



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:13 PM UTC

PDB ID : 9FKA / pdb_00009fka
EMDB ID : EMD-50520
Title : Cryo-EM structure of the reduced cytochrome bd oxidase from M. tuberculosis
Authors : Kayastha, K.; Bruenle, S.
Deposited on : 2024-06-03
Resolution : 2.96 Å(reported)
Based on initial model : 7NKZ

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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 EMD 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) : 2.49

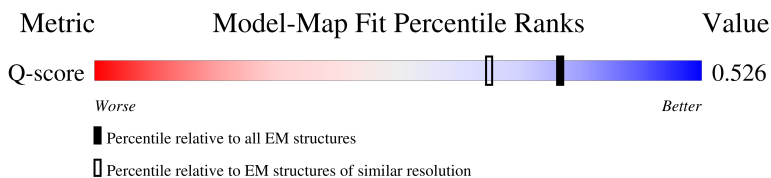
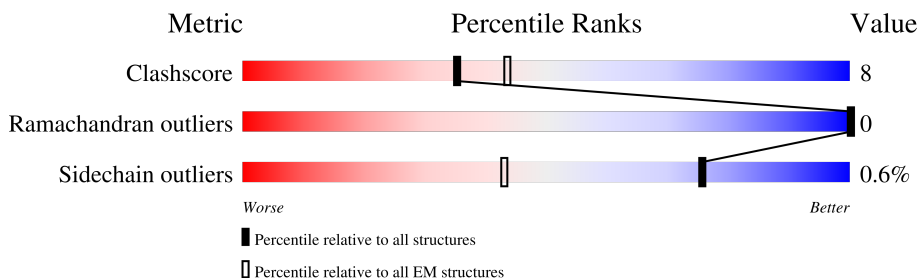
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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	13155 (2.46 - 3.46)

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 $\leq 5\%$. 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	485	 83% 11% • 5%
2	B	346	 91% 9%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 6694 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.

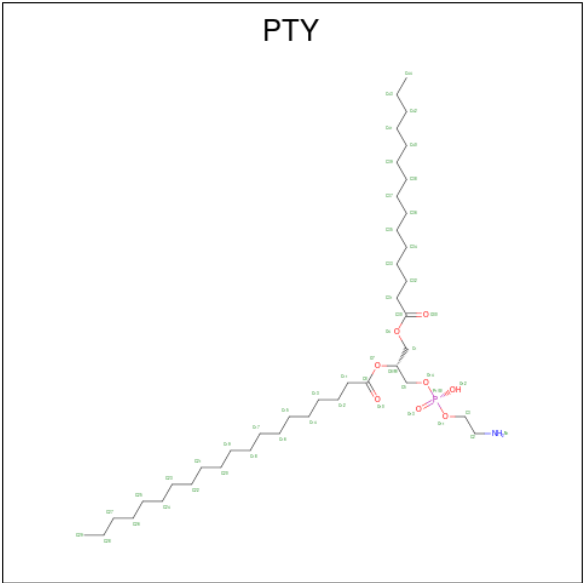
- Molecule 1 is a protein called Probable integral membrane cytochrome D ubiquinol oxidase (Subunit I) CydA (Cytochrome BD-I oxidase subunit I).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	460	Total	C	N	O	S	0	0
			3618	2384	596	619	19		

- Molecule 2 is a protein called Probable integral membrane cytochrome D ubiquinol oxidase (Subunit II) CydB (Cytochrome BD-I oxidase subunit II).

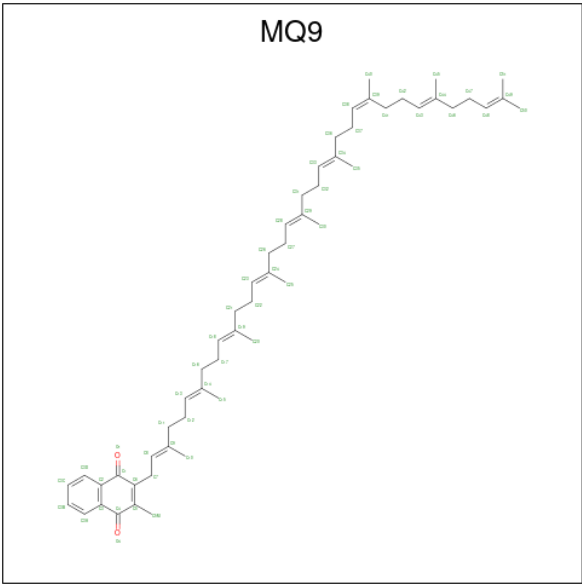
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	346	Total	C	N	O	S	0	0
			2673	1788	435	441	9		

- Molecule 3 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



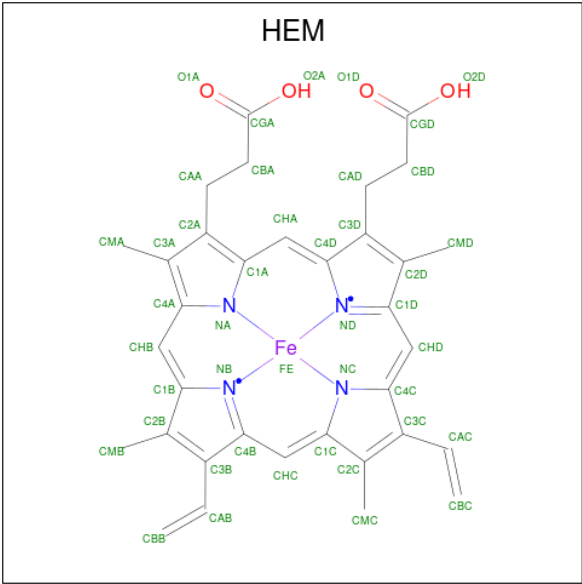
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 4 is MENAQUINONE-9 (CCD ID: MQ9) (formula: C₅₆H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O		0
			58	56	2		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



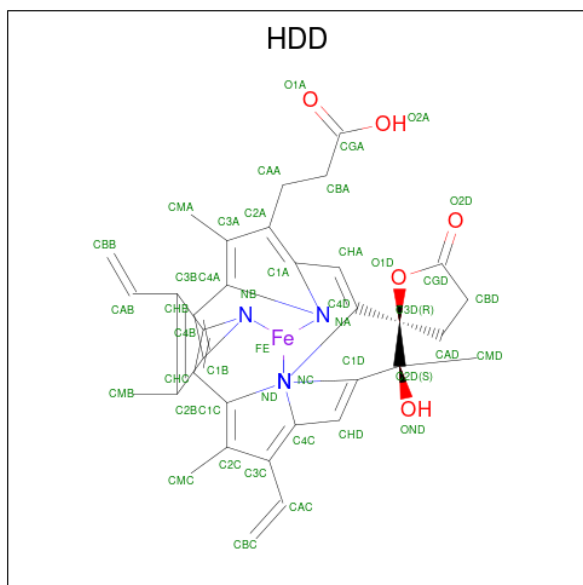
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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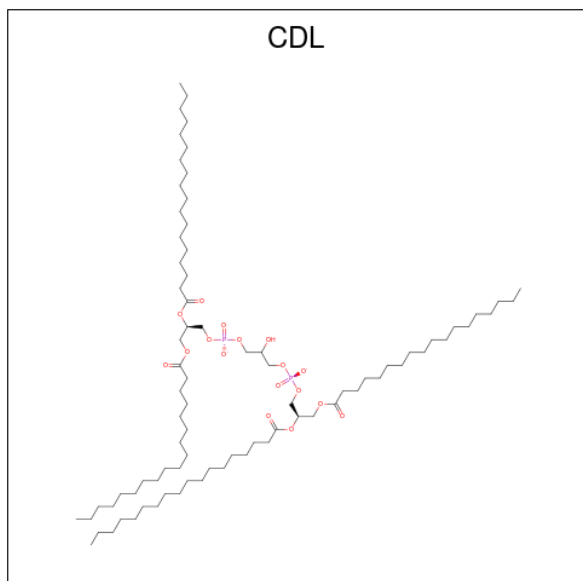
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 6 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: $C_{34}H_{32}FeN_4O_5$) (labeled as "Ligand of Interest" by depositor).



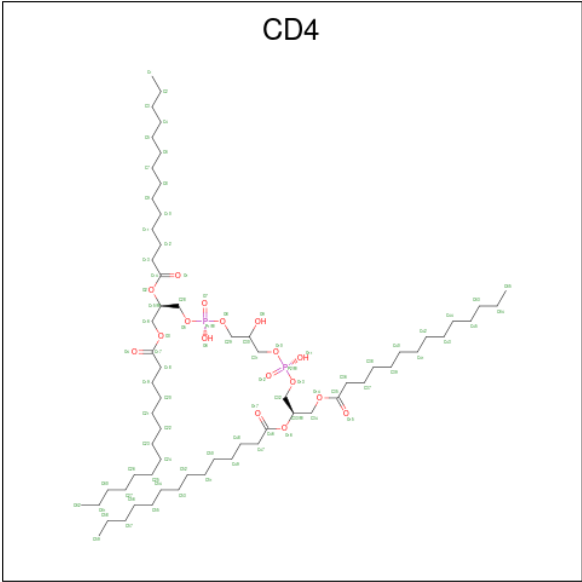
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	Fe	N	O	0
			44	34	1	4	5	

- Molecule 7 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	O	P	0
			81	62	17	2	

- Molecule 8 is (2R,5R,11R,14R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-2,14-bis(tetradecano yloxy)-4,6,10,12,16-pentaoxa-5,11-diphosphatriacont-1-yl tetradecanoate (CCD ID: CD4) (formula: C₆₅H₁₂₆O₁₇P₂).

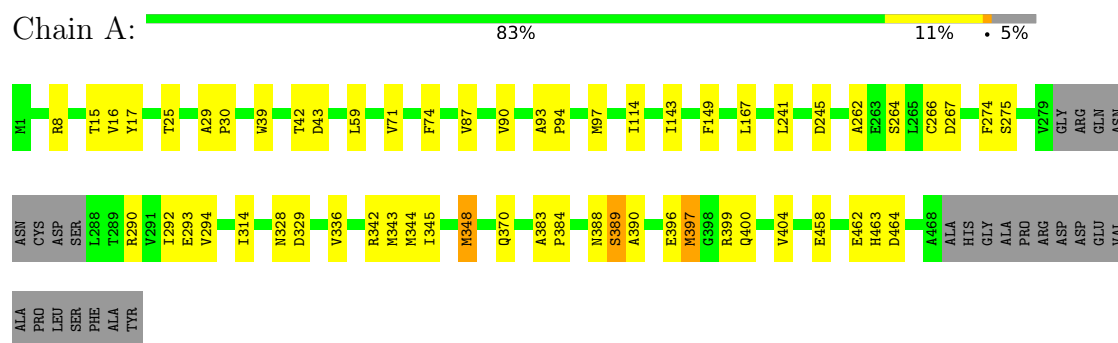


Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	O	P	0
			84	65	17	2	

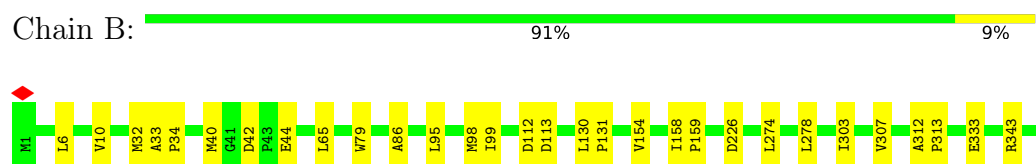
3 Residue-property plots [i](#)

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: Probable integral membrane cytochrome D ubiquinol oxidase (Subunit I) CydA (Cytochrome BD-I oxidase subunit I)



- Molecule 2: Probable integral membrane cytochrome D ubiquinol oxidase (Subunit II) CydB (Cytochrome BD-I oxidase subunit II)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1277019	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.436	Depositor
Minimum map value	-0.221	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0657	Depositor
Map size (Å)	214.016, 214.016, 214.016	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.836, 0.836, 0.836	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: HDD, HEM, CD4, CDL, PTY, MQ9

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	0/3728	0.31	2/5104 (0.0%)
2	B	0.15	0/2764	0.25	0/3797
All	All	0.15	0/6492	0.29	2/8901 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	ILE	CA-C-N	8.09	131.12	120.28
1	A	314	ILE	C-N-CA	8.09	131.12	120.28

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	3618	0	3612	55	0
2	B	2673	0	2695	26	0
3	A	50	0	79	1	0
4	A	58	0	80	12	0
5	A	86	0	60	30	0
6	A	44	0	30	10	0
7	B	81	0	112	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	84	0	124	3	0
All	All	6694	0	6792	107	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 (107) 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:344:MET:HE3	5:A:504:HEM:NB	1.74	0.99
1:A:344:MET:HE3	5:A:504:HEM:C4B	2.01	0.95
1:A:344:MET:CE	5:A:504:HEM:NB	2.39	0.86
5:A:503:HEM:C3B	6:A:505:HDD:HBB2	2.15	0.81
5:A:503:HEM:HH A	5:A:503:HEM:O1A	1.79	0.79
4:A:502:MQ9:H103	4:A:502:MQ9:H13	1.65	0.79
5:A:503:HEM:CAB	6:A:505:HDD:CBB	2.63	0.76
5:A:504:HEM:HBB2	5:A:504:HEM:HMB1	1.68	0.75
1:A:16:VAL:HG21	4:A:502:MQ9:H102	1.69	0.74
1:A:293:GLU:N	1:A:293:GLU:OE1	2.22	0.73
1:A:143:ILE:CG2	5:A:503:HEM:HBB1	2.19	0.72
1:A:343:MET:HE3	4:A:502:MQ9:H412	1.72	0.72
1:A:463:HIS:ND1	1:A:464:ASP:OD1	2.23	0.71
1:A:8:ARG:NH2	1:A:400:GLN:OE1	2.25	0.69
1:A:143:ILE:HG22	5:A:503:HEM:HBB1	1.76	0.68
8:B:402:CD4:H56	8:B:402:CD4:P1	2.17	0.68
5:A:504:HEM:HBC2	5:A:504:HEM:HMC2	1.77	0.67
1:A:17:TYR:CZ	4:A:502:MQ9:H161	2.30	0.66
1:A:262:ALA:O	1:A:342:ARG:NH1	2.29	0.66
1:A:396:GLU:OE1	1:A:399:ARG:NH2	2.28	0.65
2:B:86:ALA:HB2	2:B:154:VAL:HG21	1.78	0.65
6:A:505:HDD:HBC1	6:A:505:HDD:HMC3	1.77	0.65
5:A:504:HEM:HH A	5:A:504:HEM:HBD1	1.79	0.65
5:A:503:HEM:HMB2	5:A:503:HEM:HBB2	1.80	0.63
6:A:505:HDD:HBB1	6:A:505:HDD:HHC	1.79	0.63
1:A:292:ILE:HG23	1:A:292:ILE:O	2.00	0.62
1:A:370:GLN:N	1:A:370:GLN:OE1	2.33	0.62
1:A:274:PHE:O	1:A:294:VAL:N	2.33	0.61
2:B:113:ASP:OD2	2:B:343:ARG:NE	2.34	0.61
1:A:71:VAL:CG2	2:B:99:ILE:HD11	2.31	0.60
2:B:40:MET:SD	2:B:40:MET:N	2.74	0.60
8:B:402:CD4:O5	8:B:402:CD4:O9	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ALA:HA	4:A:502:MQ9:H302	1.84	0.58
2:B:333:GLU:OE2	2:B:333:GLU:N	2.33	0.58
1:A:328:ASN:OD1	1:A:329:ASP:N	2.37	0.58
5:A:503:HEM:CAB	6:A:505:HDD:HBB2	2.33	0.57
1:A:267:ASP:OD1	1:A:267:ASP:N	2.37	0.57
2:B:65:LEU:HD23	2:B:98:MET:HE1	1.86	0.57
1:A:8:ARG:NH2	3:A:501:PTY:O30	2.37	0.57
1:A:264:SER:O	1:A:290:ARG:NH2	2.38	0.54
2:B:79:TRP:CE3	2:B:278:LEU:HD22	2.43	0.54
1:A:343:MET:SD	4:A:502:MQ9:H301	2.48	0.54
1:A:143:ILE:HG23	5:A:503:HEM:HBB1	1.90	0.53
5:A:503:HEM:HBB2	5:A:503:HEM:CMB	2.37	0.53
4:A:502:MQ9:H103	4:A:502:MQ9:C13	2.32	0.53
1:A:74:PHE:CD2	2:B:95:LEU:HD21	2.44	0.53
5:A:504:HEM:HBB2	5:A:504:HEM:CMB	2.37	0.52
1:A:343:MET:CE	4:A:502:MQ9:H412	2.40	0.52
1:A:345:ILE:HD13	5:A:504:HEM:CAB	2.40	0.52
1:A:336:VAL:HG11	1:A:397:MET:SD	2.51	0.51
5:A:503:HEM:HBC2	5:A:503:HEM:HMC2	1.93	0.51
1:A:245:ASP:C	1:A:245:ASP:OD1	2.54	0.51
2:B:226:ASP:OD1	2:B:226:ASP:C	2.53	0.51
2:B:65:LEU:HD23	2:B:98:MET:CE	2.42	0.50
1:A:344:MET:HE1	5:A:504:HEM:C1B	2.46	0.50
1:A:389:SER:OG	4:A:502:MQ9:H253	2.11	0.50
1:A:25:THR:HG21	6:A:505:HDD:HBD2	1.94	0.49
2:B:33:ALA:HB3	2:B:34:PRO:HD3	1.95	0.49
2:B:42:ASP:OD1	2:B:42:ASP:O	2.31	0.49
1:A:344:MET:HE1	5:A:504:HEM:NB	2.26	0.48
1:A:93:ALA:HB3	1:A:94:PRO:HD3	1.95	0.48
1:A:388:ASN:OD1	5:A:504:HEM:HBC1	2.14	0.48
1:A:97:MET:HG2	2:B:307:VAL:HG11	1.96	0.47
1:A:39:TRP:O	1:A:43:ASP:N	2.47	0.47
1:A:42:THR:O	1:A:43:ASP:OD1	2.33	0.47
2:B:112:ASP:OD1	2:B:112:ASP:C	2.58	0.47
1:A:383:ALA:HB3	1:A:384:PRO:HD3	1.96	0.47
5:A:503:HEM:HBC2	5:A:503:HEM:CMC	2.45	0.46
7:B:401:CDL:H202	7:B:401:CDL:H232	1.38	0.46
5:A:503:HEM:HHA	5:A:503:HEM:CGA	2.45	0.46
1:A:29:ALA:HB3	1:A:30:PRO:HD3	1.97	0.46
1:A:87:VAL:HG11	1:A:404:VAL:HG21	1.98	0.46
1:A:345:ILE:HD13	5:A:504:HEM:C3B	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:505:HDD:CGD	6:A:505:HDD:HHA	2.47	0.45
2:B:6:LEU:O	2:B:6:LEU:HD23	2.17	0.45
6:A:505:HDD:HBC1	6:A:505:HDD:CMC	2.46	0.45
2:B:44:GLU:OE2	2:B:44:GLU:HA	2.16	0.45
1:A:74:PHE:HD2	2:B:95:LEU:HD21	1.81	0.44
1:A:43:ASP:OD1	1:A:43:ASP:C	2.61	0.44
2:B:130:LEU:HB2	2:B:131:PRO:HD3	1.99	0.44
2:B:158:ILE:N	2:B:159:PRO:HD2	2.33	0.44
1:A:462:GLU:HA	1:A:462:GLU:OE1	2.18	0.43
5:A:504:HEM:HBC2	5:A:504:HEM:CMC	2.46	0.43
4:A:502:MQ9:H303	4:A:502:MQ9:H322	1.67	0.43
2:B:6:LEU:HD23	2:B:6:LEU:C	2.44	0.43
1:A:294:VAL:O	1:A:294:VAL:HG12	2.17	0.43
5:A:504:HEM:HHA	5:A:504:HEM:CBD	2.47	0.43
6:A:505:HDD:HBB1	6:A:505:HDD:CHC	2.47	0.43
1:A:241:LEU:HD21	1:A:348:MET:HE1	2.01	0.42
1:A:344:MET:CE	5:A:504:HEM:C1B	2.98	0.42
1:A:458:GLU:HA	1:A:458:GLU:OE1	2.18	0.42
1:A:389:SER:OG	4:A:502:MQ9:H28	2.19	0.42
2:B:10:VAL:HG22	8:B:402:CD4:H82	2.01	0.42
1:A:59:LEU:HD22	1:A:114:ILE:HD11	2.02	0.41
4:A:502:MQ9:H171	4:A:502:MQ9:H153	1.68	0.41
2:B:32:MET:HB3	2:B:32:MET:HE3	1.81	0.41
1:A:90:VAL:HG12	1:A:167:LEU:N	2.35	0.41
5:A:504:HEM:HHD	5:A:504:HEM:HAC	1.83	0.41
6:A:505:HDD:HMD2	6:A:505:HDD:HAD2	1.79	0.41
2:B:312:ALA:HB3	2:B:313:PRO:HD3	2.01	0.41
1:A:90:VAL:HG21	1:A:149:PHE:CZ	2.56	0.40
2:B:274:LEU:O	2:B:274:LEU:HG	2.21	0.40
1:A:15:THR:HG21	5:A:503:HEM:C1C	2.56	0.40
2:B:303:ILE:HD13	2:B:303:ILE:HA	1.99	0.40
1:A:275:SER:HA	1:A:293:GLU:HA	2.03	0.40
5:A:504:HEM:HHA	5:A:504:HEM:HAA1	1.81	0.40
2:B:6:LEU:O	2:B:10:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	456/485 (94%)	452 (99%)	4 (1%)	0	100	100
2	B	344/346 (99%)	337 (98%)	7 (2%)	0	100	100
All	All	800/831 (96%)	789 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	380/399 (95%)	376 (99%)	4 (1%)	65	80
2	B	264/264 (100%)	264 (100%)	0	100	100
All	All	644/663 (97%)	640 (99%)	4 (1%)	76	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	266	CYS
1	A	348	MET
1	A	389	SER
1	A	397	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	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](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	HDD	A	505	1	46,52,52	3.25	25 (54%)	62,89,89	3.24	27 (43%)
5	HEM	A	503	1	50,50,50	3.28	34 (68%)	67,82,82	2.24	22 (32%)
4	MQ9	A	502	-	59,59,59	0.32	0	73,75,75	2.91	4 (5%)
5	HEM	A	504	-	50,50,50	3.50	34 (68%)	67,82,82	2.97	26 (38%)
7	CDL	B	401	-	80,80,99	1.25	9 (11%)	86,92,111	1.27	4 (4%)
3	PTY	A	501	-	49,49,49	1.17	5 (10%)	52,54,54	1.03	2 (3%)
8	CD4	B	402	-	83,83,83	0.96	8 (9%)	89,95,95	1.07	4 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HDD	A	505	1	-	3/9/89/89	0/1/9/9
5	HEM	A	503	1	-	1/14/54/54	-
4	MQ9	A	502	-	-	12/53/73/73	0/2/2/2
5	HEM	A	504	-	-	6/14/54/54	-
7	CDL	B	401	-	-	47/91/91/110	-
3	PTY	A	501	-	-	26/53/53/53	-
8	CD4	B	402	-	-	35/94/94/94	-

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	505	HDD	O1D-C3D	-8.66	1.32	1.46
5	A	504	HEM	C1B-NB	-7.54	1.27	1.40
5	A	503	HEM	C4D-ND	-7.18	1.27	1.40
6	A	505	HDD	C4C-NC	-7.11	1.26	1.39
5	A	503	HEM	C3C-C4C	-6.94	1.33	1.46
5	A	504	HEM	C4D-ND	-6.90	1.28	1.40
5	A	503	HEM	C1B-NB	-6.66	1.28	1.40
5	A	504	HEM	C3C-C4C	-6.53	1.34	1.46
5	A	503	HEM	C4B-NB	-5.87	1.27	1.38
5	A	504	HEM	C4B-NB	-5.85	1.27	1.38
6	A	505	HDD	C1C-NC	-5.78	1.28	1.39
6	A	505	HDD	C1A-NA	-5.76	1.28	1.39
5	A	504	HEM	C3D-C2D	-5.74	1.24	1.36
6	A	505	HDD	C4A-NA	-5.73	1.28	1.39
5	A	503	HEM	C1D-ND	-5.69	1.27	1.38
5	A	503	HEM	C1C-C2C	-5.42	1.34	1.45
5	A	503	HEM	C1C-NC	-5.36	1.29	1.39
6	A	505	HDD	C1D-ND	-5.33	1.28	1.37
5	A	504	HEM	FE-ND	-5.26	1.78	1.94
5	A	504	HEM	C1D-ND	-5.25	1.28	1.38
5	A	504	HEM	C1C-NC	-5.24	1.29	1.39
6	A	505	HDD	C4D-ND	-5.03	1.29	1.37
6	A	505	HDD	C1B-NB	-4.92	1.30	1.39
6	A	505	HDD	C4B-NB	-4.80	1.30	1.39
5	A	504	HEM	C1B-C2B	-4.72	1.34	1.44
5	A	503	HEM	FE-ND	-4.67	1.80	1.94
5	A	503	HEM	C3D-C2D	-4.65	1.26	1.36
5	A	504	HEM	C1A-NA	-4.57	1.31	1.39
5	A	504	HEM	C4A-NA	-4.45	1.31	1.39
5	A	504	HEM	C4C-NC	-4.39	1.31	1.39
6	A	505	HDD	CMD-C2D	-4.32	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	505	HDD	C3D-C2D	-4.32	1.44	1.55
5	A	504	HEM	CHD-C4C	-4.22	1.30	1.38
5	A	504	HEM	C1A-C2A	-3.91	1.36	1.44
5	A	503	HEM	C4C-NC	-3.90	1.32	1.39
5	A	504	HEM	C1C-C2C	-3.90	1.37	1.45
5	A	504	HEM	CMC-C2C	-3.67	1.43	1.50
5	A	503	HEM	C2A-C3A	-3.66	1.29	1.38
5	A	503	HEM	C3B-C2B	-3.63	1.29	1.37
5	A	503	HEM	C1B-C2B	-3.61	1.37	1.44
5	A	503	HEM	C1A-C2A	-3.53	1.37	1.44
5	A	504	HEM	CBD-CGD	-3.52	1.42	1.50
5	A	503	HEM	C4A-NA	-3.49	1.33	1.39
6	A	505	HDD	OND-C2D	-3.49	1.36	1.42
5	A	504	HEM	C2A-C3A	-3.40	1.30	1.38
5	A	504	HEM	CHA-C1A	-3.32	1.32	1.39
3	A	501	PTY	O7-C8	3.32	1.43	1.34
5	A	503	HEM	C1A-NA	-3.26	1.33	1.39
6	A	505	HDD	CBD-CGD	-3.25	1.43	1.50
7	B	401	CDL	OB6-CB5	3.24	1.43	1.34
7	B	401	CDL	OB8-CB7	3.21	1.42	1.33
5	A	503	HEM	C4D-C3D	-3.19	1.39	1.45
5	A	504	HEM	FE-NC	3.17	2.05	1.95
5	A	504	HEM	CAD-C3D	-3.16	1.43	1.51
5	A	504	HEM	C1D-C2D	-3.13	1.38	1.44
5	A	504	HEM	CHD-C1D	-3.11	1.32	1.39
5	A	504	HEM	O2D-CGD	-3.05	1.20	1.30
5	A	504	HEM	O2A-CGA	-2.96	1.21	1.30
7	B	401	CDL	OA6-CA4	-2.96	1.39	1.46
5	A	504	HEM	CHB-C4A	-2.96	1.32	1.39
5	A	503	HEM	CMD-C2D	-2.92	1.44	1.50
5	A	504	HEM	C3B-C2B	-2.87	1.31	1.37
5	A	503	HEM	CHA-C1A	-2.85	1.33	1.39
7	B	401	CDL	OA8-CA7	2.84	1.41	1.33
6	A	505	HDD	O2A-CGA	-2.81	1.21	1.30
5	A	503	HEM	CHA-C4D	-2.75	1.33	1.38
6	A	505	HDD	CMC-C2C	-2.74	1.45	1.50
5	A	504	HEM	C4A-C3A	-2.72	1.36	1.43
5	A	503	HEM	C4A-C3A	-2.69	1.36	1.43
6	A	505	HDD	CMA-C3A	-2.68	1.45	1.50
5	A	503	HEM	CAB-C3B	-2.68	1.40	1.47
6	A	505	HDD	CAD-CBD	-2.65	1.46	1.52
8	B	402	CD4	O16-C33	-2.64	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	503	HEM	CHB-C4A	-2.62	1.33	1.39
5	A	504	HEM	FE-NB	2.60	2.02	1.94
8	B	402	CD4	O2-C15	-2.58	1.40	1.46
6	A	505	HDD	CHD-C1D	-2.54	1.30	1.37
5	A	503	HEM	O2A-CGA	-2.50	1.22	1.30
8	B	402	CD4	O14-C35	2.50	1.40	1.33
5	A	503	HEM	FE-NC	2.49	2.03	1.95
7	B	401	CDL	OB6-CB4	-2.44	1.40	1.46
5	A	504	HEM	C3C-C2C	-2.41	1.32	1.37
8	B	402	CD4	O3-C17	2.41	1.40	1.33
6	A	505	HDD	CAA-C2A	-2.40	1.45	1.51
7	B	401	CDL	OA6-CA5	2.40	1.41	1.34
6	A	505	HDD	CHA-C1A	2.39	1.44	1.39
7	B	401	CDL	OA8-CA6	-2.38	1.39	1.45
5	A	503	HEM	CAC-C3C	-2.37	1.41	1.47
3	A	501	PTY	O4-C30	2.36	1.40	1.33
5	A	503	HEM	C1D-C2D	-2.31	1.39	1.44
5	A	503	HEM	FE-NB	2.30	2.02	1.94
5	A	504	HEM	CHA-C4D	-2.29	1.33	1.38
6	A	505	HDD	CMB-C2B	-2.29	1.46	1.50
5	A	503	HEM	CAD-C3D	-2.24	1.45	1.51
5	A	503	HEM	CAA-C2A	-2.24	1.45	1.51
5	A	503	HEM	CMA-C3A	-2.22	1.46	1.50
5	A	504	HEM	CMD-C2D	-2.22	1.46	1.50
6	A	505	HDD	CHC-C4B	2.21	1.42	1.38
3	A	501	PTY	C11-C8	2.20	1.57	1.50
8	B	402	CD4	O2-C14	2.20	1.40	1.34
5	A	504	HEM	CMA-C3A	-2.19	1.46	1.50
8	B	402	CD4	O3-C16	-2.19	1.40	1.45
3	A	501	PTY	O7-C6	-2.17	1.41	1.46
5	A	504	HEM	CAB-C3B	-2.17	1.41	1.47
5	A	503	HEM	CHD-C1D	-2.15	1.34	1.39
8	B	402	CD4	O16-C46	2.15	1.40	1.34
6	A	505	HDD	CAD-C3D	-2.15	1.49	1.53
8	B	402	CD4	O14-C34	-2.09	1.40	1.45
3	A	501	PTY	P1-O14	2.09	1.67	1.59
6	A	505	HDD	CHA-C4D	-2.07	1.31	1.37
5	A	503	HEM	CHB-C1B	-2.06	1.34	1.38
7	B	401	CDL	C51-CB5	2.03	1.56	1.50
5	A	503	HEM	O2D-CGD	-2.03	1.24	1.30
7	B	401	CDL	OB8-CB6	-2.01	1.40	1.45
6	A	505	HDD	O2D-CGD	-2.01	1.16	1.22

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	MQ9	C51-C49-C50	-16.68	76.21	114.59
4	A	502	MQ9	C51-C49-C48	13.39	162.85	122.66
4	A	502	MQ9	C50-C49-C48	-12.00	86.64	122.66
6	A	505	HDD	CAD-CBD-CGD	-11.57	87.29	104.48
6	A	505	HDD	C3D-O1D-CGD	-9.77	102.04	111.14
5	A	504	HEM	CHD-C1D-ND	8.34	133.40	124.42
5	A	504	HEM	C3B-C4B-NB	-8.04	103.70	109.47
5	A	504	HEM	CAD-C3D-C4D	7.93	138.52	124.70
5	A	504	HEM	CAD-C3D-C2D	-7.73	113.38	127.87
6	A	505	HDD	CBD-CAD-C3D	7.49	114.66	103.98
5	A	503	HEM	CHC-C4B-NB	7.14	132.11	124.42
5	A	504	HEM	CHD-C1D-C2D	-6.80	114.30	125.03
6	A	505	HDD	C3B-C2B-C1B	-6.62	100.78	107.05
6	A	505	HDD	O1D-CGD-CBD	6.56	116.15	110.17
5	A	504	HEM	C1B-NB-C4B	6.46	112.85	105.21
5	A	504	HEM	CHC-C4B-NB	6.42	131.34	124.42
6	A	505	HDD	C3C-C2C-C1C	-5.66	100.50	107.17
5	A	504	HEM	CHB-C1B-NB	5.35	130.98	124.37
5	A	503	HEM	CBD-CAD-C3D	-4.87	99.06	112.53
5	A	503	HEM	CHA-C4D-ND	4.73	130.21	124.37
6	A	505	HDD	CHB-C1B-C2B	-4.72	115.67	125.49
6	A	505	HDD	CAB-C3B-C4B	4.69	136.01	124.82
6	A	505	HDD	C2B-C1B-NB	4.45	117.87	109.64
7	B	401	CDL	OB6-CB5-C51	4.43	121.07	111.48
7	B	401	CDL	OA6-CA5-C11	4.41	121.03	111.48
5	A	503	HEM	CHB-C1B-NB	4.19	129.55	124.37
5	A	503	HEM	CHD-C4C-NC	4.10	128.92	124.45
3	A	501	PTY	O7-C8-C11	4.03	120.21	111.48
5	A	503	HEM	CHA-C4D-C3D	-4.03	117.79	125.23
8	B	402	CD4	O2-C14-C13	3.99	120.11	111.48
8	B	402	CD4	O16-C46-C47	3.92	119.97	111.48
6	A	505	HDD	C4A-C3A-C2A	-3.78	102.49	106.82
5	A	503	HEM	O2D-CGD-CBD	3.65	125.52	114.00
5	A	503	HEM	CAC-C3C-C4C	-3.61	116.20	124.82
6	A	505	HDD	C3A-C4A-NA	3.58	115.89	110.14
6	A	505	HDD	CHD-C1D-ND	3.49	129.09	124.28
5	A	504	HEM	O2D-CGD-CBD	3.47	124.95	114.00
6	A	505	HDD	C3C-C4C-NC	3.42	112.68	109.80
5	A	504	HEM	C4C-CHD-C1D	-3.40	118.79	126.02
5	A	503	HEM	C3B-C4B-NB	-3.37	107.04	109.47
6	A	505	HDD	CAA-C2A-C1A	3.25	131.29	124.94
5	A	504	HEM	CBA-CAA-C2A	3.24	121.49	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	HEM	CHD-C4C-NC	3.20	127.94	124.45
5	A	504	HEM	C3C-C2C-C1C	3.16	110.04	107.05
5	A	503	HEM	C4C-NC-C1C	3.16	110.97	105.82
5	A	503	HEM	C4C-C3C-C2C	3.14	109.54	106.81
5	A	504	HEM	CMD-C2D-C1D	3.10	129.88	125.03
6	A	505	HDD	C2A-C1A-NA	3.07	113.56	110.15
6	A	505	HDD	CAB-C3B-C2B	-3.06	118.48	128.43
5	A	503	HEM	C1B-NB-C4B	3.01	108.77	105.21
7	B	401	CDL	OA8-CA7-C31	3.00	120.97	111.83
6	A	505	HDD	CMB-C2B-C1B	2.98	129.98	124.73
7	B	401	CDL	OB8-CB7-C71	2.89	120.63	111.83
5	A	503	HEM	CHD-C1D-ND	2.88	127.53	124.42
5	A	504	HEM	C4C-C3C-C2C	-2.88	104.32	106.81
5	A	504	HEM	O1D-CGD-CBD	-2.88	113.96	123.09
5	A	503	HEM	CHB-C1B-C2B	-2.87	118.78	126.95
5	A	504	HEM	O2A-CGA-O1A	-2.84	116.03	123.33
5	A	503	HEM	C3B-C2B-C1B	-2.82	104.29	106.41
5	A	503	HEM	CAA-C2A-C1A	2.80	130.40	124.94
6	A	505	HDD	CHB-C4A-C3A	-2.76	119.42	127.43
5	A	503	HEM	C4A-CHB-C1B	-2.70	119.90	126.25
5	A	504	HEM	CHB-C1B-C2B	-2.70	119.28	126.95
8	B	402	CD4	O3-C17-C18	2.68	120.02	111.83
3	A	501	PTY	O4-C30-C31	2.62	119.82	111.83
6	A	505	HDD	CAA-CBA-CGA	-2.61	106.74	113.67
5	A	504	HEM	C4A-CHB-C1B	-2.60	120.14	126.25
6	A	505	HDD	CBA-CAA-C2A	-2.53	105.52	112.53
5	A	503	HEM	O2A-CGA-O1A	-2.45	117.02	123.33
5	A	503	HEM	CAA-CBA-CGA	-2.43	107.22	113.67
5	A	503	HEM	O2D-CGD-O1D	-2.43	117.09	123.33
6	A	505	HDD	C1A-C2A-C3A	-2.38	103.19	106.87
5	A	503	HEM	C4C-CHD-C1D	-2.35	121.02	126.02
6	A	505	HDD	CMC-C2C-C3C	2.35	132.07	126.55
8	B	402	CD4	O14-C35-C36	2.33	118.95	111.83
6	A	505	HDD	C2C-C1C-NC	2.33	113.87	110.14
4	A	502	MQ9	C7-C6-C1	-2.31	116.15	118.58
5	A	504	HEM	C2C-C1C-NC	-2.28	105.42	109.64
6	A	505	HDD	C2D-C1D-CHD	-2.21	120.84	124.27
5	A	504	HEM	CHC-C1C-C2C	2.21	130.07	125.49
5	A	503	HEM	CHC-C4B-C3B	-2.15	120.79	125.07
5	A	504	HEM	CHD-C4C-C3C	-2.13	121.61	125.21
6	A	505	HDD	CMA-C3A-C2A	2.10	130.08	125.62
5	A	504	HEM	O2A-CGA-CBA	2.10	120.64	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	505	HDD	CHC-C1C-C2C	-2.09	121.36	127.43
6	A	505	HDD	CHC-C4B-NB	-2.09	122.18	124.45
5	A	504	HEM	CHA-C1A-NA	2.07	127.62	123.86
5	A	504	HEM	C4C-NC-C1C	2.04	109.14	105.82
5	A	504	HEM	C2D-C1D-ND	2.03	112.25	109.90

There are no chirality outliers.

All (130) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	PTY	O10-C8-O7-C6
3	A	501	PTY	C3-O11-P1-O12
3	A	501	PTY	C3-O11-P1-O13
3	A	501	PTY	C3-O11-P1-O14
5	A	504	HEM	C2D-C3D-CAD-CBD
5	A	504	HEM	C4D-C3D-CAD-CBD
7	B	401	CDL	CB2-C1-CA2-OA2
7	B	401	CDL	CA3-OA5-PA1-OA3
7	B	401	CDL	C11-CA5-OA6-CA4
7	B	401	CDL	CB3-OB5-PB2-OB2
7	B	401	CDL	CB3-OB5-PB2-OB3
8	B	402	CD4	C13-C14-O2-C15
8	B	402	CD4	C29-O8-P1-O5
8	B	402	CD4	C29-O8-P1-O6
8	B	402	CD4	C29-O8-P1-O7
8	B	402	CD4	C30-C29-O8-P1
8	B	402	CD4	O9-C30-C31-O10
8	B	402	CD4	C32-O13-P2-O11
8	B	402	CD4	C32-O13-P2-O12
8	B	402	CD4	O17-C46-O16-C33
8	B	402	CD4	C47-C46-O16-C33
7	B	401	CDL	C31-CA7-OA8-CA6
3	A	501	PTY	O30-C30-O4-C1
7	B	401	CDL	OA9-CA7-OA8-CA6
7	B	401	CDL	OA7-CA5-OA6-CA4
8	B	402	CD4	O1-C14-O2-C15
3	A	501	PTY	C31-C30-O4-C1
3	A	501	PTY	C11-C8-O7-C6
4	A	502	MQ9	C30-C29-C31-C32
4	A	502	MQ9	C28-C29-C31-C32
7	B	401	CDL	O1-C1-CA2-OA2
4	A	502	MQ9	C24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
4	A	502	MQ9	C29-C31-C32-C33
8	B	402	CD4	C29-C30-C31-O10
7	B	401	CDL	C20-C21-C22-C23
4	A	502	MQ9	C15-C14-C16-C17
3	A	501	PTY	C8-C11-C12-C13
3	A	501	PTY	C30-C31-C32-C33
7	B	401	CDL	O1-C1-CB2-OB2
7	B	401	CDL	CA5-C11-C12-C13
7	B	401	CDL	C51-CB5-OB6-CB4
7	B	401	CDL	C23-C24-C25-C26
8	B	402	CD4	C24-C25-C26-C27
3	A	501	PTY	C19-C20-C21-C22
7	B	401	CDL	C12-C13-C14-C15
4	A	502	MQ9	C13-C14-C16-C17
7	B	401	CDL	C31-C32-C33-C34
7	B	401	CDL	C15-C16-C17-C18
7	B	401	CDL	C36-C37-C38-C39
7	B	401	CDL	C38-C39-C40-C41
8	B	402	CD4	C10-C11-C12-C13
7	B	401	CDL	OB7-CB5-OB6-CB4
7	B	401	CDL	C51-C52-C53-C54
8	B	402	CD4	C51-C52-C53-C54
8	B	402	CD4	C23-C24-C25-C26
7	B	401	CDL	C17-C18-C19-C20
8	B	402	CD4	C6-C7-C8-C9
8	B	402	CD4	C53-C54-C55-C56
3	A	501	PTY	C32-C33-C34-C35
7	B	401	CDL	C14-C15-C16-C17
8	B	402	CD4	C21-C22-C23-C24
3	A	501	PTY	C34-C35-C36-C37
7	B	401	CDL	C57-C58-C59-C60
7	B	401	CDL	C42-C43-C44-C45
3	A	501	PTY	C39-C40-C41-C42
7	B	401	CDL	C43-C44-C45-C46
8	B	402	CD4	C18-C17-O3-C16
3	A	501	PTY	C23-C24-C25-C26
7	B	401	CDL	CA3-CA4-CA6-OA8
7	B	401	CDL	CB3-CB4-CB6-OB8
7	B	401	CDL	C16-C17-C18-C19
3	A	501	PTY	C41-C42-C43-C44
7	B	401	CDL	C59-C60-C61-C62
7	B	401	CDL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
4	A	502	MQ9	C33-C34-C36-C37
3	A	501	PTY	O14-C5-C6-C1
8	B	402	CD4	O4-C17-O3-C16
8	B	402	CD4	C7-C8-C9-C10
4	A	502	MQ9	C20-C19-C21-C22
4	A	502	MQ9	C35-C34-C36-C37
4	A	502	MQ9	C18-C19-C21-C22
8	B	402	CD4	C56-C57-C58-C59
7	B	401	CDL	OA6-CA4-CA6-OA8
8	B	402	CD4	C11-C10-C9-C8
7	B	401	CDL	C13-C14-C15-C16
3	A	501	PTY	C15-C16-C17-C18
3	A	501	PTY	C13-C14-C15-C16
8	B	402	CD4	C16-C15-O2-C14
3	A	501	PTY	O14-C5-C6-O7
6	A	505	HDD	C4B-C3B-CAB-CBB
7	B	401	CDL	OB6-CB4-CB6-OB8
7	B	401	CDL	C37-C38-C39-C40
8	B	402	CD4	C40-C41-C42-C43
3	A	501	PTY	C24-C25-C26-C27
3	A	501	PTY	C14-C15-C16-C17
3	A	501	PTY	N1-C2-C3-O11
7	B	401	CDL	CA2-OA2-PA1-OA3
7	B	401	CDL	CA2-OA2-PA1-OA5
7	B	401	CDL	CA3-OA5-PA1-OA2
8	B	402	CD4	C32-O13-P2-O10
5	A	504	HEM	C1A-C2A-CAA-CBA
7	B	401	CDL	C33-C34-C35-C36
7	B	401	CDL	C1-CB2-OB2-PB2
7	B	401	CDL	C41-C42-C43-C44
8	B	402	CD4	C18-C19-C20-C21
7	B	401	CDL	C40-C41-C42-C43
5	A	503	HEM	C3D-CAD-CBD-CGD
8	B	402	CD4	C46-C47-C48-C49
3	A	501	PTY	C22-C23-C24-C25
5	A	504	HEM	CAD-CBD-CGD-O1D
5	A	504	HEM	CAD-CBD-CGD-O2D
4	A	502	MQ9	C9-C11-C12-C13
8	B	402	CD4	C48-C49-C50-C51
8	B	402	CD4	C42-C43-C44-C45
7	B	401	CDL	C18-C19-C20-C21
4	A	502	MQ9	C25-C24-C26-C27

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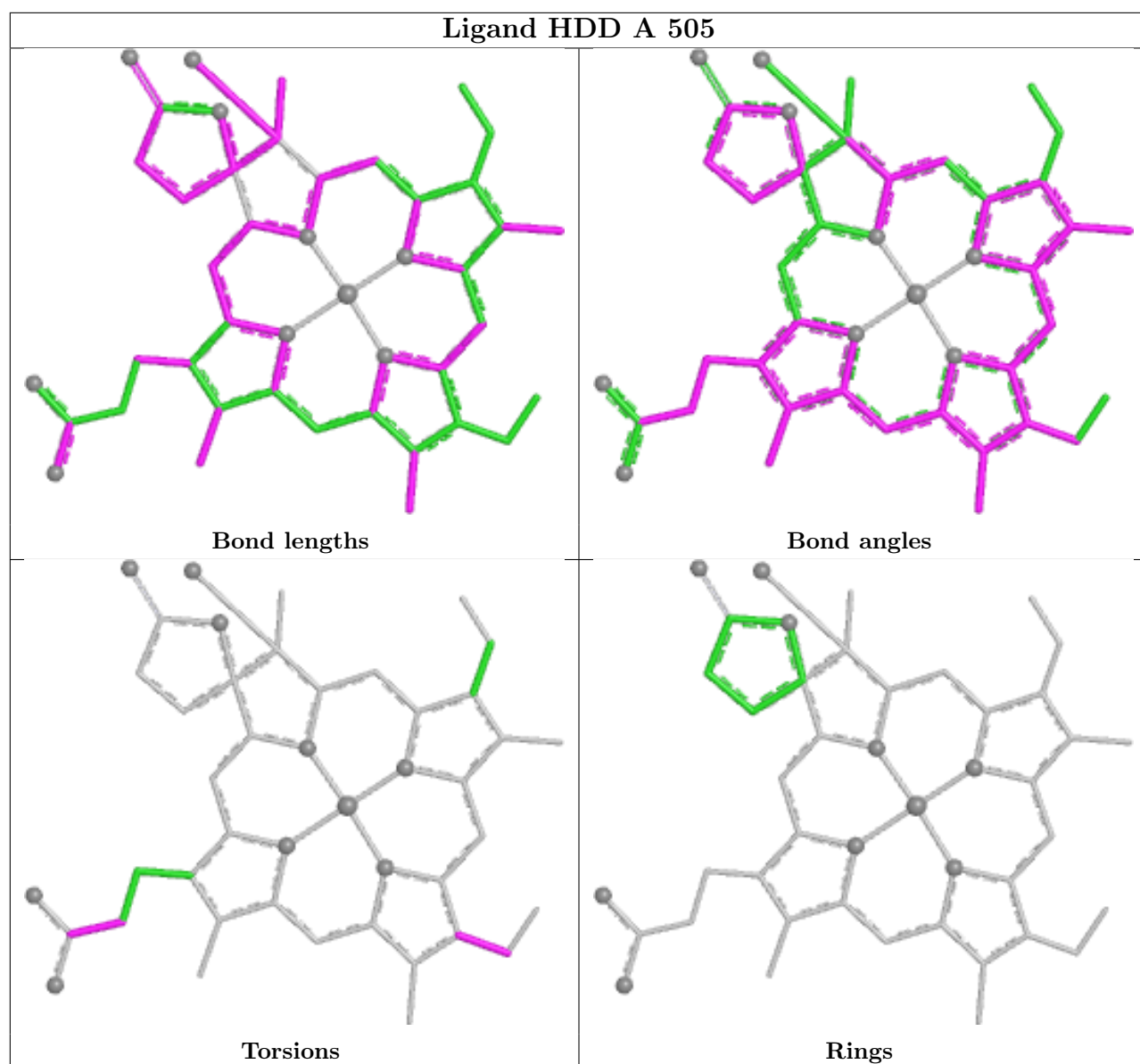
Mol	Chain	Res	Type	Atoms
3	A	501	PTY	C16-C17-C18-C19
7	B	401	CDL	C35-C36-C37-C38
7	B	401	CDL	C56-C57-C58-C59
8	B	402	CD4	C41-C42-C43-C44
8	B	402	CD4	C49-C50-C51-C52
7	B	401	CDL	OB5-CB3-CB4-OB6
6	A	505	HDD	CAA-CBA-CGA-O1A
6	A	505	HDD	CAA-CBA-CGA-O2A
3	A	501	PTY	C20-C21-C22-C23
8	B	402	CD4	C22-C23-C24-C25
3	A	501	PTY	C12-C13-C14-C15
8	B	402	CD4	C9-C10-C11-C12
7	B	401	CDL	C12-C11-CA5-OA6
5	A	504	HEM	CAA-CBA-CGA-O2A

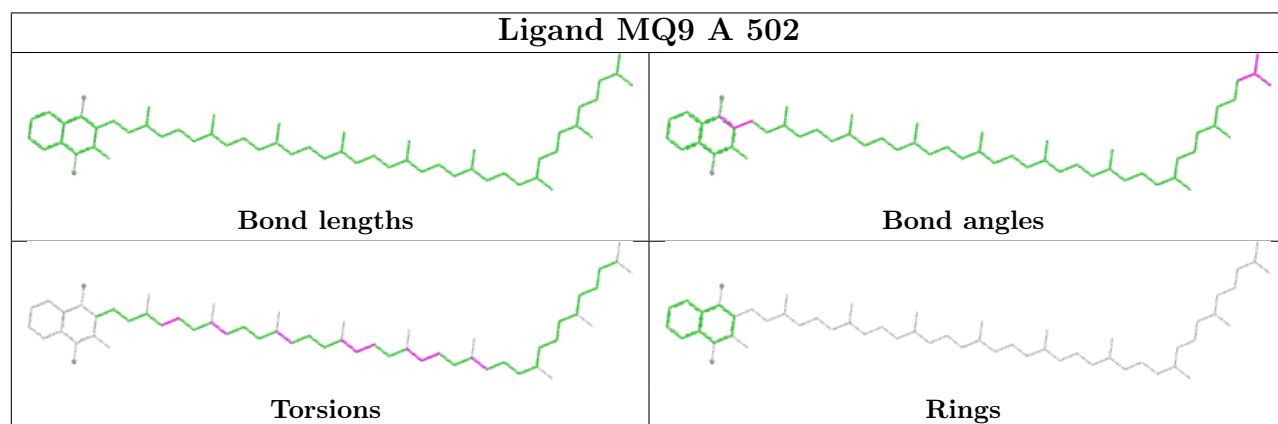
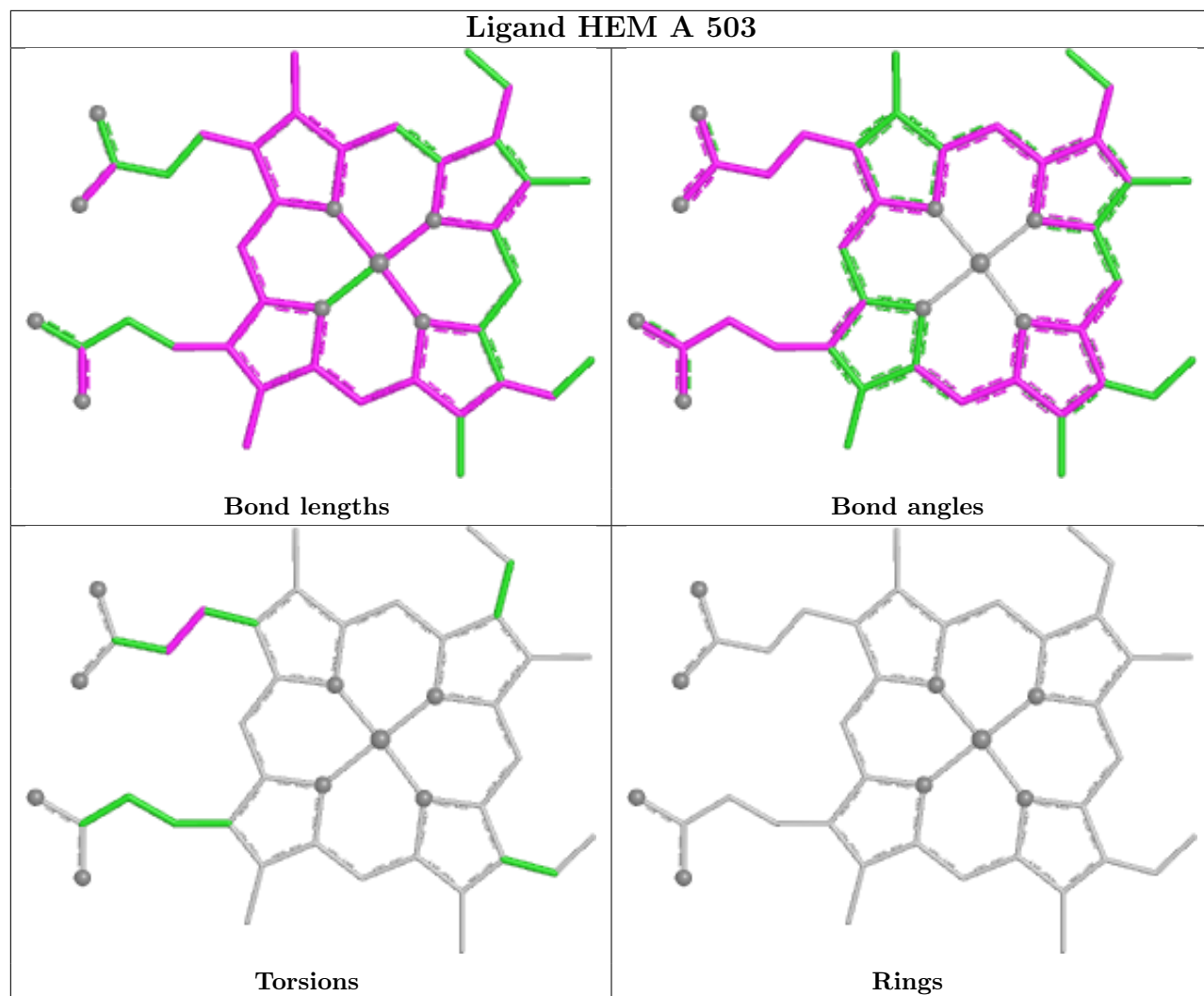
There are no ring outliers.

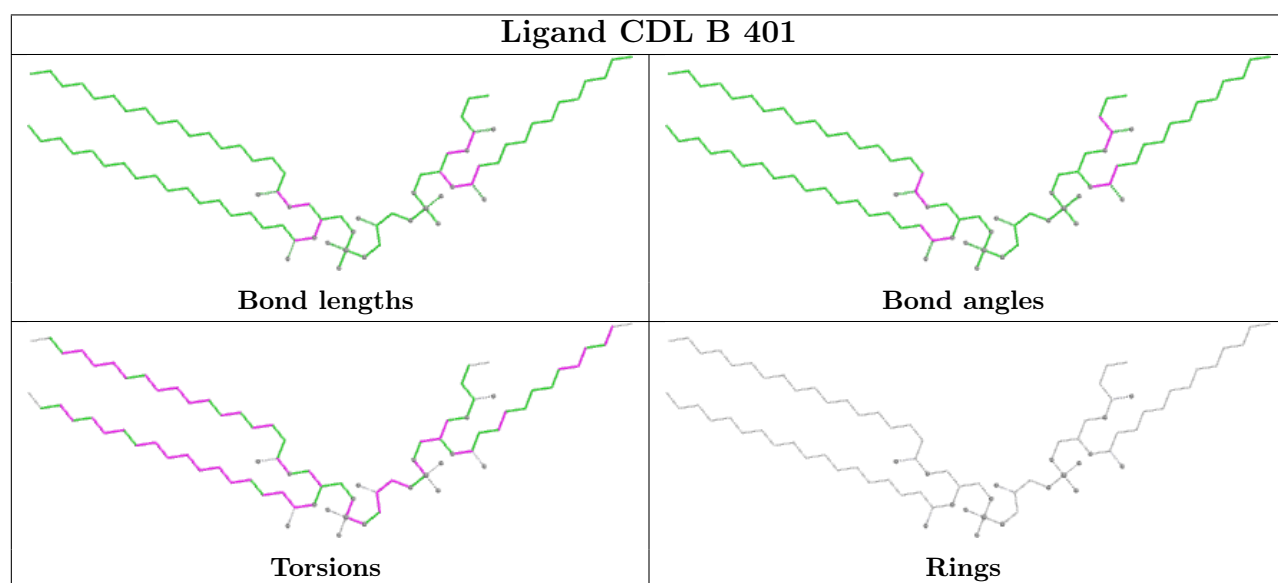
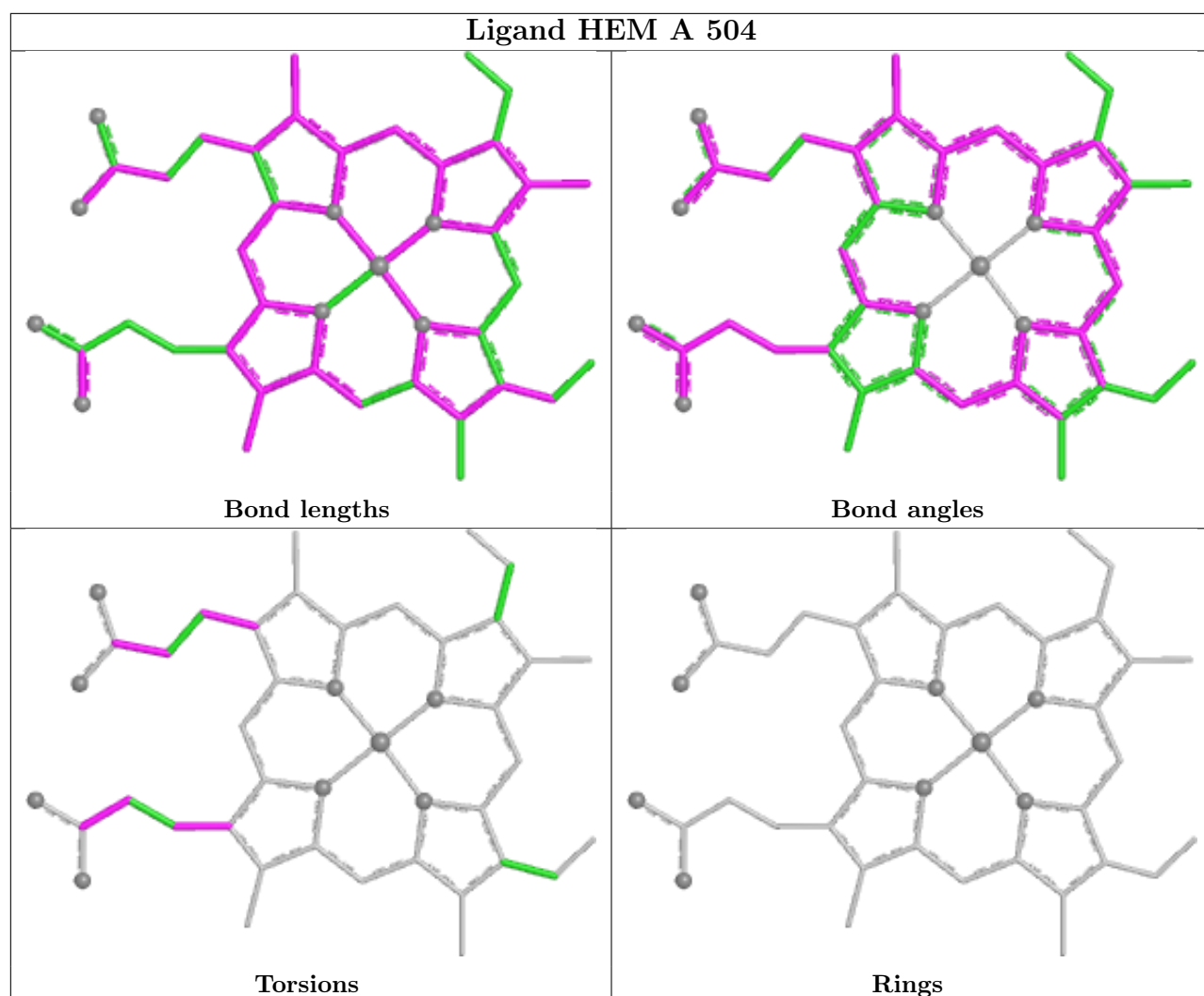
7 monomers are involved in 54 short contacts:

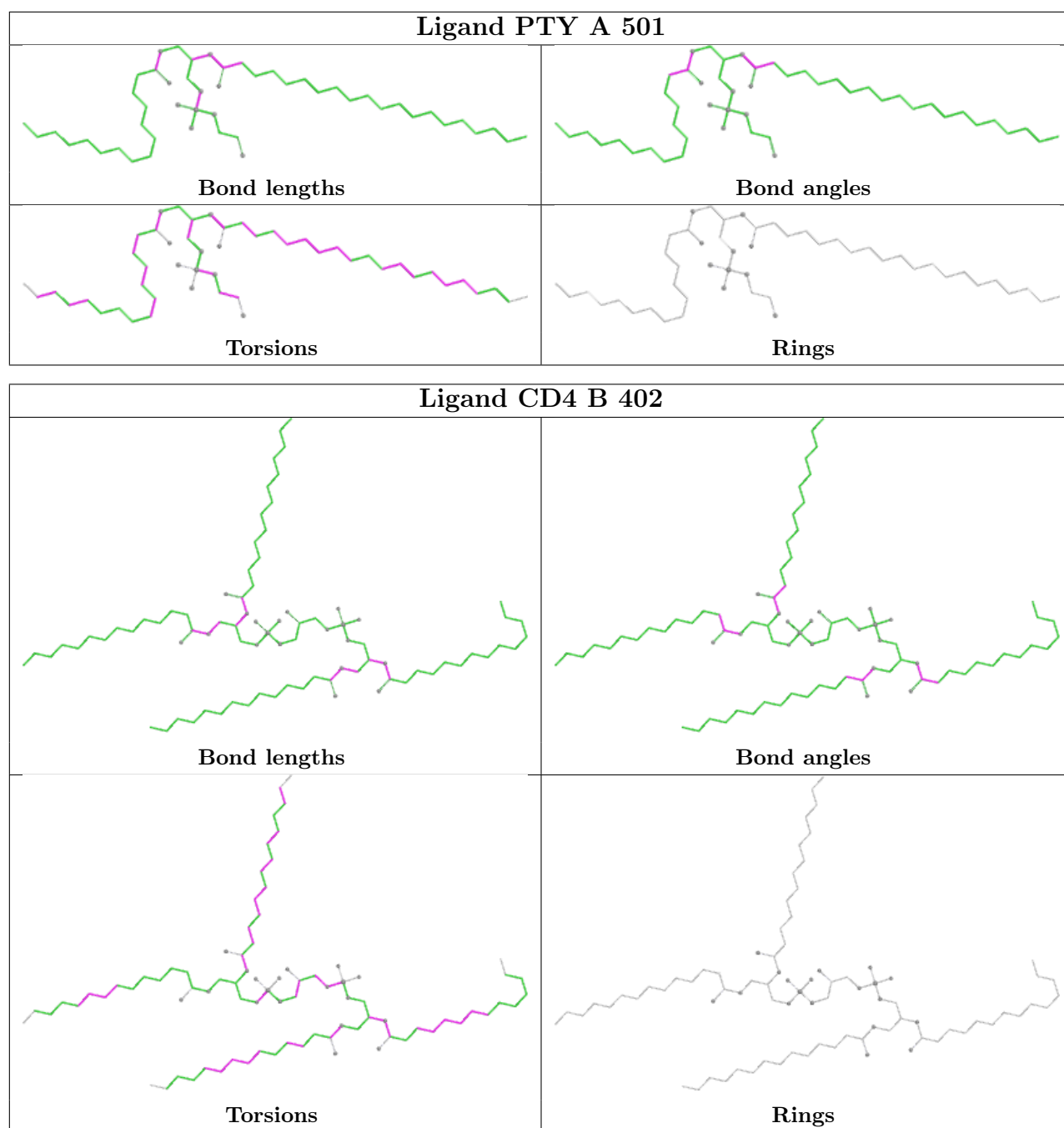
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	505	HDD	10	0
5	A	503	HEM	13	0
4	A	502	MQ9	12	0
5	A	504	HEM	17	0
7	B	401	CDL	1	0
3	A	501	PTY	1	0
8	B	402	CD4	3	0

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 than 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.









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.

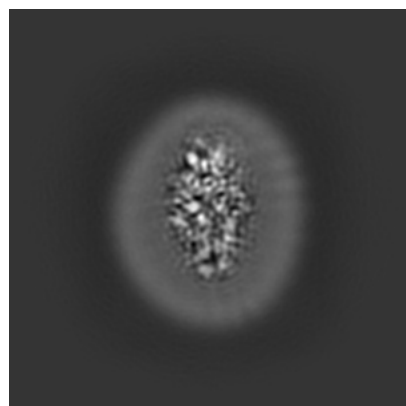
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50520. These allow visual inspection of the internal detail of the map and identification of artifacts.

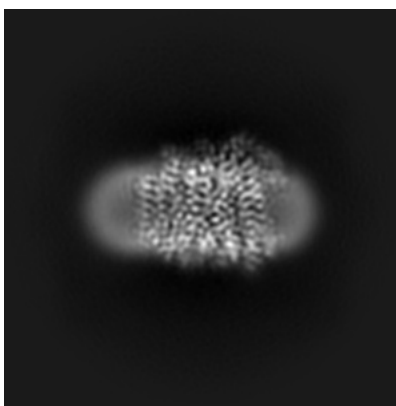
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

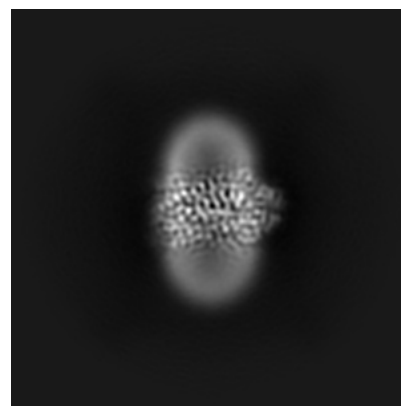
6.1.1 Primary map



X

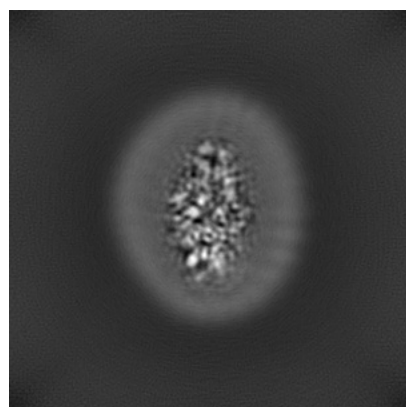


Y

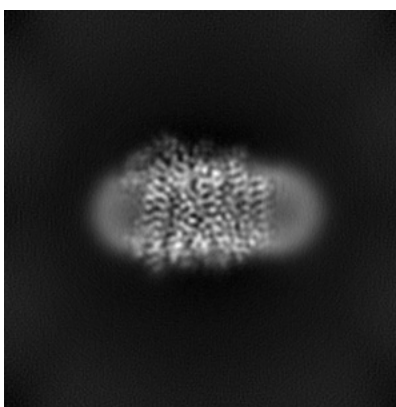


Z

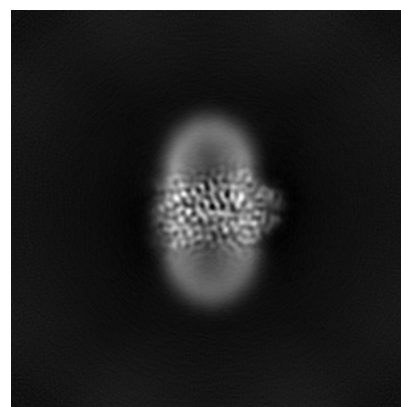
6.1.2 Raw map



X



Y

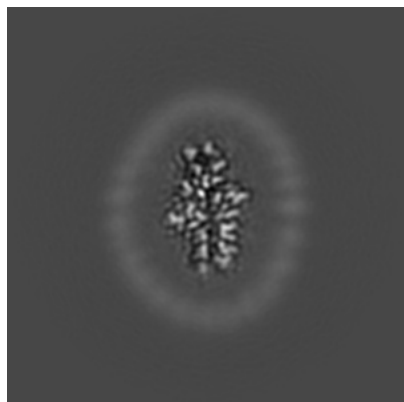


Z

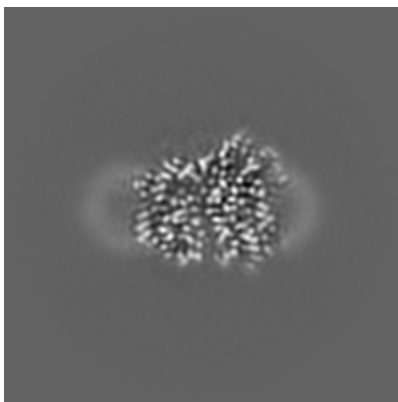
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

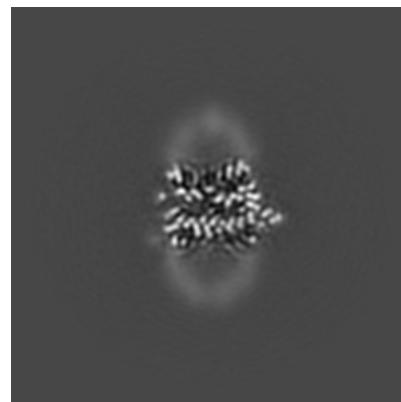
6.2.1 Primary map



X Index: 128

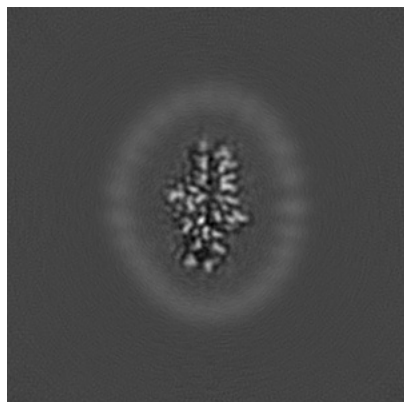


Y Index: 128

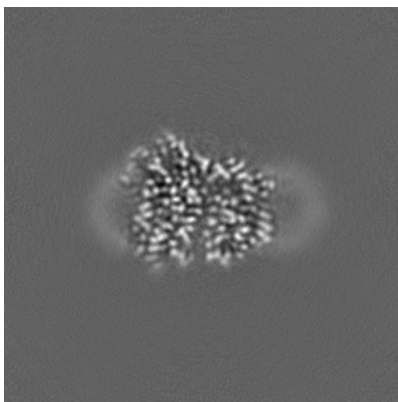


Z Index: 128

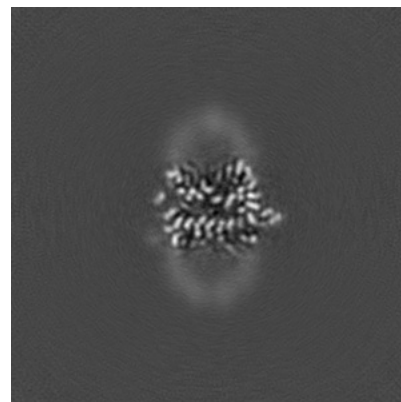
6.2.2 Raw map



X Index: 128



Y Index: 128

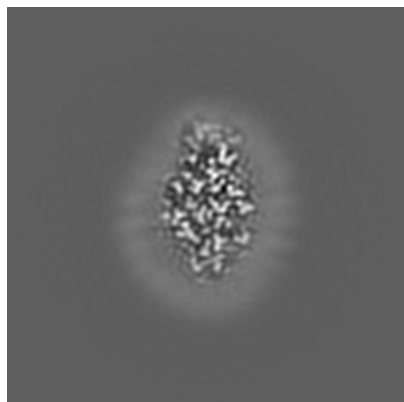


Z Index: 128

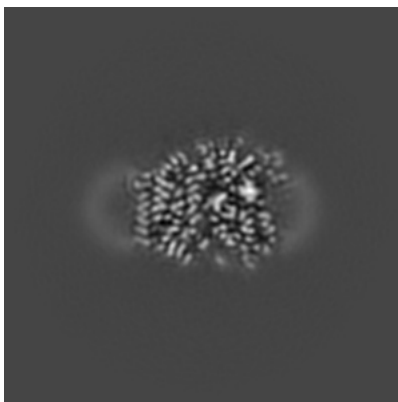
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

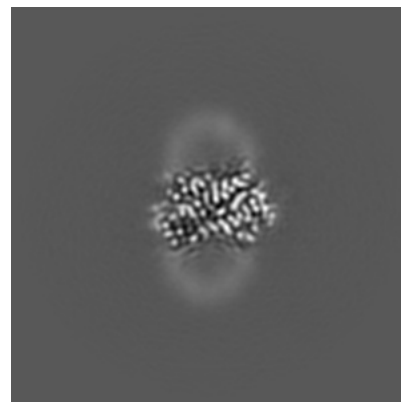
6.3.1 Primary map



X Index: 146

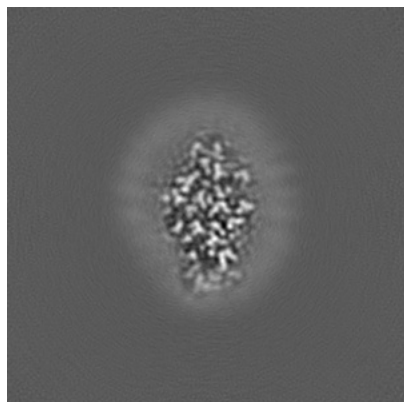


Y Index: 125

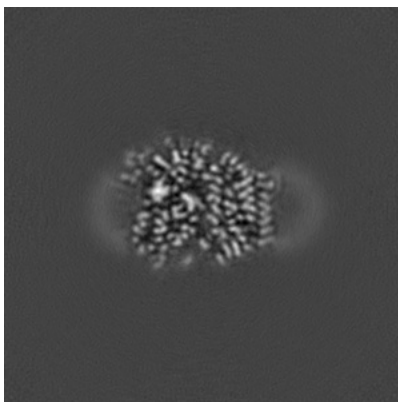


Z Index: 140

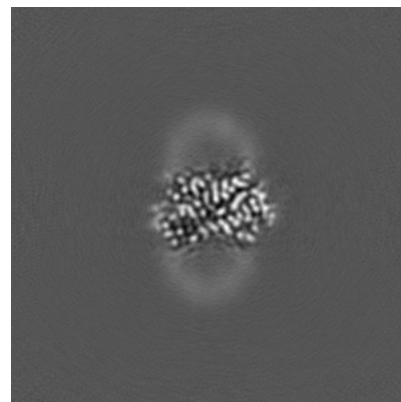
6.3.2 Raw map



X Index: 146



Y Index: 125

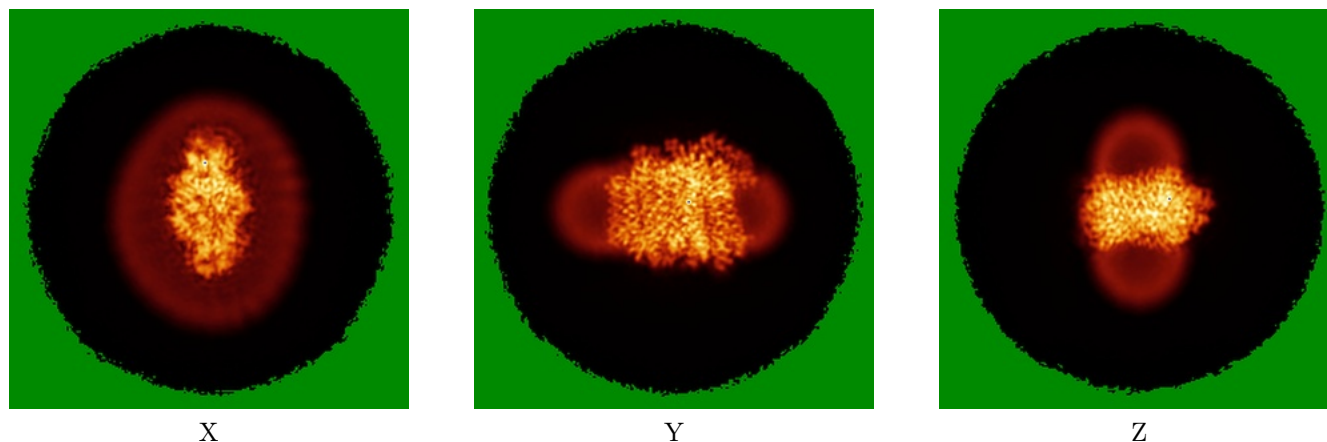


Z Index: 115

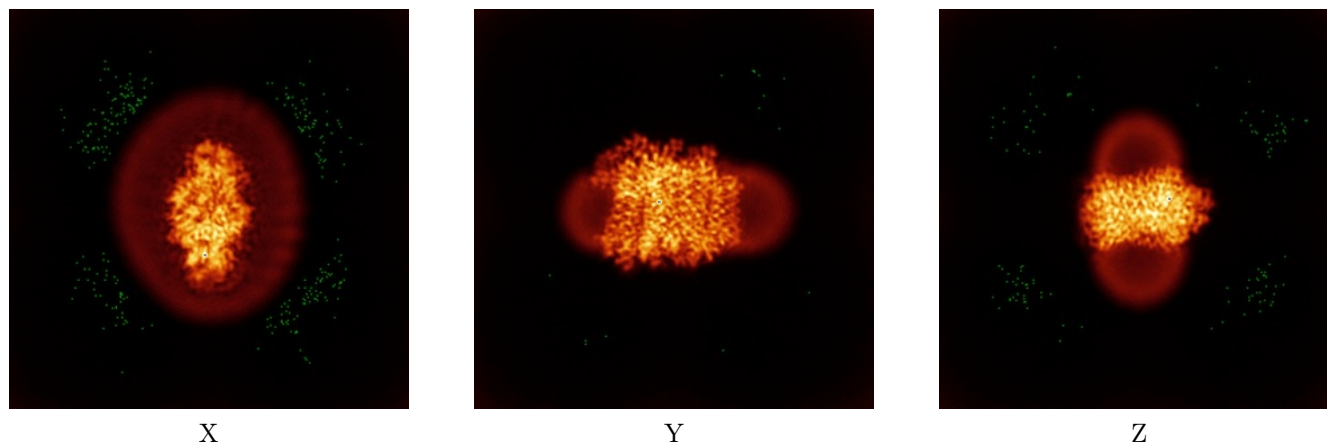
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



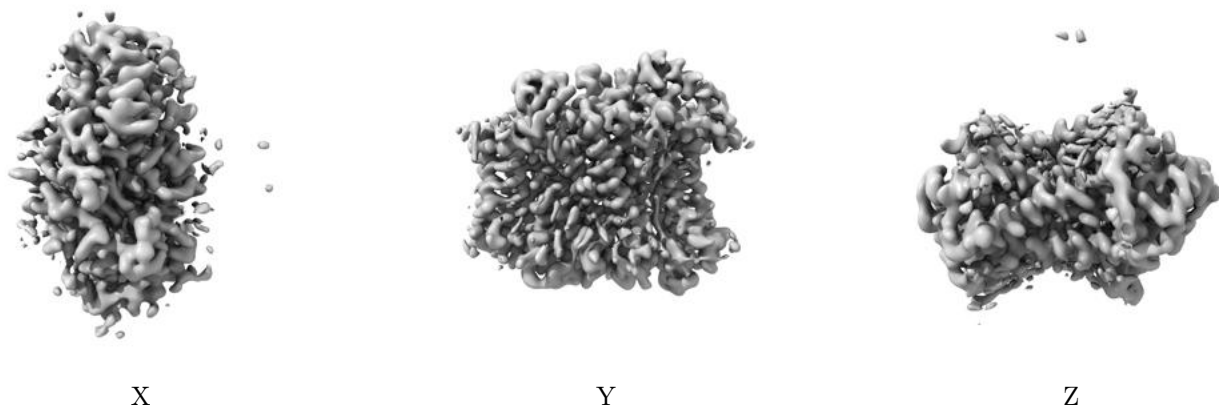
6.4.2 Raw map



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.

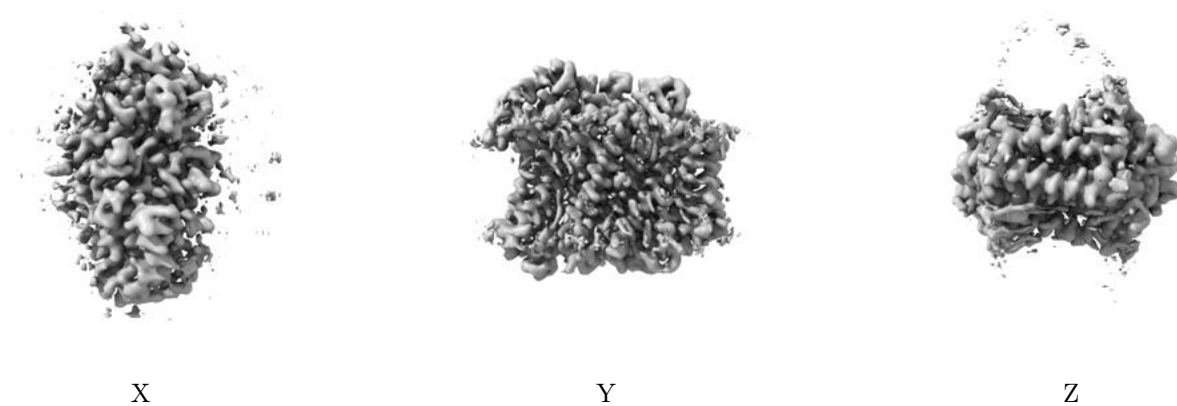
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0657. 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



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.

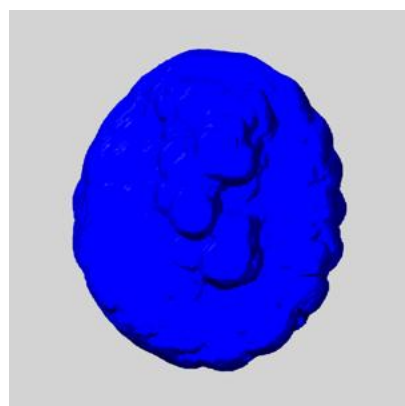
6.6 Mask visualisation [i](#)

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

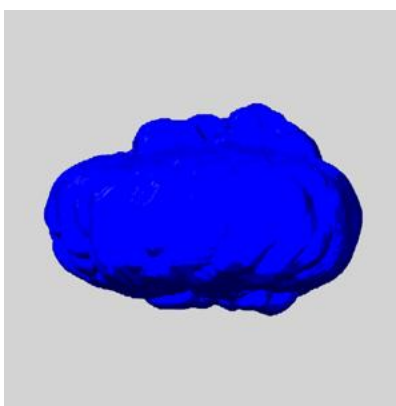
A mask typically either:

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

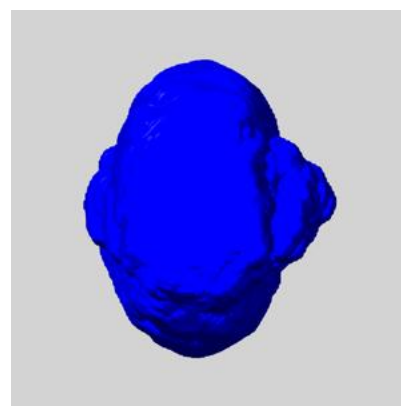
6.6.1 emd_50520_msk_1.map [i](#)



X



Y

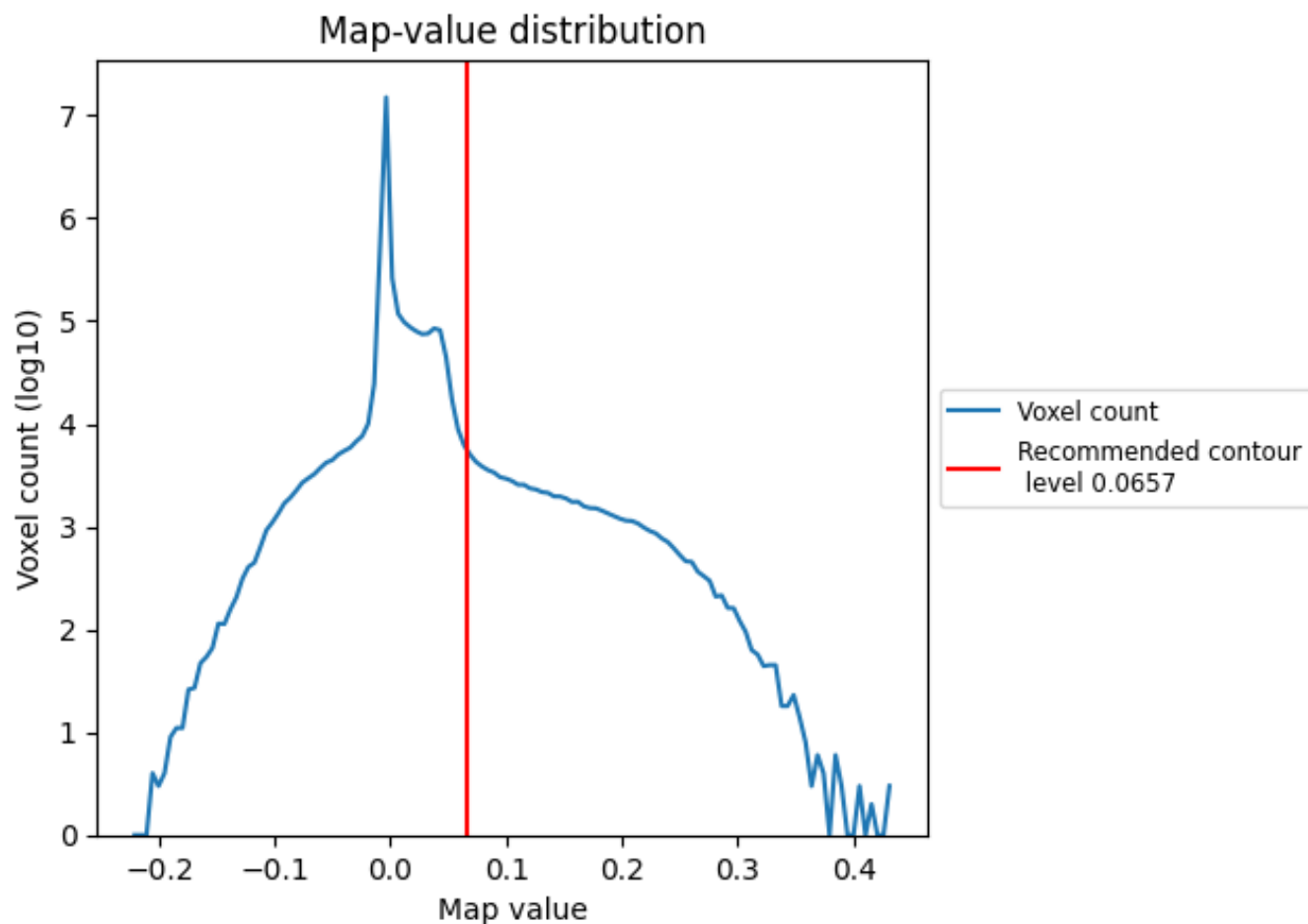


Z

7 Map analysis [i](#)

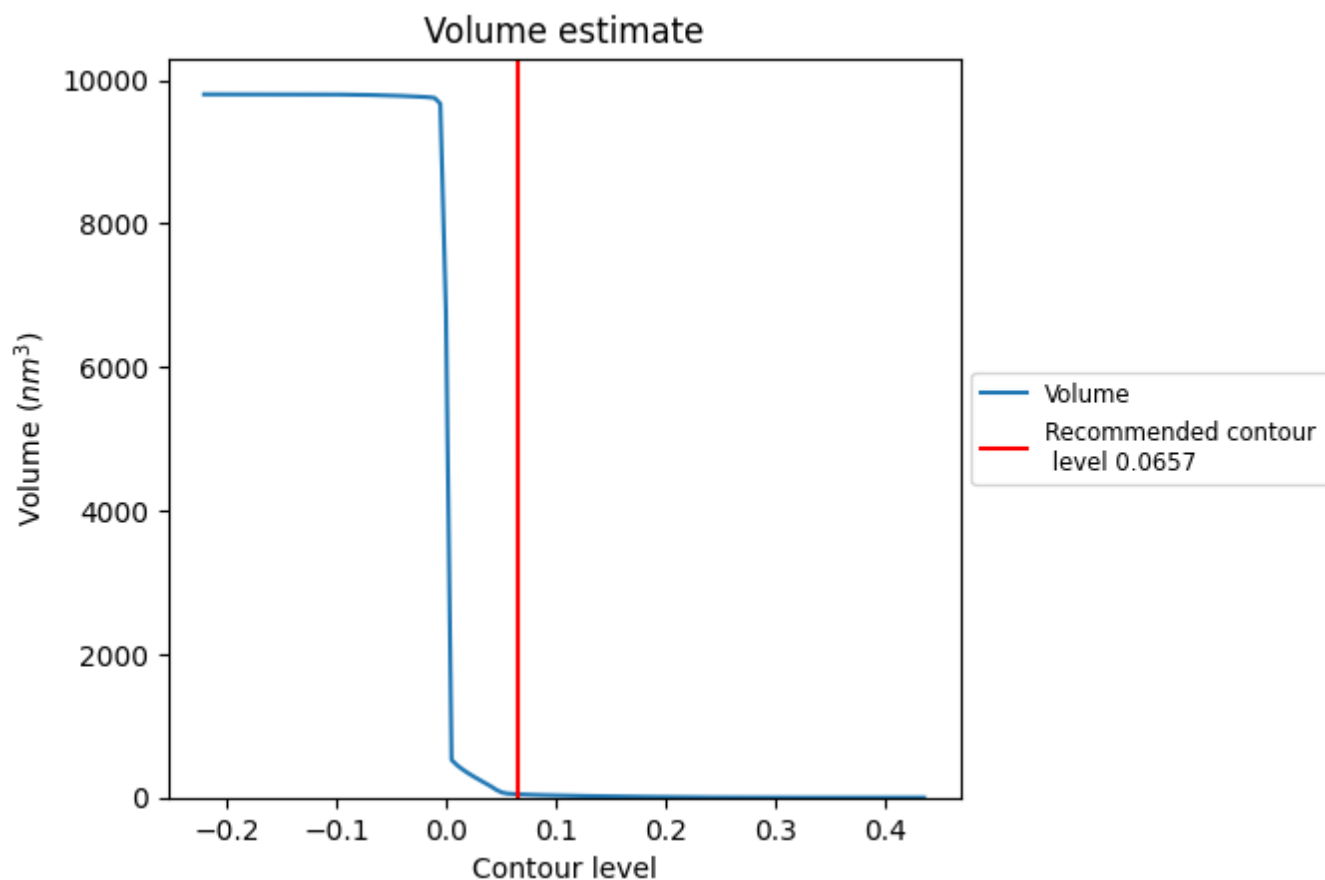
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

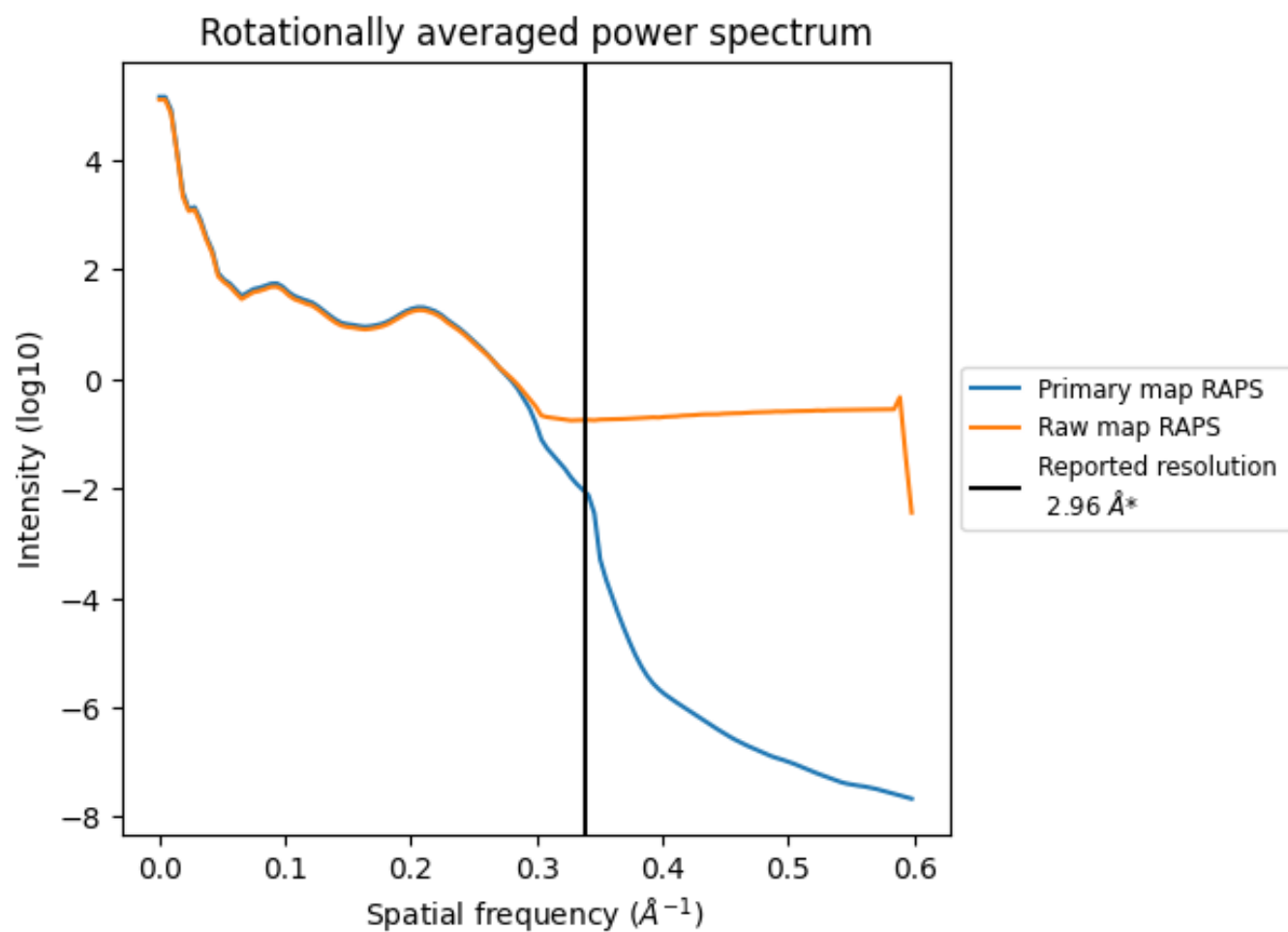
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm³; this corresponds to an approximate mass of 41 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 ⓘ

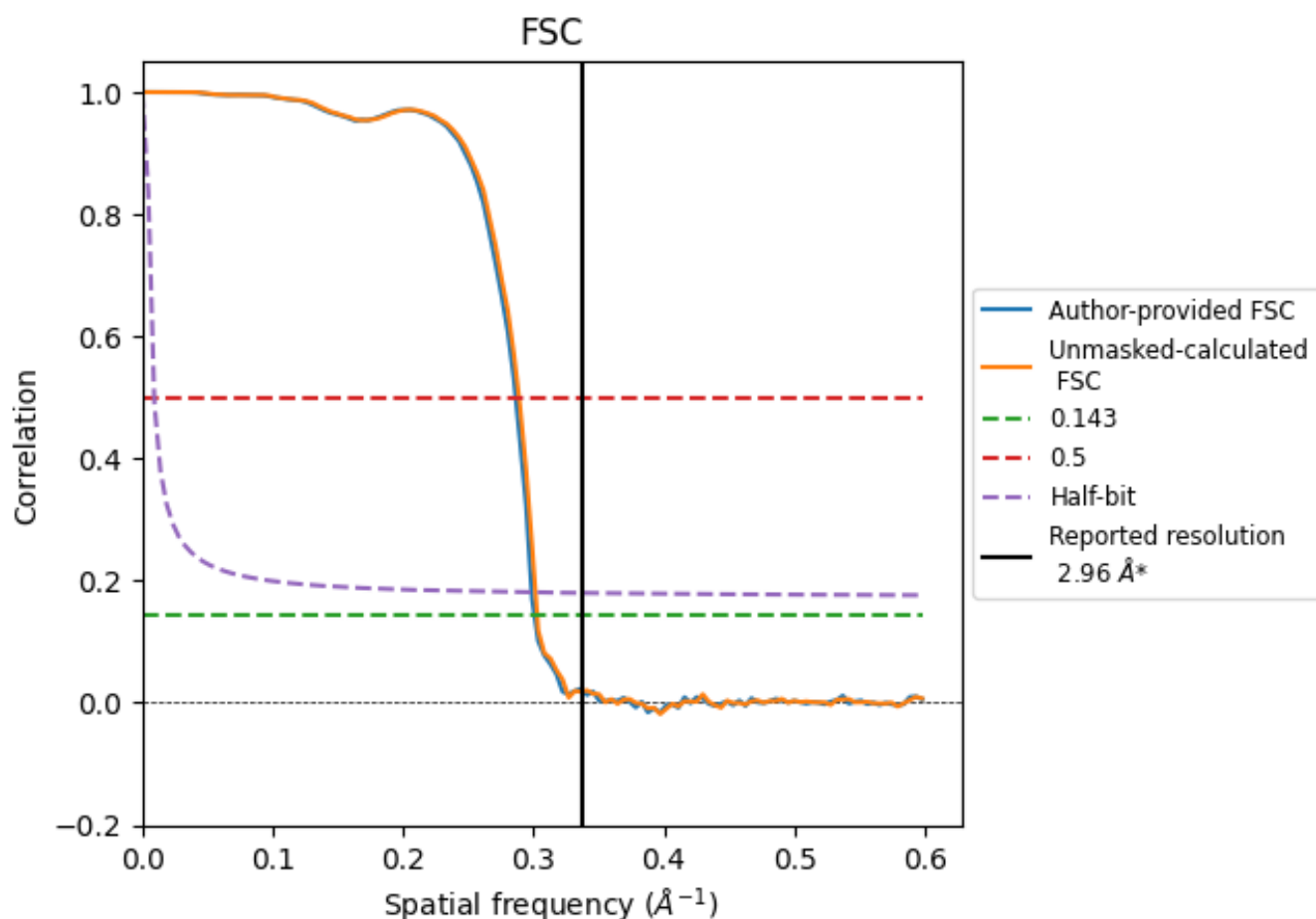


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

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 0.338 $\text{\AA}^{-1}$

8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	3.32	3.49	3.35
Unmasked-calculated*	3.30	3.46	3.32

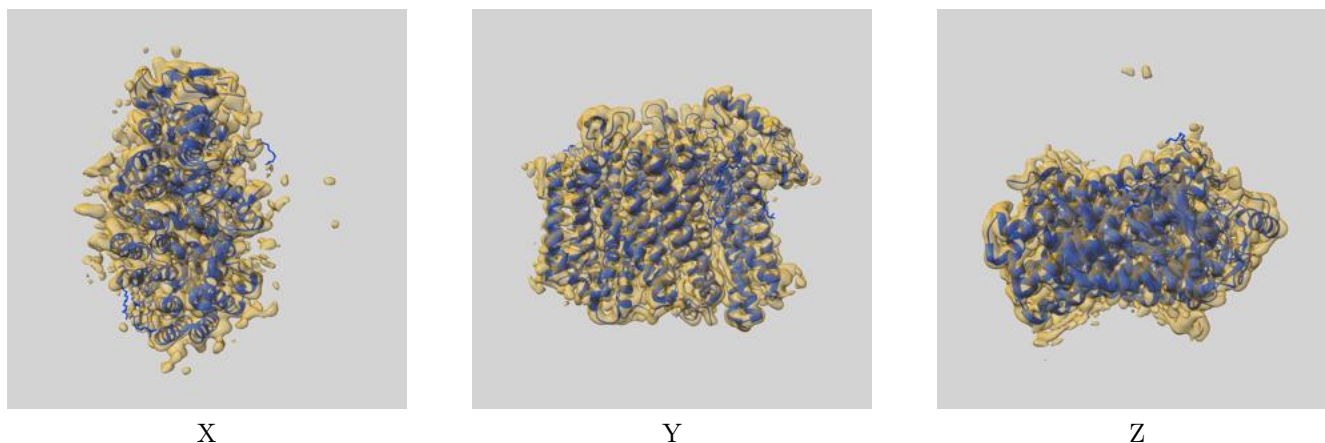
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.32 differs from the reported value 2.96 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.30 differs from the reported value 2.96 by more than 10 %

9 Map-model fit [i](#)

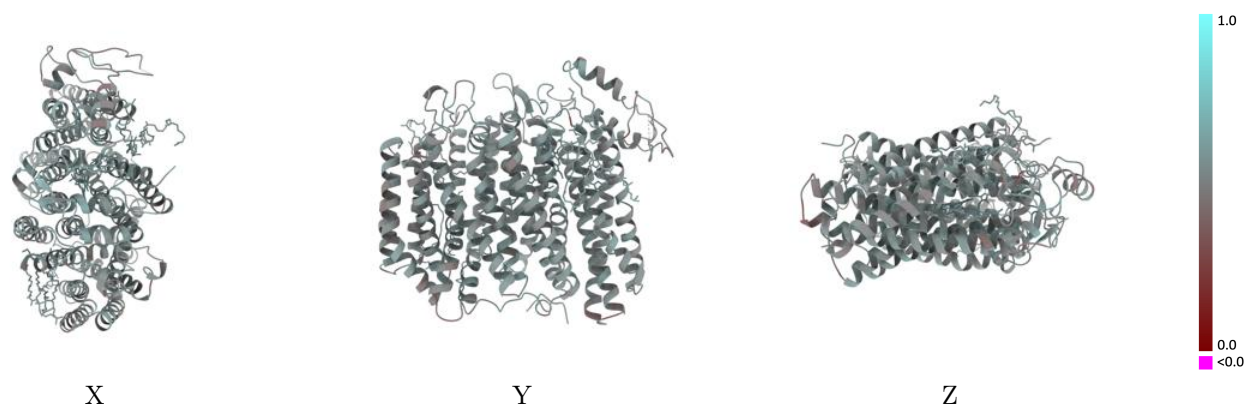
This section contains information regarding the fit between EMDB map EMD-50520 and PDB model 9FKA. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



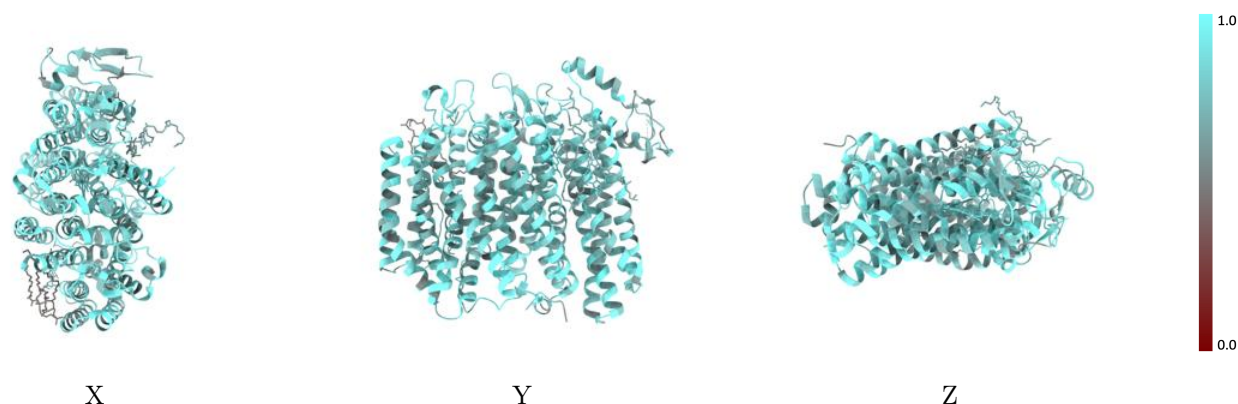
The images above show the 3D surface view of the map at the recommended contour level 0.0657 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



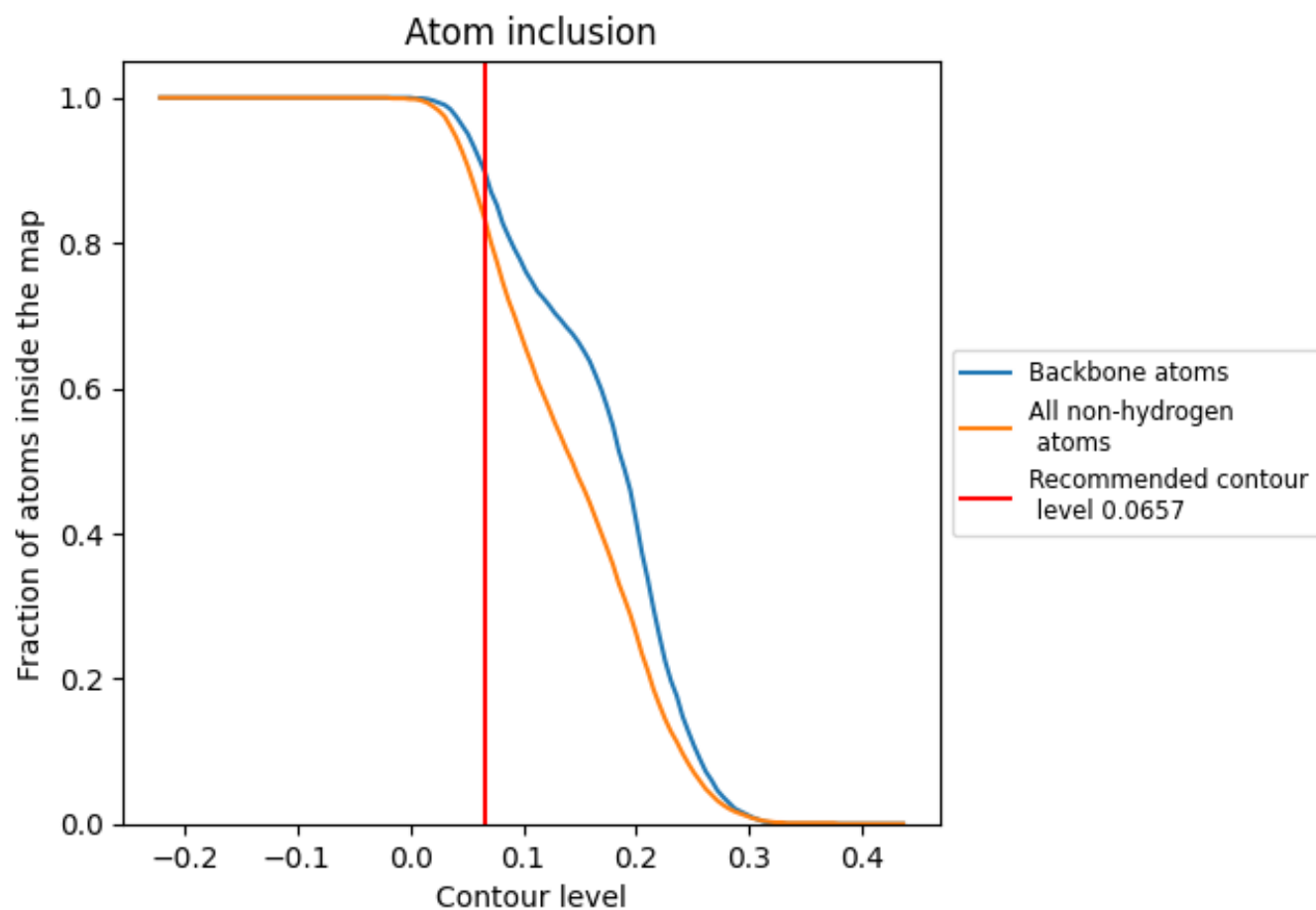
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.0657).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0657) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8340	0.5260
A	0.8400	0.5270
B	0.8270	0.5240

