Full wwPDB EM Validation Report

Aug 26, 2026 – 11:43 am BST

PDB ID	:	32FI / pdb_000032fi
EMDB ID	:	EMD-58853
Title	:	CryoEM structure of the E494A Quinol-Dependent Nitric Oxide Reductase
Authors	:	Khaja, F.; Antonyuk, S.V.; Muench, S.P.; Hsanain, S.S.
Deposited on	:	2026-07-08
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 (1)) were used in the production of this report:

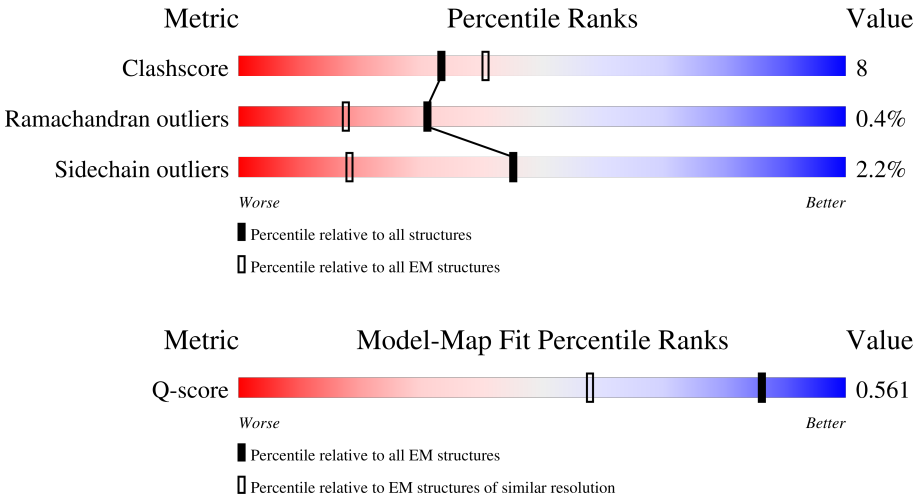
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

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	761	78% 19%
1	B	761	76% 22%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12155 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.

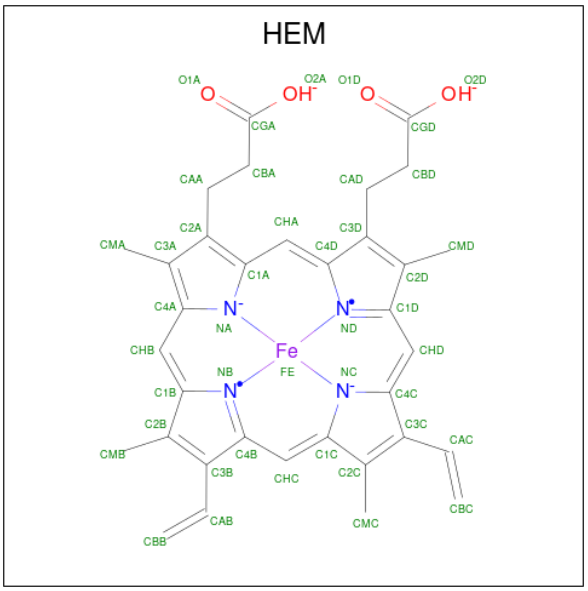
- Molecule 1 is a protein called Nitric oxide reductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	750	Total	C	N	O	S	0	0
			5878	3879	987	989	23		
1	B	750	Total	C	N	O	S	0	0
			5897	3889	990	995	23		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	494	ALA	GLU	engineered mutation	UNP A0ABF7PH53
B	494	ALA	GLU	engineered mutation	UNP A0ABF7PH53

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

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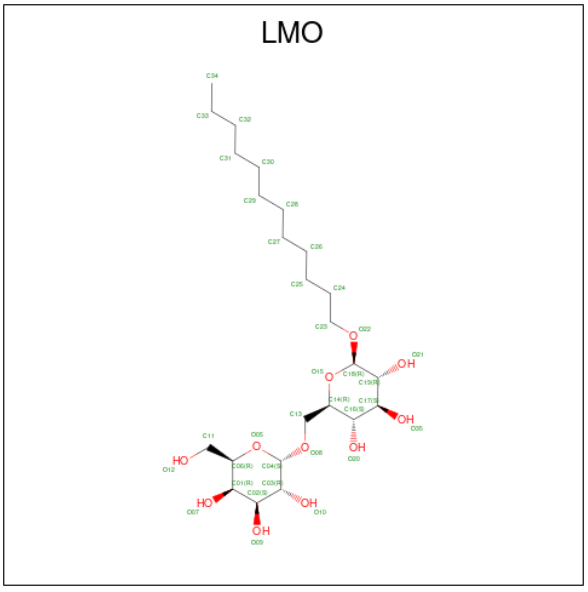
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Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

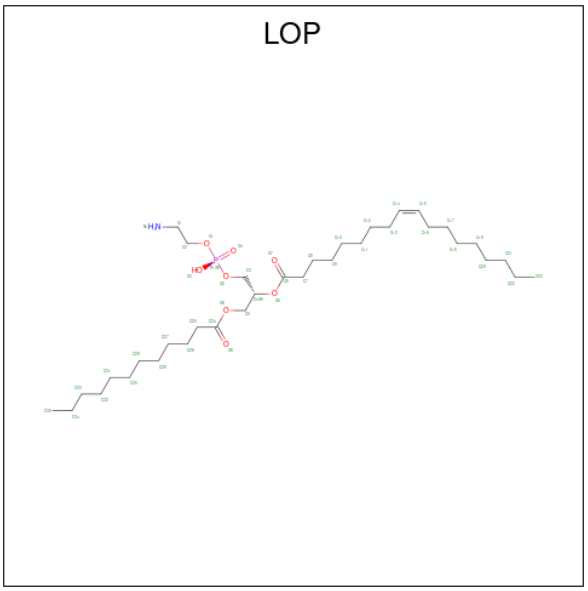
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	
3	B	1	Total	Ca	0
			1	1	

- Molecule 4 is dodecyl 6-O-alpha-D-galactopyranosyl-beta-D-glucopyranoside (CCD ID: LMO) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			35	24	11	
4	B	1	Total	C	O	0
			35	24	11	

- Molecule 5 is (1R)-2-{[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (CCD ID: LOP) (formula: $C_{35}H_{68}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	50	Total	O	0
			50	50	
6	B	48	Total	O	0
			48	48	

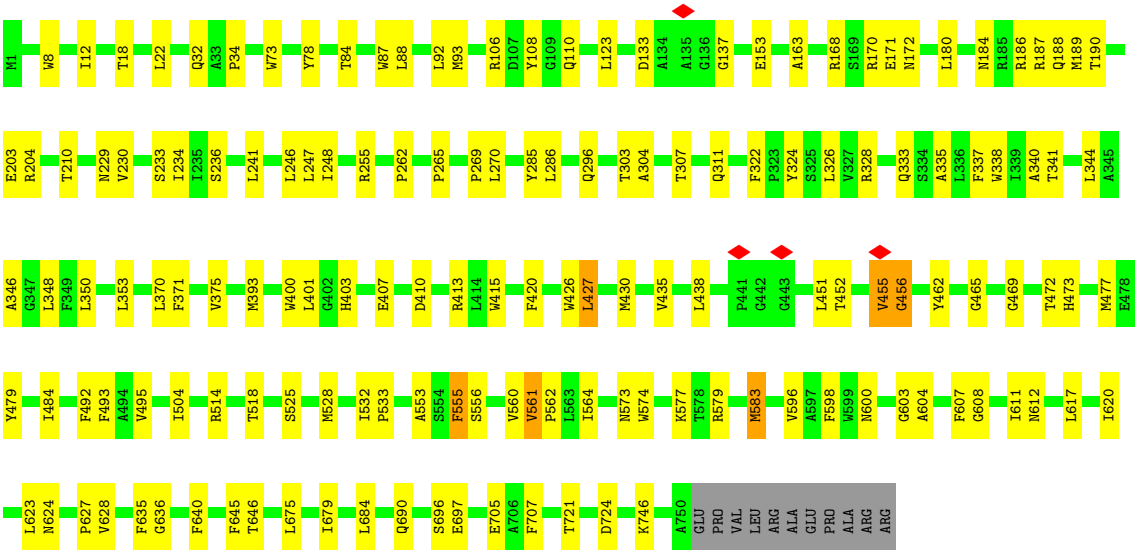
3 Residue-property plots (i)

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: Nitric oxide reductase subunit B

Chain A:

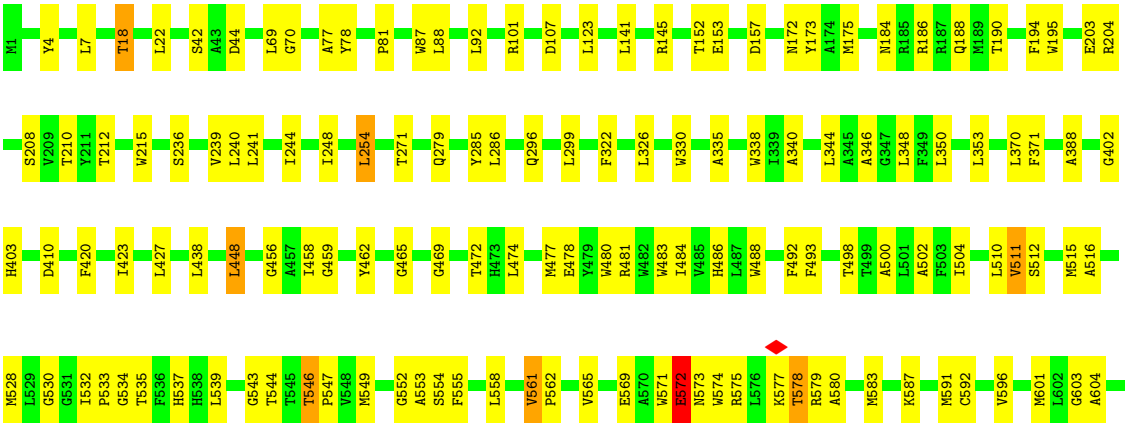




• Molecule 1: Nitric oxide reductase subunit B

Chain B:






F607
M610
I611
P614
I620
L623
N624
P627
V628
H629
L634
F635
G636
F640
L641
A642
L643
G644
F645
T646
R654
L673
G674
L675
M678
I679
L684
L688
I689
Q690
E705
M708
R720
L732
A733
M734
V735
I739
K746
P747
A748
A749
A750
GLU
PRO
VAL
LEU
ARG
ALA
GLU
PRO
ALA
ARG
ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	417968	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.660	Depositor
Minimum map value	-0.402	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.0567	Depositor
Map size (Å)	278.4, 278.4, 278.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, HEM, LMO, LOP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.15	0/6069	0.33	1/8285 (0.0%)
1	B	0.16	0/6089	0.32	0/8311
All	All	0.15	0/12158	0.32	1/16596 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	262	PRO	N-CA-CB	7.67	110.52	103.08

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5878	0	5797	93	0
1	B	5897	0	5824	102	0
2	A	86	0	60	6	0
2	B	86	0	60	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	35	0	0	1	0
4	B	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	38	0	50	3	0
6	A	50	0	0	0	0
6	B	48	0	0	1	0
All	All	12155	0	11791	199	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 8.

All (199) 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:393:MET:HE1	1:A:401:LEU:HB2	1.56	0.88
1:B:18:THR:HG23	1:B:532:ILE:HD11	1.62	0.81
1:B:427:LEU:HD21	1:B:456:GLY:HA2	1.67	0.74
1:B:549:MET:HE2	1:B:614:PRO:HB3	1.71	0.73
1:B:236:SER:HB2	1:B:553:ALA:HB1	1.73	0.71
1:A:92:LEU:HD22	1:A:123:LEU:HD11	1.74	0.70
1:B:533:PRO:HB3	1:B:552:GLY:HA2	1.73	0.69
1:B:279:GLN:HE22	1:B:353:LEU:HD13	1.58	0.69
1:B:571:TRP:O	1:B:573:ASN:N	2.29	0.66
1:A:492:PHE:HA	1:A:495:VAL:HG12	1.77	0.66
1:B:561:VAL:HG13	1:B:562:PRO:HD3	1.78	0.65
1:A:22:LEU:HD13	1:A:532:ILE:HG13	1.78	0.64
1:A:430:MET:SD	1:A:455:VAL:HG11	2.37	0.64
1:B:101:ARG:NH2	1:B:107:ASP:OD1	2.31	0.63
1:B:674:GLY:O	1:B:678:MET:HG3	1.98	0.63
1:A:203:GLU:HA	1:A:210:THR:HA	1.81	0.62
1:A:236:SER:HB3	1:A:553:ALA:HB1	1.81	0.62
1:A:106:ARG:NH2	1:A:110:GLN:O	2.32	0.62
2:B:801:HEM:HMC2	2:B:801:HEM:HBC2	1.83	0.61
2:B:802:HEM:HMB1	2:B:802:HEM:HBB2	1.83	0.60
1:B:604:ALA:HA	1:B:629:HIS:HE1	1.66	0.60
1:A:465:GLY:HA2	1:A:484:ILE:HD11	1.82	0.59
2:A:802:HEM:HMB1	2:A:802:HEM:HBB2	1.84	0.59
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.85	0.59
1:B:157:ASP:OD1	1:B:186:ARG:NH1	2.32	0.59
1:A:172:ASN:ND2	1:A:705:GLU:OE2	2.34	0.59
1:B:240:LEU:O	1:B:244:ILE:HG13	2.03	0.58
1:B:510:LEU:O	1:B:512:SER:N	2.31	0.58
1:A:230:VAL:O	1:A:234:ILE:HG12	2.05	0.57
1:A:350:LEU:HD21	1:A:504:ILE:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:GLU:HA	1:B:210:THR:HA	1.86	0.57
1:A:533:PRO:HG2	1:A:555:PHE:HB2	1.85	0.56
2:B:802:HEM:HMC1	2:B:802:HEM:HBC2	1.88	0.56
2:B:801:HEM:HMB1	2:B:801:HEM:HBB2	1.87	0.56
5:B:804:LOP:H272	5:B:804:LOP:H92	1.88	0.56
1:B:636:GLY:HA2	1:B:640:PHE:HD2	1.71	0.56
1:A:561:VAL:HG13	1:A:562:PRO:HD3	1.88	0.56
1:B:634:LEU:HD23	2:B:801:HEM:HAC	1.88	0.55
1:B:172:ASN:ND2	1:B:705:GLU:OE2	2.37	0.55
1:A:324:TYR:OH	2:A:801:HEM:O1A	2.24	0.55
2:A:801:HEM:HMB1	2:A:801:HEM:HBB2	1.88	0.55
1:B:510:LEU:C	1:B:512:SER:H	2.14	0.55
2:A:802:HEM:HMC2	2:A:802:HEM:HBC2	1.89	0.54
1:A:32:GLN:O	1:A:204:ARG:NH2	2.37	0.54
1:B:22:LEU:HD13	1:B:532:ILE:HD12	1.90	0.53
1:A:635:PHE:HD2	1:A:675:LEU:HD22	1.73	0.53
1:B:335:ALA:HA	1:B:338:TRP:CD1	2.44	0.53
1:B:486:HIS:HB2	1:B:535:THR:HG22	1.91	0.53
1:B:532:ILE:HB	1:B:533:PRO:HD3	1.90	0.53
1:A:400:TRP:HA	1:A:413:ARG:HB3	1.91	0.53
1:B:42:SER:OG	1:B:44:ASP:OD1	2.20	0.53
1:A:344:LEU:HD22	1:A:426:TRP:CD2	2.44	0.53
1:B:611:ILE:HA	1:B:620:ILE:HD11	1.91	0.53
1:A:333:GLN:NE2	1:A:410:ASP:OD1	2.37	0.52
1:B:423:ILE:HG22	1:B:459:GLY:HA2	1.91	0.52
1:B:286:LEU:HD22	1:B:646:THR:HG23	1.92	0.52
1:A:335:ALA:HA	1:A:338:TRP:CD1	2.45	0.52
1:A:22:LEU:O	1:A:479:TYR:OH	2.26	0.52
1:B:4:TYR:HB3	1:B:7:LEU:HD12	1.92	0.51
1:B:322:PHE:HA	1:B:326:LEU:HD23	1.92	0.51
1:B:635:PHE:HD2	1:B:675:LEU:HD22	1.75	0.51
1:A:420:PHE:HD1	1:A:462:TYR:HB3	1.76	0.51
1:B:528:MET:HE3	1:B:528:MET:HA	1.93	0.50
1:B:571:TRP:O	1:B:572:GLU:C	2.54	0.50
1:B:578:THR:O	1:B:580:ALA:N	2.45	0.50
1:A:304:ALA:O	1:A:307:THR:OG1	2.22	0.50
1:B:285:TYR:CE1	1:B:371:PHE:HB2	2.47	0.50
1:A:180:LEU:O	1:A:186:ARG:NH1	2.40	0.49
1:A:328:ARG:NH1	1:A:407:GLU:OE2	2.32	0.49
1:B:141:LEU:HD22	1:B:145:ARG:HD3	1.94	0.49
1:B:678:MET:HE3	1:B:720:ARG:HH21	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:ILE:HA	1:A:620:ILE:HD11	1.95	0.49
1:B:195:TRP:HZ3	1:B:474:LEU:HD12	1.77	0.49
1:B:69:LEU:HD11	1:B:175:MET:HG2	1.94	0.49
1:A:469:GLY:H	1:A:472:THR:HG1	1.59	0.49
1:A:18:THR:HB	1:A:532:ILE:HD13	1.95	0.49
1:A:184:ASN:O	1:A:188:GLN:HG2	2.13	0.48
1:B:271:THR:O	1:B:271:THR:OG1	2.30	0.48
1:B:628:VAL:HG13	1:B:679:ILE:HG23	1.95	0.48
1:B:92:LEU:HD22	1:B:123:LEU:HD11	1.95	0.48
1:B:403:HIS:CE1	1:B:410:ASP:HB3	2.48	0.48
1:B:478:GLU:OE1	1:B:481:ARG:NH2	2.44	0.48
1:A:168:ARG:NH1	1:A:171:GLU:OE1	2.46	0.47
1:A:403:HIS:CE1	1:A:410:ASP:HB3	2.49	0.47
1:B:511:VAL:HG12	1:B:569:GLU:HG3	1.95	0.47
1:A:617:LEU:HA	1:A:620:ILE:HG12	1.95	0.47
1:A:8:TRP:O	1:A:12:ILE:HD12	2.14	0.47
1:A:265:PRO:HG2	1:A:269:PRO:HG3	1.96	0.47
1:B:239:VAL:HG21	1:B:554:SER:O	2.14	0.47
1:B:469:GLY:N	1:B:472:THR:OG1	2.37	0.47
1:B:587:LYS:HE2	1:B:591:MET:HE2	1.97	0.47
1:A:596:VAL:HA	1:A:636:GLY:O	2.15	0.47
1:A:600:ASN:O	1:A:604:ALA:HB3	2.15	0.47
1:A:34:PRO:O	1:A:473:HIS:NE2	2.44	0.46
1:A:340:ALA:O	1:A:344:LEU:HG	2.16	0.46
1:A:598:PHE:HD1	1:B:248:ILE:HG22	1.81	0.46
1:A:574:TRP:CD1	1:A:583:MET:HG2	2.51	0.46
1:A:636:GLY:HA2	1:A:640:PHE:HD2	1.80	0.46
1:A:346:ALA:HB2	1:A:645:PHE:HB3	1.98	0.46
1:A:573:ASN:HA	1:A:577:LYS:HG2	1.97	0.46
1:A:285:TYR:CE1	1:A:371:PHE:HB2	2.50	0.46
1:B:350:LEU:HD21	1:B:504:ILE:HD11	1.98	0.46
1:B:546:THR:N	1:B:547:PRO:HD2	2.31	0.46
1:A:603:GLY:HA2	1:A:607:PHE:CD2	2.52	0.45
1:B:78:TYR:OH	2:B:801:HEM:O2D	2.33	0.45
1:B:596:VAL:HG21	1:B:641:LEU:HG	1.98	0.45
1:A:348:LEU:HD11	1:A:370:LEU:HD23	1.98	0.45
1:A:88:LEU:O	1:A:92:LEU:HG	2.17	0.45
1:A:573:ASN:OD1	1:A:573:ASN:N	2.49	0.45
1:B:346:ALA:HB2	1:B:645:PHE:HB3	1.99	0.45
1:B:530:GLY:HA3	1:B:558:LEU:HB2	1.96	0.45
1:A:255:ARG:O	1:B:575:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:LEU:HD13	1:B:734:MET:HE3	1.98	0.45
1:A:133:ASP:OD1	1:A:137:GLY:N	2.50	0.45
1:A:286:LEU:HD22	1:A:646:THR:HG23	1.98	0.45
1:B:88:LEU:O	1:B:92:LEU:HG	2.17	0.45
1:B:184:ASN:O	1:B:188:GLN:HG2	2.16	0.45
1:A:560:VAL:HG12	1:A:564:ILE:HD11	1.99	0.45
1:B:488:TRP:O	1:B:493:PHE:HB2	2.17	0.45
1:A:624:ASN:HA	1:A:627:PRO:HD2	1.98	0.45
5:B:804:LOP:H14	5:B:804:LOP:H322	1.99	0.45
1:A:153:GLU:HG2	1:A:190:THR:HB	1.98	0.44
1:A:533:PRO:HB2	1:A:556:SER:HA	1.99	0.44
1:B:603:GLY:HA2	1:B:607:PHE:CD2	2.53	0.44
1:B:87:TRP:CZ2	1:B:194:PHE:HB2	2.53	0.44
1:A:270:LEU:HD22	1:A:353:LEU:HD11	1.99	0.44
1:B:511:VAL:O	1:B:515:MET:HB3	2.17	0.44
1:A:435:VAL:HA	1:A:438:LEU:HD12	1.99	0.44
1:B:212:THR:HG22	1:B:215:TRP:HB3	1.99	0.44
1:A:303:THR:O	1:A:307:THR:HG23	2.18	0.44
1:A:187:ARG:O	1:A:190:THR:OG1	2.31	0.43
1:A:696:SER:OG	1:A:697:GLU:HG2	2.18	0.43
1:B:70:GLY:O	1:B:77:ALA:N	2.49	0.43
1:A:624:ASN:C	1:A:627:PRO:HD2	2.43	0.43
1:A:248:ILE:HG21	1:B:601:MET:HB3	2.01	0.43
1:A:514:ARG:O	1:A:518:THR:HG23	2.18	0.43
1:A:579:ARG:HB2	1:A:583:MET:HE3	2.00	0.43
1:A:684:LEU:HD21	1:B:241:LEU:HD12	1.99	0.43
1:A:623:LEU:HD13	1:A:690:GLN:HB3	1.99	0.43
1:B:577:LYS:O	1:B:578:THR:HG22	2.19	0.43
1:A:229:ASN:O	1:A:233:SER:OG	2.31	0.43
1:B:438:LEU:HD21	1:B:448:LEU:HB3	2.00	0.43
1:A:241:LEU:HD11	1:B:610:MET:HE1	2.01	0.43
1:A:322:PHE:HA	1:A:326:LEU:HD23	1.99	0.43
1:B:465:GLY:HA2	1:B:484:ILE:HD11	2.01	0.43
1:B:22:LEU:HD23	1:B:483:TRP:NE1	2.34	0.43
1:B:502:ALA:HB1	1:B:516:ALA:HB1	2.00	0.43
1:A:583:MET:HE2	1:A:583:MET:HB2	1.87	0.43
1:B:296:GLN:NE2	1:B:335:ALA:HB2	2.34	0.43
1:B:624:ASN:C	1:B:627:PRO:HD2	2.44	0.43
1:A:78:TYR:OH	2:A:801:HEM:O2D	2.37	0.42
1:B:533:PRO:HG2	1:B:555:PHE:O	2.19	0.42
1:B:572:GLU:O	1:B:575:ARG:N	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:LEU:HD11	1:B:370:LEU:HD23	2.01	0.42
1:A:371:PHE:O	1:A:375:VAL:HG13	2.19	0.42
1:B:340:ALA:O	1:B:344:LEU:HG	2.19	0.42
1:B:534:GLY:HA2	1:B:537:HIS:CE1	2.55	0.42
1:B:153:GLU:HG2	1:B:190:THR:HB	2.01	0.42
1:B:458:ILE:HG13	1:B:492:PHE:HB3	2.01	0.42
1:A:163:ALA:O	1:A:170:ARG:NH2	2.41	0.42
1:A:189:MET:HE2	1:A:189:MET:HB3	1.74	0.42
1:A:628:VAL:HG13	1:A:679:ILE:HG23	2.01	0.42
1:B:204:ARG:NH2	1:B:543:GLY:O	2.53	0.42
1:A:427:LEU:HD11	1:A:456:GLY:HA2	2.02	0.41
1:A:93:MET:HE3	1:A:93:MET:HA	2.02	0.41
1:A:337:PHE:O	1:A:341:THR:OG1	2.35	0.41
1:A:690:GLN:HG2	1:A:707:PHE:HE2	1.84	0.41
1:B:654:ARG:HH22	1:B:748:ALA:HB3	1.84	0.41
1:A:87:TRP:HH2	1:A:153:GLU:HG3	1.86	0.41
1:A:234:ILE:HD12	1:B:688:LEU:HB3	2.01	0.41
1:A:561:VAL:HA	1:A:564:ILE:HD12	2.02	0.41
1:B:574:TRP:CD1	1:B:583:MET:HG2	2.55	0.41
1:A:241:LEU:HD12	1:B:684:LEU:HD21	2.02	0.41
1:A:477:MET:C	1:A:477:MET:SD	3.04	0.41
1:B:592:CYS:O	1:B:596:VAL:HG23	2.21	0.41
1:A:93:MET:HE1	1:A:108:TYR:CD2	2.55	0.41
1:B:420:PHE:CD1	1:B:462:TYR:HB3	2.56	0.41
1:B:532:ILE:HD13	1:B:532:ILE:HA	1.85	0.41
4:A:804:LMO:O35	5:B:804:LOP:N1	2.53	0.41
1:B:539:LEU:O	1:B:544:THR:OG1	2.29	0.41
1:A:73:TRP:CD1	1:A:84:THR:HG21	2.56	0.41
1:A:401:LEU:O	1:A:415:TRP:NE1	2.46	0.41
1:A:608:GLY:O	1:A:612:ASN:HB2	2.21	0.41
1:B:477:MET:SD	1:B:477:MET:C	3.04	0.41
1:A:420:PHE:CD1	1:A:462:TYR:HB3	2.56	0.41
1:B:145:ARG:NH2	6:B:916:HOH:O	2.53	0.41
1:B:480:TRP:O	1:B:484:ILE:HG13	2.21	0.41
1:B:254:LEU:HD22	1:B:254:LEU:HA	1.81	0.40
1:B:500:ALA:O	1:B:504:ILE:HG12	2.21	0.40
1:B:623:LEU:HD13	1:B:690:GLN:HB3	2.03	0.40
1:B:708:MET:HE3	1:B:708:MET:HB3	1.91	0.40
1:B:18:THR:CG2	1:B:532:ILE:HD11	2.43	0.40
1:A:18:THR:HG21	1:A:528:MET:O	2.22	0.40
1:A:296:GLN:NE2	1:A:335:ALA:HB2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:THR:HA	1:A:724:ASP:HB2	2.03	0.40
1:B:299:LEU:HD13	1:B:330:TRP:HB3	2.04	0.40
1:B:388:ALA:HB2	1:B:402:GLY:HA3	2.04	0.40
1:B:735:VAL:O	1:B:739:ILE:HG12	2.21	0.40
1:B:81:PRO:HD3	1:B:173:TYR:CD1	2.56	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	748/761 (98%)	717 (96%)	29 (4%)	2 (0%)	36	55
1	B	748/761 (98%)	716 (96%)	28 (4%)	4 (0%)	24	43
All	All	1496/1522 (98%)	1433 (96%)	57 (4%)	6 (0%)	31	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	511	VAL
1	B	572	GLU
1	B	579	ARG
1	B	746	LYS
1	A	456	GLY
1	A	746	LYS

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	578/595 (97%)	566 (98%)	12 (2%)	47	74
1	B	583/595 (98%)	570 (98%)	13 (2%)	45	73
All	All	1161/1190 (98%)	1136 (98%)	25 (2%)	45	73

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	LEU
1	A	247	LEU
1	A	311	GLN
1	A	427	LEU
1	A	451	LEU
1	A	452	THR
1	A	455	VAL
1	A	493	PHE
1	A	525	SER
1	A	555	PHE
1	A	561	VAL
1	A	583	MET
1	B	18	THR
1	B	152	THR
1	B	208	SER
1	B	254	LEU
1	B	448	LEU
1	B	498	THR
1	B	546	THR
1	B	561	VAL
1	B	565	VAL
1	B	572	GLU
1	B	578	THR
1	B	673	LEU
1	B	732	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	311	GLN

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Mol	Chain	Res	Type
1	A	320	GLN
1	A	355	ASN
1	A	446	ASN
1	B	158	GLN
1	B	538	HIS
1	B	585	ASN
1	B	612	ASN
1	B	624	ASN
1	B	709	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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	LOP	B	804	-	37,37,44	0.54	0	40,42,49	0.48	0
2	HEM	B	801	1,3	50,50,50	1.36	6 (12%)	66,82,82	1.20	7 (10%)
4	LMO	B	805	-	36,36,36	0.56	0	47,47,47	1.02	3 (6%)
2	HEM	A	801	1,3	50,50,50	1.36	6 (12%)	66,82,82	1.18	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	LMO	A	804	-	36,36,36	0.57	0	47,47,47	0.95	1 (2%)
2	HEM	B	802	1,3,6	50,50,50	1.44	6 (12%)	66,82,82	1.15	6 (9%)
2	HEM	A	802	1,3,6	50,50,50	1.37	6 (12%)	66,82,82	1.21	8 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LOP	B	804	-	-	22/41/41/48	-
2	HEM	B	801	1,3	-	0/14/54/54	-
4	LMO	B	805	-	-	15/20/60/60	0/2/2/2
2	HEM	A	801	1,3	-	0/14/54/54	-
4	LMO	A	804	-	-	12/20/60/60	0/2/2/2
2	HEM	B	802	1,3,6	-	1/14/54/54	-
2	HEM	A	802	1,3,6	-	0/14/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	HEM	FE-NB	3.66	2.06	1.94
2	B	802	HEM	FE-ND	3.49	2.05	1.94
2	B	802	HEM	FE-NC	3.37	2.06	1.95
2	A	802	HEM	FE-NB	3.23	2.04	1.94
2	A	801	HEM	FE-NB	3.22	2.04	1.94
2	A	802	HEM	FE-ND	3.20	2.04	1.94
2	A	801	HEM	FE-ND	3.06	2.04	1.94
2	B	801	HEM	FE-ND	3.04	2.04	1.94
2	B	801	HEM	FE-NB	3.03	2.04	1.94
2	B	802	HEM	CAB-C3B	3.02	1.55	1.47
2	A	802	HEM	CAC-C3C	2.99	1.55	1.47
2	B	801	HEM	CAC-C3C	2.98	1.55	1.47
2	A	801	HEM	CAC-C3C	2.98	1.55	1.47
2	B	802	HEM	CAC-C3C	2.98	1.55	1.47
2	A	802	HEM	CAB-C3B	2.97	1.55	1.47
2	B	801	HEM	CAB-C3B	2.96	1.55	1.47
2	B	801	HEM	FE-NA	2.96	2.05	1.95
2	A	801	HEM	CAB-C3B	2.96	1.55	1.47
2	B	802	HEM	FE-NA	2.90	2.05	1.95
2	A	802	HEM	FE-NC	2.86	2.04	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	FE-NA	2.80	2.04	1.95
2	B	801	HEM	FE-NC	2.79	2.04	1.95
2	A	802	HEM	FE-NA	2.67	2.04	1.95
2	A	801	HEM	FE-NC	2.61	2.04	1.95

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	HEM	C4D-ND-C1D	2.87	108.04	105.07
2	A	802	HEM	C4A-NA-C1A	2.85	108.14	105.35
2	A	802	HEM	C4D-ND-C1D	2.85	108.01	105.07
2	A	801	HEM	C4D-ND-C1D	2.79	107.95	105.07
4	B	805	LMO	O08-C13-C14	2.78	114.19	109.05
4	A	804	LMO	O08-C13-C14	2.71	114.06	109.05
2	B	802	HEM	C4D-ND-C1D	2.67	107.83	105.07
2	B	802	HEM	C4A-NA-C1A	2.62	107.91	105.35
2	A	802	HEM	C1B-NB-C4B	2.60	107.76	105.07
2	B	801	HEM	C4C-NC-C1C	2.53	107.83	105.35
2	B	801	HEM	C1B-NB-C4B	2.52	107.68	105.07
2	A	801	HEM	C4A-NA-C1A	2.50	107.80	105.35
2	B	801	HEM	C4A-NA-C1A	2.48	107.77	105.35
2	A	802	HEM	C4C-NC-C1C	2.47	107.77	105.35
2	A	801	HEM	C1B-NB-C4B	2.46	107.61	105.07
2	A	801	HEM	C4C-NC-C1C	2.44	107.74	105.35
2	B	802	HEM	C1B-NB-C4B	2.34	107.49	105.07
2	A	802	HEM	CAD-CBD-CGD	-2.32	108.61	113.60
2	A	801	HEM	CAA-CBA-CGA	-2.22	108.82	113.60
2	B	802	HEM	C4C-NC-C1C	2.22	107.52	105.35
4	B	805	LMO	C23-O22-C18	2.20	117.48	113.84
2	B	801	HEM	CAA-CBA-CGA	-2.16	108.94	113.60
2	A	802	HEM	C2A-C1A-NA	-2.13	107.77	110.15
2	B	801	HEM	C3B-C2B-C1B	2.12	108.06	106.49
2	B	802	HEM	C3B-C2B-C1B	2.12	108.06	106.49
4	B	805	LMO	O20-C16-C17	-2.11	105.46	110.35
2	A	802	HEM	C3B-C2B-C1B	2.10	108.04	106.49
2	B	801	HEM	C3D-C4D-ND	-2.09	107.84	110.17
2	A	802	HEM	C3D-C4D-ND	-2.05	107.88	110.17
2	A	801	HEM	C3B-C2B-C1B	2.04	108.00	106.49
2	A	801	HEM	C3D-C4D-ND	-2.02	107.91	110.17
2	B	802	HEM	CAD-CBD-CGD	-2.02	109.25	113.60

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	804	LMO	O08-C13-C14-C16
4	A	804	LMO	C19-C18-O22-C23
4	A	804	LMO	O15-C18-O22-C23
4	A	804	LMO	C24-C23-O22-C18
4	B	805	LMO	O08-C13-C14-C16
4	B	805	LMO	C24-C23-O22-C18
5	B	804	LOP	C2-O1-P1-O4
5	B	804	LOP	C3-O2-P1-O1
5	B	804	LOP	C3-O2-P1-O4
5	B	804	LOP	O8-C24-O6-C5
5	B	804	LOP	C25-C24-O6-C5
4	B	805	LMO	O08-C13-C14-O15
4	B	805	LMO	C23-C24-C25-C26
4	A	804	LMO	O08-C13-C14-O15
5	B	804	LOP	C7-C6-O5-C4
5	B	804	LOP	C7-C8-C9-C10
4	B	805	LMO	O22-C23-C24-C25
5	B	804	LOP	O7-C6-O5-C4
5	B	804	LOP	C2-O1-P1-O2
4	B	805	LMO	C29-C30-C31-C32
5	B	804	LOP	C24-C25-C26-C27
4	B	805	LMO	C24-C25-C26-C27
4	A	804	LMO	C03-C04-O08-C13
4	B	805	LMO	C03-C04-O08-C13
4	A	804	LMO	C26-C27-C28-C29
4	B	805	LMO	O05-C04-O08-C13
4	B	805	LMO	C25-C26-C27-C28
4	A	804	LMO	C28-C29-C30-C31
5	B	804	LOP	C27-C28-C29-C30
4	A	804	LMO	O05-C04-O08-C13
4	B	805	LMO	O15-C18-O22-C23
4	A	804	LMO	O22-C23-C24-C25
4	B	805	LMO	C30-C31-C32-C33
5	B	804	LOP	C4-C3-O2-P1
5	B	804	LOP	C32-C33-C34-C35
4	A	804	LMO	C25-C26-C27-C28
4	B	805	LMO	C19-C18-O22-C23
5	B	804	LOP	C25-C26-C27-C28
5	B	804	LOP	C2-O1-P1-O3
5	B	804	LOP	C3-O2-P1-O3
4	B	805	LMO	C28-C29-C30-C31
5	B	804	LOP	O5-C4-C5-O6

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Mol	Chain	Res	Type	Atoms
4	B	805	LMO	C26-C27-C28-C29
5	B	804	LOP	C5-C4-O5-C6
5	B	804	LOP	C28-C29-C30-C31
4	A	804	LMO	C30-C31-C32-C33
5	B	804	LOP	C12-C13-C14-C15
5	B	804	LOP	C3-C4-C5-O6
5	B	804	LOP	O5-C6-C7-C8
2	B	802	HEM	C1A-C2A-CAA-CBA

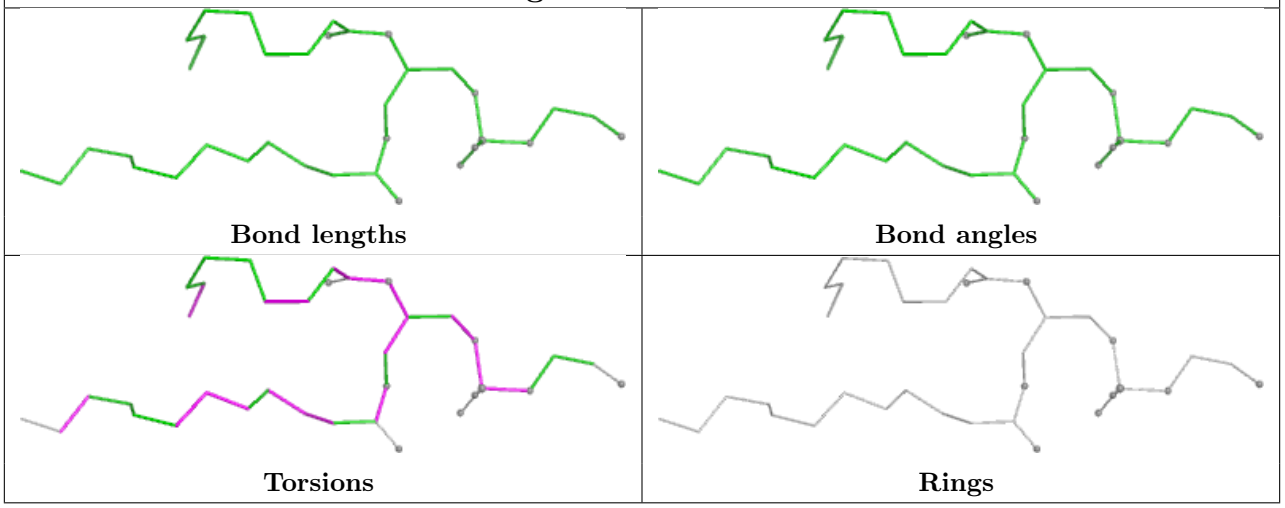
There are no ring outliers.

6 monomers are involved in 15 short contacts:

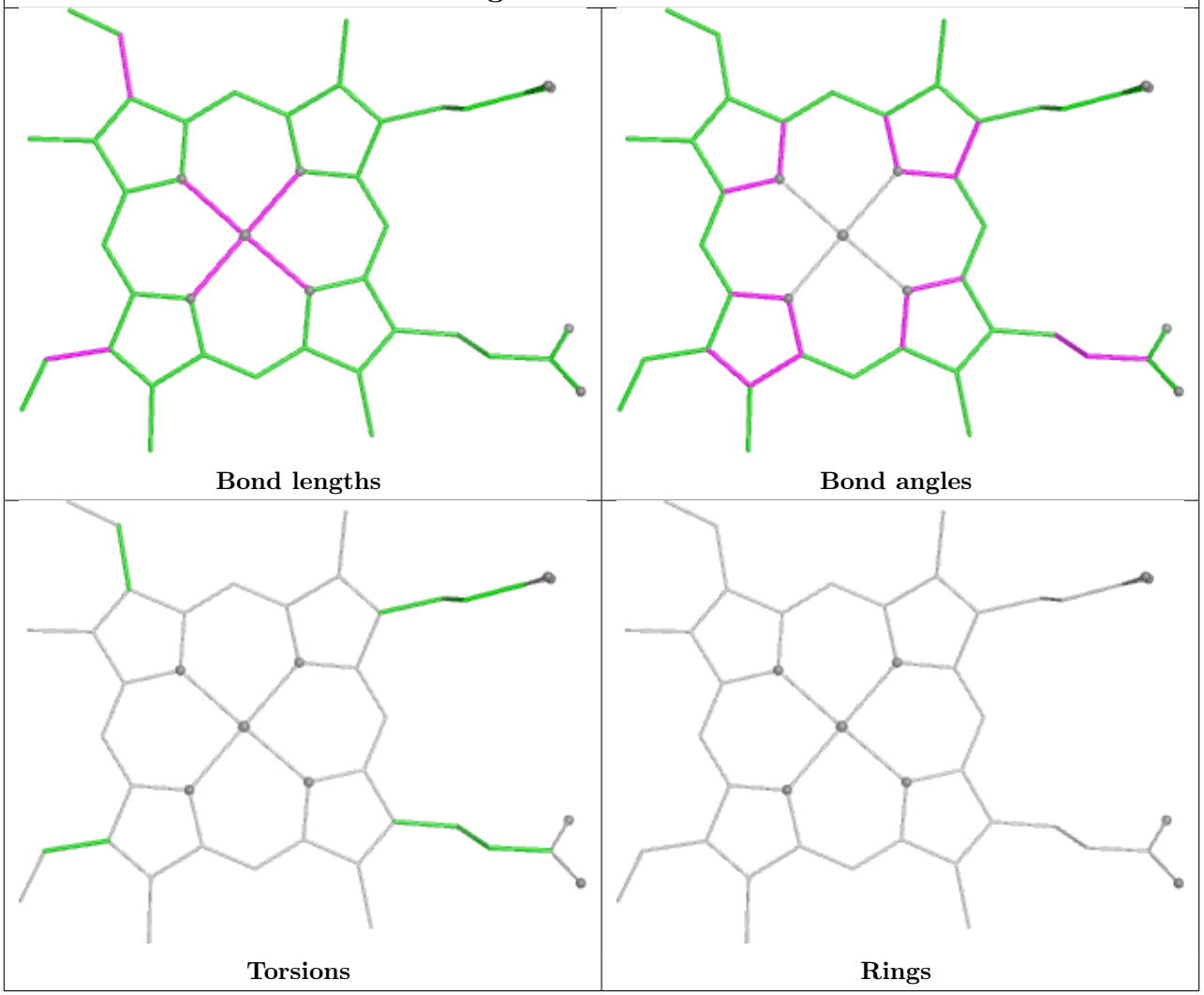
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	804	LOP	3	0
2	B	801	HEM	4	0
2	A	801	HEM	4	0
4	A	804	LMO	1	0
2	B	802	HEM	2	0
2	A	802	HEM	2	0

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.

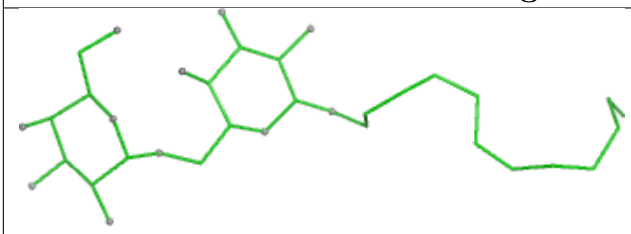
Ligand LOP B 804



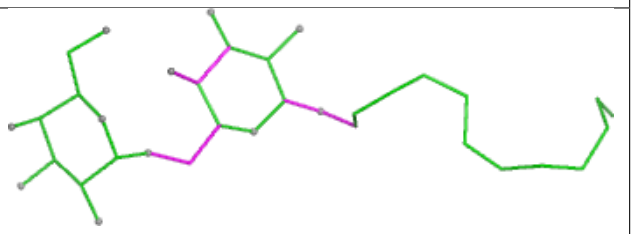
Ligand HEM B 801



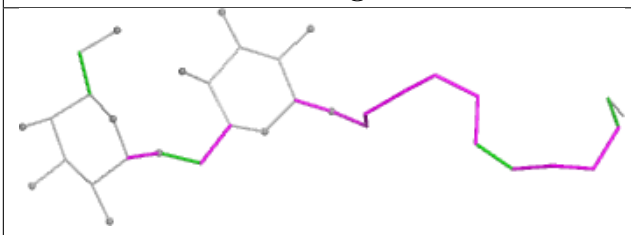
Ligand LMO B 805



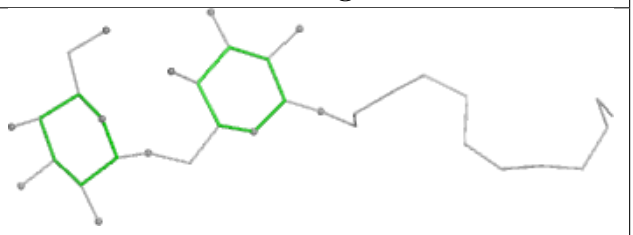
Bond lengths



Bond angles

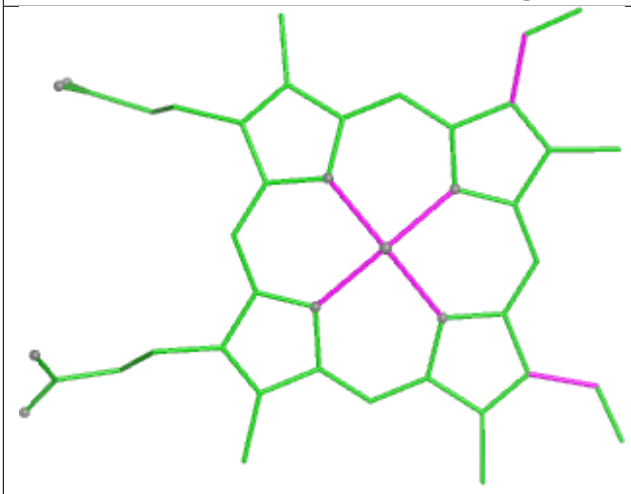


Torsions

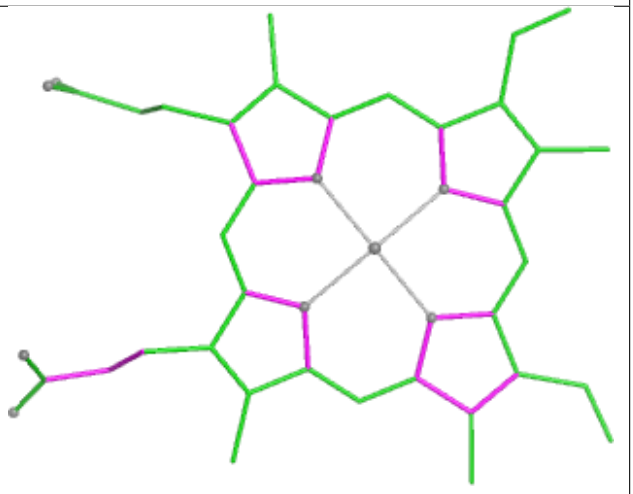


Rings

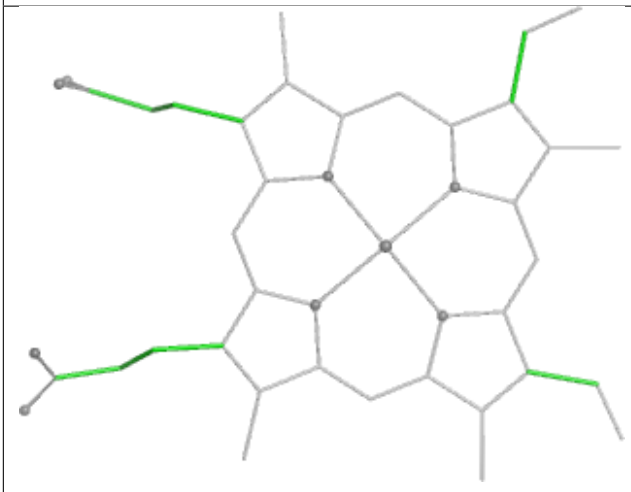
Ligand HEM A 801



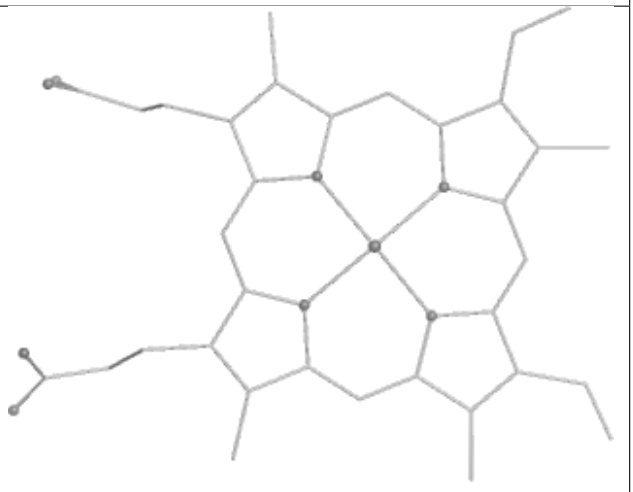
Bond lengths



Bond angles

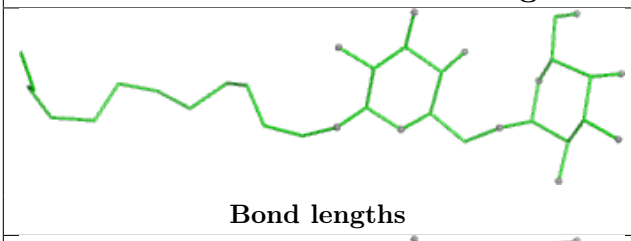


Torsions

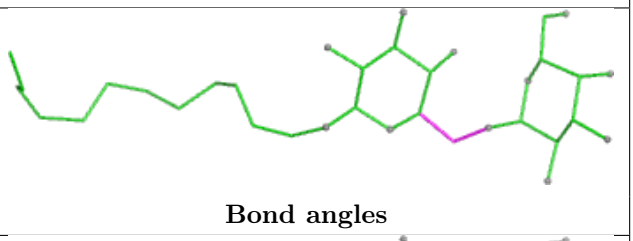


Rings

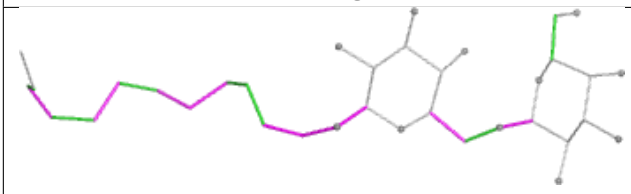
Ligand LMO A 804



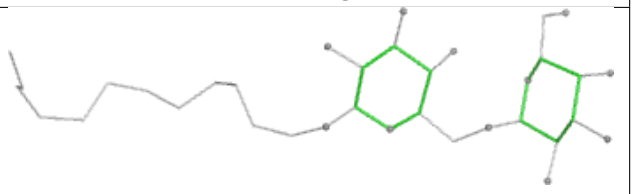
Bond lengths



Bond angles

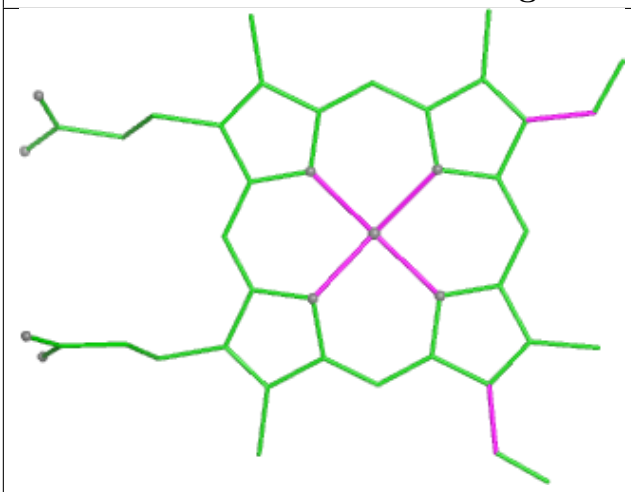


Torsions

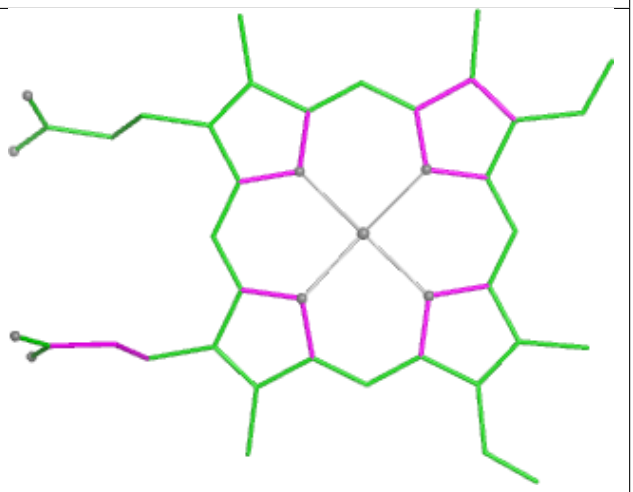


Rings

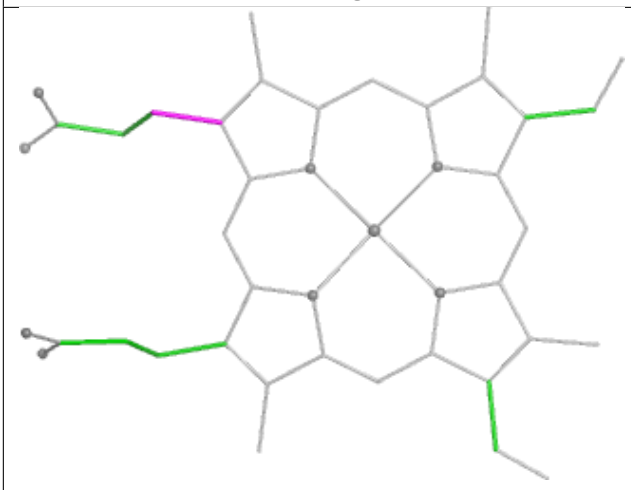
Ligand HEM B 802



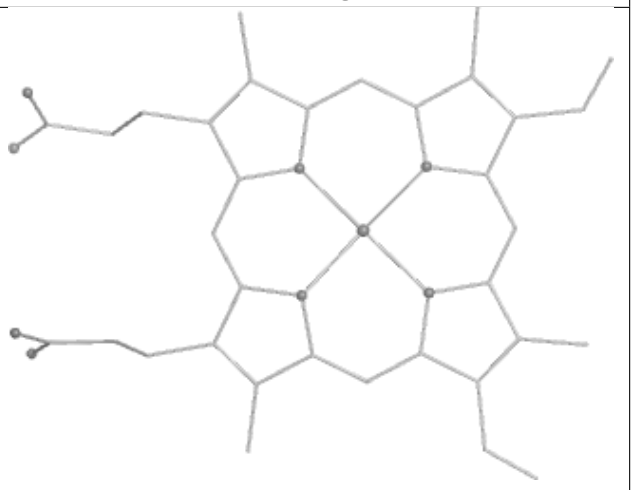
Bond lengths



Bond angles

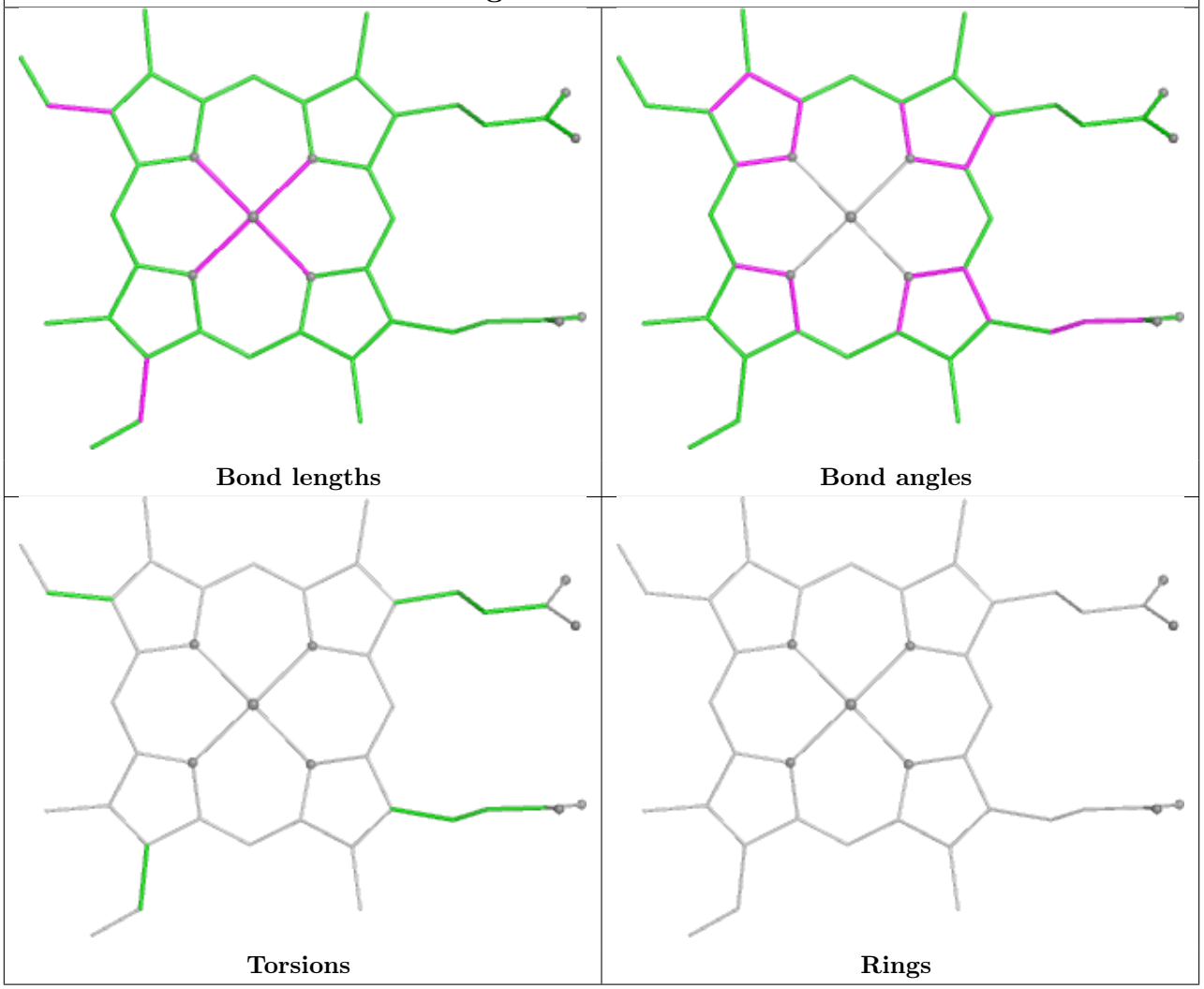


Torsions



Rings

Ligand HEM A 802



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

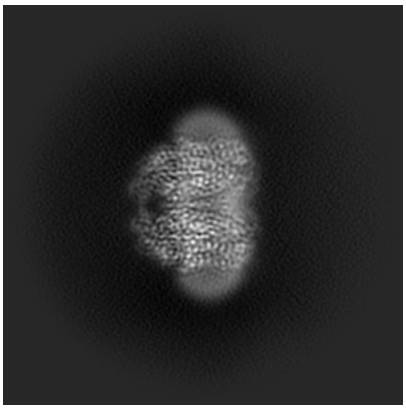
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-58853. These allow visual inspection of the internal detail of the map and identification of artifacts.

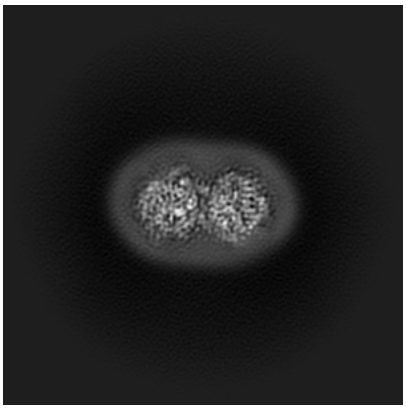
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

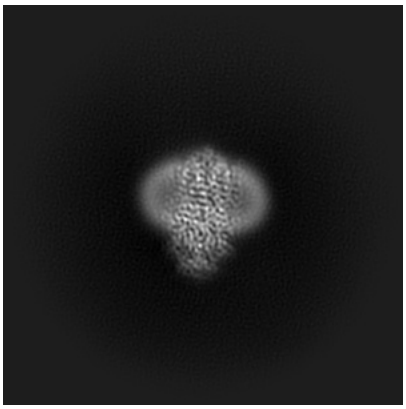
6.1.1 Primary map



X

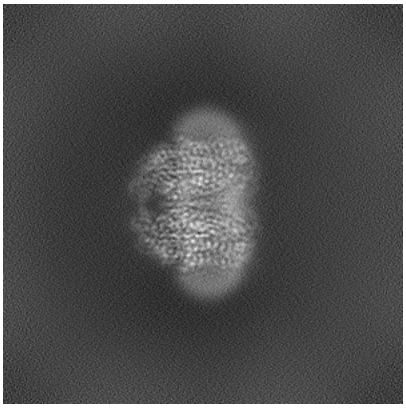


Y

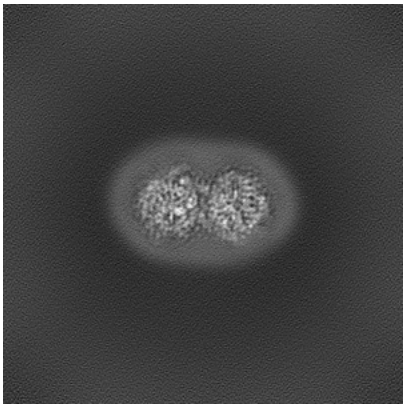


Z

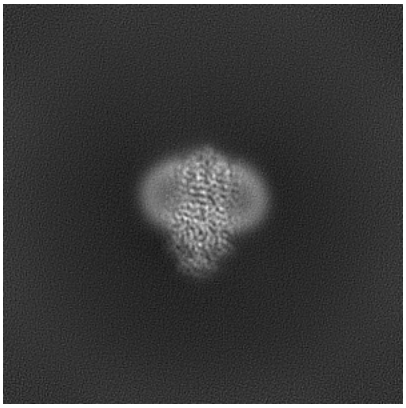
6.1.2 Raw map



X



Y

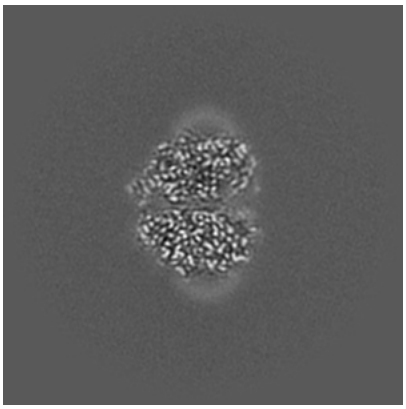


Z

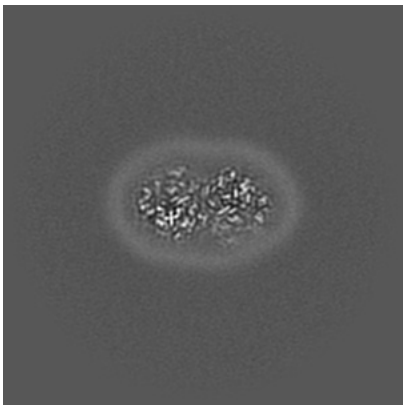
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

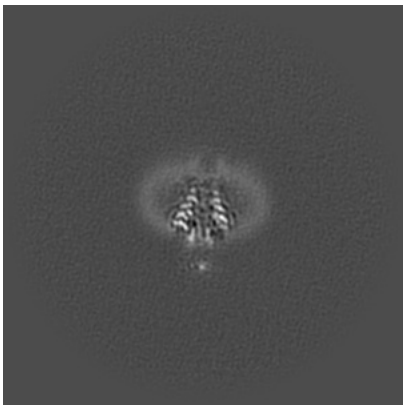
6.2.1 Primary map



X Index: 160

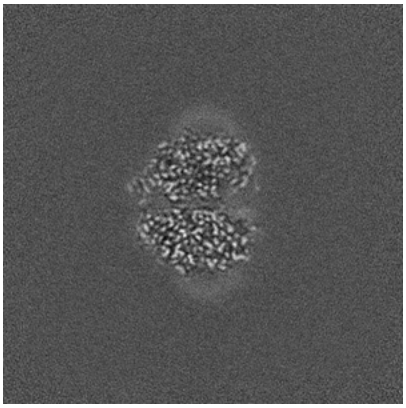


Y Index: 160

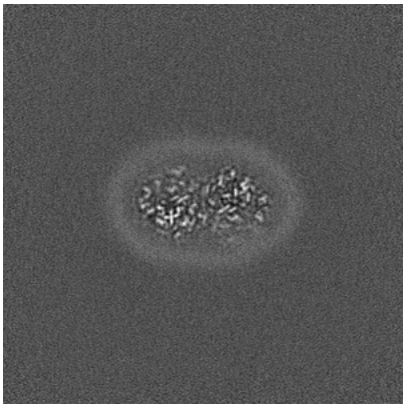


Z Index: 160

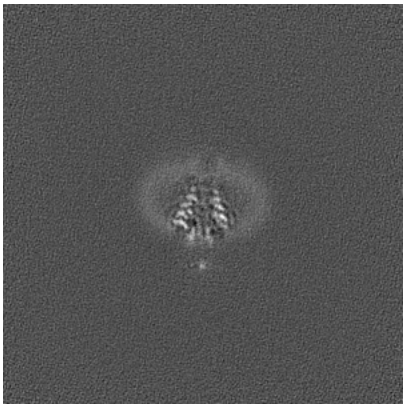
6.2.2 Raw map



X Index: 160



Y Index: 160

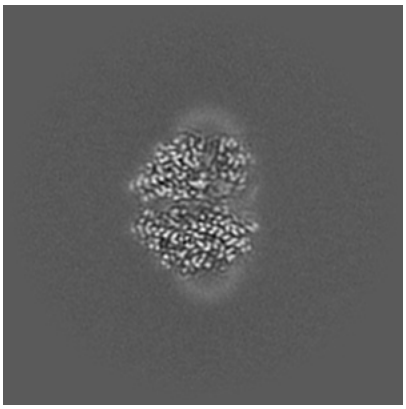


Z Index: 160

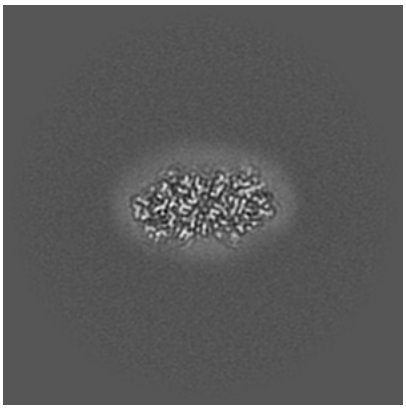
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

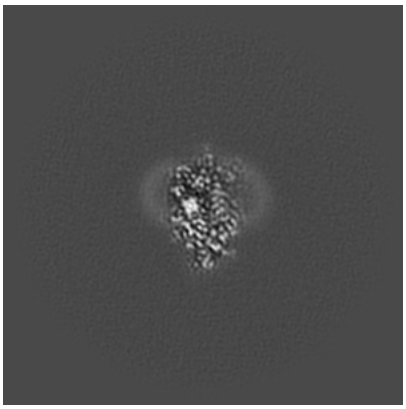
6.3.1 Primary map



X Index: 155

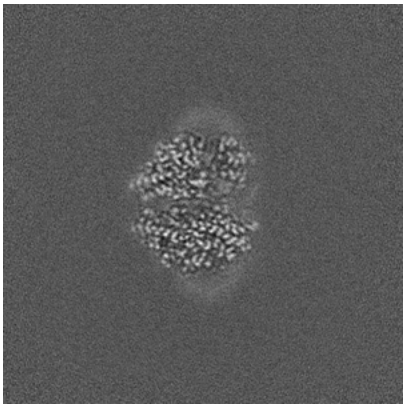


Y Index: 145

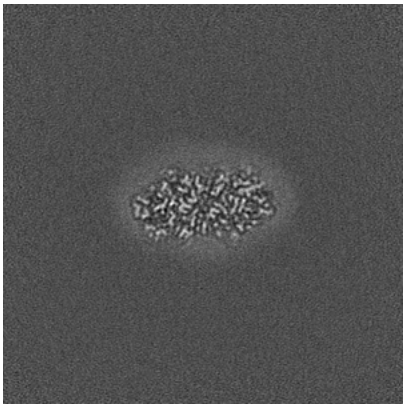


Z Index: 134

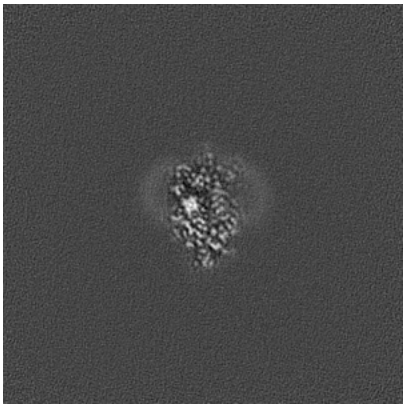
6.3.2 Raw map



X Index: 155



Y Index: 145

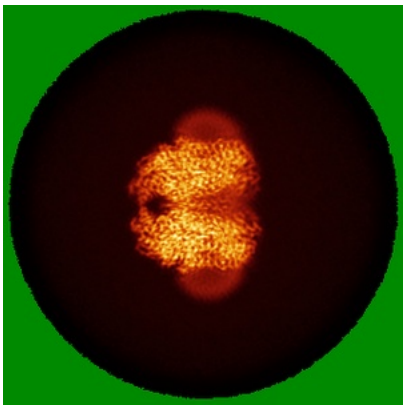


Z Index: 134

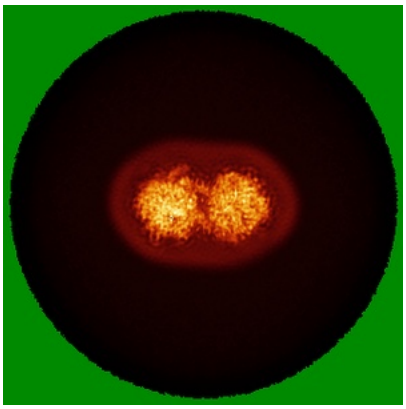
The images above show the largest variance slices of the map in three orthogonal directions.

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

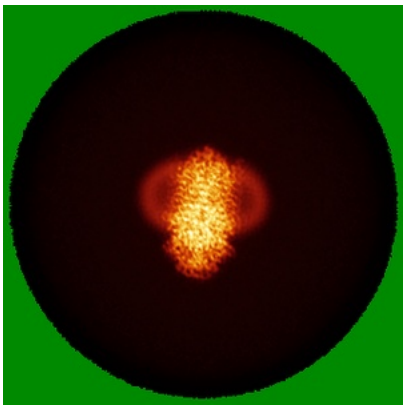
6.4.1 Primary map



X

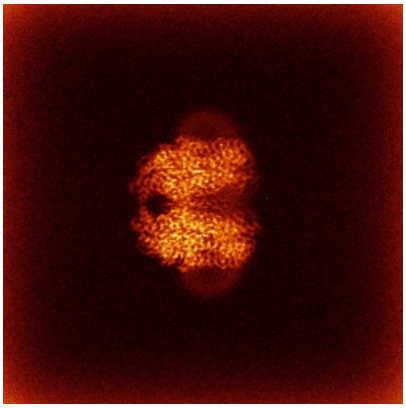


Y

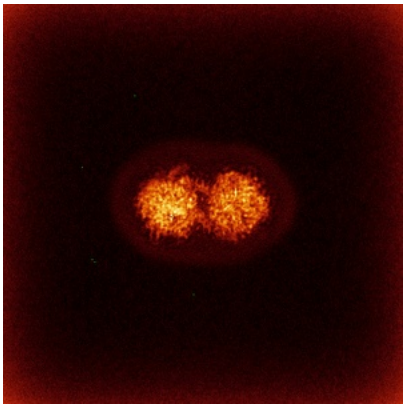


Z

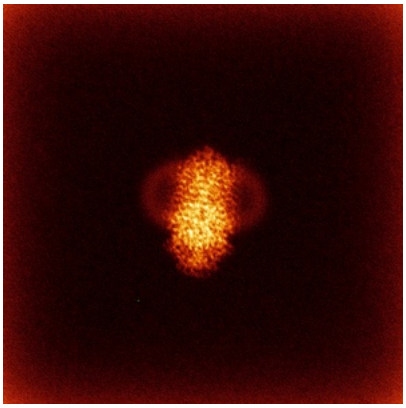
6.4.2 Raw map



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)

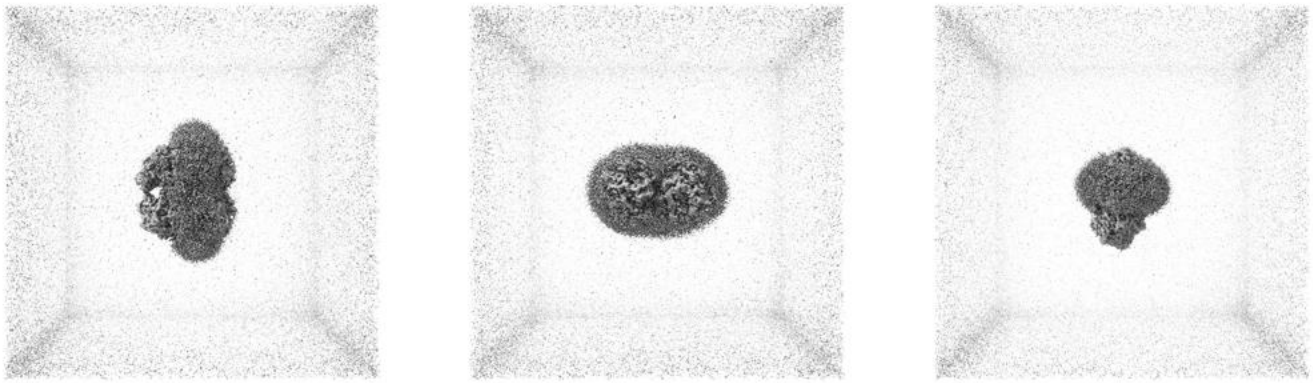
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0567. 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.

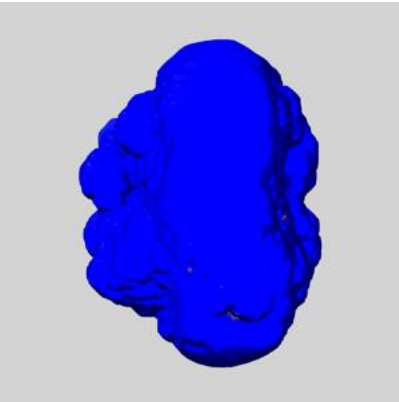
6.6 Mask visualisation (i)

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

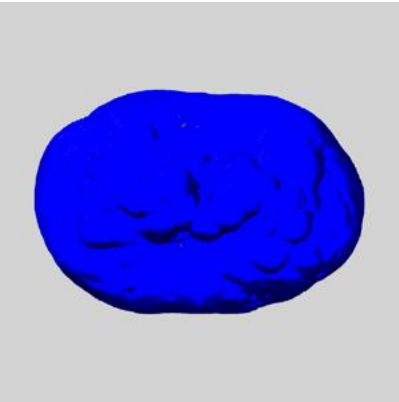
A mask typically either:

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

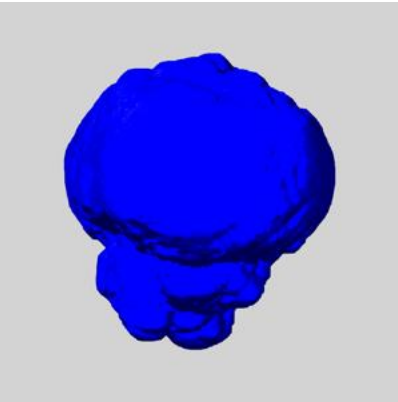
6.6.1 emd_58853_msk_1.map (i)



X



Y

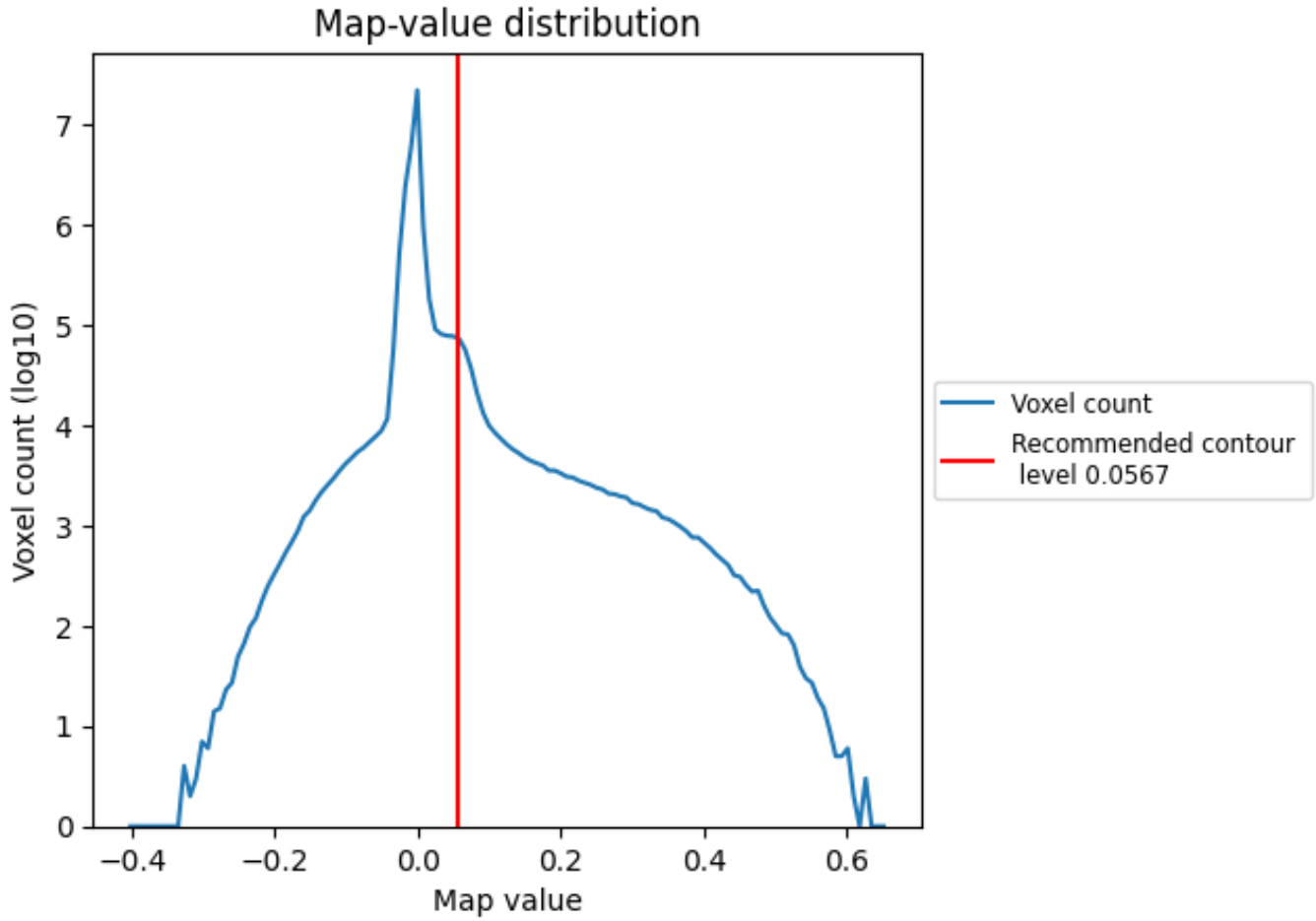


Z

7 Map analysis

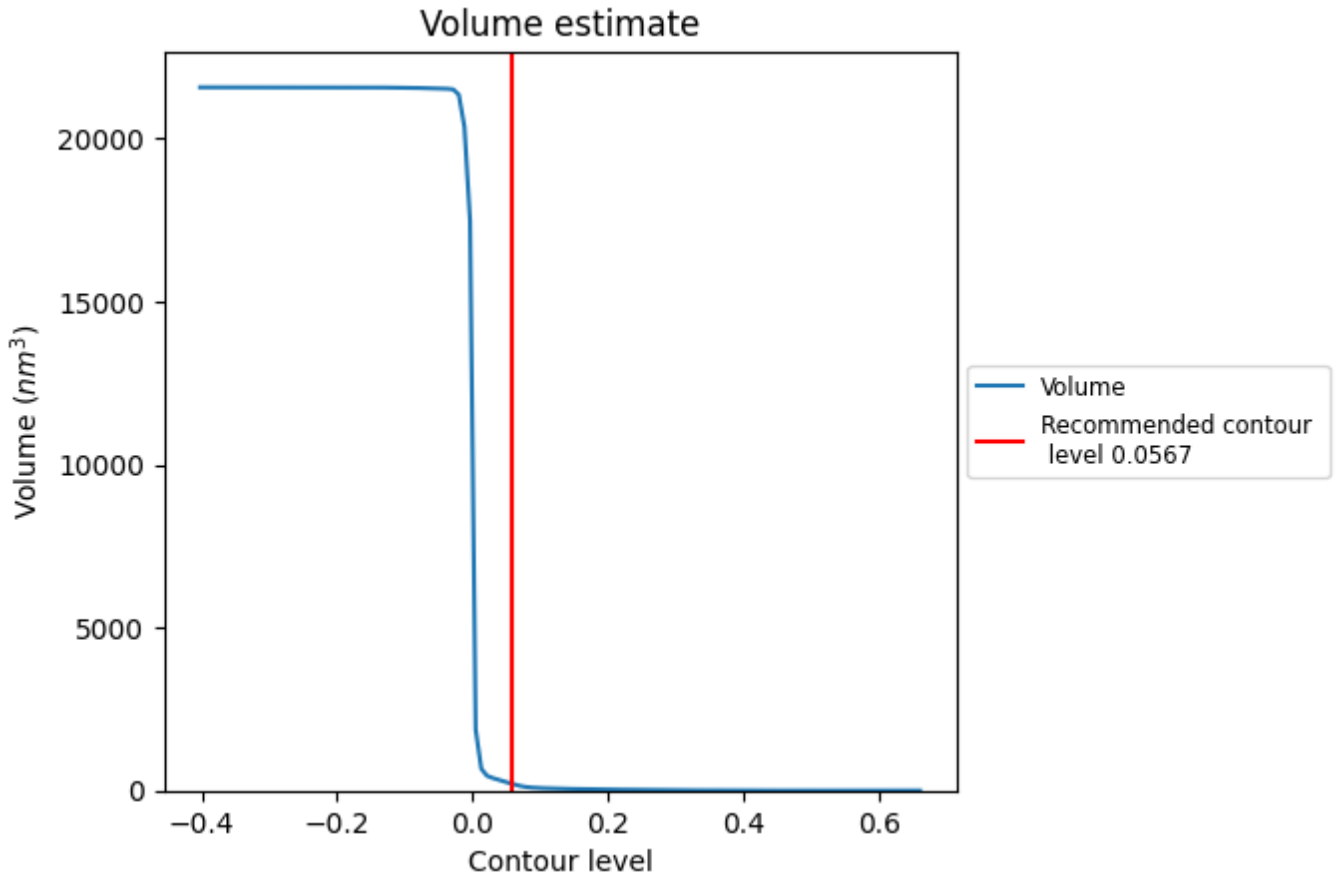
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

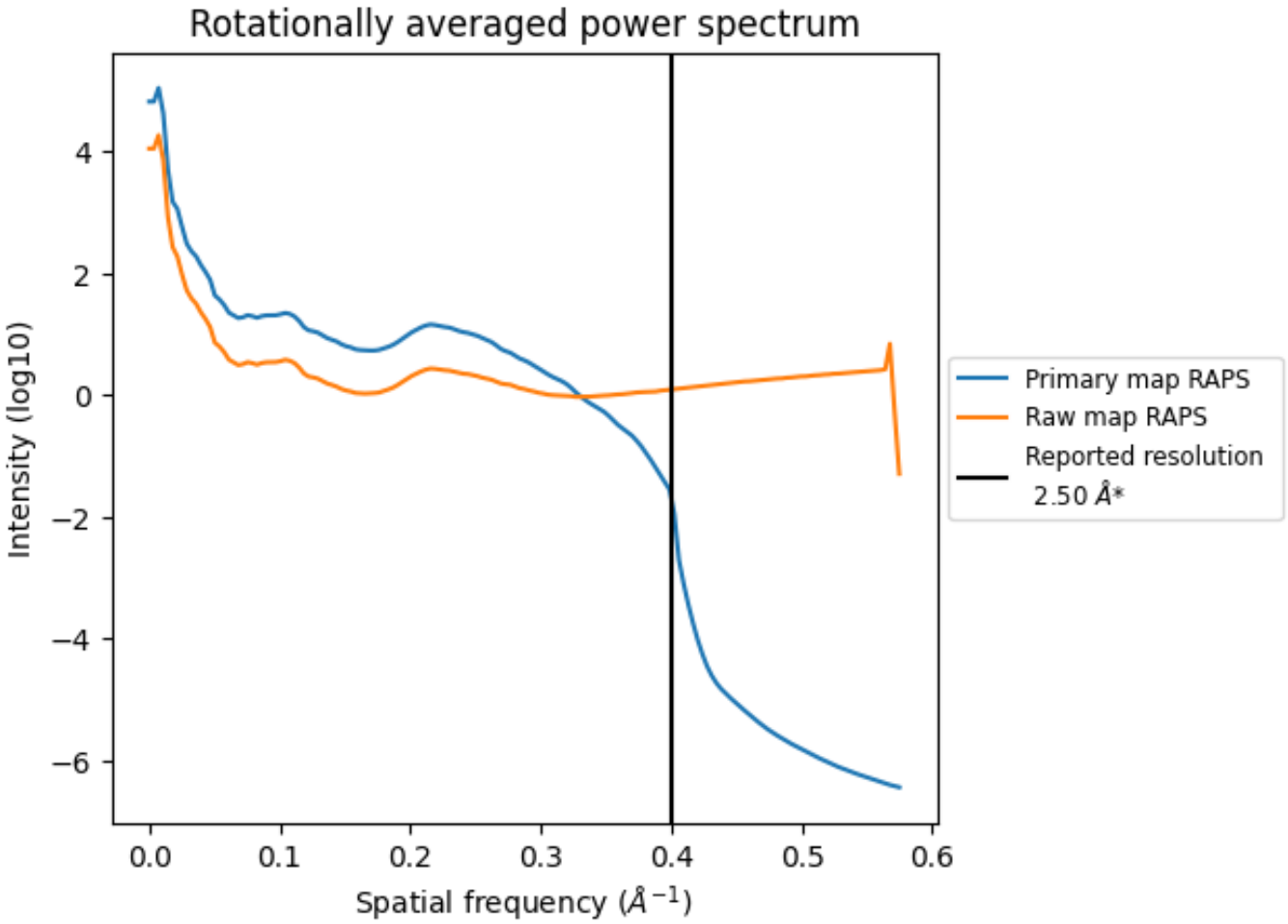
7.2 Volume estimate



The volume at the recommended contour level is 216 nm^3; this corresponds to an approximate mass of 195 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)

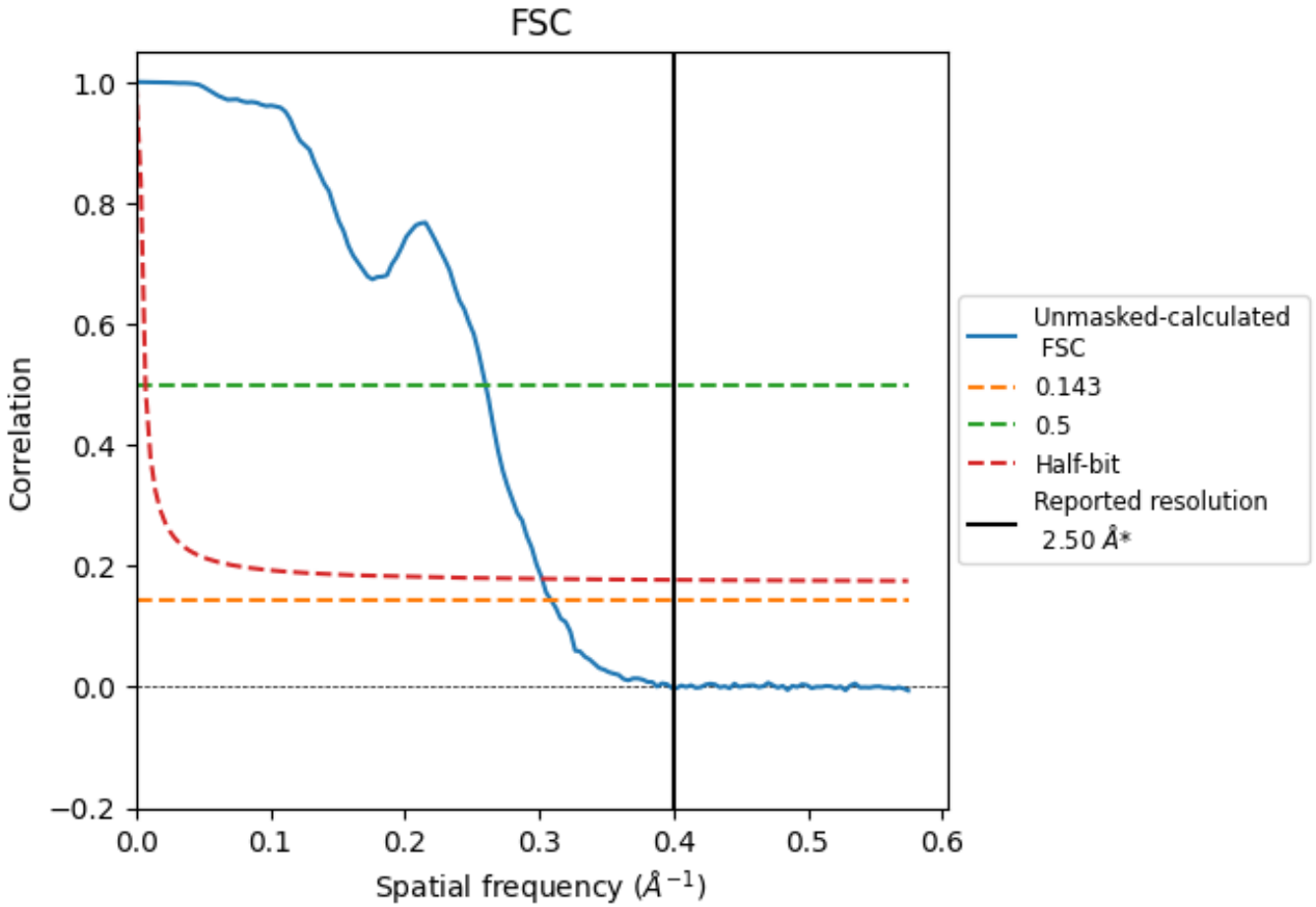


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



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

8.2 Resolution estimates (i)

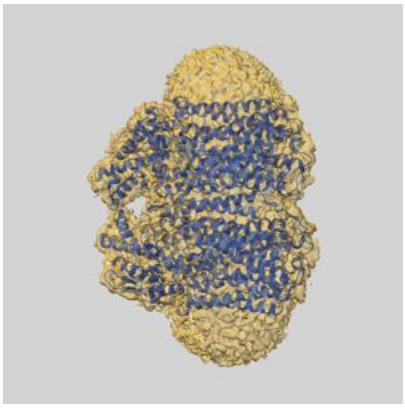
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.24	3.84	3.31

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

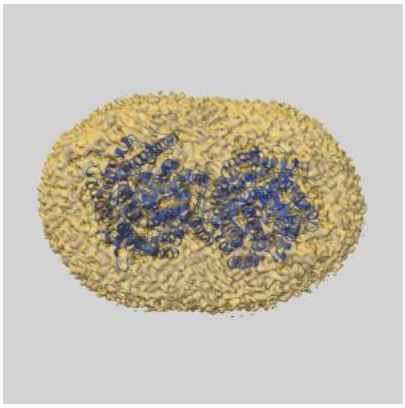
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-58853 and PDB model 32FI. Per-residue inclusion information can be found in section 3 on page 6.

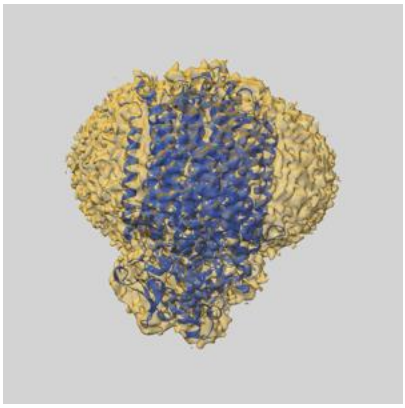
9.1 Map-model overlay



X



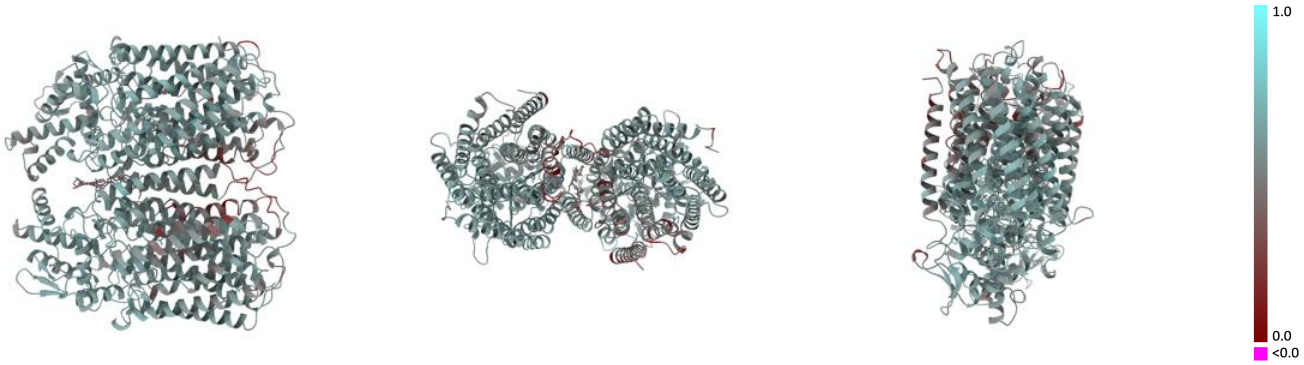
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0567 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.

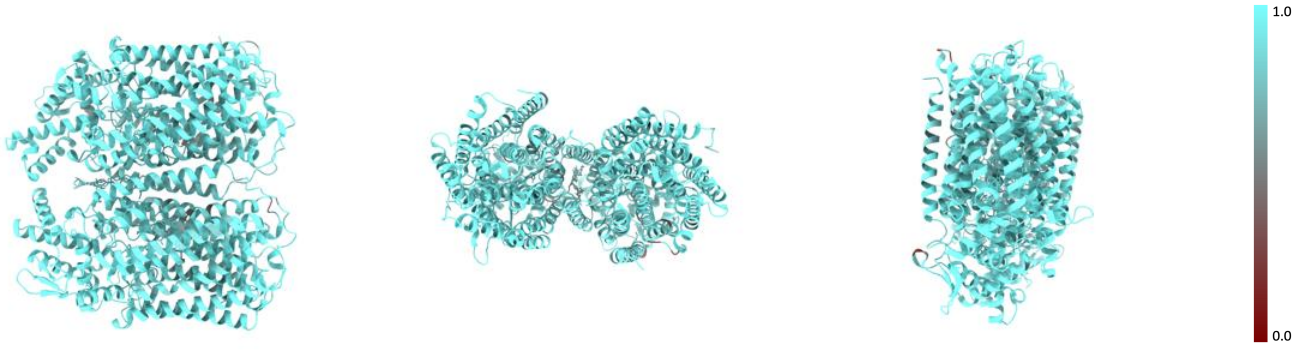
9.2 Q-score mapped to coordinate model (i)



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.

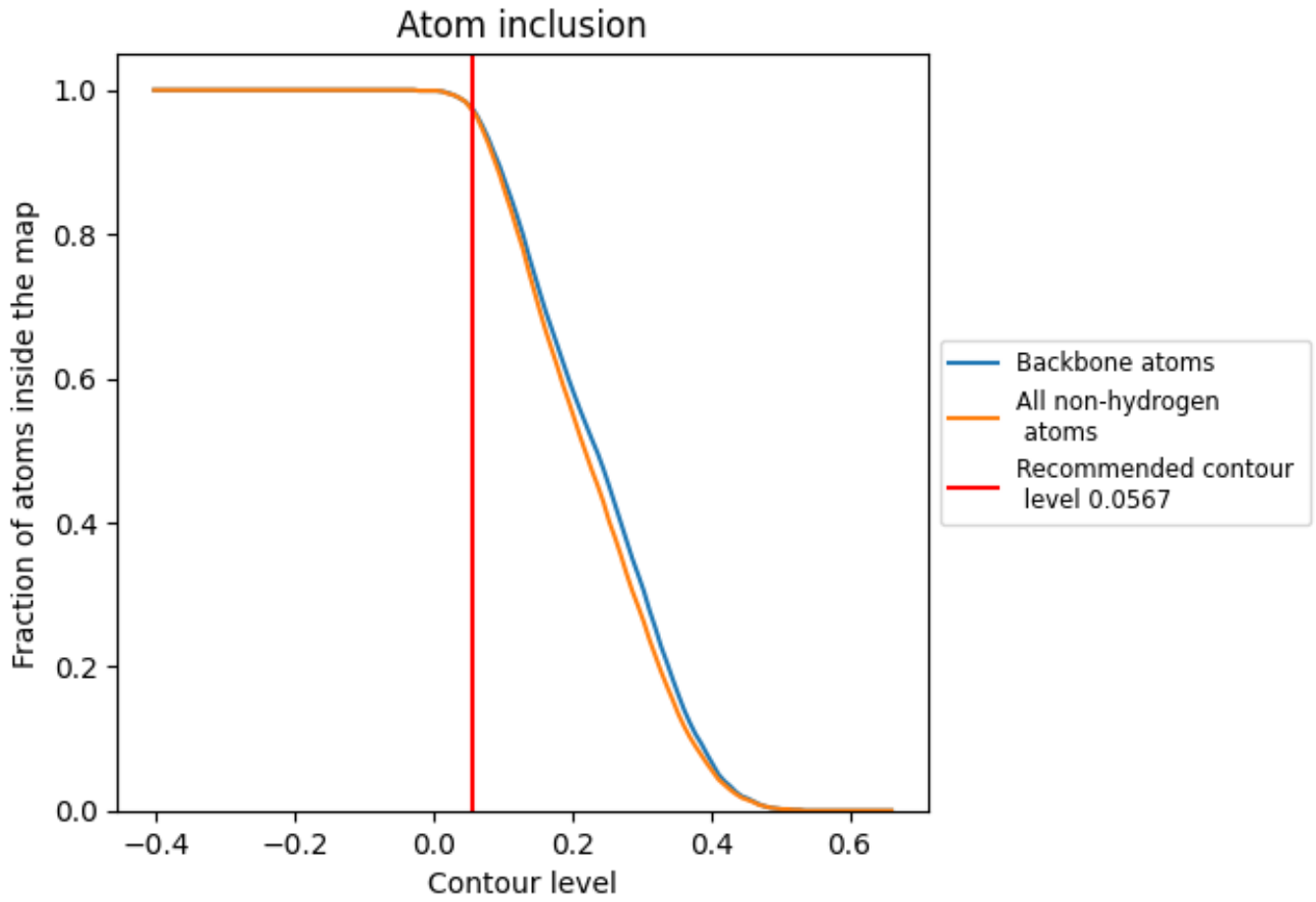
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0567).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.0567) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.9710	0.5610
A	0.9690	0.5540
B	0.9750	0.5670