



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 11:56 PM UTC

PDB ID : 9R2G / pdb_00009r2g
EMDB ID : EMD-53529
Title : Cytochrome bd II oxidase qOR-2 type from Mycobacterium smegmatis
Authors : Kovalova, T.; Janczak, M.; Adelroth, P.; Hogbom, M.
Deposited on : 2025-04-30
Resolution : 2.80 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 ⓘ 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 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) : 2.49

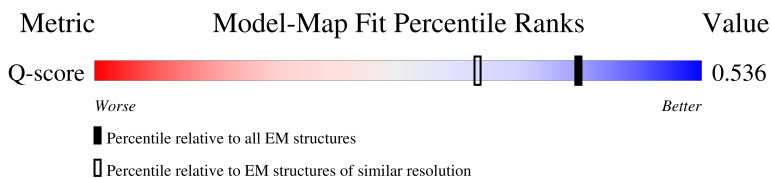
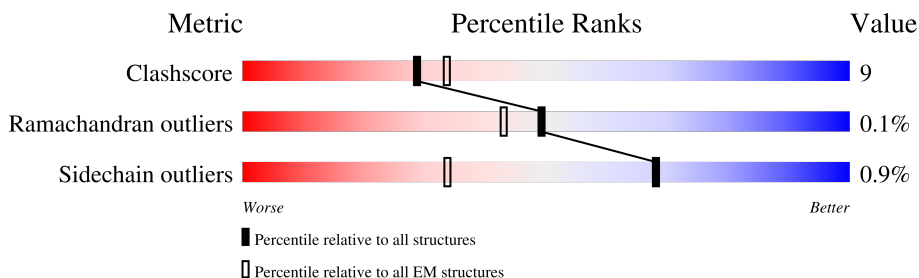
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

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	462	 68% 13% 18%
2	D	374	 73% 15% 12%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	HEB	A	503	X	-	-	-
5	HEB	A	504	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5774 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome bd menaquinol oxidase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	377	Total	C	N	O	S	1	0
			2933	1939	507	470	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	330	Total	C	N	O	S	0	0
			2451	1616	408	423	4		

There are 42 discrepancies between the modelled and reference sequences:

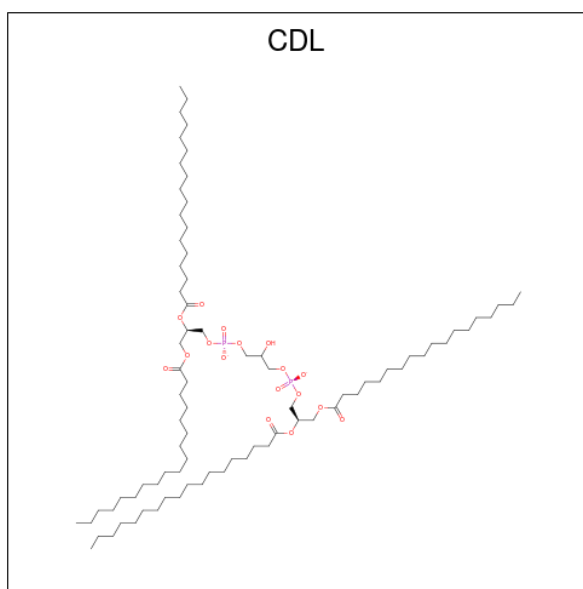
Chain	Residue	Modelled	Actual	Comment	Reference
D	333	LYS	-	expression tag	UNP A0A2U9PXA2
D	334	LEU	-	expression tag	UNP A0A2U9PXA2
D	335	SER	-	expression tag	UNP A0A2U9PXA2
D	336	GLY	-	expression tag	UNP A0A2U9PXA2
D	337	GLY	-	expression tag	UNP A0A2U9PXA2
D	338	SER	-	expression tag	UNP A0A2U9PXA2
D	339	ALA	-	expression tag	UNP A0A2U9PXA2
D	340	GLU	-	expression tag	UNP A0A2U9PXA2
D	341	ASN	-	expression tag	UNP A0A2U9PXA2
D	342	LEU	-	expression tag	UNP A0A2U9PXA2
D	343	TYR	-	expression tag	UNP A0A2U9PXA2
D	344	PHE	-	expression tag	UNP A0A2U9PXA2
D	345	GLN	-	expression tag	UNP A0A2U9PXA2
D	346	GLY	-	expression tag	UNP A0A2U9PXA2
D	347	TRP	-	expression tag	UNP A0A2U9PXA2
D	348	SER	-	expression tag	UNP A0A2U9PXA2
D	349	HIS	-	expression tag	UNP A0A2U9PXA2
D	350	PRO	-	expression tag	UNP A0A2U9PXA2
D	351	GLN	-	expression tag	UNP A0A2U9PXA2
D	352	PHE	-	expression tag	UNP A0A2U9PXA2
D	353	GLU	-	expression tag	UNP A0A2U9PXA2

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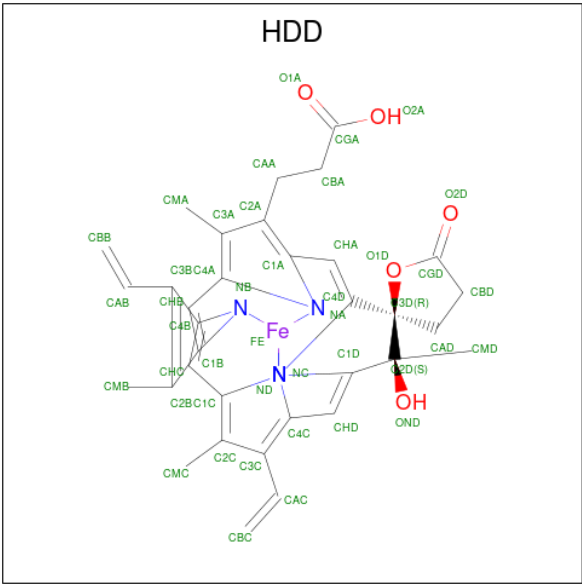
Chain	Residue	Modelled	Actual	Comment	Reference
D	354	LYS	-	expression tag	UNP A0A2U9PXA2
D	355	GLY	-	expression tag	UNP A0A2U9PXA2
D	356	GLY	-	expression tag	UNP A0A2U9PXA2
D	357	GLY	-	expression tag	UNP A0A2U9PXA2
D	358	SER	-	expression tag	UNP A0A2U9PXA2
D	359	GLY	-	expression tag	UNP A0A2U9PXA2
D	360	GLY	-	expression tag	UNP A0A2U9PXA2
D	361	GLY	-	expression tag	UNP A0A2U9PXA2
D	362	SER	-	expression tag	UNP A0A2U9PXA2
D	363	GLY	-	expression tag	UNP A0A2U9PXA2
D	364	GLY	-	expression tag	UNP A0A2U9PXA2
D	365	SER	-	expression tag	UNP A0A2U9PXA2
D	366	ALA	-	expression tag	UNP A0A2U9PXA2
D	367	TRP	-	expression tag	UNP A0A2U9PXA2
D	368	SER	-	expression tag	UNP A0A2U9PXA2
D	369	HIS	-	expression tag	UNP A0A2U9PXA2
D	370	PRO	-	expression tag	UNP A0A2U9PXA2
D	371	GLN	-	expression tag	UNP A0A2U9PXA2
D	372	PHE	-	expression tag	UNP A0A2U9PXA2
D	373	GLU	-	expression tag	UNP A0A2U9PXA2
D	374	LYS	-	expression tag	UNP A0A2U9PXA2

- Molecule 3 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



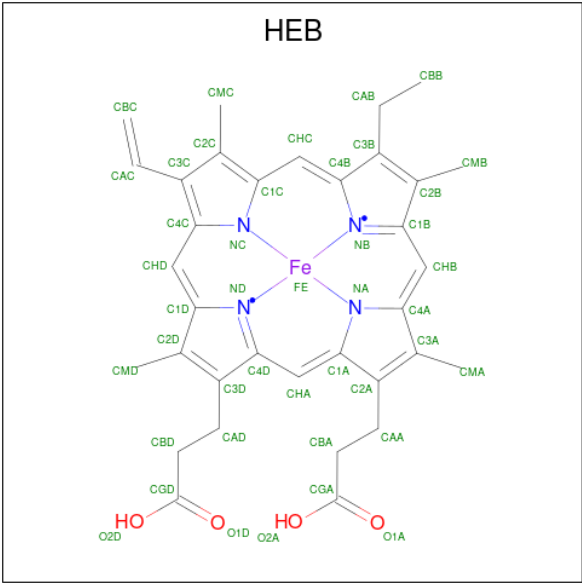
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			79	60	17	2	

- Molecule 4 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: C₃₄H₃₂FeN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is HEME B/C (CCD ID: HEB) (formula: C₃₄H₃₄FeN₄O₄).



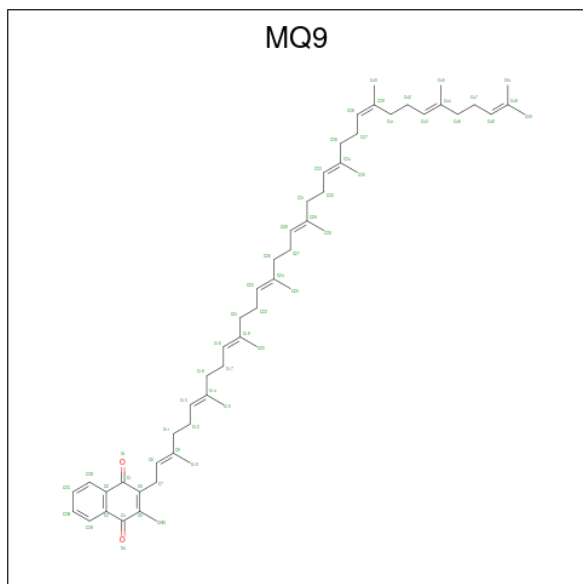
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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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 MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$).



Mol	Chain	Residues	Atoms			AltConf
6	D	1	Total	C	O	0
			58	56	2	
6	D	1	Total	C	O	0
			58	56	2	
6	D	1	Total	C	O	0
			58	56	2	

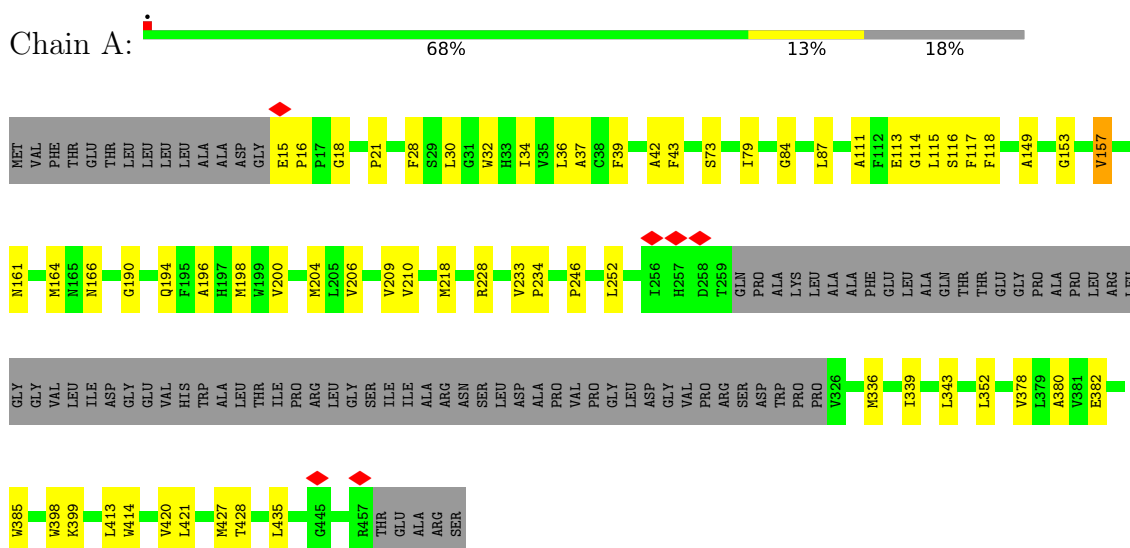
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	5	Total	O	0
			5	5	
7	D	2	Total	O	0
			2	2	

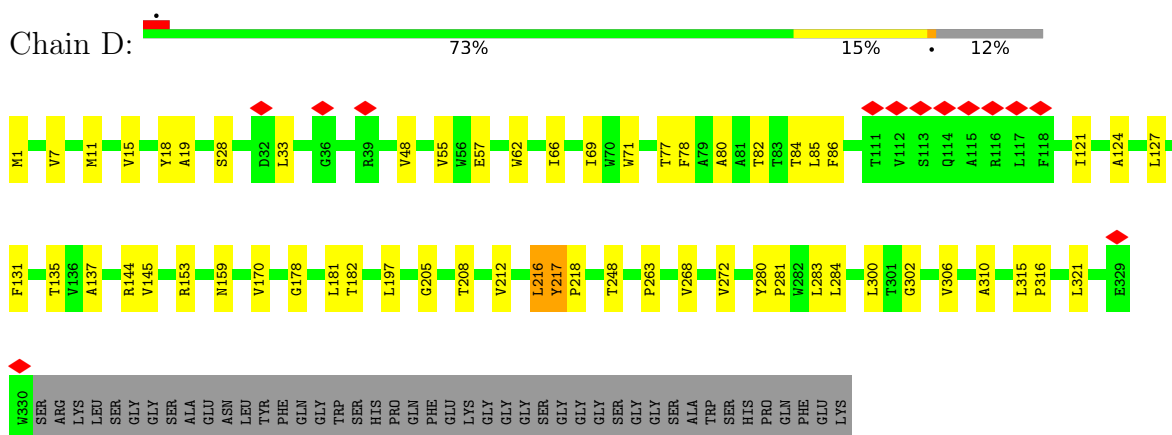
3 Residue-property plots

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

• Molecule 1: Cytochrome bd menaquinol oxidase subunit I



• Molecule 2: Cytochrome bd-I oxidase subunit II



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	200084	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 ($e^-/\text{\AA}^2$)	93.4	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.120	Depositor
Minimum map value	-0.561	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.208	Depositor
Map size (Å)	233.99998, 233.99998, 233.99998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MQ9, CDL, HDD, HEB

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	0/3027	0.31	0/4134
2	D	0.21	0/2512	0.37	0/3446
All	All	0.18	0/5539	0.34	0/7580

There are no bond length outliers.

There are no bond angle outliers.

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	2933	0	2978	57	0
2	D	2451	0	2519	44	0
3	A	79	0	105	1	0
4	A	44	0	31	10	0
5	A	86	0	64	10	0
6	D	174	0	240	19	0
7	A	5	0	0	0	0
7	D	2	0	0	0	0
All	All	5774	0	5937	110	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 9.

All (110) 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:117[A]:PHE:CZ	4:A:502:HDD:OND	2.23	0.91
2:D:217:TYR:H	2:D:218:PRO:CD	1.89	0.84
1:A:385:TRP:HB3	5:A:503:HEB:HAC	1.60	0.83
2:D:315:LEU:HD12	6:D:401:MQ9:H23	1.59	0.82
1:A:117[A]:PHE:CE2	4:A:502:HDD:OND	2.33	0.81
2:D:144:ARG:HE	2:D:159:ASN:HD22	1.30	0.80
2:D:216:LEU:HD13	2:D:216:LEU:O	1.86	0.75
1:A:117[A]:PHE:CE1	4:A:502:HDD:OND	2.49	0.66
1:A:385:TRP:CB	5:A:503:HEB:HAC	2.28	0.64
2:D:18:TYR:HB2	2:D:62:TRP:HB2	1.80	0.64
2:D:217:TYR:H	2:D:218:PRO:HD2	1.63	0.62
2:D:217:TYR:N	2:D:218:PRO:CD	2.57	0.61
2:D:55:VAL:HG21	2:D:321:LEU:HD21	1.84	0.59
2:D:310:ALA:HB1	6:D:401:MQ9:H8	1.83	0.59
2:D:216:LEU:HD23	6:D:403:MQ9:H111	1.84	0.59
2:D:217:TYR:H	2:D:218:PRO:HD3	1.65	0.58
1:A:164:MET:HE1	5:A:503:HEB:HHB	1.87	0.57
1:A:198:MET:HE1	5:A:504:HEB:HMD1	1.85	0.57
1:A:246:PRO:HA	5:A:504:HEB:HBB2	1.89	0.55
2:D:19:ALA:HA	6:D:402:MQ9:H502	1.88	0.55
1:A:114:GLY:HA2	1:A:117[B]:PHE:CZ	2.40	0.55
1:A:427:MET:HE3	1:A:427:MET:HA	1.90	0.54
2:D:217:TYR:CD1	2:D:217:TYR:C	2.85	0.53
2:D:144:ARG:NE	2:D:159:ASN:HD22	2.02	0.52
4:A:502:HDD:HHD	4:A:502:HDD:HBC1	1.91	0.52
1:A:84:GLY:HA3	4:A:502:HDD:C2A	2.39	0.52
1:A:194:GLN:HG2	1:A:252:LEU:HD11	1.91	0.52
1:A:37:ALA:HA	4:A:502:HDD:HMD2	1.92	0.51
2:D:144:ARG:HE	2:D:159:ASN:ND2	2.04	0.51
2:D:145:VAL:HG21	2:D:284:LEU:HD22	1.93	0.51
1:A:233:VAL:HB	1:A:234:PRO:HD3	1.93	0.50
1:A:339:ILE:HG21	1:A:380:ALA:HB2	1.94	0.49
2:D:127:LEU:HD12	2:D:170:VAL:HG13	1.95	0.49
1:A:113:GLU:HG2	1:A:117[A]:PHE:CE2	2.48	0.49
1:A:198:MET:HE2	1:A:198:MET:HA	1.95	0.48
2:D:212:VAL:HG11	6:D:403:MQ9:H311	1.95	0.48
2:D:178:GLY:O	2:D:182:THR:HG22	2.13	0.48
1:A:378:VAL:O	1:A:382:GLU:HG2	2.14	0.48
1:A:111:ALA:HB1	2:D:306:VAL:HG11	1.95	0.48
1:A:32:TRP:CZ3	1:A:36:LEU:HD11	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117[A]:PHE:CD2	4:A:502:HDD:OND	2.67	0.47
1:A:435:LEU:HB3	3:A:501:CDL:H721	1.96	0.47
2:D:216:LEU:CD2	6:D:403:MQ9:H111	2.43	0.47
2:D:7:VAL:HG21	2:D:300:LEU:HG	1.95	0.47
1:A:79:ILE:HG23	1:A:427:MET:HE2	1.97	0.47
1:A:113:GLU:HG3	1:A:157:VAL:HB	1.97	0.47
1:A:190:GLY:O	1:A:194:GLN:HG3	2.15	0.47
1:A:161:ASN:HB2	5:A:503:HEB:HBB3	1.97	0.47
1:A:398:TRP:CD1	1:A:399:LYS:HG3	2.49	0.46
1:A:114:GLY:HA2	1:A:117[B]:PHE:CE2	2.51	0.46
1:A:198:MET:HE1	5:A:504:HEB:CMD	2.45	0.46
1:A:385:TRP:HA	5:A:504:HEB:HAD2	1.96	0.46
6:D:402:MQ9:H103	6:D:402:MQ9:H121	1.71	0.46
6:D:402:MQ9:H422	6:D:402:MQ9:H461	1.64	0.46
4:A:502:HDD:HMD2	4:A:502:HDD:HAD2	1.59	0.46
6:D:403:MQ9:H18	6:D:403:MQ9:H222	1.52	0.46
1:A:39:PHE:HZ	1:A:209:VAL:HG11	1.81	0.46
1:A:339:ILE:O	1:A:343:LEU:HG	2.16	0.46
1:A:42:ALA:HB3	1:A:206:VAL:HG21	1.97	0.45
2:D:315:LEU:CD1	6:D:401:MQ9:H23	2.39	0.45
1:A:115:LEU:HA	6:D:401:MQ9:H71	1.97	0.45
1:A:21:PRO:HG3	1:A:414:TRP:CE2	2.52	0.45
1:A:198:MET:CE	5:A:504:HEB:HMD1	2.47	0.45
2:D:131:PHE:O	2:D:135:THR:HG23	2.17	0.45
1:A:28:PHE:C	1:A:28:PHE:CD1	2.96	0.44
1:A:30:LEU:HG	1:A:87:LEU:HD21	2.00	0.44
2:D:137:ALA:HB3	6:D:402:MQ9:H352	1.99	0.44
1:A:218:MET:HE1	1:A:228:ARG:HD3	1.99	0.44
2:D:84:THR:HG23	2:D:85:LEU:HG	1.99	0.44
1:A:30:LEU:HD13	5:A:503:HEB:NC	2.32	0.44
1:A:336:MET:HE2	1:A:336:MET:HB3	1.68	0.44
2:D:181:LEU:HB3	2:D:197:LEU:HD13	1.99	0.44
2:D:77:THR:HG21	2:D:283:LEU:HD23	2.00	0.44
2:D:86:PHE:HB3	2:D:153:ARG:HH21	1.81	0.44
2:D:268:VAL:O	2:D:272:VAL:HG23	2.18	0.44
2:D:71:TRP:C	2:D:71:TRP:CD1	2.95	0.43
6:D:401:MQ9:H272	6:D:401:MQ9:H253	1.65	0.43
1:A:117[B]:PHE:CZ	4:A:502:HDD:HBA1	2.53	0.43
2:D:248:THR:HB	2:D:263:PRO:HB2	2.01	0.43
1:A:15:GLU:HB2	1:A:16:PRO:HD3	2.00	0.43
1:A:117[A]:PHE:CZ	1:A:153:GLY:HA3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:302:GLY:O	2:D:306:VAL:HG23	2.19	0.43
1:A:18:GLY:HA3	1:A:413:LEU:HD12	2.01	0.43
1:A:34:ILE:HD13	4:A:502:HDD:HMC3	2.00	0.42
6:D:403:MQ9:H322	6:D:403:MQ9:H303	1.54	0.42
1:A:118:PHE:CE1	2:D:57:GLU:HB3	2.54	0.42
1:A:421:LEU:HD23	1:A:421:LEU:HA	1.86	0.42
2:D:205:GLY:O	2:D:208:THR:HG22	2.20	0.42
6:D:401:MQ9:H462	6:D:401:MQ9:H421	1.79	0.42
2:D:280:TYR:CD1	2:D:281:PRO:HA	2.54	0.42
2:D:33:LEU:HD22	2:D:124:ALA:HB2	2.01	0.42
6:D:401:MQ9:H403	6:D:401:MQ9:H422	1.59	0.42
1:A:204:MET:HE2	1:A:204:MET:HB3	1.98	0.42
2:D:28:SER:HB3	2:D:48:VAL:HG21	2.01	0.42
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.89	0.42
2:D:15:VAL:HA	2:D:66:ILE:HD11	2.02	0.41
1:A:32:TRP:HZ2	1:A:428:THR:HB	1.85	0.41
1:A:43:PHE:HD2	1:A:73:SER:HB2	1.86	0.41
2:D:316:PRO:HG3	6:D:401:MQ9:H33	2.01	0.41
2:D:80:ALA:O	2:D:84:THR:HG22	2.20	0.41
1:A:18:GLY:C	1:A:21:PRO:HD2	2.45	0.41
1:A:116:SER:O	1:A:149:ALA:HB1	2.21	0.41
1:A:196:ALA:O	1:A:200:VAL:HG22	2.21	0.41
6:D:402:MQ9:H272	6:D:402:MQ9:H253	1.92	0.41
2:D:1:MET:HE2	2:D:1:MET:HB2	1.83	0.40
1:A:43:PHE:HE1	1:A:210:VAL:HG21	1.87	0.40
1:A:228:ARG:HD3	1:A:228:ARG:HA	1.94	0.40
2:D:11:MET:HB2	2:D:69:ILE:HG21	2.02	0.40
2:D:78:PHE:O	2:D:82:THR:HG23	2.21	0.40
6:D:401:MQ9:H153	6:D:401:MQ9:H171	1.75	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	374/462 (81%)	369 (99%)	5 (1%)	0	100	100
2	D	328/374 (88%)	317 (97%)	10 (3%)	1 (0%)	36	66
All	All	702/836 (84%)	686 (98%)	15 (2%)	1 (0%)	49	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	217	TYR

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	298/363 (82%)	295 (99%)	3 (1%)	68	88
2	D	240/271 (89%)	238 (99%)	2 (1%)	73	90
All	All	538/634 (85%)	533 (99%)	5 (1%)	68	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	VAL
1	A	166	ASN
1	A	420	VAL
2	D	121	ILE
2	D	216	LEU

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

5.3.3 RNA ⓘ

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	MQ9	D	401	-	59,59,59	1.59	5 (8%)	73,75,75	1.67	22 (30%)
5	HEB	A	503	1	50,50,50	1.43	6 (12%)	66,82,82	1.85	19 (28%)
5	HEB	A	504	1	50,50,50	2.79	25 (50%)	66,82,82	2.21	24 (36%)
4	HDD	A	502	1	46,52,52	2.51	21 (45%)	62,89,89	2.26	23 (37%)
6	MQ9	D	402	-	59,59,59	1.59	5 (8%)	73,75,75	1.74	21 (28%)
3	CDL	A	501	-	78,78,99	1.02	7 (8%)	84,90,111	1.14	4 (4%)
6	MQ9	D	403	-	59,59,59	1.59	5 (8%)	73,75,75	1.62	20 (27%)

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	MQ9	D	401	-	-	17/53/73/73	0/2/2/2
5	HEB	A	503	1	1/1/3/8	6/14/54/54	-
5	HEB	A	504	1	1/1/3/8	6/14/54/54	-
4	HDD	A	502	1	-	5/9/89/89	0/1/9/9
6	MQ9	D	402	-	-	11/53/73/73	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CDL	A	501	-	-	42/89/89/110	-
6	MQ9	D	403	-	-	12/53/73/73	0/2/2/2

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	402	MQ9	C6-C5	7.51	1.48	1.35
6	D	403	MQ9	C6-C5	7.45	1.48	1.35
6	D	401	MQ9	C6-C5	7.39	1.48	1.35
4	A	502	HDD	O1D-CGD	5.53	1.44	1.35
4	A	502	HDD	C3B-C2B	5.07	1.47	1.37
4	A	502	HDD	CHC-C4B	5.01	1.48	1.38
5	A	503	HEB	FE-ND	5.00	2.10	1.94
5	A	504	HEB	C3B-C2B	4.99	1.47	1.36
5	A	504	HEB	C3D-C2D	4.92	1.47	1.36
5	A	504	HEB	C2A-C3A	4.83	1.47	1.36
5	A	504	HEB	CHB-C4A	4.78	1.47	1.38
5	A	504	HEB	CHC-C4B	4.72	1.47	1.38
4	A	502	HDD	CHB-C1B	4.72	1.47	1.38
5	A	504	HEB	CHA-C1A	4.66	1.47	1.38
6	D	403	MQ9	C2-C1	4.65	1.57	1.48
6	D	402	MQ9	C3-C4	4.61	1.57	1.48
6	D	402	MQ9	C2-C1	4.61	1.57	1.48
6	D	401	MQ9	C3-C4	4.60	1.57	1.48
5	A	504	HEB	CHD-C1D	4.57	1.47	1.38
6	D	403	MQ9	C3-C4	4.52	1.56	1.48
5	A	504	HEB	FE-NB	4.48	2.08	1.94
6	D	401	MQ9	C2-C1	4.43	1.56	1.48
5	A	504	HEB	FE-ND	4.37	2.08	1.94
5	A	504	HEB	FE-NC	4.18	2.09	1.95
5	A	504	HEB	FE-NA	4.17	2.08	1.95
5	A	504	HEB	CHB-C1B	3.88	1.48	1.39
4	A	502	HDD	CHB-C4A	3.84	1.48	1.39
4	A	502	HDD	CHC-C1C	3.77	1.47	1.39
4	A	502	HDD	CHD-C4C	3.77	1.47	1.39
5	A	504	HEB	CHC-C1C	3.75	1.47	1.39
4	A	502	HDD	C1A-NA	-3.74	1.32	1.39
4	A	502	HDD	C2A-C3A	3.67	1.48	1.38
4	A	502	HDD	CHA-C1A	3.66	1.47	1.39
5	A	504	HEB	CHD-C4C	3.57	1.47	1.39
5	A	503	HEB	FE-NC	3.57	2.06	1.95
5	A	503	HEB	FE-NA	3.52	2.06	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	504	HEB	C1D-ND	-3.51	1.34	1.40
5	A	504	HEB	CHA-C4D	3.47	1.47	1.39
5	A	504	HEB	C4B-NB	-3.39	1.34	1.40
4	A	502	HDD	C4C-NC	-3.27	1.33	1.39
4	A	502	HDD	C4A-NA	-3.20	1.33	1.39
5	A	503	HEB	C4B-NB	-3.02	1.35	1.40
4	A	502	HDD	O1D-C3D	-2.91	1.42	1.46
4	A	502	HDD	C1C-NC	-2.86	1.34	1.39
5	A	504	HEB	C1A-NA	-2.82	1.34	1.39
4	A	502	HDD	C1B-NB	-2.78	1.34	1.39
4	A	502	HDD	C4B-NB	-2.78	1.34	1.39
3	A	501	CDL	OA6-CA4	-2.78	1.40	1.46
4	A	502	HDD	C1D-ND	-2.70	1.33	1.37
5	A	504	HEB	C4C-NC	-2.70	1.34	1.39
3	A	501	CDL	OB8-CB7	2.65	1.41	1.33
5	A	504	HEB	C4A-NA	-2.64	1.34	1.39
3	A	501	CDL	OB6-CB5	2.58	1.41	1.34
5	A	504	HEB	C4D-ND	-2.55	1.33	1.38
5	A	504	HEB	C1C-NC	-2.46	1.35	1.39
5	A	504	HEB	C1C-C2C	2.45	1.48	1.43
4	A	502	HDD	C1C-C2C	2.43	1.48	1.43
6	D	401	MQ9	O1-C1	-2.42	1.18	1.23
3	A	501	CDL	OA8-CA7	2.40	1.40	1.33
6	D	403	MQ9	O4-C4	-2.34	1.18	1.23
6	D	403	MQ9	O1-C1	-2.33	1.18	1.23
3	A	501	CDL	OB6-CB4	-2.33	1.41	1.46
5	A	503	HEB	C1C-NC	-2.30	1.35	1.39
5	A	504	HEB	C1B-NB	-2.26	1.34	1.38
6	D	402	MQ9	O1-C1	-2.24	1.18	1.23
4	A	502	HDD	C4A-C3A	2.22	1.48	1.43
4	A	502	HDD	C4D-ND	-2.22	1.33	1.37
5	A	503	HEB	C1A-NA	-2.21	1.35	1.39
6	D	401	MQ9	O4-C4	-2.20	1.18	1.23
3	A	501	CDL	OA8-CA6	-2.19	1.40	1.45
6	D	402	MQ9	O4-C4	-2.13	1.18	1.23
3	A	501	CDL	OA6-CA5	2.09	1.40	1.34
5	A	504	HEB	C4B-C3B	2.02	1.48	1.45
4	A	502	HDD	C3D-C2D	-2.01	1.50	1.55

All (133) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	HDD	C3B-C2B-C1B	-6.95	100.47	107.05
4	A	502	HDD	CHB-C1B-NB	-5.66	118.30	124.45
5	A	504	HEB	C3C-C2C-C1C	-5.06	101.21	107.17
4	A	502	HDD	C3C-C2C-C1C	-4.92	101.37	107.17
5	A	504	HEB	C2A-C1A-NA	4.81	114.97	110.32
5	A	503	HEB	C4B-NB-C1B	4.47	110.50	105.21
5	A	504	HEB	C3D-C4D-ND	4.40	114.60	110.35
5	A	504	HEB	C3C-C4C-NC	4.23	113.36	109.80
5	A	503	HEB	C3C-C4C-NC	-4.18	106.28	109.80
5	A	504	HEB	C2D-C1D-ND	4.15	114.61	109.84
3	A	501	CDL	OB6-CB5-C51	4.09	120.32	111.48
5	A	504	HEB	C3B-C4B-NB	4.09	114.65	110.17
5	A	504	HEB	C2B-C1B-NB	4.08	114.61	109.90
6	D	402	MQ9	C7-C8-C9	-4.02	119.91	126.83
5	A	504	HEB	C1D-C2D-C3D	-4.00	102.78	106.98
5	A	503	HEB	CHA-C1A-NA	3.94	128.74	124.45
5	A	503	HEB	C1D-ND-C4D	3.94	109.87	105.21
5	A	504	HEB	C1B-C2B-C3B	-3.88	102.89	106.98
4	A	502	HDD	C4A-C3A-C2A	-3.87	102.39	106.82
3	A	501	CDL	OA6-CA5-C11	3.83	119.77	111.48
5	A	503	HEB	CHA-C4D-ND	3.82	128.53	124.42
4	A	502	HDD	CBD-CAD-C3D	3.78	109.37	103.98
5	A	503	HEB	CHC-C4B-NB	3.62	128.85	124.37
6	D	402	MQ9	C37-C38-C39	-3.48	119.67	127.62
6	D	402	MQ9	C12-C13-C14	-3.44	119.76	127.62
4	A	502	HDD	C3C-C4C-NC	3.38	112.64	109.80
5	A	503	HEB	CHB-C1B-NB	3.37	128.04	124.42
6	D	402	MQ9	C42-C43-C44	-3.33	119.99	127.62
6	D	401	MQ9	C7-C6-C5	-3.31	119.21	124.89
5	A	503	HEB	CHD-C1D-ND	3.31	128.46	124.37
4	A	502	HDD	C2A-C1A-NA	3.30	113.81	110.15
6	D	402	MQ9	C27-C28-C29	-3.28	120.11	127.62
6	D	403	MQ9	C37-C38-C39	-3.27	120.13	127.62
6	D	402	MQ9	C22-C23-C24	-3.25	120.19	127.62
4	A	502	HDD	O1D-CGD-CBD	3.24	113.13	110.17
6	D	403	MQ9	C17-C18-C19	-3.24	120.20	127.62
6	D	403	MQ9	C32-C33-C34	-3.20	120.29	127.62
6	D	403	MQ9	C7-C8-C9	-3.20	121.32	126.83
4	A	502	HDD	CHA-C1A-NA	-3.18	118.10	123.86
5	A	504	HEB	C1A-C2A-C3A	-3.17	102.93	107.11
6	D	403	MQ9	C27-C28-C29	-3.16	120.39	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	401	MQ9	C27-C28-C29	-3.10	120.52	127.62
6	D	402	MQ9	C7-C6-C5	-3.09	119.59	124.89
6	D	401	MQ9	C32-C33-C34	-3.09	120.55	127.62
5	A	504	HEB	C2C-C1C-NC	3.08	115.07	110.14
6	D	401	MQ9	C12-C13-C14	-3.07	120.61	127.62
4	A	502	HDD	CHD-C4C-NC	-3.01	118.40	123.86
4	A	502	HDD	C2B-C1B-NB	3.00	115.19	109.64
6	D	401	MQ9	C22-C23-C24	-3.00	120.76	127.62
4	A	502	HDD	CHB-C4A-NA	-2.97	118.47	123.86
6	D	401	MQ9	C15-C14-C16	2.95	120.35	115.23
6	D	402	MQ9	C32-C33-C34	-2.95	120.88	127.62
6	D	401	MQ9	C37-C38-C39	-2.94	120.89	127.62
6	D	401	MQ9	C40-C39-C41	2.91	120.29	115.23
5	A	504	HEB	C4A-C3A-C2A	-2.90	102.67	106.97
5	A	503	HEB	C4A-NA-C1A	2.88	110.51	105.82
6	D	401	MQ9	C7-C8-C9	-2.87	121.88	126.83
5	A	504	HEB	CAB-C3B-C4B	2.87	128.52	124.79
6	D	402	MQ9	C45-C44-C46	2.86	120.20	115.23
5	A	504	HEB	C4B-C3B-C2B	-2.86	102.72	106.89
6	D	401	MQ9	C25-C24-C26	2.86	120.19	115.23
6	D	403	MQ9	C12-C13-C14	-2.84	121.13	127.62
6	D	403	MQ9	C42-C43-C44	-2.83	121.14	127.62
3	A	501	CDL	OB8-CB7-C71	2.83	120.47	111.83
6	D	402	MQ9	C25-C24-C26	2.83	120.13	115.23
6	D	402	MQ9	C10-C9-C11	2.83	120.13	115.23
6	D	403	MQ9	C30-C29-C31	2.82	120.12	115.23
6	D	401	MQ9	C10-C9-C11	2.80	120.09	115.23
6	D	402	MQ9	C40-C39-C41	2.80	120.09	115.23
6	D	402	MQ9	C17-C18-C19	-2.79	121.24	127.62
5	A	504	HEB	C4D-C3D-C2D	-2.78	102.85	106.89
5	A	504	HEB	C3A-C4A-NA	2.76	114.75	109.64
5	A	503	HEB	CHB-C4A-NA	2.75	127.45	124.45
6	D	401	MQ9	C17-C18-C19	-2.75	121.34	127.62
6	D	403	MQ9	C10-C9-C11	2.72	119.95	115.23
6	D	403	MQ9	C7-C6-C5	-2.72	120.23	124.89
6	D	403	MQ9	C15-C14-C16	2.72	119.94	115.23
6	D	401	MQ9	C42-C43-C44	-2.71	121.42	127.62
6	D	401	MQ9	C20-C19-C21	2.71	119.93	115.23
6	D	402	MQ9	C20-C19-C21	2.69	119.90	115.23
4	A	502	HDD	CMB-C2B-C1B	2.69	129.46	124.73
6	D	401	MQ9	C5M-C5-C6	-2.66	120.08	124.45
5	A	504	HEB	CMC-C2C-C1C	2.66	129.47	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	HEB	CHB-C4A-NA	-2.65	121.56	124.45
4	A	502	HDD	C3D-O1D-CGD	-2.65	108.67	111.14
6	D	401	MQ9	C7-C6-C1	2.65	121.37	118.58
6	D	402	MQ9	C30-C29-C31	2.64	119.81	115.23
5	A	503	HEB	CHC-C1C-NC	2.63	128.63	123.86
4	A	502	HDD	C2C-C1C-NC	2.62	114.35	110.14
5	A	503	HEB	C2A-C1A-NA	-2.59	107.82	110.32
6	D	403	MQ9	C40-C39-C41	2.59	119.72	115.23
6	D	402	MQ9	C5M-C5-C6	-2.58	120.21	124.45
6	D	402	MQ9	C15-C14-C16	2.58	119.70	115.23
4	A	502	HDD	CHA-C4D-ND	2.57	127.83	124.28
3	A	501	CDL	OA8-CA7-C31	2.57	119.67	111.83
6	D	401	MQ9	C30-C29-C31	2.56	119.67	115.23
6	D	402	MQ9	C35-C34-C36	2.56	119.67	115.23
6	D	403	MQ9	C35-C34-C36	2.56	119.66	115.23
4	A	502	HDD	C1A-C2A-C3A	-2.52	102.97	106.87
6	D	401	MQ9	C35-C34-C36	2.51	119.59	115.23
6	D	403	MQ9	C20-C19-C21	2.51	119.58	115.23
6	D	403	MQ9	C25-C24-C26	2.50	119.56	115.23
4	A	502	HDD	O1D-CGD-O2D	2.48	122.90	120.81
6	D	402	MQ9	C47-C48-C49	-2.44	119.52	127.64
6	D	401	MQ9	C45-C44-C46	2.44	119.45	115.23
5	A	503	HEB	C4C-NC-C1C	2.40	109.74	105.82
5	A	503	HEB	C2B-C1B-NB	-2.40	107.13	109.90
5	A	504	HEB	CAA-CBA-CGA	-2.40	107.31	113.67
4	A	502	HDD	C3A-C4A-NA	2.39	113.98	110.14
4	A	502	HDD	CMC-C2C-C1C	2.39	129.06	125.42
5	A	504	HEB	CMA-C3A-C4A	2.39	128.93	124.73
6	D	403	MQ9	C22-C23-C24	-2.39	122.16	127.62
4	A	502	HDD	CAD-CBD-CGD	-2.36	100.98	104.48
5	A	503	HEB	O1D-CGD-CBD	-2.36	115.62	123.09
6	D	403	MQ9	C45-C44-C46	2.34	119.29	115.23
5	A	503	HEB	C3D-C4D-ND	-2.33	108.11	110.35
5	A	503	HEB	CHD-C4C-NC	2.32	128.07	123.86
6	D	403	MQ9	C51-C49-C50	2.30	119.88	114.59
6	D	403	MQ9	C5M-C5-C6	-2.28	120.70	124.45
5	A	503	HEB	C2D-C1D-ND	-2.25	107.25	109.84
4	A	502	HDD	CAA-CBA-CGA	-2.25	107.70	113.67
4	A	502	HDD	O1D-C3D-CAD	2.18	107.10	103.06
5	A	504	HEB	CBD-CAD-C3D	-2.18	106.50	112.53
6	D	401	MQ9	C51-C49-C50	2.18	119.61	114.59
6	D	402	MQ9	C51-C49-C50	2.18	119.60	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	402	MQ9	C7-C6-C1	2.15	120.84	118.58
5	A	504	HEB	CHC-C4B-NB	-2.08	121.80	124.37
6	D	401	MQ9	C47-C48-C49	-2.05	120.80	127.64
6	D	403	MQ9	C47-C48-C49	-2.05	120.82	127.64
5	A	503	HEB	C4C-CHD-C1D	-2.03	121.47	126.25
5	A	504	HEB	CHB-C1B-NB	-2.02	122.25	124.42
5	A	504	HEB	CHA-C1A-NA	-2.02	122.25	124.45
6	D	401	MQ9	O1-C1-C2	-2.01	118.36	121.57

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	503	HEB	NA
5	A	504	HEB	NA

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	CDL	CA2-OA2-PA1-OA3
3	A	501	CDL	CA2-OA2-PA1-OA4
3	A	501	CDL	CA2-OA2-PA1-OA5
3	A	501	CDL	CB2-OB2-PB2-OB3
3	A	501	CDL	CB2-OB2-PB2-OB5
3	A	501	CDL	CB3-OB5-PB2-OB3
3	A	501	CDL	OB9-CB7-OB8-CB6
6	D	401	MQ9	C24-C26-C27-C28
6	D	403	MQ9	C44-C46-C47-C48
3	A	501	CDL	OA9-CA7-OA8-CA6
3	A	501	CDL	OB7-CB5-OB6-CB4
3	A	501	CDL	C71-CB7-OB8-CB6
3	A	501	CDL	C51-CB5-OB6-CB4
6	D	401	MQ9	C15-C14-C16-C17
6	D	401	MQ9	C25-C24-C26-C27
6	D	401	MQ9	C40-C39-C41-C42
6	D	402	MQ9	C12-C11-C9-C10
6	D	402	MQ9	C25-C24-C26-C27
6	D	401	MQ9	C13-C14-C16-C17
6	D	401	MQ9	C23-C24-C26-C27
6	D	402	MQ9	C12-C11-C9-C8
6	D	402	MQ9	C23-C24-C26-C27
3	A	501	CDL	C31-CA7-OA8-CA6
6	D	403	MQ9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
6	D	403	MQ9	C30-C29-C31-C32
6	D	403	MQ9	C13-C14-C16-C17
6	D	403	MQ9	C28-C29-C31-C32
6	D	401	MQ9	C9-C11-C12-C13
6	D	401	MQ9	C19-C21-C22-C23
6	D	401	MQ9	C29-C31-C32-C33
6	D	401	MQ9	C39-C41-C42-C43
6	D	402	MQ9	C19-C21-C22-C23
6	D	402	MQ9	C29-C31-C32-C33
3	A	501	CDL	CB2-C1-CA2-OA2
6	D	401	MQ9	C38-C39-C41-C42
6	D	401	MQ9	C14-C16-C17-C18
6	D	401	MQ9	C44-C46-C47-C48
6	D	403	MQ9	C14-C16-C17-C18
6	D	403	MQ9	C19-C21-C22-C23
6	D	403	MQ9	C29-C31-C32-C33
3	A	501	CDL	CB5-C51-C52-C53
5	A	503	HEB	C3D-CAD-CBD-CGD
3	A	501	CDL	O1-C1-CA2-OA2
5	A	503	HEB	C2A-CAA-CBA-CGA
3	A	501	CDL	C76-C77-C78-C79
5	A	504	HEB	C4C-C3C-CAC-CBC
3	A	501	CDL	C72-C73-C74-C75
3	A	501	CDL	C80-C81-C82-C83
3	A	501	CDL	C79-C80-C81-C82
3	A	501	CDL	C11-C12-C13-C14
3	A	501	CDL	C78-C79-C80-C81
3	A	501	CDL	C11-CA5-OA6-CA4
4	A	502	HDD	C2A-CAA-CBA-CGA
3	A	501	CDL	C75-C76-C77-C78
3	A	501	CDL	OA7-CA5-OA6-CA4
3	A	501	CDL	OA5-CA3-CA4-OA6
3	A	501	CDL	C73-C74-C75-C76
6	D	403	MQ9	C43-C44-C46-C47
3	A	501	CDL	CA7-C31-C32-C33
6	D	403	MQ9	C45-C44-C46-C47
3	A	501	CDL	C12-C13-C14-C15
3	A	501	CDL	C53-C54-C55-C56
6	D	403	MQ9	C12-C11-C9-C10
5	A	503	HEB	C4C-C3C-CAC-CBC
3	A	501	CDL	OA5-CA3-CA4-CA6
6	D	403	MQ9	C12-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
3	A	501	CDL	C71-C72-C73-C74
5	A	503	HEB	C2C-C3C-CAC-CBC
3	A	501	CDL	C51-C52-C53-C54
3	A	501	CDL	C17-C18-C19-C20
3	A	501	CDL	C55-C56-C57-C58
3	A	501	CDL	CB6-CB4-OB6-CB5
6	D	401	MQ9	C1-C6-C7-C8
3	A	501	CDL	C14-C15-C16-C17
6	D	402	MQ9	C30-C29-C31-C32
6	D	401	MQ9	C34-C36-C37-C38
4	A	502	HDD	C3A-C2A-CAA-CBA
3	A	501	CDL	CB2-OB2-PB2-OB4
5	A	504	HEB	C2C-C3C-CAC-CBC
6	D	402	MQ9	C28-C29-C31-C32
4	A	502	HDD	C4B-C3B-CAB-CBB
5	A	504	HEB	C2B-C3B-CAB-CBB
4	A	502	HDD	C1A-C2A-CAA-CBA
5	A	503	HEB	CAD-CBD-CGD-O1D
6	D	402	MQ9	C40-C39-C41-C42
6	D	402	MQ9	C38-C39-C41-C42
6	D	401	MQ9	C12-C11-C9-C10
5	A	503	HEB	CAD-CBD-CGD-O2D
5	A	504	HEB	C2D-C3D-CAD-CBD
4	A	502	HDD	C2B-C3B-CAB-CBB
3	A	501	CDL	C72-C71-CB7-OB8
3	A	501	CDL	C12-C11-CA5-OA6
3	A	501	CDL	CA3-CA4-CA6-OA8
5	A	504	HEB	CAA-CBA-CGA-O2A
5	A	504	HEB	CAA-CBA-CGA-O1A
3	A	501	CDL	C12-C11-CA5-OA7
3	A	501	CDL	C72-C71-CB7-OB9
6	D	401	MQ9	C5-C6-C7-C8
6	D	402	MQ9	C16-C17-C18-C19

There are no ring outliers.

7 monomers are involved in 40 short contacts:

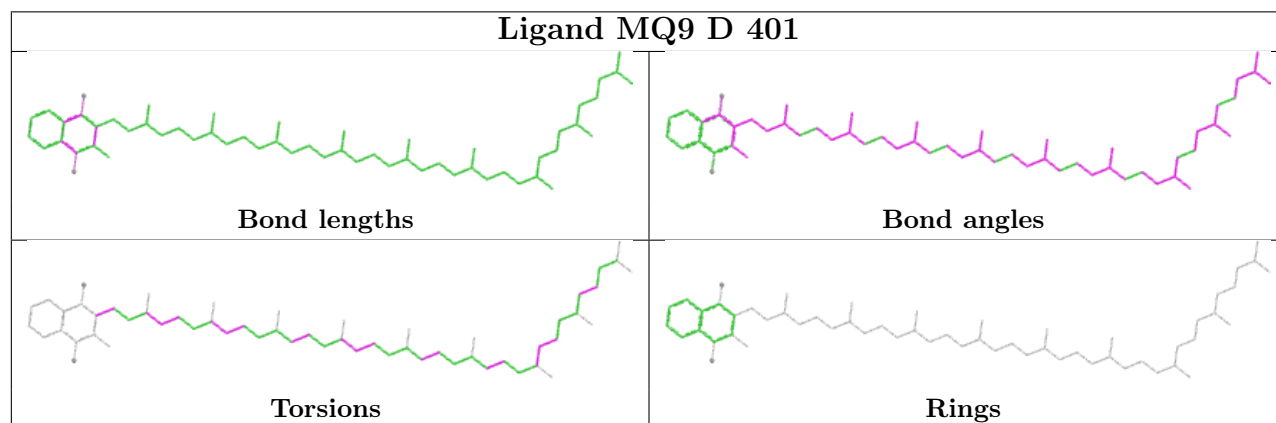
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	401	MQ9	9	0
5	A	503	HEB	5	0
5	A	504	HEB	5	0
4	A	502	HDD	10	0

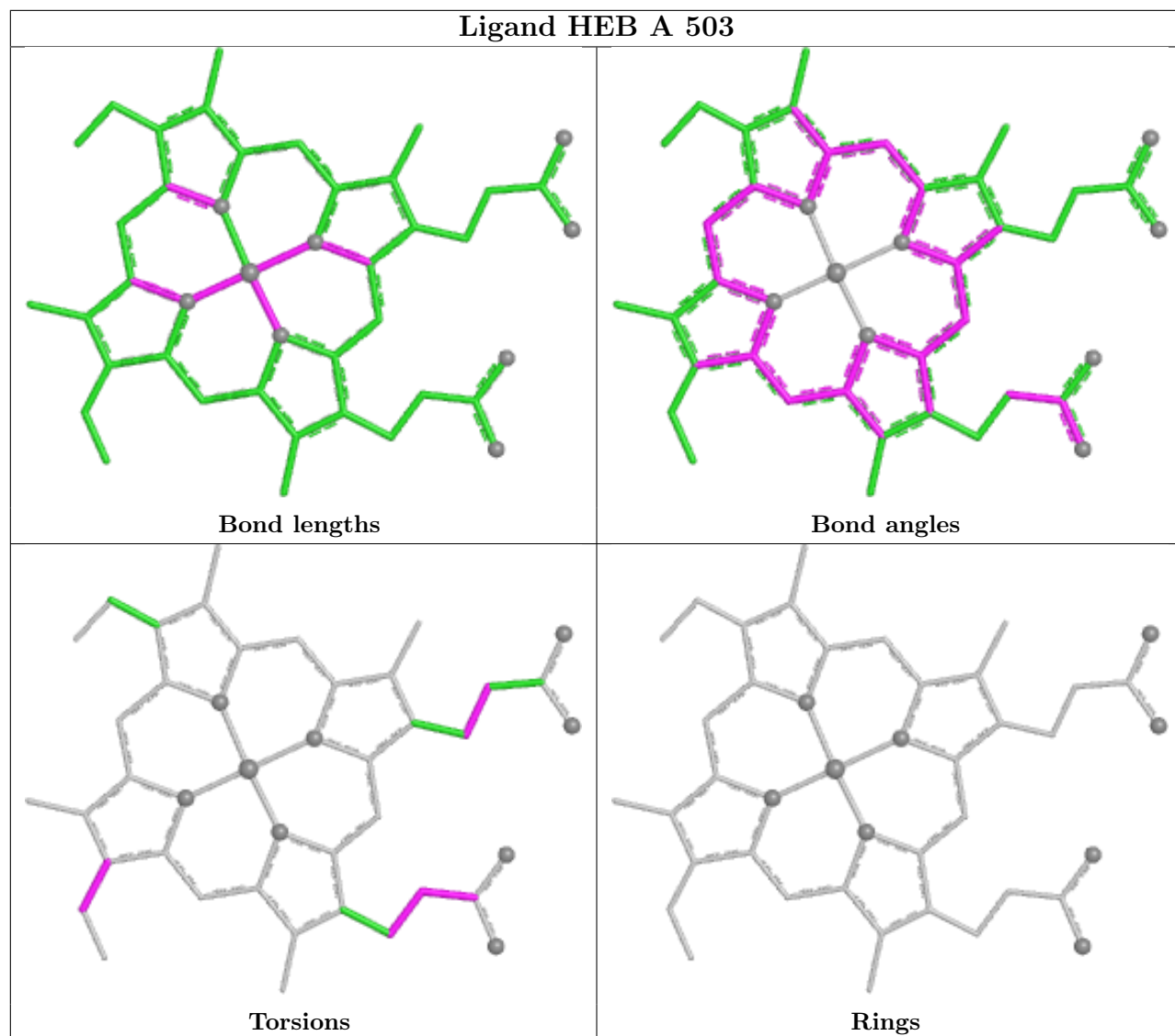
Continued on next page...

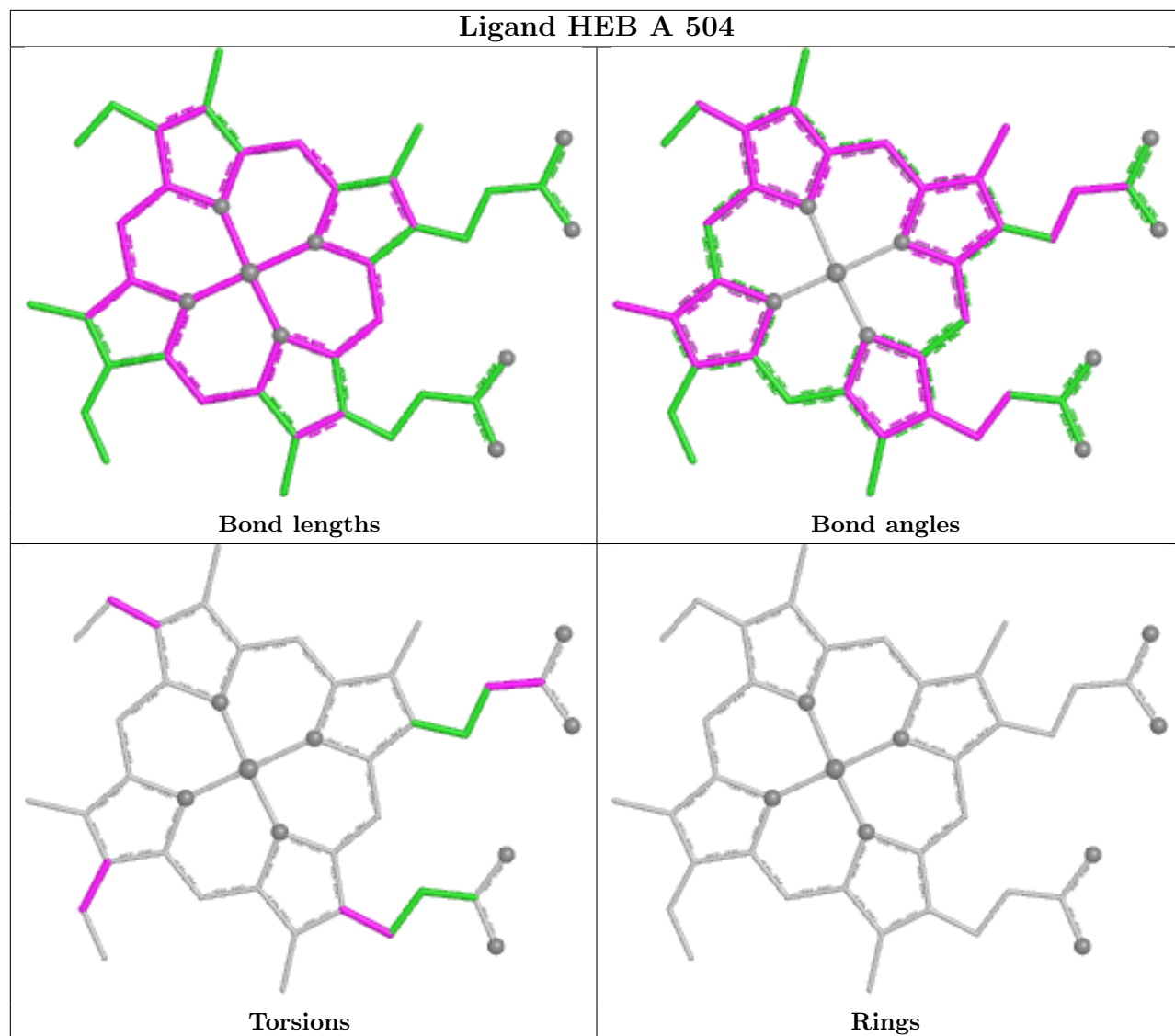
Continued from previous page...

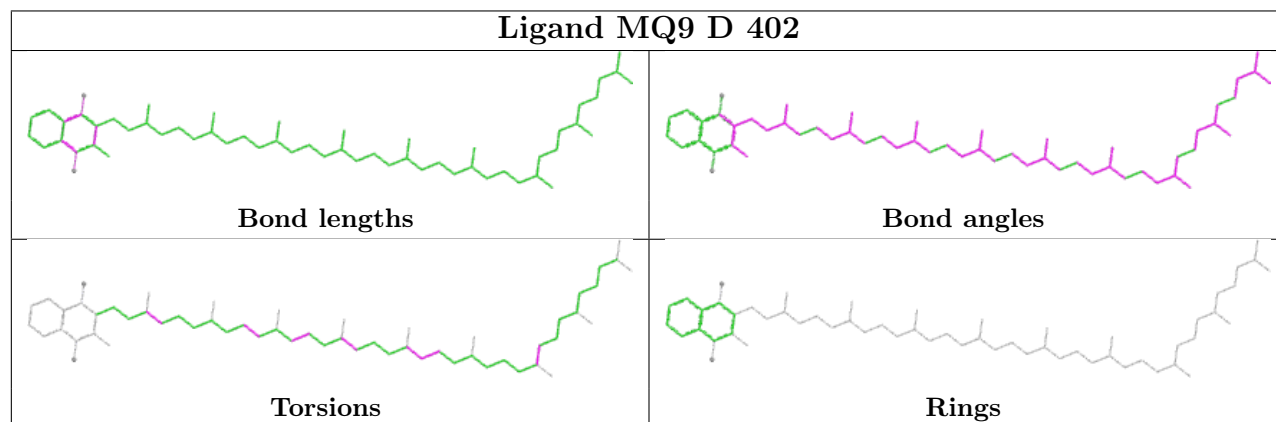
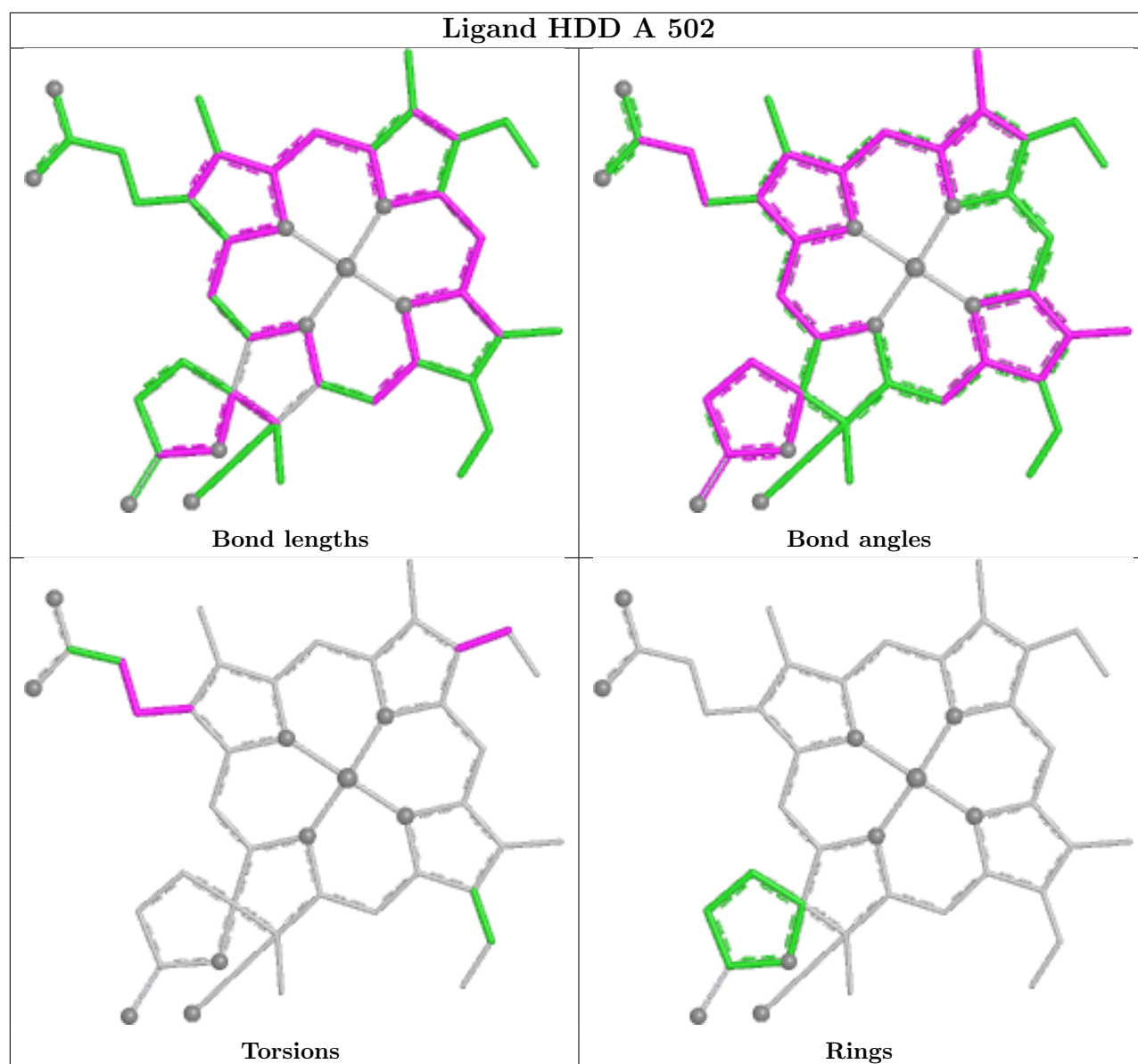
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	402	MQ9	5	0
3	A	501	CDL	1	0
6	D	403	MQ9	5	0

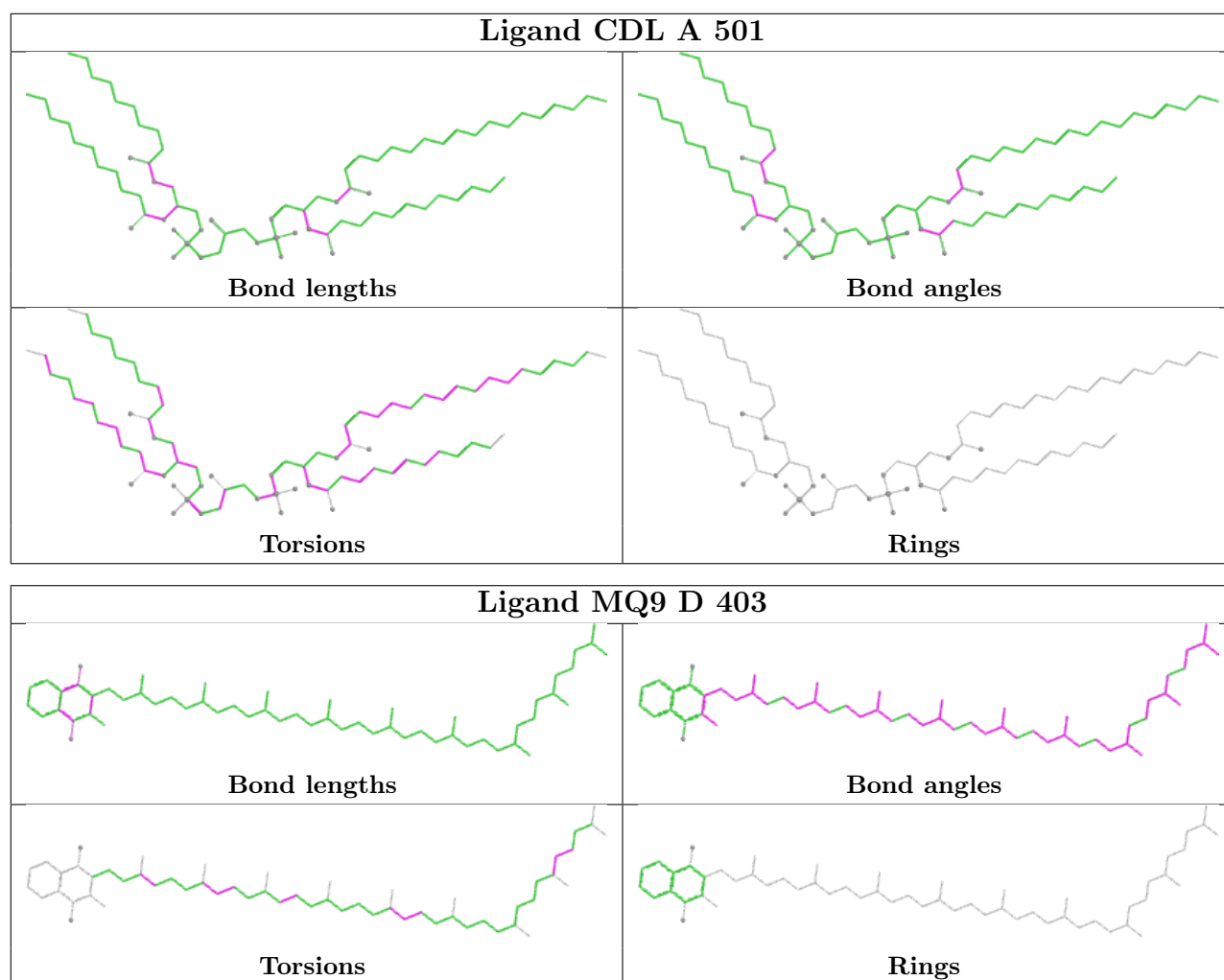
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

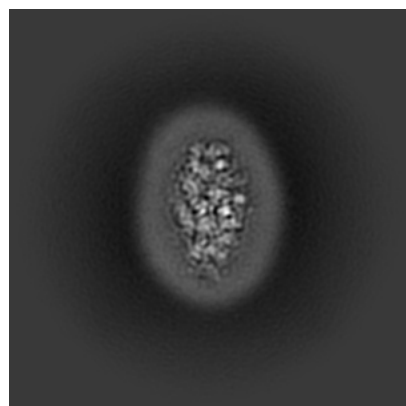
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53529. These allow visual inspection of the internal detail of the map and identification of artifacts.

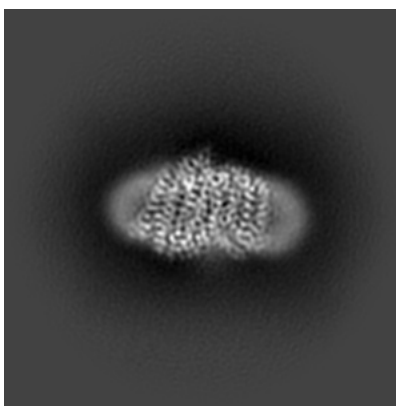
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

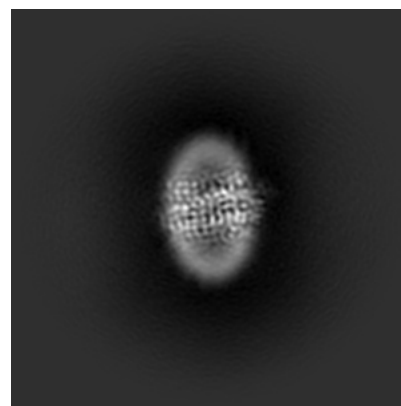
6.1.1 Primary map



X

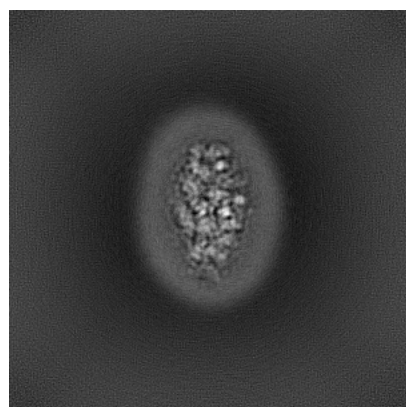


Y

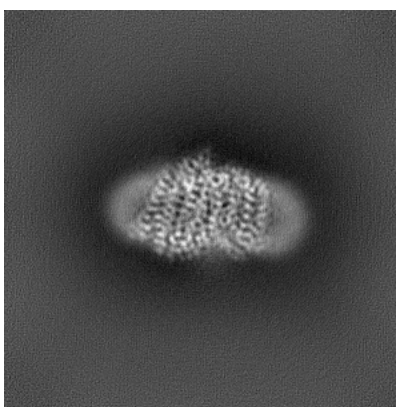


Z

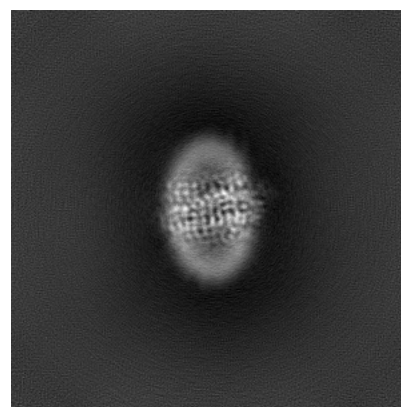
6.1.2 Raw map



X



Y

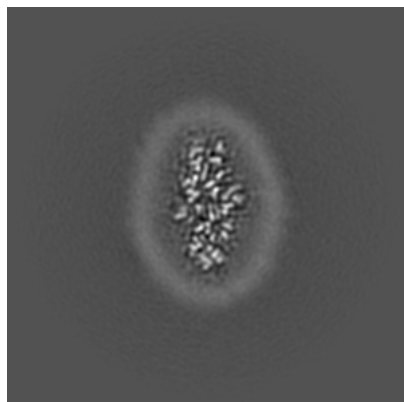


Z

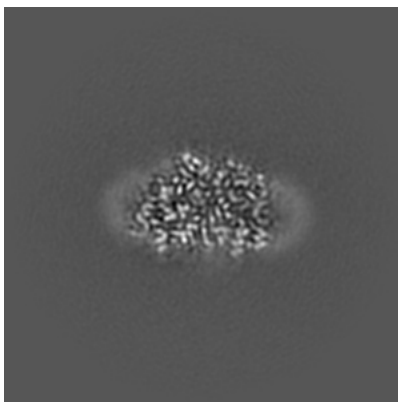
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

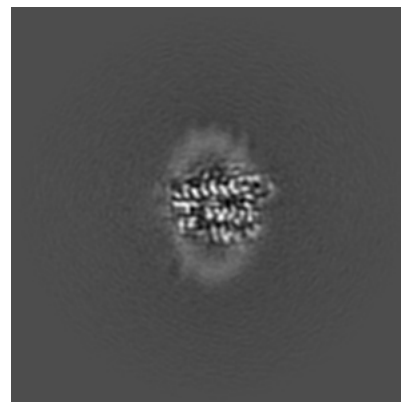
6.2.1 Primary map



X Index: 180

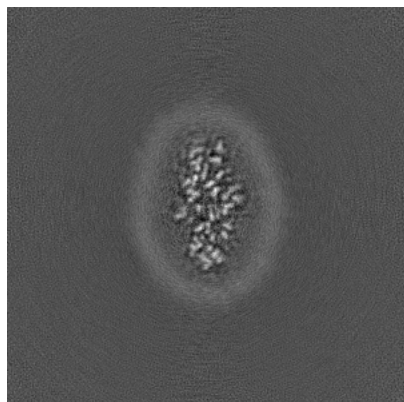


Y Index: 180

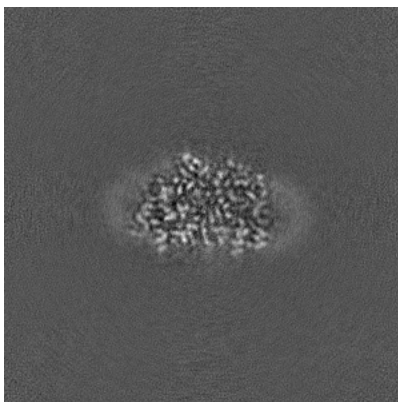


Z Index: 180

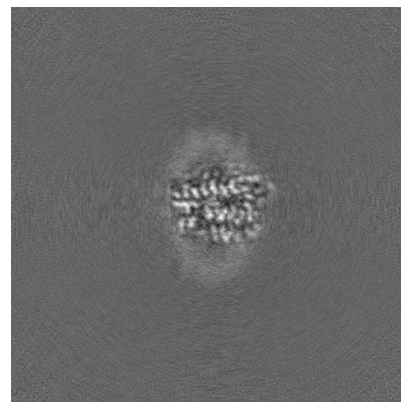
6.2.2 Raw map



X Index: 180



Y Index: 180

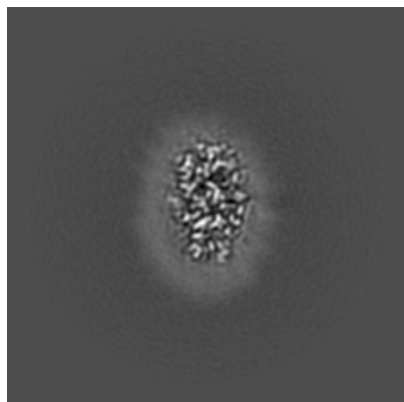


Z Index: 180

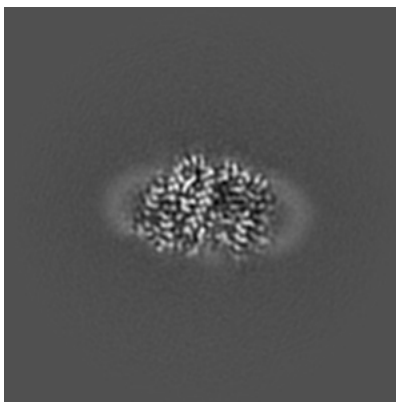
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

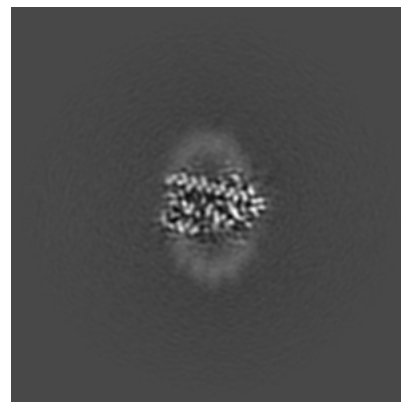
6.3.1 Primary map



X Index: 201

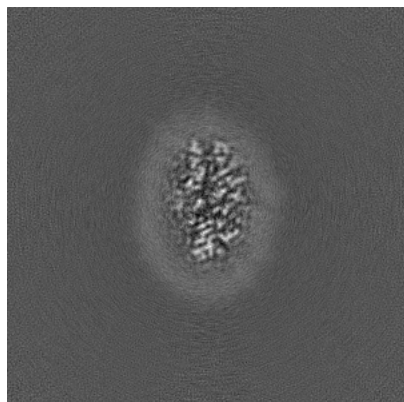


Y Index: 175

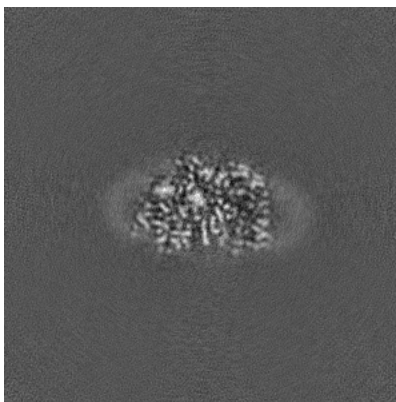


Z Index: 165

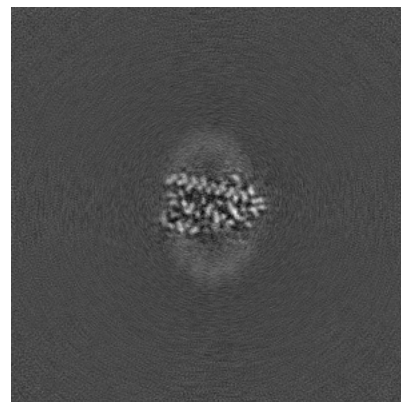
6.3.2 Raw map



X Index: 196



Y Index: 182

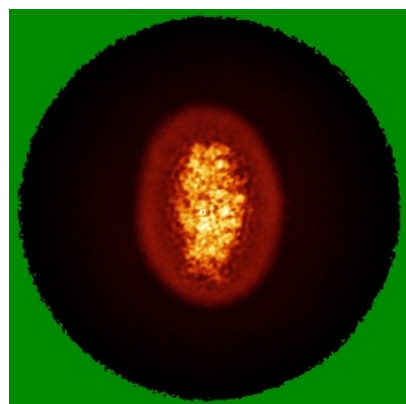


Z Index: 165

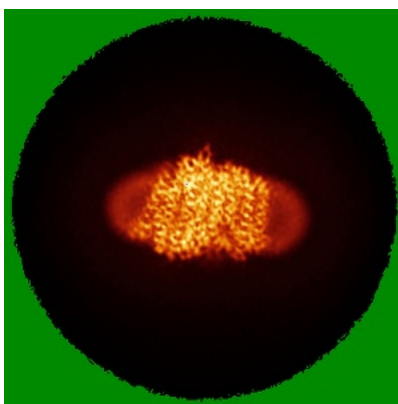
The images above show the largest variance slices of the map in three orthogonal directions.

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

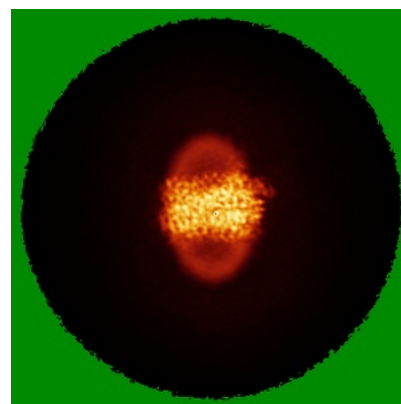
6.4.1 Primary map



X

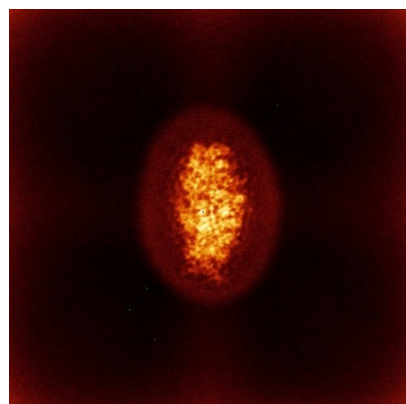


Y

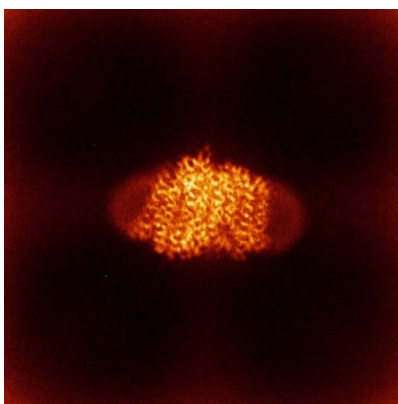


Z

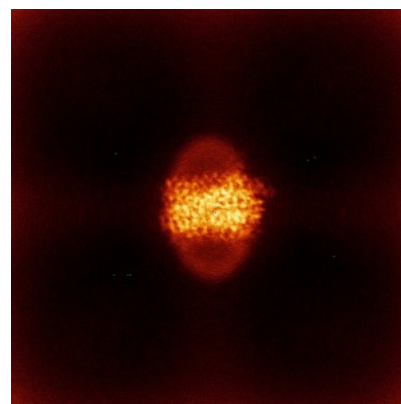
6.4.2 Raw map



X



Y

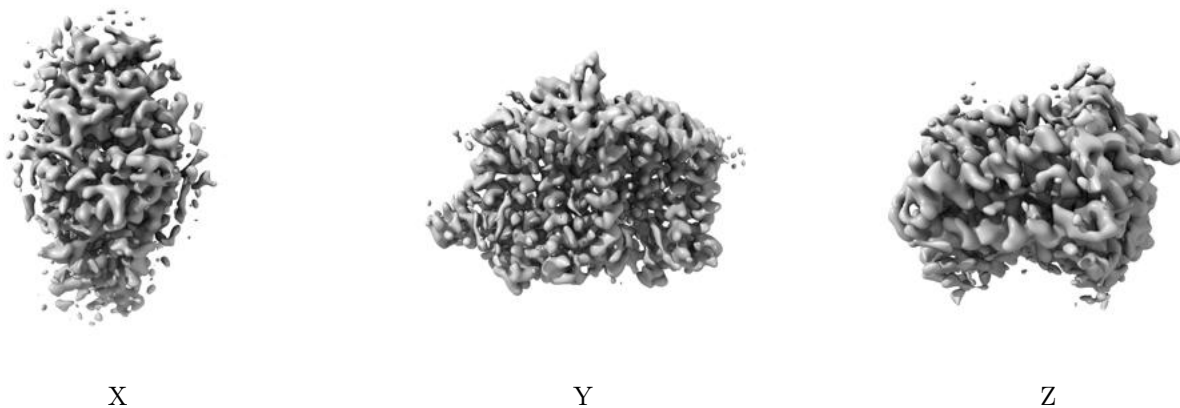


Z

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.

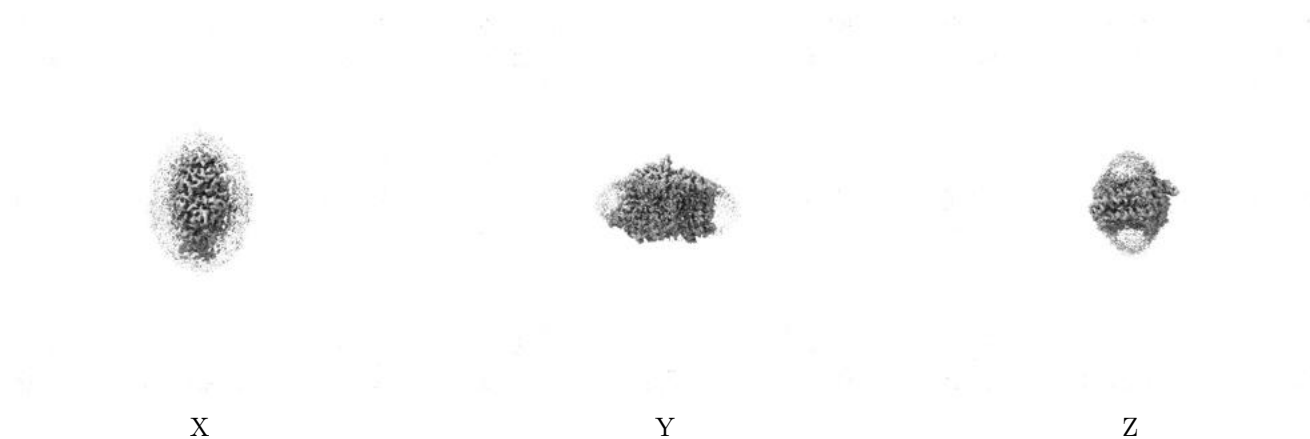
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.208. 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.

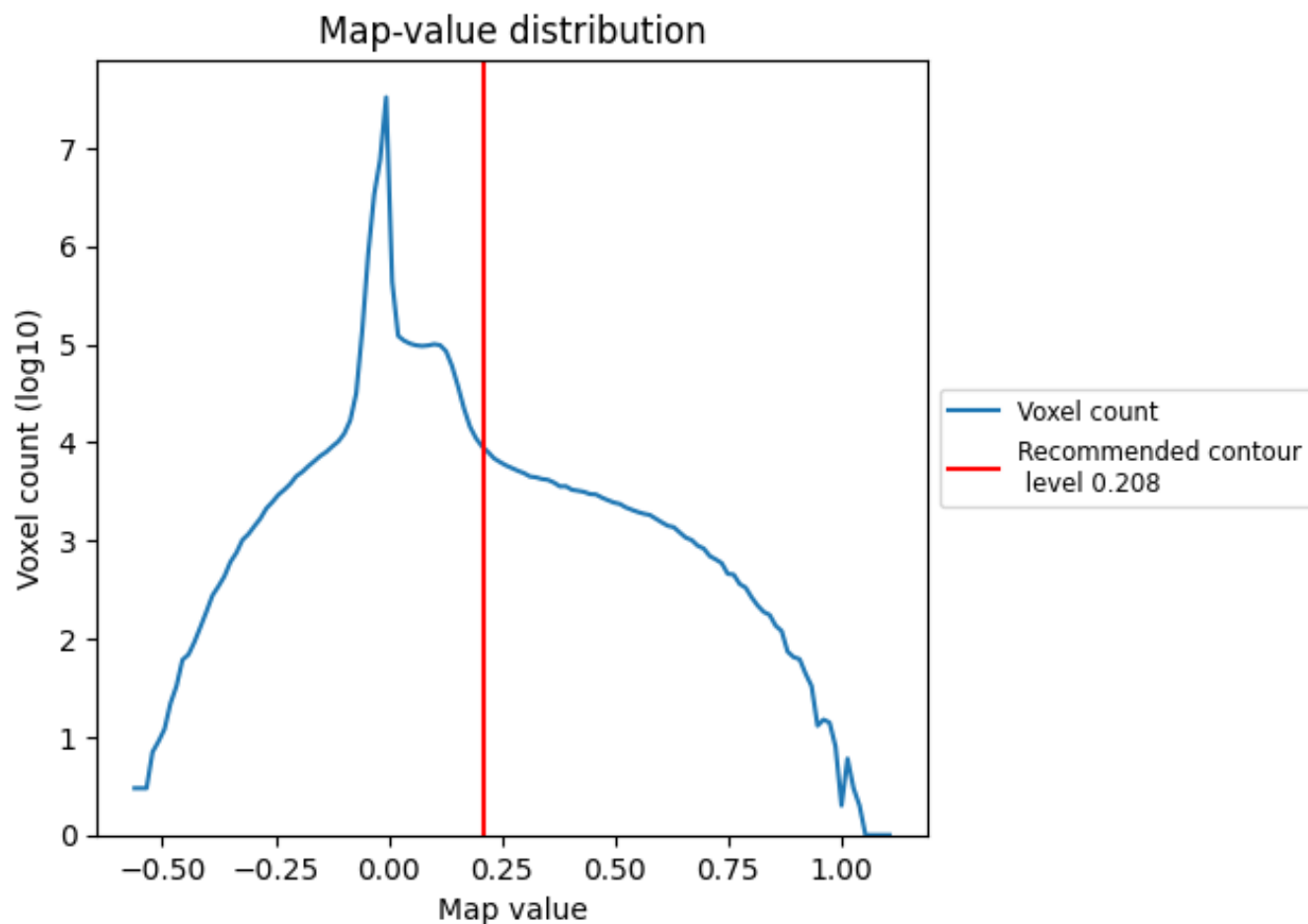
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

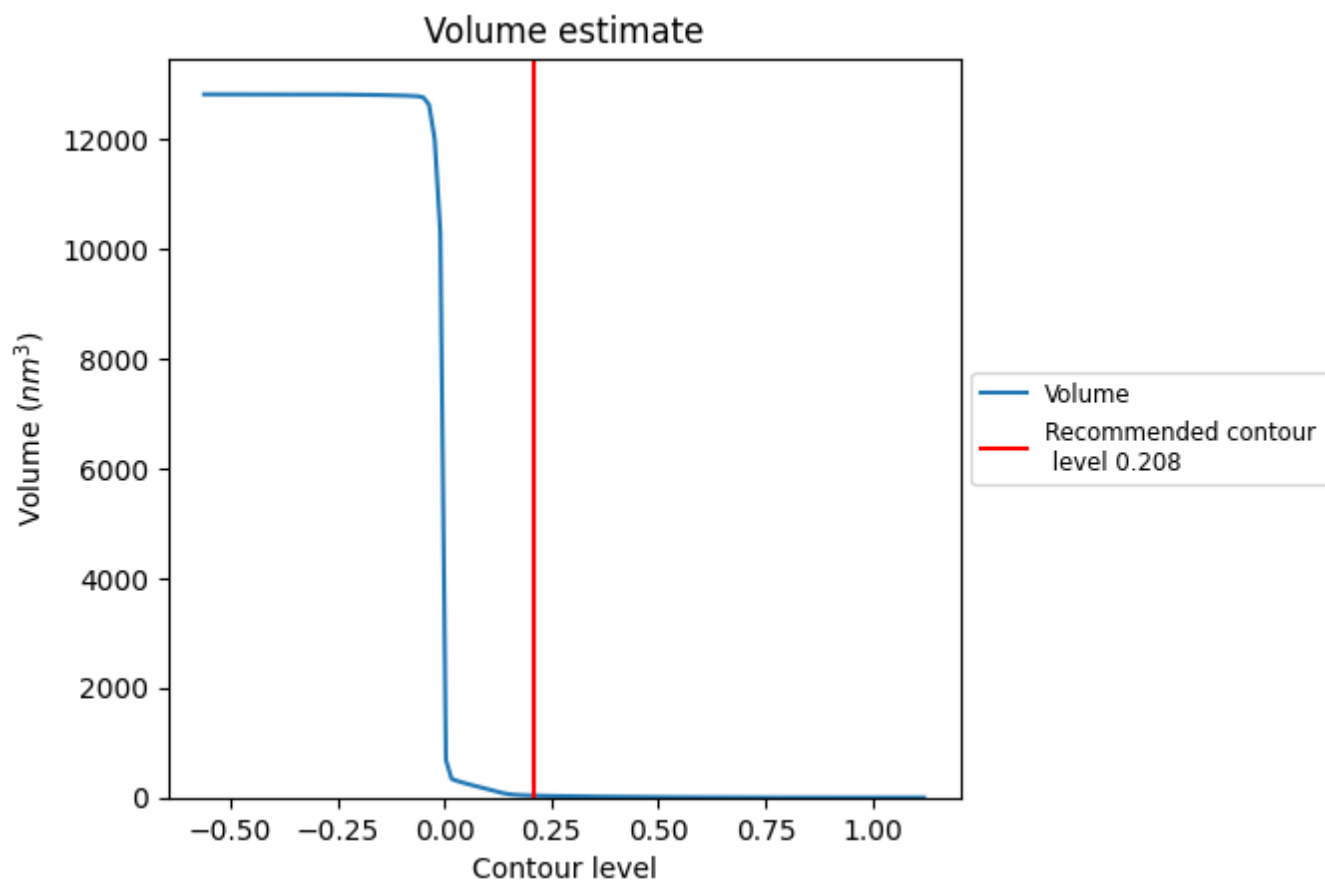
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

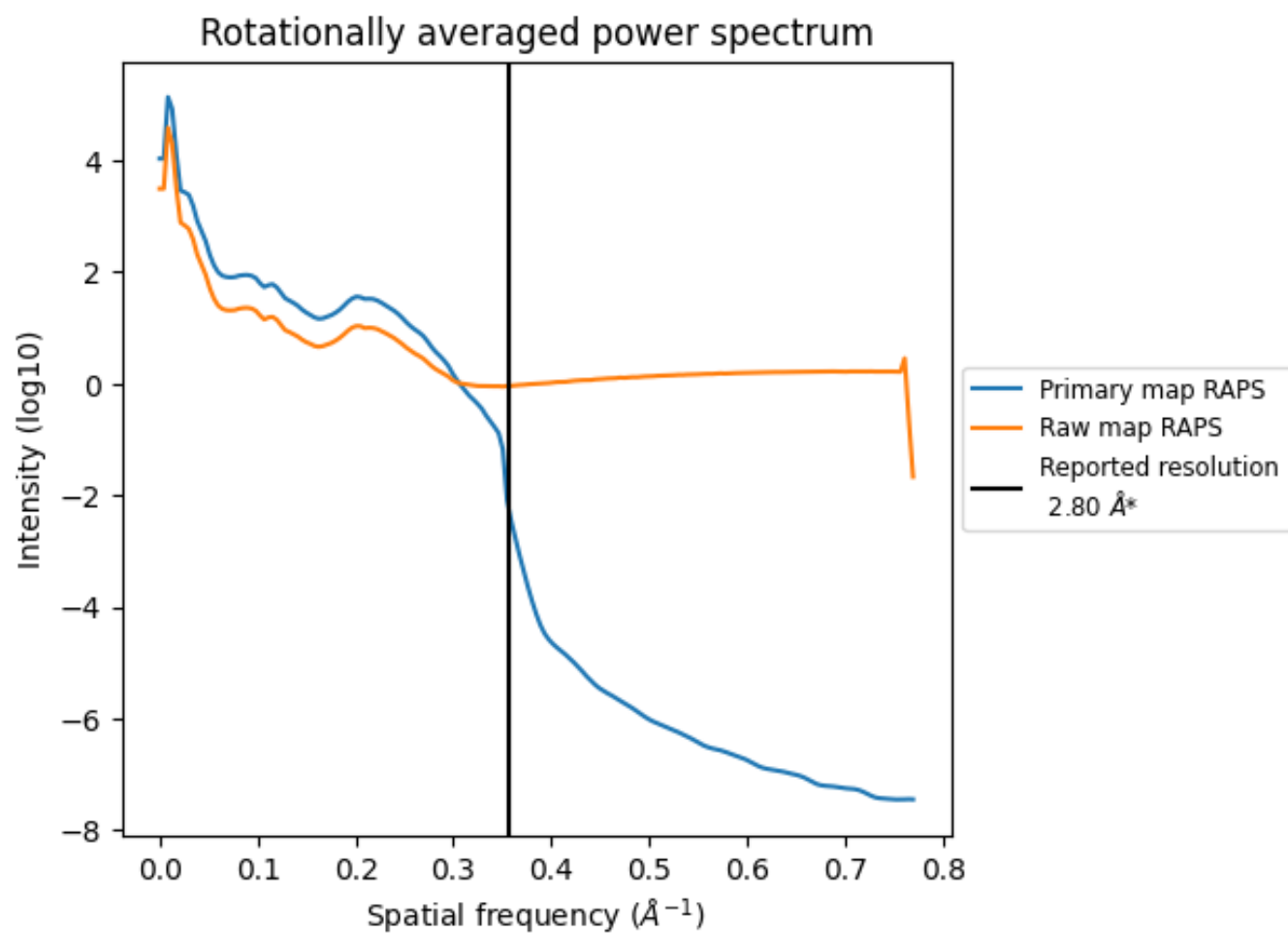
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 36 nm^3 ; this corresponds to an approximate mass of 32 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 ⓘ

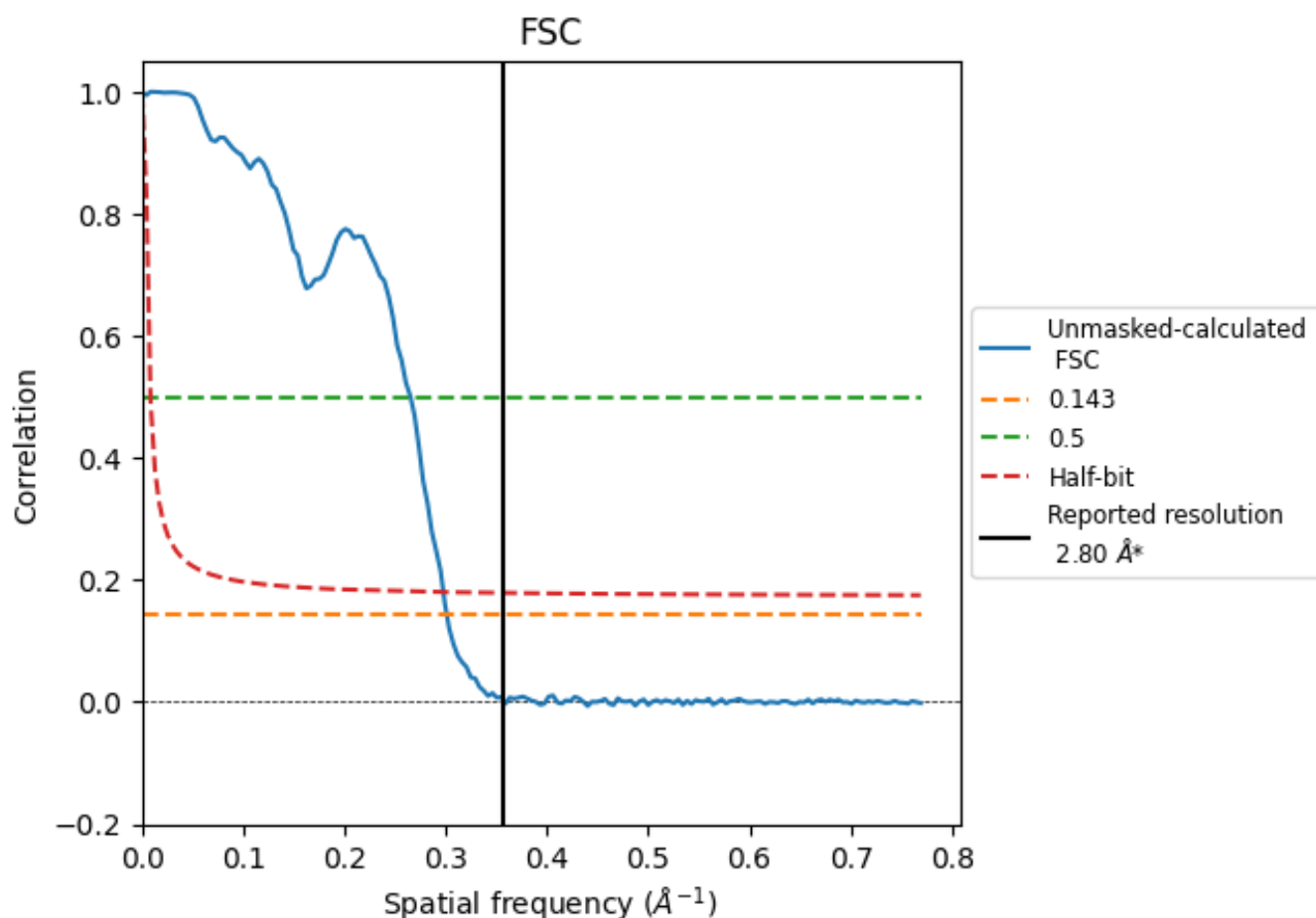


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 \AA^{-1}

8.2 Resolution estimates [i](#)

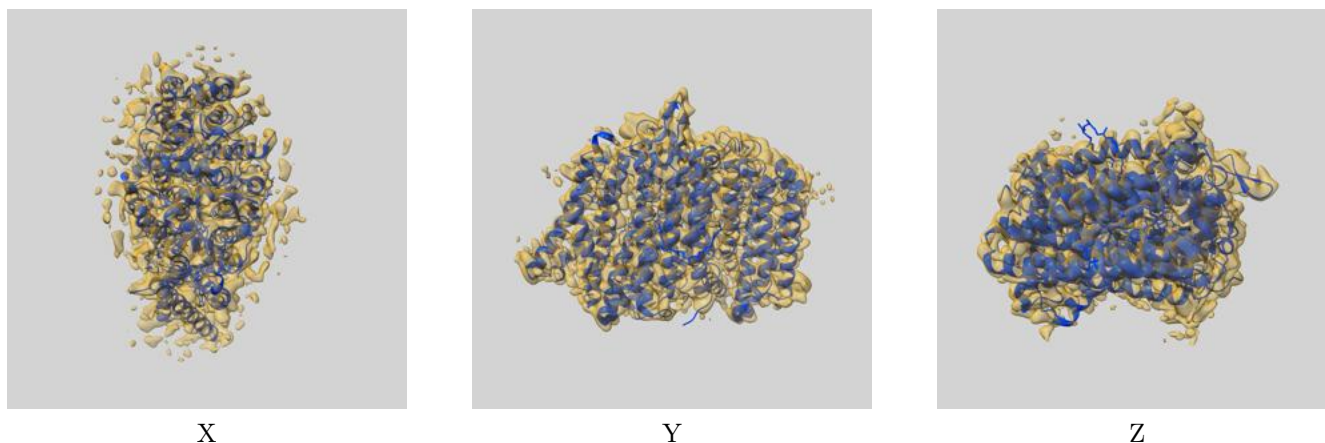
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.32	3.77	3.36

*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 3.32 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

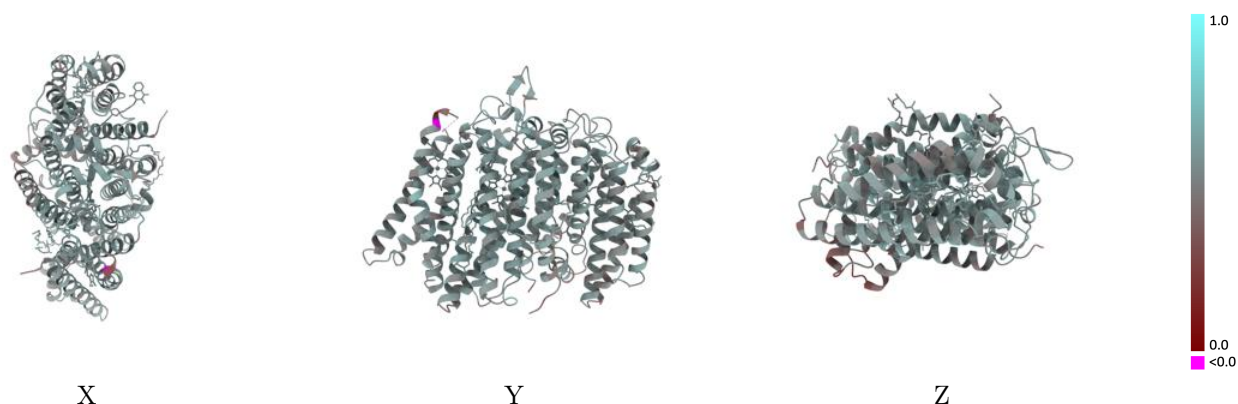
This section contains information regarding the fit between EMDB map EMD-53529 and PDB model 9R2G. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



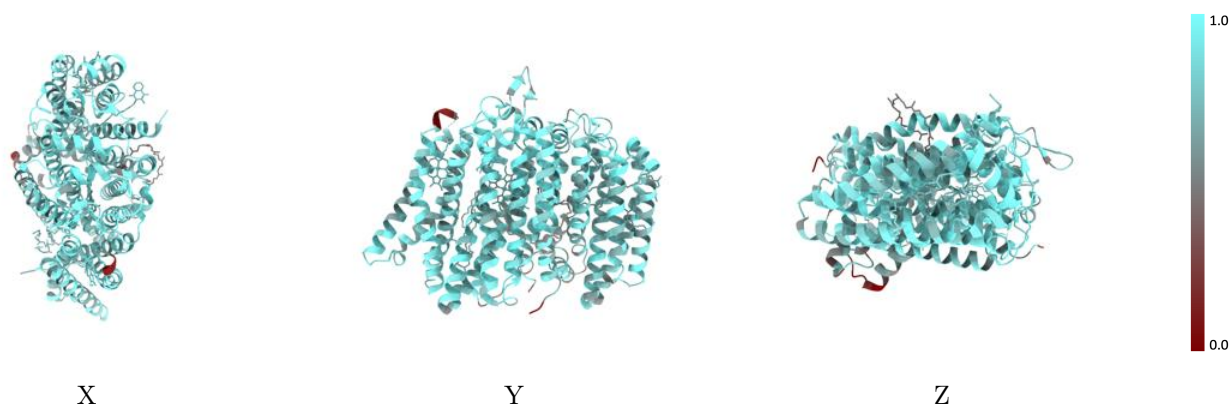
The images above show the 3D surface view of the map at the recommended contour level 0.208 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



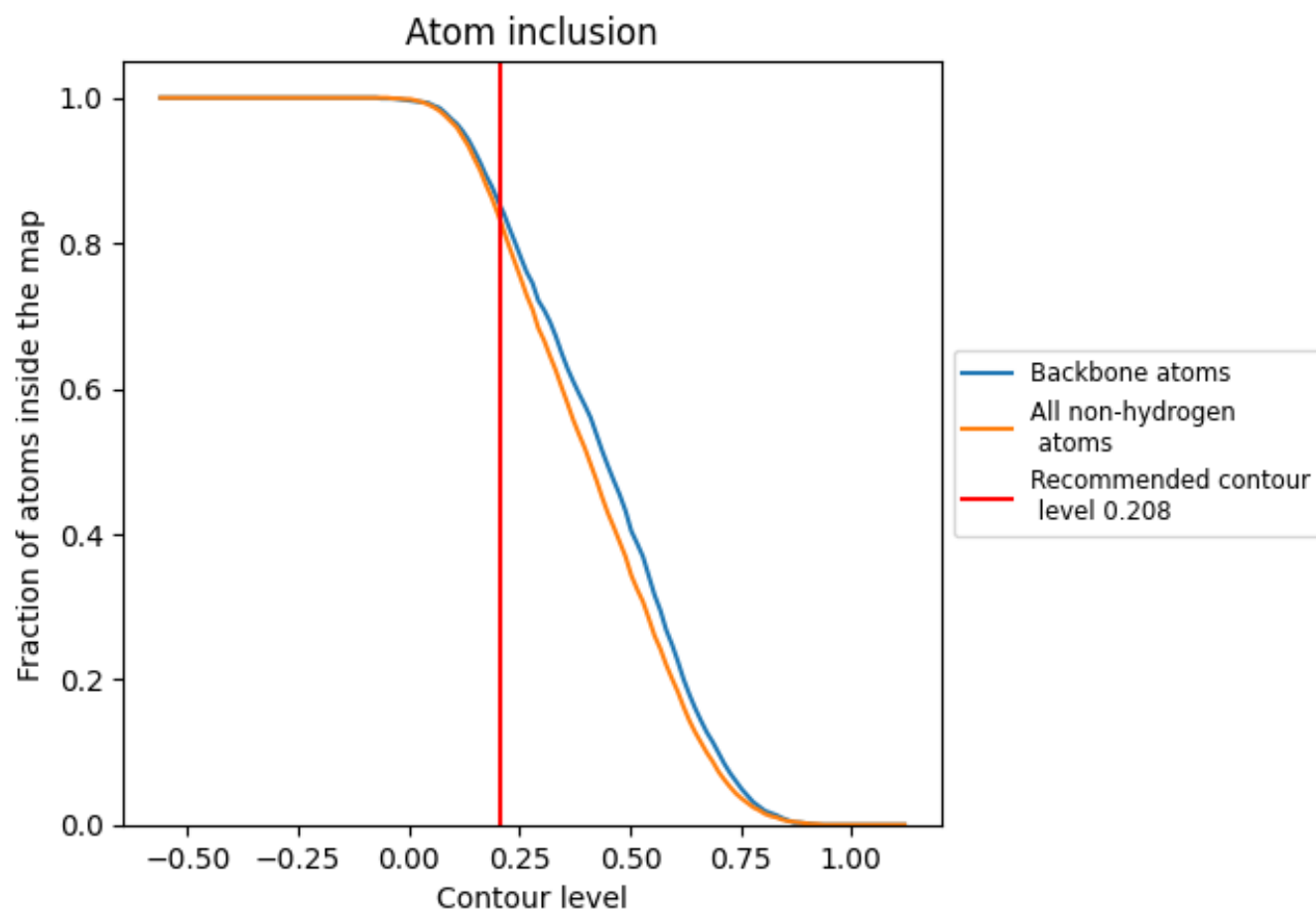
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.208).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% 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 (0.208) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8290	<div><div></div></div> 0.5360
A	<div><div></div></div> 0.8520	<div><div></div></div> 0.5440
D	<div><div></div></div> 0.8090	<div><div></div></div> 0.5260

