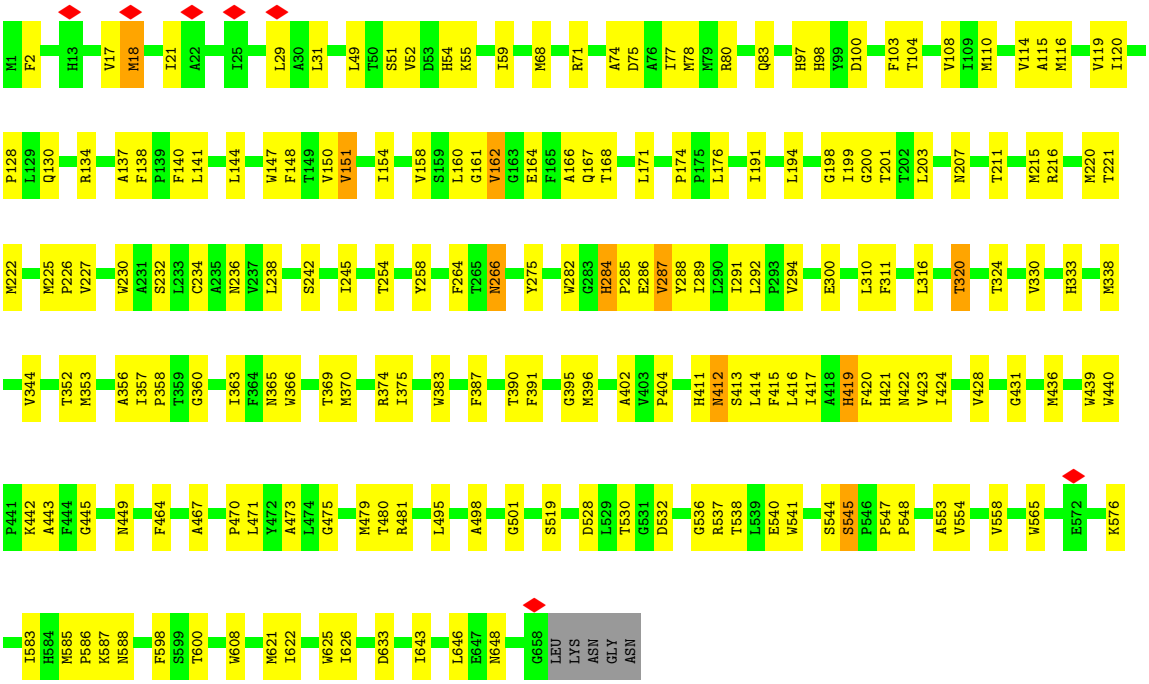
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	A	1	51	41	1	8	1	0
			Total	C	N	O	P	
9	C	1	51	41	1	8	1	0

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.

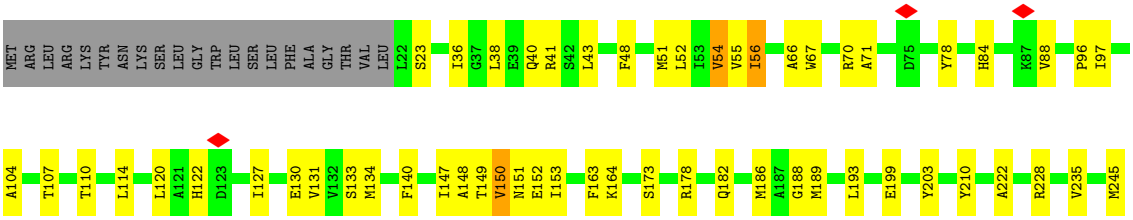
• Molecule 1: Cytochrome bo(3) ubiquinol oxidase subunit 1

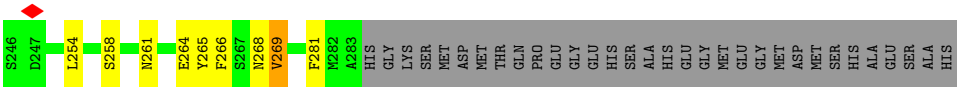
Chain A:



• Molecule 2: Cytochrome bo(3) ubiquinol oxidase subunit 2

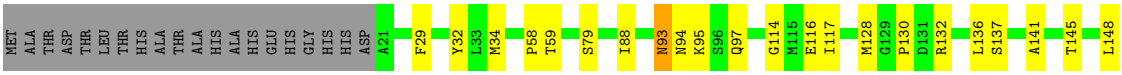
Chain B:





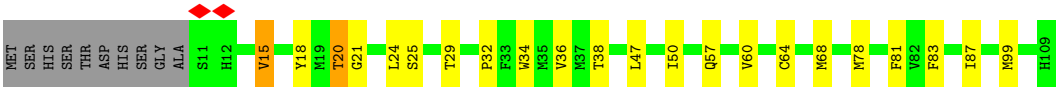
- Molecule 3: ubiquinol oxidase

Chain C:



- Molecule 4: Cytochrome bo(3) ubiquinol oxidase subunit 4

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	538627	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 ($e^-/Å^2$)	50.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.841	Depositor
Minimum map value	-1.192	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.31	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: HEO, 3PE, HEM, UQ8, CU

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	0.24	1/5401 (0.0%)	0.37	2/7364 (0.0%)
2	B	0.14	0/2106	0.32	0/2868
3	C	0.15	0/1483	0.28	0/2014
4	D	0.13	0/789	0.32	0/1077
All	All	0.20	1/9779 (0.0%)	0.34	2/13323 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	HIS	N-CA	-6.50	1.42	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	421	HIS	N-CA-C	-11.44	99.86	114.04
1	A	419	HIS	N-CA-C	-5.55	105.54	112.93

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	5224	0	5226	165	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2047	0	2046	41	0
3	C	1441	0	1456	28	0
4	D	769	0	800	14	0
5	A	43	0	30	5	0
6	A	59	0	56	17	0
7	A	1	0	0	0	0
8	A	53	0	74	9	0
9	A	51	0	82	31	0
9	C	51	0	82	24	0
All	All	9739	0	9852	254	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (254) 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:A:621:MET:CE	9:A:705:3PE:H3A2	1.76	1.14
1:A:199:ILE:HD11	9:A:705:3PE:C3H	1.81	1.10
1:A:199:ILE:HD11	9:A:705:3PE:H3H2	1.36	1.04
1:A:621:MET:HE3	9:A:705:3PE:H3A2	1.50	0.93
3:C:176:ARG:HG2	9:C:301:3PE:H12	1.49	0.92
1:A:621:MET:CE	9:A:705:3PE:C3A	2.48	0.91
1:A:621:MET:HE2	9:A:705:3PE:C3A	2.05	0.86
1:A:311:PHE:H	1:A:369:THR:HG22	1.40	0.86
1:A:199:ILE:HD11	9:A:705:3PE:H3H1	1.60	0.81
1:A:284:HIS:HB3	1:A:285:PRO:HD3	1.65	0.79
1:A:625:TRP:CZ3	9:C:301:3PE:H391	2.18	0.79
1:A:621:MET:HE2	9:A:705:3PE:H3A1	1.65	0.78
3:C:159:VAL:HG11	9:C:301:3PE:H331	1.67	0.77
1:A:199:ILE:CD1	9:A:705:3PE:H3H2	2.15	0.76
1:A:174:PRO:HB3	1:A:264:PHE:HB3	1.66	0.76
1:A:310:LEU:HD21	1:A:316:LEU:HD12	1.70	0.73
1:A:439:TRP:NE1	1:A:540:GLU:OE1	2.22	0.71
1:A:626:ILE:CD1	9:C:301:3PE:H342	2.21	0.71
1:A:415:PHE:HB2	1:A:475:GLY:HA3	1.73	0.70
9:A:705:3PE:HN2	9:C:301:3PE:H112	1.55	0.70
1:A:626:ILE:HD12	9:C:301:3PE:H342	1.72	0.70
1:A:294:VAL:HG21	1:A:428:VAL:HA	1.73	0.69
1:A:130:GLN:HB3	1:A:226:PRO:HG2	1.75	0.68
1:A:232:SER:O	1:A:236:ASN:ND2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HD21	9:A:705:3PE:H281	1.75	0.66
9:A:705:3PE:N	9:C:301:3PE:H112	2.10	0.66
6:A:702:HEO:H251	2:B:51:MET:HE3	1.78	0.65
1:A:284:HIS:NE2	1:A:288:TYR:HE2	1.94	0.65
1:A:338:MET:HG3	2:B:186:MET:HE1	1.80	0.64
9:C:301:3PE:H2C1	9:C:301:3PE:H3G1	1.80	0.64
3:C:34:MET:HE2	4:D:81:PHE:HA	1.79	0.64
3:C:163:GLN:OE1	3:C:176:ARG:NH1	2.30	0.64
1:A:168:THR:HG22	1:A:176:LEU:HG	1.80	0.63
1:A:294:VAL:HG13	1:A:431:GLY:HA3	1.81	0.63
6:A:702:HEO:H252	6:A:702:HEO:H18	1.79	0.62
1:A:220:MET:HE3	1:A:225:MET:HA	1.81	0.61
1:A:587:LYS:NZ	1:A:633:ASP:OD2	2.30	0.61
1:A:199:ILE:HG12	9:A:705:3PE:H2G1	1.83	0.61
3:C:95:LYS:HE2	3:C:168:GLY:HA2	1.82	0.61
3:C:204:MET:HE1	4:D:47:LEU:HD13	1.82	0.61
1:A:144:LEU:HD23	9:A:705:3PE:H342	1.81	0.61
1:A:199:ILE:CD1	9:A:705:3PE:H3F2	2.31	0.60
1:A:174:PRO:HG3	1:A:275:TYR:HB3	1.84	0.60
1:A:352:THR:HG23	1:A:402:ALA:HB1	1.83	0.60
1:A:141:LEU:HD13	9:A:705:3PE:H321	1.82	0.60
1:A:227:VAL:HG21	1:A:310:LEU:HD22	1.83	0.59
1:A:442:LYS:NZ	1:A:544:SER:O	2.30	0.59
4:D:68:MET:HE3	4:D:78:MET:HA	1.85	0.58
3:C:176:ARG:NE	9:C:301:3PE:O12	2.36	0.58
9:C:301:3PE:H3G1	9:C:301:3PE:C2C	2.34	0.58
2:B:147:ILE:HD13	2:B:235:VAL:HG13	1.86	0.58
1:A:622:ILE:HD13	9:C:301:3PE:H3B2	1.86	0.58
3:C:79:SER:OG	3:C:184:TRP:NE1	2.36	0.57
1:A:141:LEU:HD11	1:A:203:LEU:HD13	1.86	0.57
4:D:25:SER:OG	4:D:57:GLN:NE2	2.37	0.57
1:A:80:ARG:NH2	1:A:83:GLN:OE1	2.39	0.56
1:A:363:ILE:HD11	1:A:391:PHE:HD2	1.70	0.56
1:A:71:ARG:HH11	1:A:160:LEU:HD22	1.70	0.56
1:A:424:ILE:HG21	5:A:701:HEM:CAC	2.35	0.56
2:B:67:TRP:O	2:B:70:ARG:NH1	2.38	0.56
1:A:417:ILE:HA	1:A:420:PHE:CE1	2.40	0.56
1:A:626:ILE:HG13	3:C:159:VAL:HG21	1.87	0.56
1:A:104:THR:HG21	1:A:166:ALA:HB3	1.88	0.56
1:A:216:ARG:NH1	1:A:220:MET:O	2.39	0.56
1:A:284:HIS:CE1	1:A:333:HIS:CE1	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:705:3PE:H3D2	9:C:301:3PE:H3F1	1.88	0.55
1:A:174:PRO:HD3	1:A:275:TYR:CD1	2.42	0.55
1:A:383:TRP:O	1:A:387:PHE:N	2.38	0.55
1:A:360:GLY:CA	6:A:702:HEO:H201	2.37	0.55
1:A:284:HIS:HB3	1:A:285:PRO:CD	2.36	0.55
4:D:21:GLY:HA3	4:D:64:CYS:SG	2.47	0.55
6:A:702:HEO:H251	2:B:51:MET:CE	2.37	0.54
1:A:144:LEU:CD2	9:A:705:3PE:H342	2.36	0.54
1:A:470:PRO:HB2	1:A:498:ALA:HB2	1.88	0.54
6:A:702:HEO:HBD2	6:A:702:HEO:HMD3	1.89	0.54
6:A:702:HEO:H261	6:A:702:HEO:C18	2.38	0.54
6:A:702:HEO:HBD2	6:A:702:HEO:CMD	2.38	0.53
1:A:130:GLN:NE2	1:A:300:GLU:OE1	2.36	0.53
3:C:159:VAL:CG1	9:C:301:3PE:H331	2.38	0.53
1:A:445:GLY:HA2	1:A:545:SER:HB2	1.89	0.53
1:A:98:HIS:CE1	8:A:704:UQ8:H3M	2.44	0.53
1:A:140:PHE:HB3	9:A:705:3PE:C11	2.39	0.53
1:A:375:ILE:N	2:B:70:ARG:O	2.41	0.53
1:A:537:ARG:HA	1:A:565:TRP:HB2	1.90	0.53
1:A:404:PRO:HD2	2:B:107:THR:HG23	1.91	0.53
2:B:173:SER:OG	2:B:182:GLN:NE2	2.42	0.53
1:A:138:PHE:HB3	9:A:705:3PE:O14	2.08	0.53
5:A:701:HEM:HBC2	5:A:701:HEM:CMC	2.39	0.53
1:A:360:GLY:HA2	6:A:702:HEO:H201	1.91	0.52
3:C:200:LEU:HG	4:D:36:VAL:HG11	1.91	0.52
1:A:74:ALA:HB3	8:A:704:UQ8:H7	1.91	0.52
1:A:198:GLY:HA2	1:A:201:THR:HG22	1.90	0.52
1:A:245:ILE:HB	1:A:282:TRP:HB2	1.90	0.52
1:A:357:ILE:HG23	2:B:96:PRO:HB2	1.90	0.52
1:A:55:LYS:HD2	1:A:547:PRO:HG2	1.90	0.52
1:A:71:ARG:HD3	8:A:704:UQ8:H1MB	1.91	0.51
1:A:203:LEU:HD21	9:A:705:3PE:C28	2.40	0.51
1:A:222:MET:O	1:A:230:TRP:NE1	2.41	0.51
3:C:152:SER:HB2	9:C:301:3PE:H3A2	1.90	0.51
1:A:625:TRP:CZ3	9:C:301:3PE:C39	2.91	0.51
1:A:110:MET:HA	1:A:114:VAL:HB	1.92	0.51
1:A:538:THR:OG1	1:A:540:GLU:OE2	2.22	0.51
1:A:100:ASP:OD2	2:B:210:TYR:OH	2.21	0.51
1:A:21:ILE:HG21	1:A:161:GLY:HA2	1.93	0.51
3:C:130:PRO:O	3:C:137:SER:OG	2.27	0.50
1:A:97:HIS:CD2	1:A:167:GLN:HE22	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:THR:O	1:A:215:MET:HB2	2.12	0.50
2:B:151:ASN:ND2	2:B:261:ASN:O	2.45	0.50
1:A:292:LEU:HD22	1:A:320:THR:HG22	1.93	0.50
1:A:310:LEU:HD12	1:A:369:THR:HG21	1.94	0.49
1:A:199:ILE:HD13	9:A:705:3PE:H3C2	1.92	0.49
1:A:288:TYR:HA	1:A:291:ILE:HG22	1.95	0.49
1:A:191:ILE:HG21	1:A:254:THR:HG22	1.94	0.49
1:A:473:ALA:HB2	2:B:23:SER:HB2	1.93	0.49
1:A:234:CYS:HB3	1:A:324:THR:OG1	2.13	0.49
3:C:169:LEU:O	3:C:174:ARG:NH2	2.45	0.49
3:C:196:THR:HA	3:C:200:LEU:HB2	1.94	0.49
1:A:284:HIS:CD2	1:A:288:TYR:HE2	2.30	0.49
1:A:413:SER:HA	1:A:480:THR:HA	1.94	0.49
2:B:40:GLN:HG2	2:B:114:LEU:HD13	1.94	0.49
1:A:80:ARG:NH1	5:A:701:HEM:HMA3	2.27	0.49
1:A:98:HIS:NE2	8:A:704:UQ8:H3M	2.28	0.49
1:A:116:MET:HE1	1:A:289:ILE:HG21	1.94	0.49
1:A:284:HIS:CD2	1:A:330:VAL:HG23	2.48	0.49
2:B:43:LEU:HD13	2:B:110:THR:HG21	1.95	0.49
1:A:395:GLY:HA3	6:A:702:HEO:C15	2.43	0.48
1:A:536:GLY:HA3	1:A:541:TRP:CD1	2.48	0.48
1:A:59:ILE:HD11	1:A:443:ALA:HB1	1.95	0.48
9:A:705:3PE:C3D	9:C:301:3PE:H3F1	2.43	0.48
3:C:132:ARG:HB3	3:C:136:LEU:HD12	1.95	0.48
1:A:420:PHE:HA	1:A:423:VAL:HG22	1.96	0.48
1:A:449:ASN:H	1:A:519:SER:HB3	1.78	0.48
2:B:70:ARG:HG3	2:B:71:ALA:H	1.79	0.48
2:B:52:LEU:HD22	2:B:56:ILE:HD13	1.96	0.48
3:C:141:ALA:O	3:C:145:THR:OG1	2.30	0.48
1:A:216:ARG:HD3	1:A:225:MET:SD	2.54	0.47
1:A:414:LEU:HD13	1:A:471:LEU:HD22	1.96	0.47
1:A:583:ILE:HG12	1:A:643:ILE:HD11	1.95	0.47
6:A:702:HEO:HMD3	6:A:702:HEO:CBD	2.44	0.47
2:B:130:GLU:HG2	2:B:164:LYS:HE3	1.95	0.47
9:A:705:3PE:H261	9:A:705:3PE:H292	1.47	0.47
1:A:287:VAL:HB	6:A:702:HEO:HAC	1.95	0.47
2:B:127:ILE:HD11	2:B:228:ARG:HH22	1.78	0.47
4:D:32:PRO:HB3	4:D:50:ILE:HG22	1.96	0.47
1:A:356:ALA:HB1	6:A:702:HEO:H262	1.96	0.47
2:B:148:ALA:O	2:B:266:PHE:HB2	2.14	0.47
2:B:150:VAL:HG13	2:B:264:GLU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:GLY:O	2:B:189:MET:HG3	2.15	0.47
2:B:199:GLU:O	2:B:203:TYR:OH	2.21	0.47
4:D:24:LEU:HD23	4:D:60:VAL:HG21	1.96	0.47
4:D:29:THR:HG23	4:D:57:GLN:HE22	1.80	0.46
1:A:100:ASP:HA	1:A:103:PHE:CE2	2.50	0.46
2:B:153:ILE:HG13	2:B:222:ALA:HA	1.97	0.46
3:C:188:ASP:O	3:C:192:ILE:HG12	2.16	0.46
1:A:51:SER:HA	1:A:588:ASN:HD22	1.79	0.46
3:C:29:PHE:CE2	3:C:183:PHE:HB2	2.51	0.46
1:A:479:MET:HE1	1:A:495:LEU:HD11	1.96	0.46
8:A:704:UQ8:H4MA	8:A:704:UQ8:O5	2.16	0.46
9:C:301:3PE:H322	9:C:301:3PE:H352	1.51	0.46
2:B:131:VAL:HG22	2:B:140:PHE:HD1	1.82	0.45
1:A:625:TRP:CZ2	9:C:301:3PE:H232	2.51	0.45
3:C:201:MET:HE3	4:D:47:LEU:HD11	1.98	0.45
1:A:116:MET:HE3	1:A:120:ILE:HD11	1.99	0.45
1:A:357:ILE:HD13	2:B:97:ILE:HG12	1.98	0.45
1:A:49:LEU:HD22	1:A:147:TRP:CZ2	2.51	0.45
1:A:115:ALA:HB2	5:A:701:HEM:HBC1	1.99	0.45
1:A:360:GLY:HA3	6:A:702:HEO:H201	1.99	0.45
1:A:370:MET:HB3	1:A:375:ILE:HD11	1.99	0.45
1:A:417:ILE:HG12	1:A:481:ARG:HG2	1.99	0.45
1:A:621:MET:HE3	9:A:705:3PE:C3A	2.29	0.45
8:A:704:UQ8:C23	8:A:704:UQ8:H18	2.46	0.44
1:A:137:ALA:HA	1:A:215:MET:HE3	1.98	0.44
1:A:626:ILE:HD11	9:C:301:3PE:H342	1.97	0.44
9:C:301:3PE:H2C1	9:C:301:3PE:C3G	2.47	0.44
1:A:134:ARG:NH2	1:A:553:ALA:O	2.50	0.44
1:A:530:THR:HG23	1:A:532:ASP:H	1.82	0.44
1:A:174:PRO:CB	1:A:264:PHE:HB3	2.44	0.44
9:A:705:3PE:H331	9:A:705:3PE:H362	1.77	0.44
2:B:36:ILE:HD11	2:B:120:LEU:HD21	1.98	0.44
2:B:178:ARG:HD2	2:B:203:TYR:HD1	1.82	0.44
1:A:467:ALA:HB2	1:A:501:GLY:HA3	1.98	0.44
3:C:114:GLY:O	3:C:117:ILE:HG13	2.17	0.44
1:A:148:PHE:HZ	9:A:705:3PE:H391	1.82	0.44
6:A:702:HEO:H211	2:B:54:VAL:HB	2.00	0.44
3:C:32:TYR:OH	9:C:301:3PE:H282	2.17	0.44
1:A:140:PHE:HB3	9:A:705:3PE:H112	2.00	0.44
1:A:316:LEU:HD21	1:A:365:ASN:HB2	1.99	0.44
1:A:141:LEU:CD1	9:A:705:3PE:H321	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:PHE:O	1:A:151:VAL:HG12	2.17	0.44
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.85	0.44
1:A:238:LEU:O	1:A:242:SER:OG	2.25	0.44
1:A:412:ASN:OD1	1:A:412:ASN:N	2.52	0.43
2:B:149:THR:OG1	2:B:152:GLU:O	2.36	0.43
2:B:134:MET:HE1	2:B:254:LEU:HD23	2.00	0.43
4:D:34:TRP:O	4:D:38:THR:HG22	2.18	0.43
1:A:108:VAL:HG13	1:A:194:LEU:HD21	2.01	0.43
1:A:74:ALA:HA	1:A:77:ILE:HG22	2.01	0.43
2:B:38:LEU:HD11	2:B:41:ARG:HH21	1.84	0.43
1:A:52:VAL:HG22	1:A:588:ASN:HA	2.01	0.43
1:A:284:HIS:O	1:A:287:VAL:HG22	2.18	0.43
1:A:422:ASN:HA	1:A:464:PHE:CZ	2.53	0.43
5:A:701:HEM:HBC2	5:A:701:HEM:HMC1	1.99	0.43
1:A:220:MET:HG3	1:A:558:VAL:HG21	2.00	0.43
1:A:141:LEU:HB3	1:A:207:ASN:HD21	1.84	0.43
1:A:576:LYS:NZ	1:A:648:ASN:HD21	2.17	0.43
1:A:585:MET:HE3	1:A:586:PRO:HD2	2.01	0.43
3:C:58:PRO:HG3	3:C:128:MET:HG2	2.01	0.43
1:A:374:ARG:NH1	2:B:78:TYR:HB2	2.34	0.42
9:A:705:3PE:H252	9:A:705:3PE:H222	1.26	0.42
1:A:338:MET:HE3	1:A:338:MET:HB2	1.88	0.42
1:A:353:MET:HE1	2:B:104:ALA:HA	2.01	0.42
1:A:366:TRP:CZ3	1:A:387:PHE:HE2	2.37	0.42
1:A:411:HIS:CG	1:A:412:ASN:H	2.37	0.42
9:C:301:3PE:H3D2	9:C:301:3PE:H3G2	1.48	0.42
4:D:18:TYR:C	4:D:20:THR:H	2.27	0.42
2:B:163:PHE:HB2	2:B:193:LEU:HB3	2.02	0.42
2:B:245:MET:O	2:B:269:VAL:HA	2.19	0.42
3:C:88:ILE:HD13	4:D:15:VAL:HG22	2.01	0.42
1:A:287:VAL:HB	6:A:702:HEO:CAC	2.50	0.42
1:A:365:ASN:O	1:A:369:THR:HG23	2.19	0.42
2:B:133:SER:O	2:B:133:SER:OG	2.35	0.42
1:A:548:PRO:HB3	1:A:646:LEU:HD13	2.01	0.42
1:A:18:MET:HE3	1:A:21:ILE:HD11	2.02	0.42
1:A:395:GLY:HA3	6:A:702:HEO:C14	2.50	0.42
3:C:148:LEU:HA	3:C:151:THR:HG22	2.01	0.41
1:A:162:VAL:HG22	1:A:608:TRP:CZ2	2.56	0.41
1:A:254:THR:O	1:A:258:TYR:N	2.53	0.41
3:C:93:ASN:OD1	3:C:93:ASN:N	2.53	0.41
1:A:266:ASN:O	2:B:281:PHE:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ILE:HB	1:A:358:PRO:HD3	2.01	0.41
1:A:51:SER:HA	1:A:588:ASN:ND2	2.34	0.41
3:C:94:ASN:O	3:C:97:GLN:N	2.54	0.41
1:A:285:PRO:O	1:A:289:ILE:HG13	2.20	0.41
2:B:152:GLU:OE2	2:B:265:TYR:OH	2.29	0.41
4:D:83:PHE:O	4:D:87:ILE:HG12	2.21	0.41
1:A:413:SER:C	1:A:415:PHE:H	2.28	0.41
1:A:411:HIS:O	1:A:412:ASN:C	2.64	0.41
1:A:436:MET:O	1:A:440:TRP:HB2	2.20	0.41
2:B:258:SER:OG	2:B:261:ASN:ND2	2.39	0.41
1:A:54:HIS:CE1	1:A:128:PRO:HB2	2.55	0.41
1:A:71:ARG:CD	8:A:704:UQ8:H1MB	2.50	0.41
1:A:75:ASP:CG	8:A:704:UQ8:H1MA	2.46	0.41
1:A:78:MET:HE1	8:A:704:UQ8:C3	2.51	0.41
1:A:150:VAL:O	1:A:154:ILE:HG13	2.21	0.41
1:A:375:ILE:HD12	2:B:66:ALA:HA	2.02	0.41
1:A:417:ILE:HA	1:A:420:PHE:HE1	1.84	0.41
9:A:705:3PE:N	9:C:301:3PE:C11	2.82	0.41
3:C:192:ILE:HA	3:C:195:PHE:CE2	2.56	0.41
1:A:282:TRP:CZ2	1:A:286:GLU:HG3	2.57	0.40
1:A:396:MET:HB2	2:B:55:VAL:HG21	2.02	0.40
9:C:301:3PE:H3A1	9:C:301:3PE:H3D1	1.25	0.40
6:A:702:HEO:H252	6:A:702:HEO:C18	2.48	0.40
1:A:148:PHE:HB3	1:A:200:GLY:HA3	2.02	0.40
1:A:416:LEU:HD23	1:A:481:ARG:HD2	2.02	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	656/663 (99%)	618 (94%)	38 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	260/315 (82%)	235 (90%)	25 (10%)	0	100	100
3	C	182/204 (89%)	171 (94%)	11 (6%)	0	100	100
4	D	97/109 (89%)	90 (93%)	7 (7%)	0	100	100
All	All	1195/1291 (93%)	1114 (93%)	81 (7%)	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	543/547 (99%)	519 (96%)	24 (4%)	25	56
2	B	219/262 (84%)	210 (96%)	9 (4%)	27	59
3	C	151/166 (91%)	148 (98%)	3 (2%)	48	72
4	D	86/94 (92%)	83 (96%)	3 (4%)	32	62
All	All	999/1069 (94%)	960 (96%)	39 (4%)	30	60

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	PHE
1	A	17	VAL
1	A	18	MET
1	A	29	LEU
1	A	31	LEU
1	A	68	MET
1	A	119	VAL
1	A	151	VAL
1	A	158	VAL
1	A	162	VAL
1	A	164	GLU
1	A	221	THR
1	A	266	ASN

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Mol	Chain	Res	Type
1	A	287	VAL
1	A	320	THR
1	A	344	VAL
1	A	390	THR
1	A	412	ASN
1	A	419	HIS
1	A	528	ASP
1	A	545	SER
1	A	554	VAL
1	A	598	PHE
1	A	600	THR
2	B	48	PHE
2	B	54	VAL
2	B	56	ILE
2	B	84	HIS
2	B	88	VAL
2	B	122	HIS
2	B	150	VAL
2	B	268	ASN
2	B	269	VAL
3	C	59	THR
3	C	93	ASN
3	C	116	GLU
4	D	15	VAL
4	D	20	THR
4	D	99	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	167	GLN
1	A	262	HIS
1	A	271	ASN
1	A	557	HIS
1	A	559	HIS
1	A	588	ASN
1	A	609	HIS
1	A	648	ASN
2	B	112	HIS
2	B	158	ASN
2	B	182	GLN

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Mol	Chain	Res	Type
2	B	194	HIS
2	B	198	ASN
2	B	240	GLN
2	B	261	ASN
3	C	97	GLN
3	C	149	HIS
3	C	185	HIS
4	D	57	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	HEO	A	702	1	65,66,66	1.05	1 (1%)	81,102,102	1.23	11 (13%)
8	UQ8	A	704	-	53,53,53	1.09	2 (3%)	64,67,67	1.75	18 (28%)
5	HEM	A	701	1	50,50,50	1.72	10 (20%)	66,82,82	1.78	15 (22%)
9	3PE	C	301	-	50,50,50	0.90	3 (6%)	53,55,55	1.01	3 (5%)
9	3PE	A	705	-	50,50,50	0.88	2 (4%)	53,55,55	1.16	3 (5%)

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	HEO	A	702	1	3/3/7/15	16/34/74/74	-
8	UQ8	A	704	-	-	17/51/75/75	0/1/1/1
5	HEM	A	701	1	-	6/14/54/54	-
9	3PE	C	301	-	-	30/54/54/54	-
9	3PE	A	705	-	-	34/54/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	704	UQ8	C6-C1	6.78	1.47	1.35
5	A	701	HEM	FE-NB	5.09	2.10	1.94
5	A	701	HEM	C4D-ND	-3.89	1.33	1.40
5	A	701	HEM	FE-NC	3.72	2.07	1.95
5	A	701	HEM	C1B-NB	-3.69	1.33	1.40
9	C	301	3PE	O21-C2	-3.27	1.38	1.46
5	A	701	HEM	C1C-C2C	-3.03	1.39	1.45
8	A	704	UQ8	C4-C3	2.98	1.48	1.36
9	A	705	3PE	O21-C2	-2.88	1.39	1.46
5	A	701	HEM	FE-ND	-2.85	1.86	1.94
6	A	702	HEO	CAC-C3C	-2.81	1.39	1.47
9	A	705	3PE	O31-C3	-2.80	1.38	1.45
5	A	701	HEM	C4B-NB	-2.58	1.33	1.38
5	A	701	HEM	C1D-ND	-2.35	1.33	1.38
9	C	301	3PE	O31-C3	-2.31	1.39	1.45
5	A	701	HEM	C3C-C4C	-2.23	1.42	1.46
5	A	701	HEM	C1A-C2A	-2.20	1.40	1.44
9	C	301	3PE	O31-C31	2.20	1.39	1.33

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	705	3PE	O21-C21-C22	5.25	122.81	111.50
5	A	701	HEM	CHC-C4B-NB	5.10	129.96	124.42
5	A	701	HEM	CHD-C1D-ND	4.65	129.47	124.42
8	A	704	UQ8	C7-C8-C9	-4.33	119.59	126.79
9	C	301	3PE	O21-C21-C22	4.15	120.44	111.50
5	A	701	HEM	CAA-CBA-CGA	-4.04	104.91	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	701	HEM	CHA-C4D-ND	3.78	129.04	124.37
5	A	701	HEM	CHB-C1B-NB	3.73	128.98	124.37
8	A	704	UQ8	C37-C38-C39	-3.56	119.09	127.66
8	A	704	UQ8	C15-C14-C16	3.56	121.25	115.27
8	A	704	UQ8	C20-C19-C21	3.48	121.12	115.27
6	A	702	HEO	C3C-C4C-NC	3.47	112.38	110.25
5	A	701	HEM	C1B-NB-C4B	3.40	108.58	105.07
8	A	704	UQ8	C12-C13-C14	-3.26	119.82	127.66
9	C	301	3PE	O31-C31-C32	3.10	121.63	111.91
5	A	701	HEM	C4C-NC-C1C	3.05	108.34	105.35
5	A	701	HEM	C4D-ND-C1D	3.03	108.20	105.07
8	A	704	UQ8	C27-C28-C29	-3.03	120.37	127.66
8	A	704	UQ8	C10-C9-C11	2.88	120.12	115.27
9	A	705	3PE	C3-C2-C1	-2.84	105.08	111.79
8	A	704	UQ8	C40-C39-C41	2.82	120.01	115.27
6	A	702	HEO	C13-C12-C11	-2.73	110.25	114.35
8	A	704	UQ8	C30-C29-C31	2.71	119.82	115.27
8	A	704	UQ8	C17-C18-C19	-2.56	121.49	127.66
8	A	704	UQ8	C32-C33-C34	-2.53	121.57	127.66
8	A	704	UQ8	C46-C44-C45	2.48	120.08	114.60
9	A	705	3PE	O31-C31-C32	2.46	119.62	111.91
6	A	702	HEO	CAD-CBD-CGD	-2.42	108.39	113.60
6	A	702	HEO	C13-C14-C15	-2.42	121.82	127.66
8	A	704	UQ8	C22-C23-C24	-2.32	122.07	127.66
5	A	701	HEM	CHD-C1D-C2D	-2.29	121.41	124.98
8	A	704	UQ8	C1M-C1-C6	-2.28	120.69	124.40
6	A	702	HEO	C21-C22-C23	-2.27	119.99	127.75
5	A	701	HEM	C4A-CHB-C1B	-2.26	120.98	126.34
5	A	701	HEM	CHB-C1B-C2B	-2.24	120.50	126.73
5	A	701	HEM	CHD-C4C-NC	2.24	126.86	124.44
8	A	704	UQ8	C35-C34-C36	2.24	119.03	115.27
8	A	704	UQ8	C42-C43-C44	-2.22	120.16	127.75
6	A	702	HEO	CBD-CAD-C3D	2.19	118.72	112.63
6	A	702	HEO	C1D-ND-C4D	-2.19	102.81	105.07
6	A	702	HEO	C4C-NC-C1C	-2.17	103.22	105.35
5	A	701	HEM	C4C-CHD-C1D	-2.15	121.41	126.06
6	A	702	HEO	O1A-CGA-CBA	-2.13	116.25	123.08
6	A	702	HEO	C17-C18-C19	-2.11	122.57	127.66
6	A	702	HEO	C3D-C4D-ND	2.10	112.39	110.36
5	A	701	HEM	CHA-C4D-C3D	-2.10	121.39	125.33
8	A	704	UQ8	C27-C26-C24	-2.10	106.07	112.98
9	C	301	3PE	O21-C21-O22	-2.08	118.68	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	704	UQ8	C8-C7-C6	-2.03	106.58	112.05
5	A	701	HEM	O2D-CGD-CBD	2.02	120.51	114.03

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	702	HEO	ND
6	A	702	HEO	NB
6	A	702	HEO	NA

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	702	HEO	C4D-C3D-CAD-CBD
6	A	702	HEO	C17-C18-C19-C20
6	A	702	HEO	C17-C18-C19-C27
8	A	704	UQ8	C25-C24-C26-C27
8	A	704	UQ8	C23-C24-C26-C27
8	A	704	UQ8	C15-C14-C16-C17
8	A	704	UQ8	C13-C14-C16-C17
9	A	705	3PE	C1-O11-P-O12
9	A	705	3PE	C1-O11-P-O13
9	A	705	3PE	O13-C11-C12-N
9	C	301	3PE	C1-O11-P-O12
9	C	301	3PE	C1-O11-P-O14
9	C	301	3PE	O13-C11-C12-N
9	C	301	3PE	C22-C21-O21-C2
9	C	301	3PE	O22-C21-O21-C2
6	A	702	HEO	C2D-C3D-CAD-CBD
9	C	301	3PE	C32-C33-C34-C35
9	C	301	3PE	C3D-C3E-C3F-C3G
9	A	705	3PE	C2D-C2E-C2F-C2G
9	C	301	3PE	C3A-C3B-C3C-C3D
8	A	704	UQ8	C30-C29-C31-C32
8	A	704	UQ8	C28-C29-C31-C32
9	A	705	3PE	C22-C23-C24-C25
6	A	702	HEO	C19-C20-C21-C22
8	A	704	UQ8	C34-C36-C37-C38
8	A	704	UQ8	C29-C31-C32-C33
8	A	704	UQ8	C24-C26-C27-C28
8	A	704	UQ8	C9-C11-C12-C13
9	A	705	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
6	A	702	HEO	C13-C14-C15-C16
9	A	705	3PE	C24-C25-C26-C27
6	A	702	HEO	C21-C22-C23-C24
9	A	705	3PE	C21-C22-C23-C24
9	C	301	3PE	C35-C36-C37-C38
8	A	704	UQ8	C3-C4-O4-C4M
9	A	705	3PE	C11-O13-P-O11
9	C	301	3PE	C1-O11-P-O13
9	A	705	3PE	O22-C21-O21-C2
9	A	705	3PE	C32-C31-O31-C3
9	A	705	3PE	C27-C28-C29-C2A
9	A	705	3PE	C22-C21-O21-C2
9	C	301	3PE	C33-C34-C35-C36
9	C	301	3PE	C2C-C2D-C2E-C2F
9	A	705	3PE	C37-C38-C39-C3A
9	A	705	3PE	C39-C3A-C3B-C3C
9	C	301	3PE	C2A-C2B-C2C-C2D
9	A	705	3PE	C3A-C3B-C3C-C3D
9	C	301	3PE	C21-C22-C23-C24
9	A	705	3PE	C2E-C2F-C2G-C2H
9	C	301	3PE	C2E-C2F-C2G-C2H
9	A	705	3PE	C29-C2A-C2B-C2C
9	C	301	3PE	C3C-C3D-C3E-C3F
9	A	705	3PE	C25-C26-C27-C28
9	A	705	3PE	O32-C31-O31-C3
9	A	705	3PE	C2C-C2D-C2E-C2F
9	C	301	3PE	C2-C1-O11-P
9	C	301	3PE	C23-C24-C25-C26
5	A	701	HEM	C2B-C3B-CAB-CBB
9	C	301	3PE	C39-C3A-C3B-C3C
5	A	701	HEM	C4B-C3B-CAB-CBB
9	A	705	3PE	C2B-C2C-C2D-C2E
9	A	705	3PE	C3E-C3F-C3G-C3H
9	A	705	3PE	C36-C37-C38-C39
9	C	301	3PE	C2F-C2G-C2H-C2I
9	A	705	3PE	C28-C29-C2A-C2B
9	A	705	3PE	C2F-C2G-C2H-C2I
9	C	301	3PE	O11-C1-C2-C3
6	A	702	HEO	C15-C16-C17-C18
9	C	301	3PE	C32-C31-O31-C3
9	A	705	3PE	C34-C35-C36-C37
9	C	301	3PE	C3B-C3C-C3D-C3E

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Mol	Chain	Res	Type	Atoms
9	C	301	3PE	C1-C2-C3-O31
9	C	301	3PE	O32-C31-O31-C3
9	A	705	3PE	C23-C24-C25-C26
9	A	705	3PE	C1-O11-P-O14
9	A	705	3PE	C11-O13-P-O12
9	A	705	3PE	C11-O13-P-O14
6	A	702	HEO	C3A-C2A-CAA-CBA
9	C	301	3PE	O11-C1-C2-O21
9	C	301	3PE	C3E-C3F-C3G-C3H
9	A	705	3PE	C3B-C3C-C3D-C3E
6	A	702	HEO	C11-C12-C13-C14
9	C	301	3PE	O21-C2-C3-O31
9	C	301	3PE	C11-O13-P-O11
6	A	702	HEO	C1A-C2A-CAA-CBA
6	A	702	HEO	CAA-CBA-CGA-O2A
6	A	702	HEO	C3D-CAD-CBD-CGD
9	C	301	3PE	C27-C28-C29-C2A
8	A	704	UQ8	C14-C16-C17-C18
8	A	704	UQ8	C35-C34-C36-C37
6	A	702	HEO	CAA-CBA-CGA-O1A
8	A	704	UQ8	C20-C19-C21-C22
6	A	702	HEO	CAD-CBD-CGD-O1D
8	A	704	UQ8	C33-C34-C36-C37
8	A	704	UQ8	C18-C19-C21-C22
6	A	702	HEO	CAD-CBD-CGD-O2D
5	A	701	HEM	CAD-CBD-CGD-O2D
8	A	704	UQ8	C40-C39-C41-C42
5	A	701	HEM	CAD-CBD-CGD-O1D
9	A	705	3PE	C33-C34-C35-C36
5	A	701	HEM	CAA-CBA-CGA-O1A
9	A	705	3PE	O21-C21-C22-C23
5	A	701	HEM	CAA-CBA-CGA-O2A

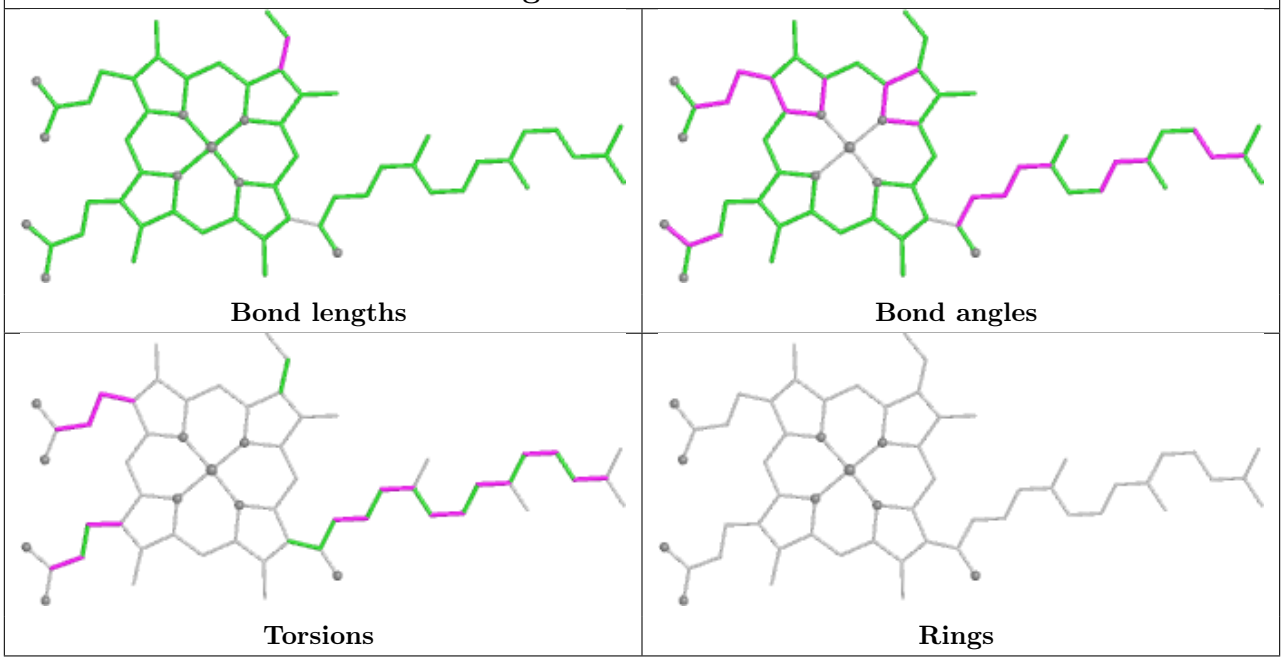
There are no ring outliers.

5 monomers are involved in 81 short contacts:

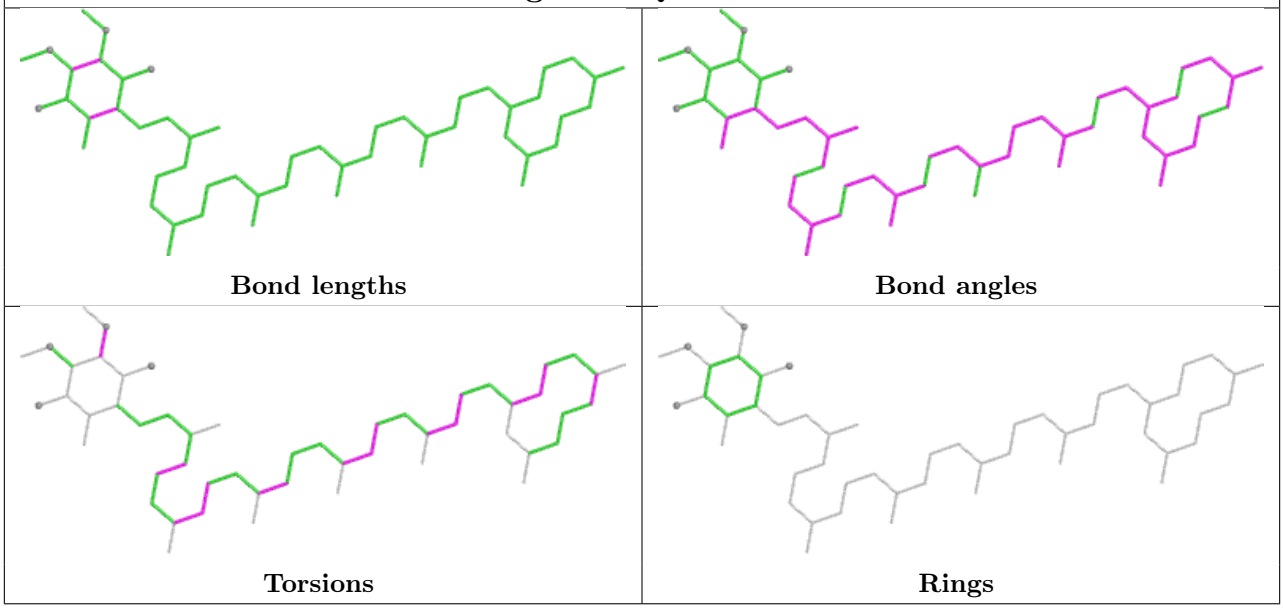
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	702	HEO	17	0
8	A	704	UQ8	9	0
5	A	701	HEM	5	0
9	C	301	3PE	24	0
9	A	705	3PE	31	0

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.

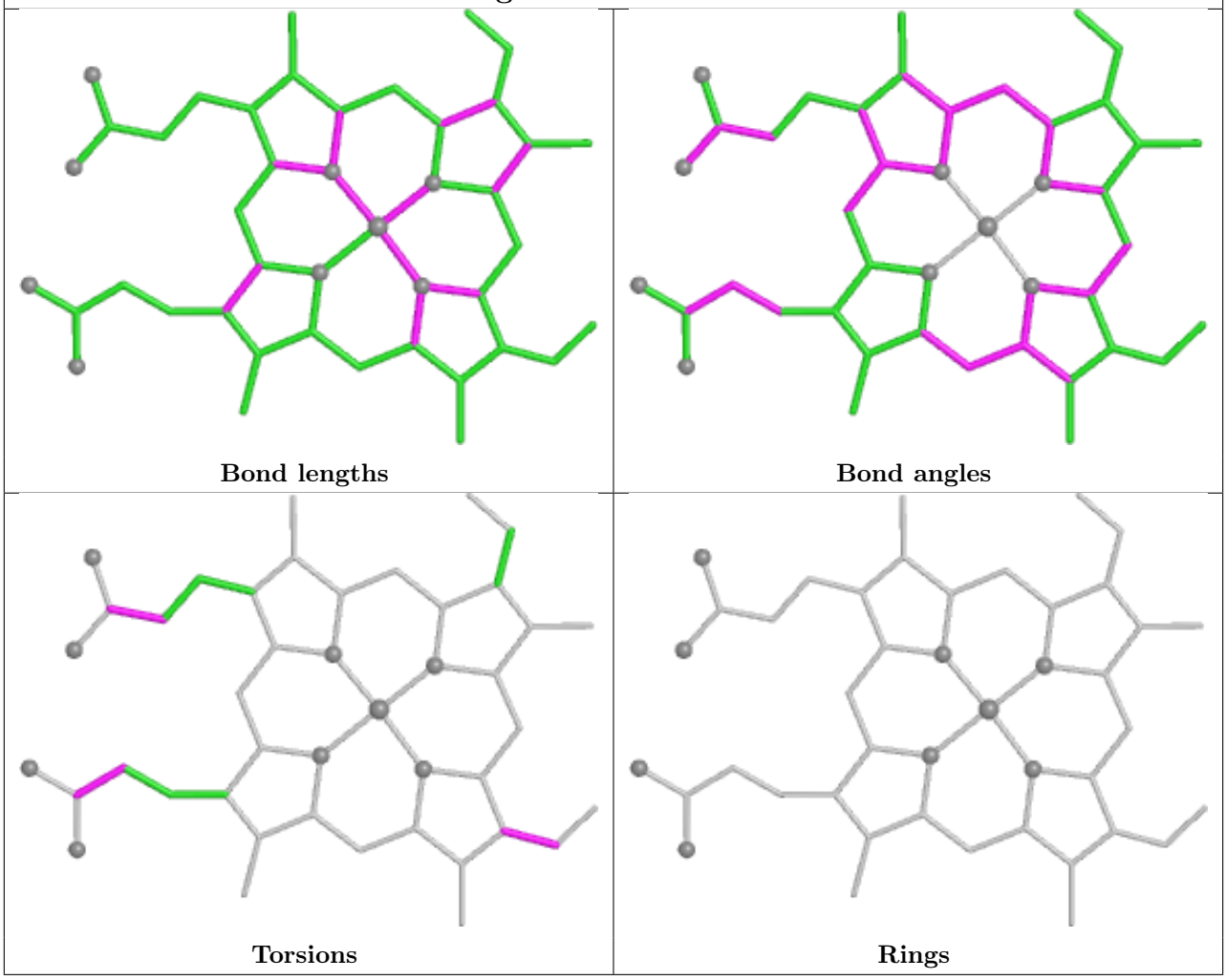
Ligand HEO A 702

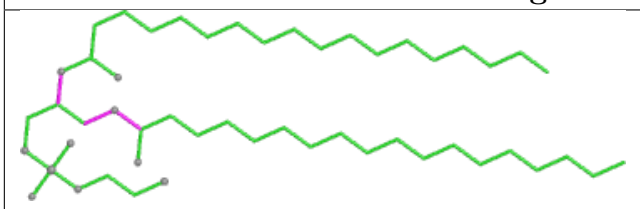
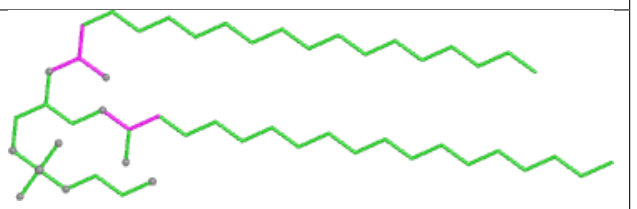
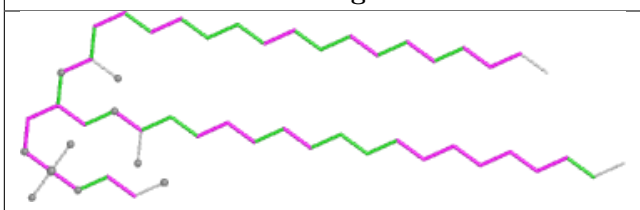
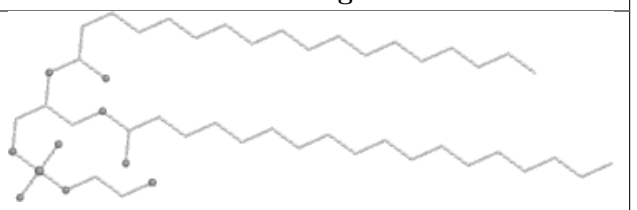


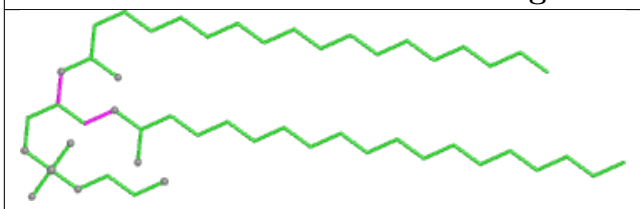
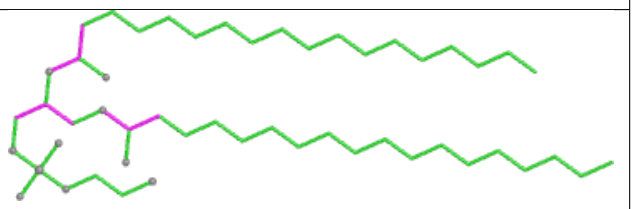
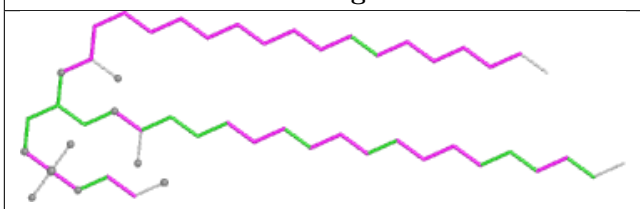
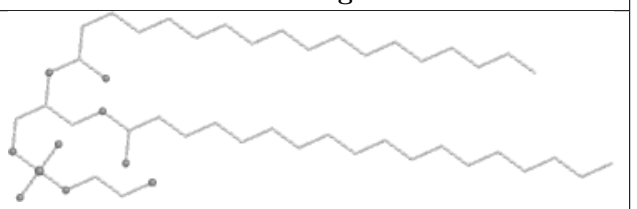
Ligand UQ8 A 704



Ligand HEM A 701



Ligand 3PE C 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE A 705	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

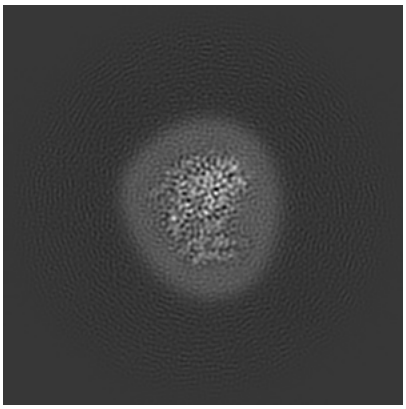
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-34171. These allow visual inspection of the internal detail of the map and identification of artifacts.

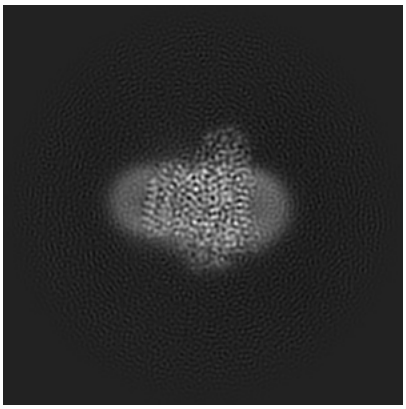
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



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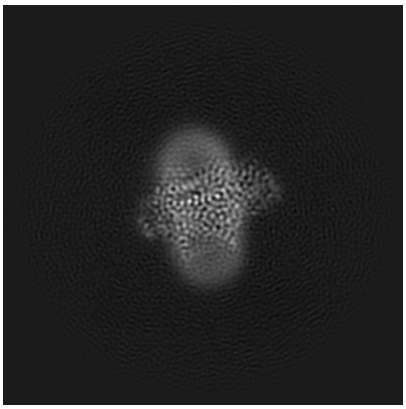
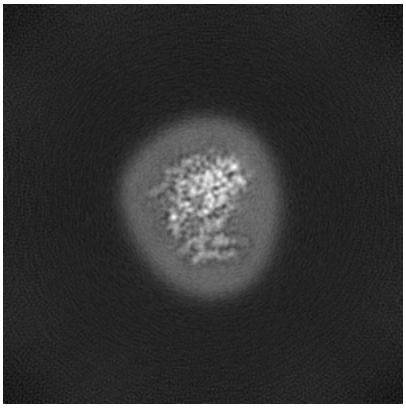


Z

6.1.2 Raw map



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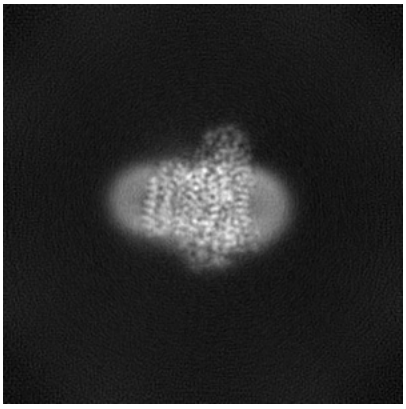
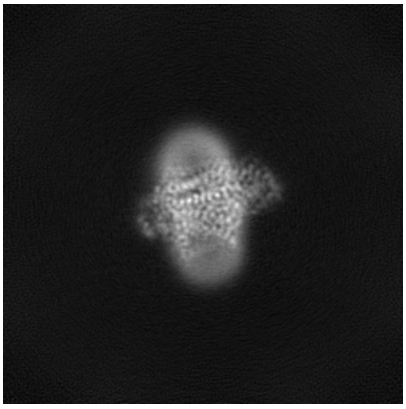


Y

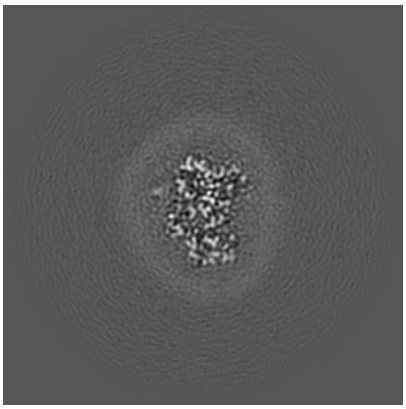


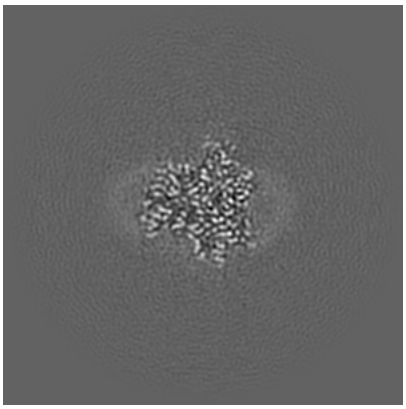
Z

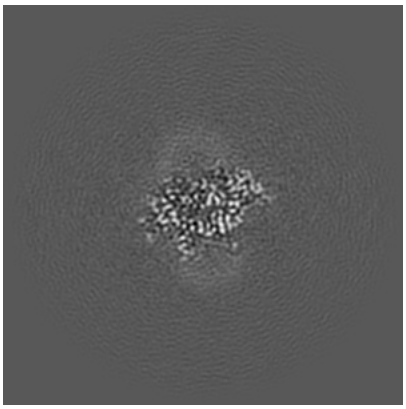
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

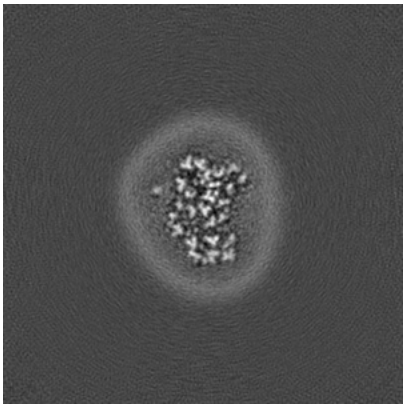
6.2.1 Primary map

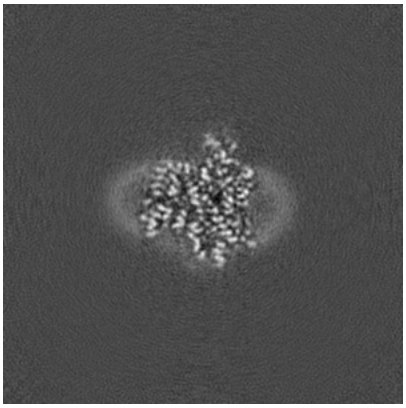

X Index: 128

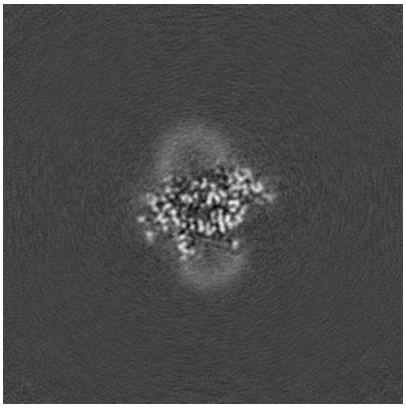

Y Index: 128


Z Index: 128

6.2.2 Raw map


X Index: 128

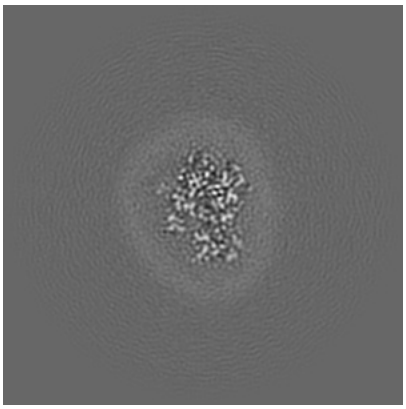

Y Index: 128

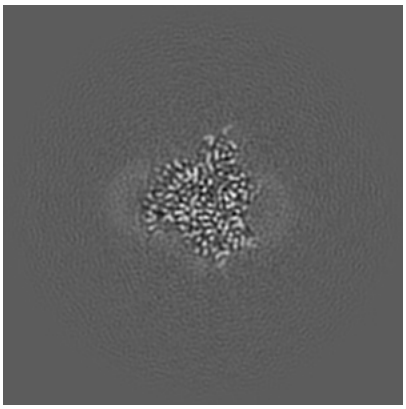

Z Index: 128

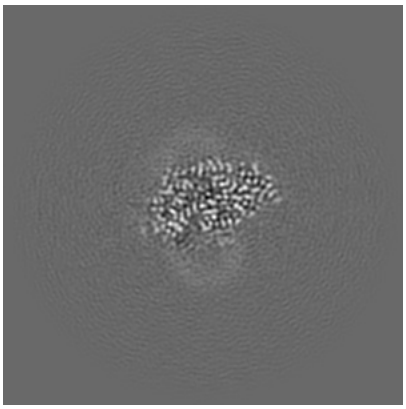
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

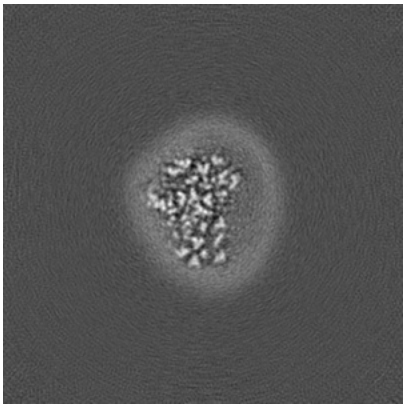
6.3.1 Primary map

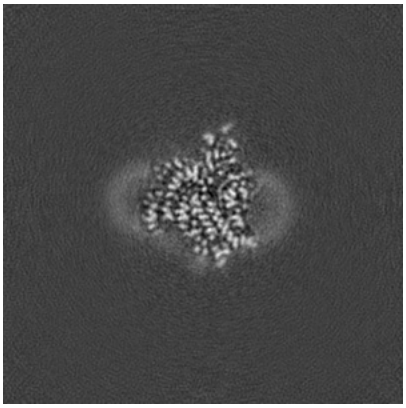

X Index: 134

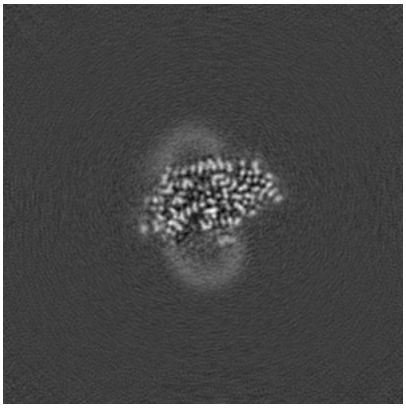

Y Index: 130


Z Index: 142

6.3.2 Raw map


X Index: 115

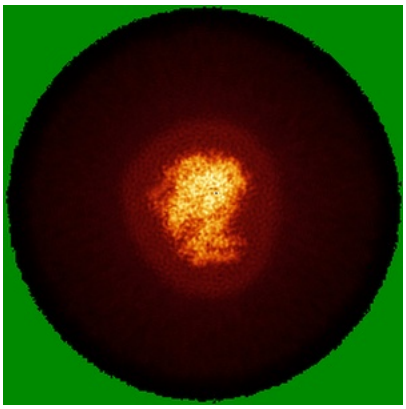

Y Index: 130

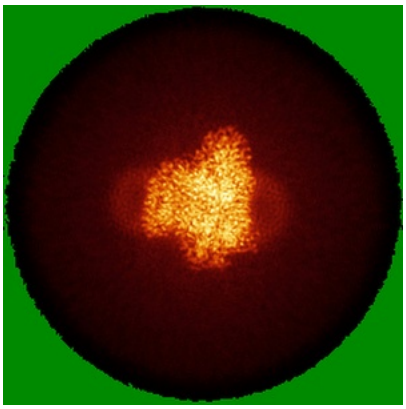

Z Index: 142

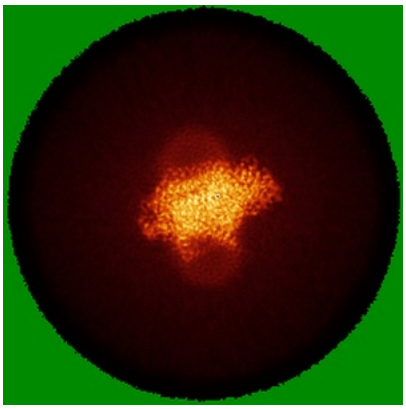
The images above show the largest variance slices of the map in three orthogonal directions.

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

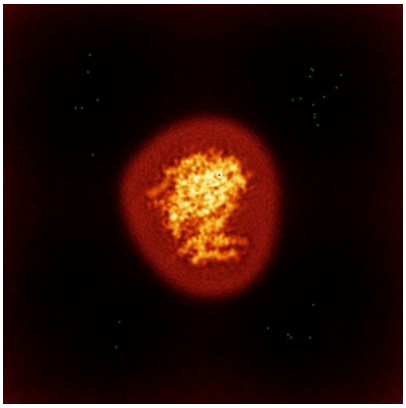
6.4.1 Primary map

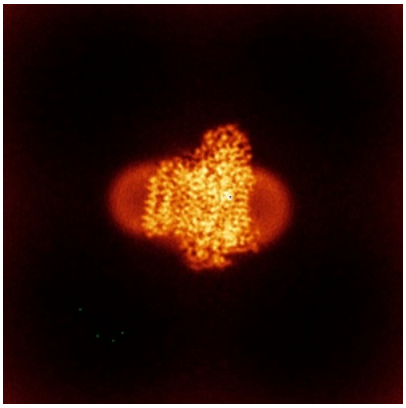

X

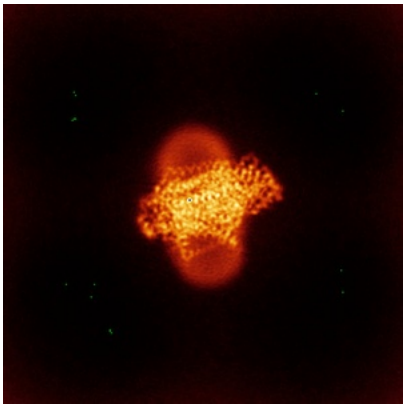

Y


Z

6.4.2 Raw map


X

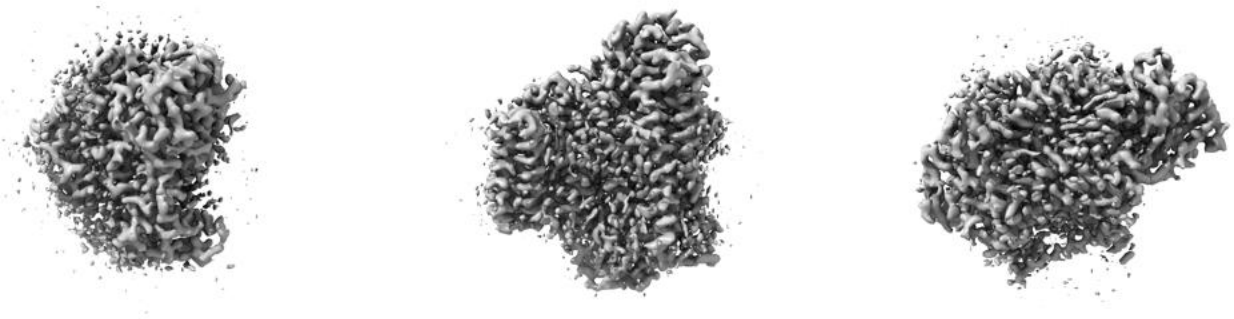

Y


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)

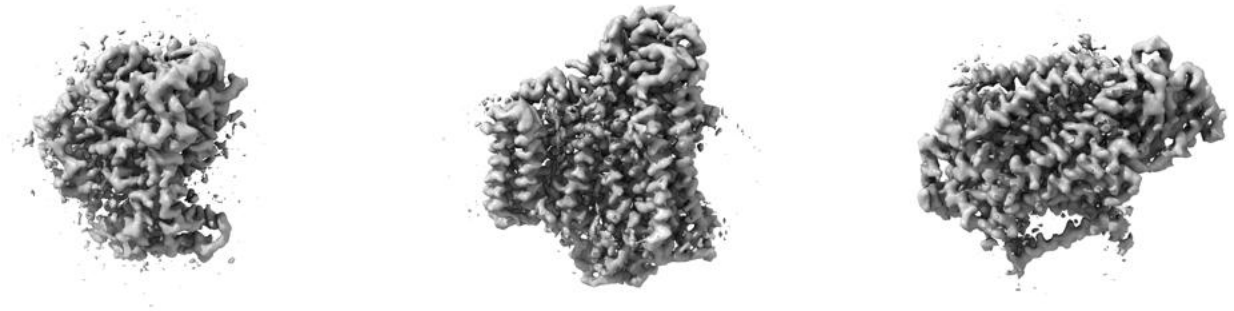
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.31. 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.

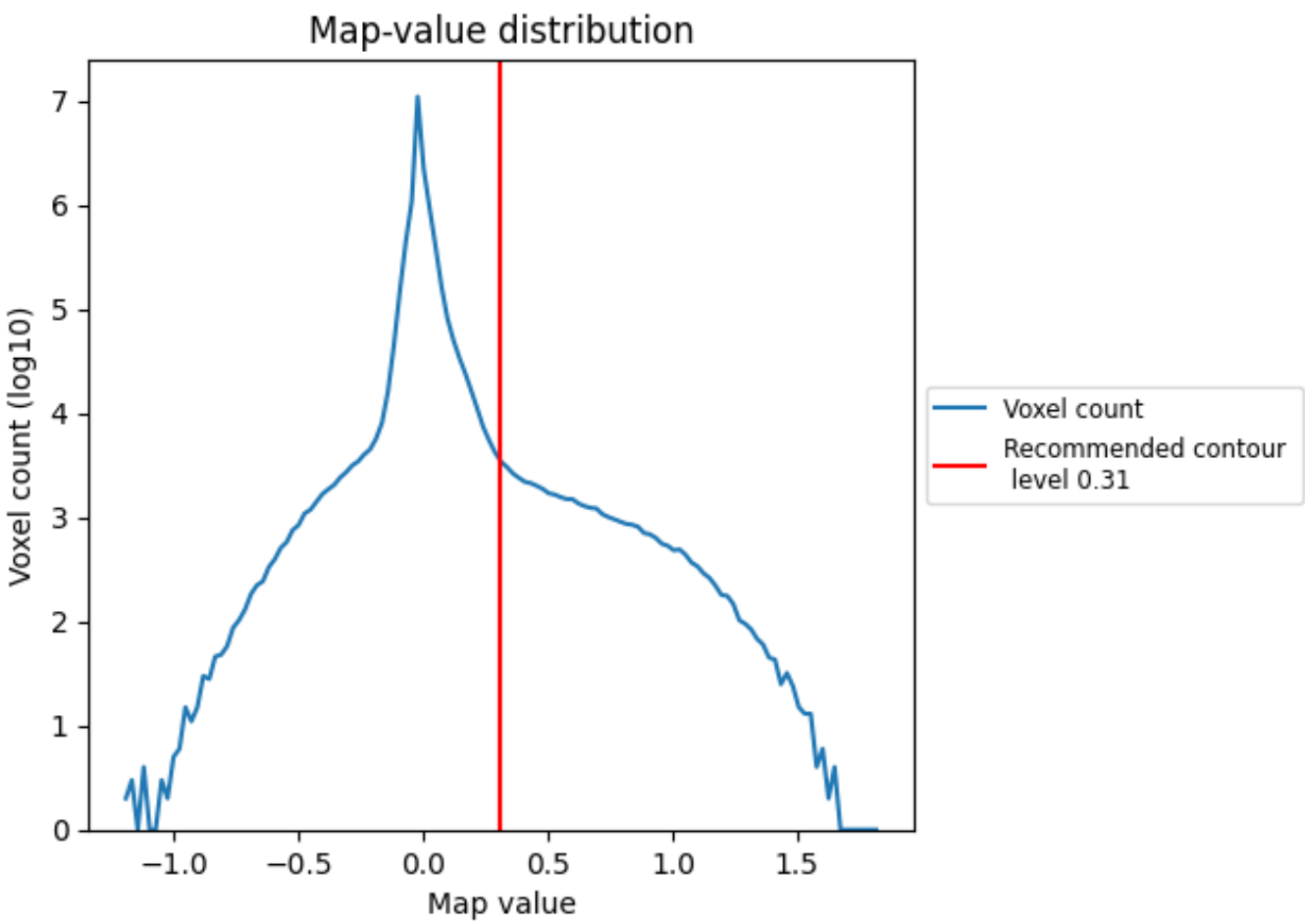
6.6 Mask visualisation (i)

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

7 Map analysis (i)

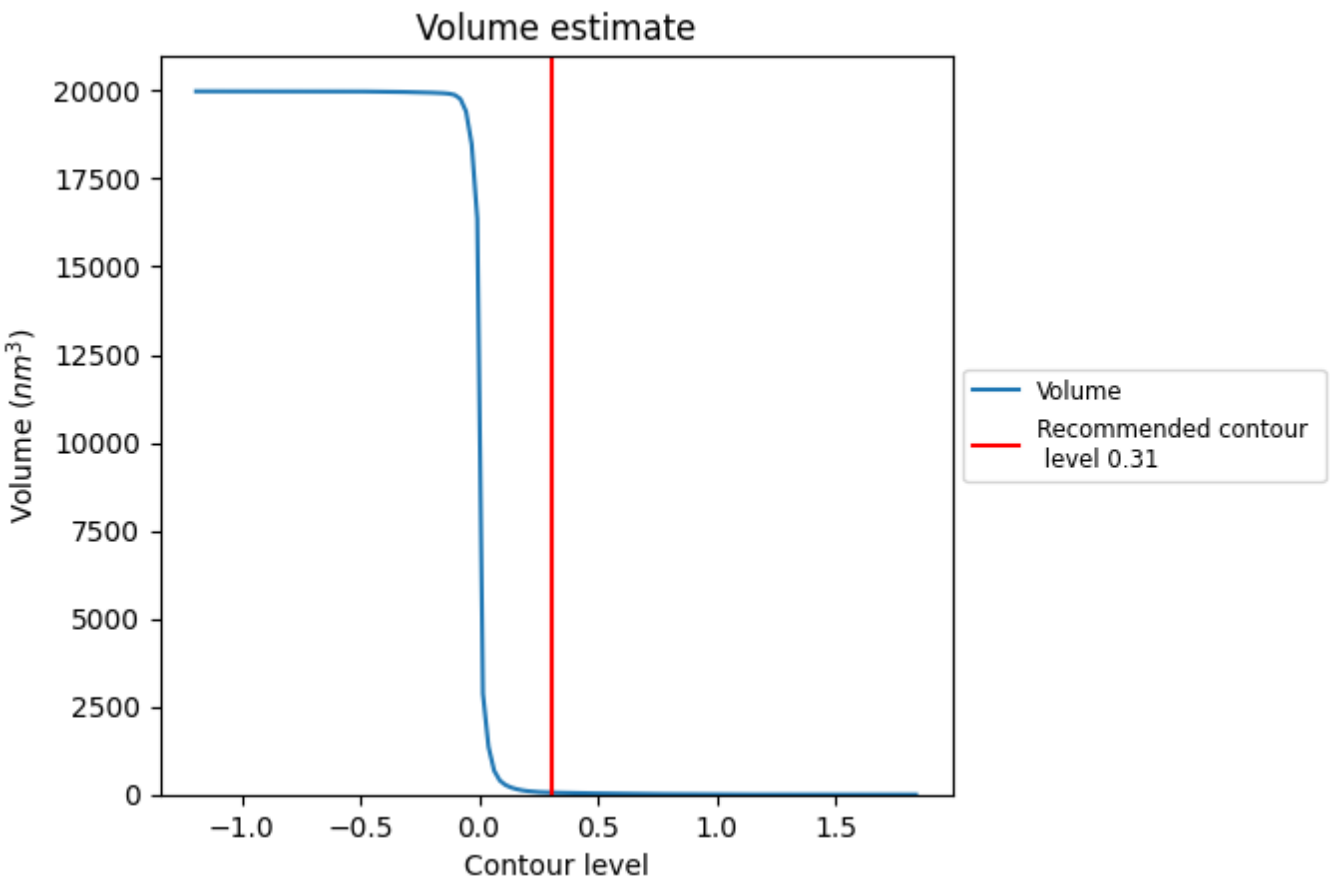
This section contains the results of statistical analysis of the map.

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.

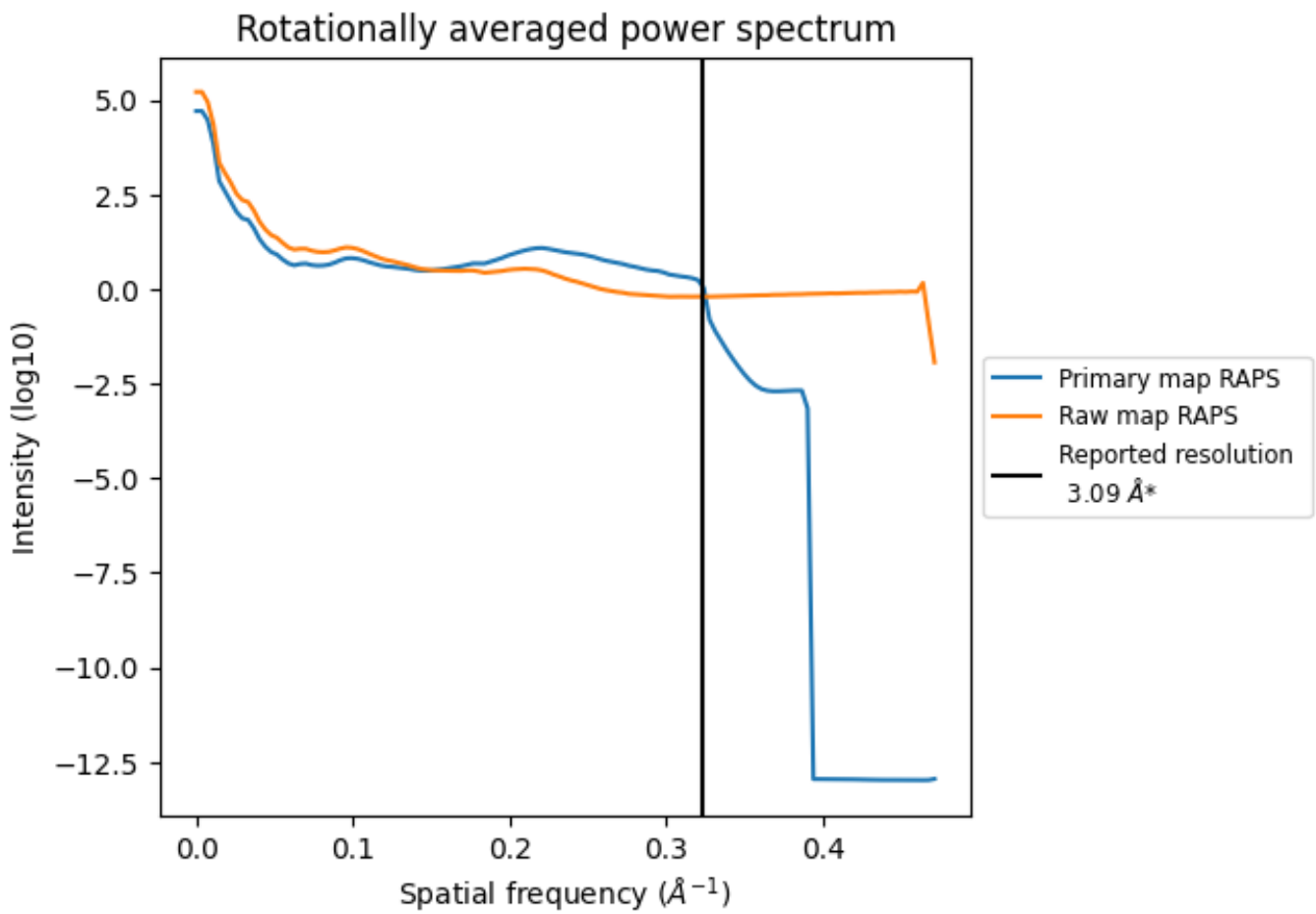
7.2 Volume estimate (i)



The volume at the recommended contour level is 56 nm^3; this corresponds to an approximate mass of 50 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)

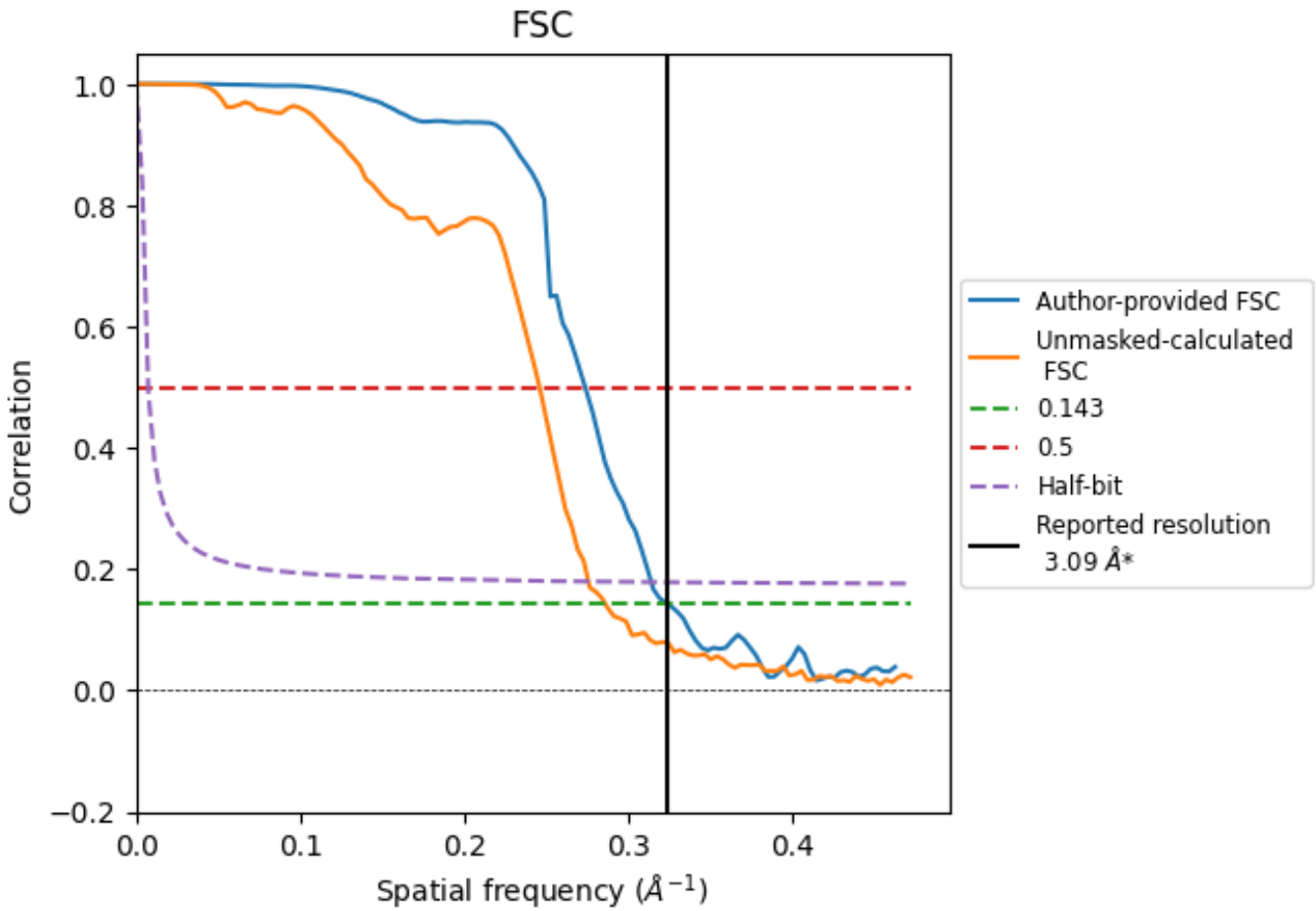


*Reported resolution corresponds to spatial frequency of 0.324 Å^{-1}

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 0.324 Å^{-1}

8.2 Resolution estimates (i)

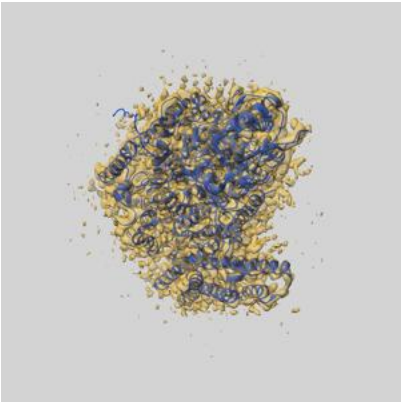
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	3.09	3.65	3.19
Unmasked-calculated*	3.50	4.07	3.63

*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 3.50 differs from the reported value 3.09 by more than 10 %

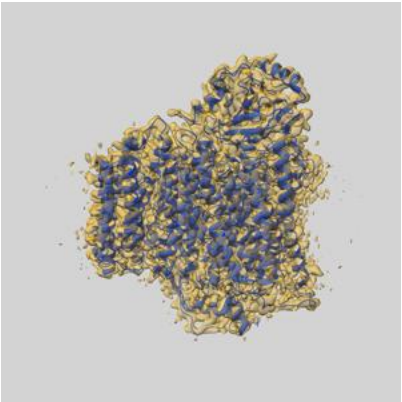
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-34171 and PDB model 8GO3. Per-residue inclusion information can be found in section 3 on page 8.

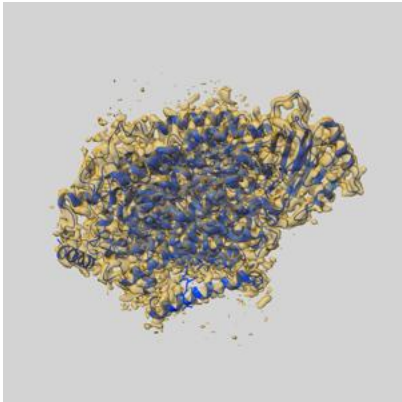
9.1 Map-model overlay (i)



X



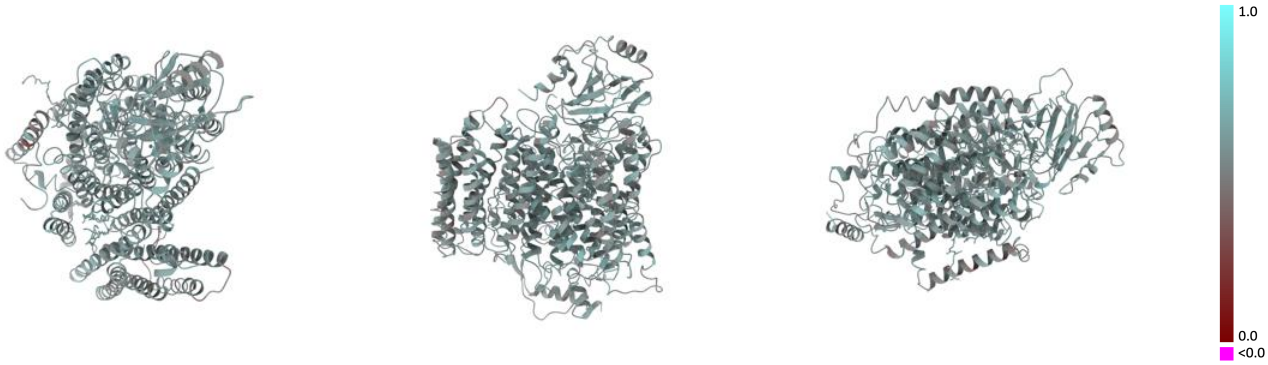
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.31 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.

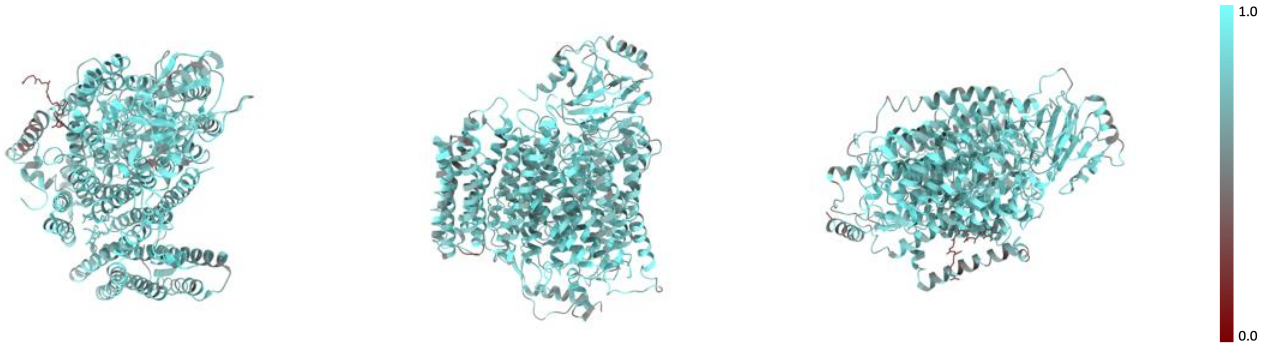
9.2 Q-score mapped to coordinate model (i)



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.

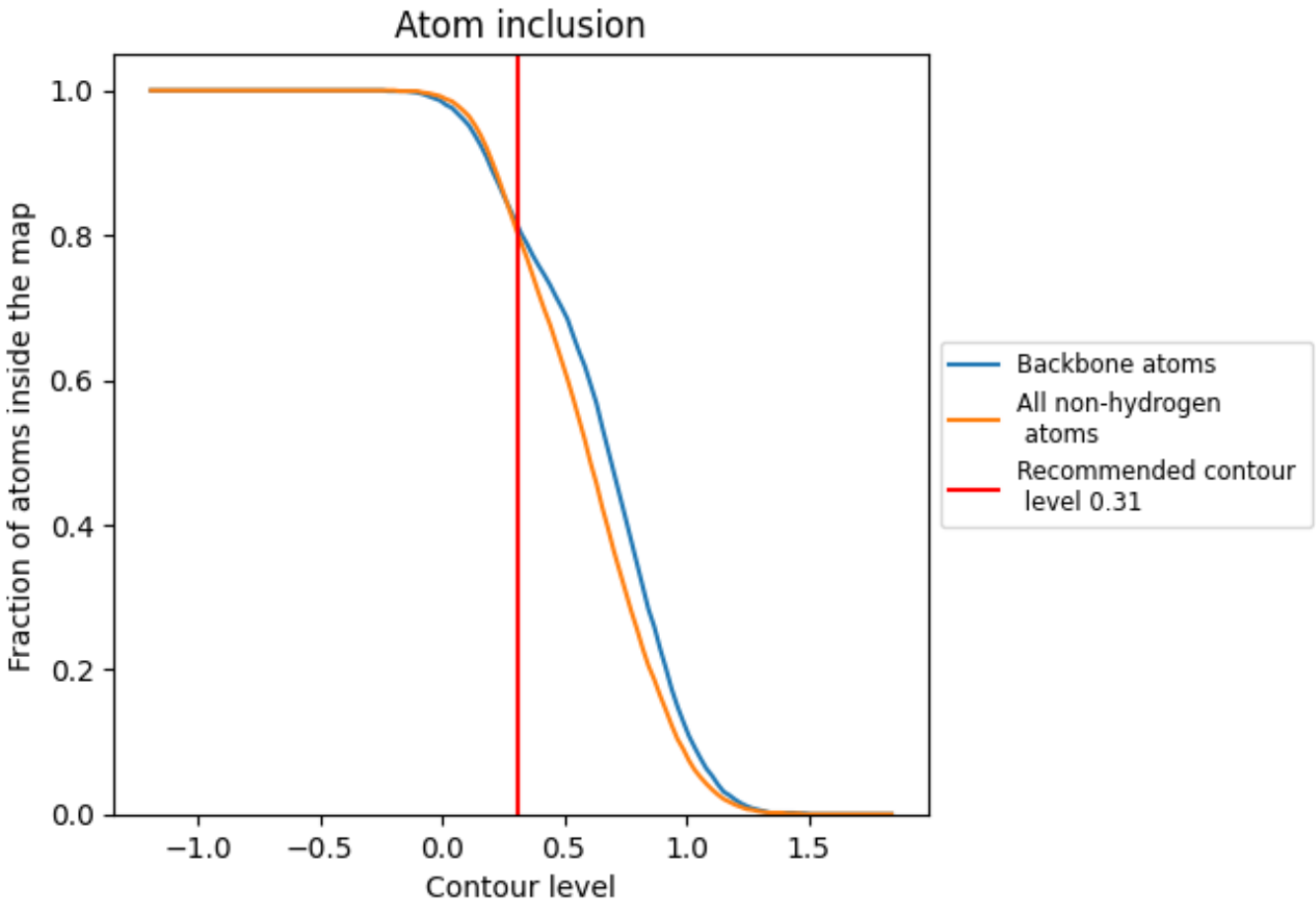
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.31).

9.4 Atom inclusion (i)



At the recommended contour level, 81% 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 (0.31) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8020	0.5530
A	0.8230	0.5600
B	0.7660	0.5430
C	0.8100	0.5500
D	0.7290	0.5330