



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:55 AM UTC

PDB ID : 6RKO / pdb_00006rko
EMDB ID : EMD-4908
Title : Cryo-EM structure of the E. coli cytochrome bd-I oxidase at 2.68 Å resolution
Authors : Safarian, S.; Hahn, A.; Kuehlbrandt, W.; Michel, H.
Deposited on : 2019-04-30
Resolution : 2.68 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

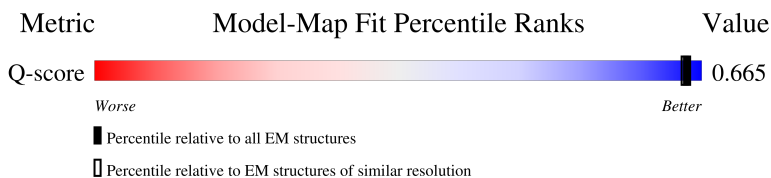
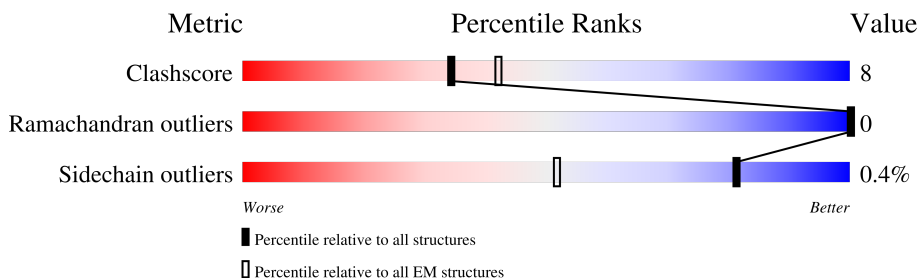
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.68 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	9255 (2.18 - 3.18)

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	B	379	
2	A	522	
3	H	29	
4	X	37	

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
8	HEB	A	604	X	-	-	-
8	HEB	A	605	X	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7289 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-I ubiquinol oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	378	Total	C	N	O	S	0	0
			2987	1981	482	503	21		

- Molecule 2 is a protein called Cytochrome bd-I ubiquinol oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	444	Total	C	N	O	S	0	0
			3518	2332	568	595	23		

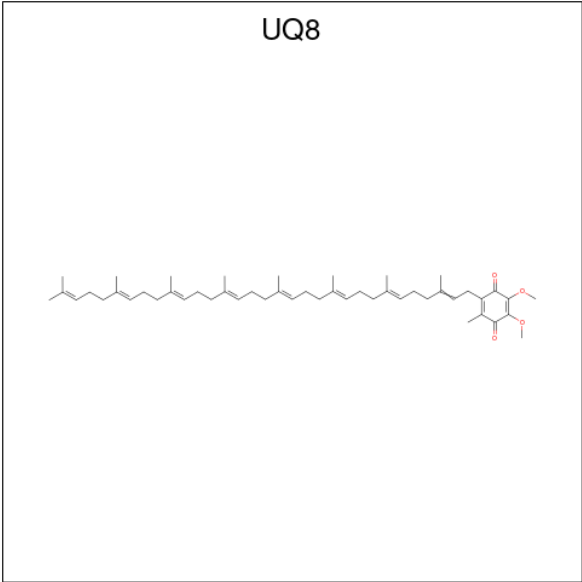
- Molecule 3 is a protein called Uncharacterized protein YnhF.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	27	Total	C	N	O	0	0
			195	131	30	34		

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

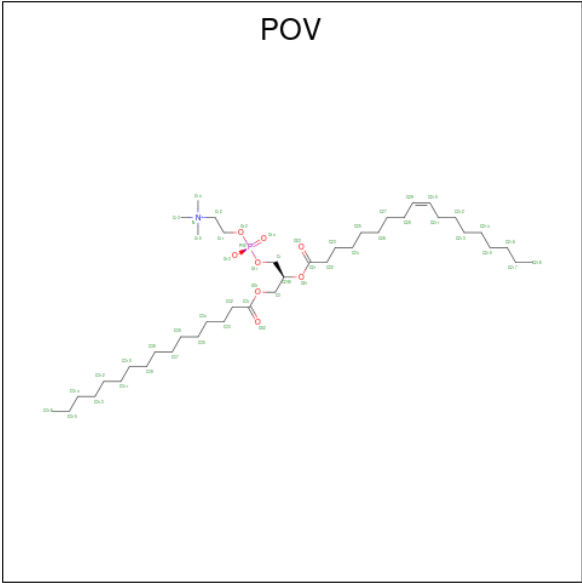
Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	26	Total	C	N	O	S	0	0
			188	125	28	34	1		

- Molecule 5 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	C	O	0
			53	49	4	

- Molecule 6 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P).



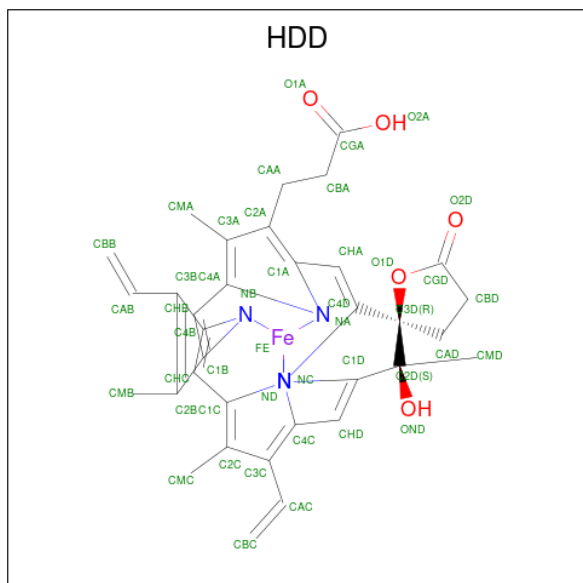
Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			52	42	1	8	1	
6	B	1	Total	C	O	P		0
			38	29	8	1		

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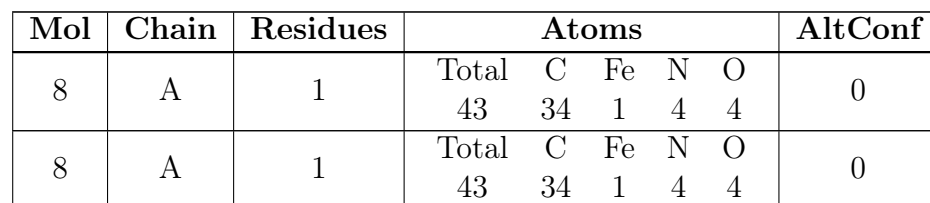
Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
6	A	1	Total	C	N	O	P	0
			43	33	1	8	1	

- Molecule 7 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).



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

- Molecule 8 is HEME B/C (CCD ID: HEB) (formula: $C_{34}H_{34}FeN_4O_4$).



- OXY
- O1 O = O O2

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

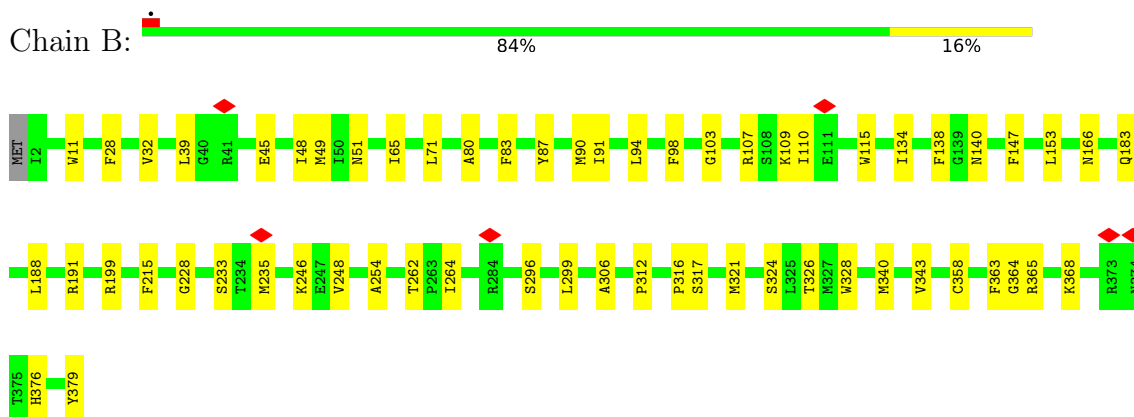
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Mol	Chain	Residues	Atoms		AltConf
10	B	13	Total 13	O 13	0
10	A	18	Total 18	O 18	0

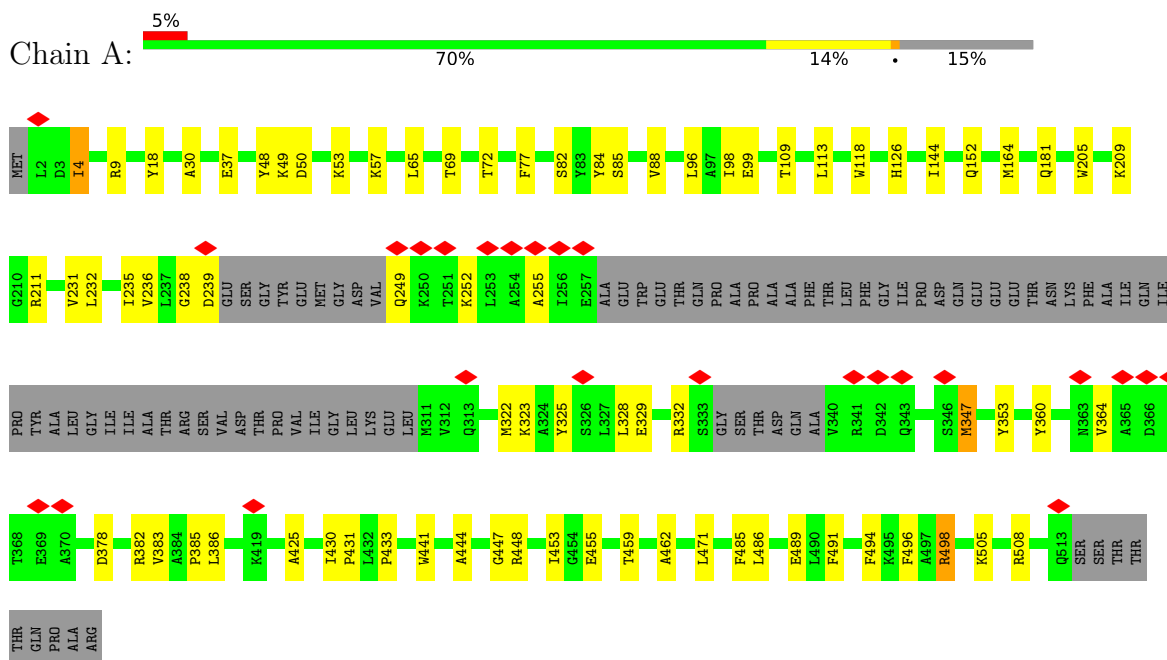
3 Residue-property plots

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.

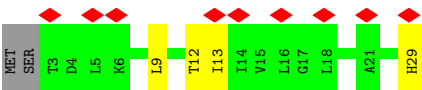
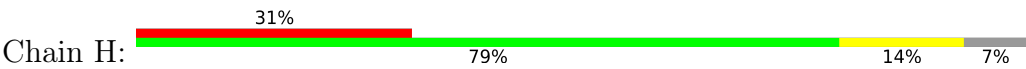
- Molecule 1: Cytochrome bd-I ubiquinol oxidase subunit 2



- Molecule 2: Cytochrome bd-I ubiquinol oxidase subunit 1



- Molecule 3: Uncharacterized protein YnhF



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	170000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.997	Depositor
Minimum map value	-0.671	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.13	Depositor
Map size ($\text{\AA}$)	249.6, 249.6, 249.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.832, 0.832, 0.832	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, HEB, POV, OXY, UQ8

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.17	0/3074	0.37	0/4202
2	A	0.23	0/3609	0.39	0/4885
3	H	0.33	0/196	0.69	0/268
4	X	0.11	0/191	0.30	0/260
All	All	0.20	0/7070	0.39	0/9615

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 [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	B	2987	0	3013	44	0
2	A	3518	0	3565	67	0
3	H	195	0	221	7	0
4	X	188	0	183	3	0
5	B	53	0	74	8	0
6	A	95	0	140	5	0
6	B	90	0	129	2	0
7	A	44	0	31	3	0
8	A	86	0	64	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	2	0	0	1	0
10	A	18	0	0	5	0
10	B	13	0	0	0	0
All	All	7289	0	7420	119	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 (119) 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)
8:A:605:HEB:HHA	8:A:605:HEB:HBA2	1.29	1.15
2:A:30:ALA:O	10:A:702:HOH:O	1.64	1.13
2:A:448:ARG:NH2	8:A:604:HEB:O1D	1.91	1.03
2:A:255:ALA:HB1	2:A:383:VAL:HG12	1.41	1.02
7:A:603:HDD:O1A	10:A:703:HOH:O	1.78	1.00
2:A:57:LYS:O	10:A:704:HOH:O	1.81	0.97
1:B:246:LYS:NZ	1:B:324:SER:O	2.04	0.91
2:A:96:LEU:HD23	10:A:717:HOH:O	1.73	0.89
8:A:605:HEB:HBB3	8:A:605:HEB:HMB1	1.58	0.83
2:A:255:ALA:CB	2:A:383:VAL:HG12	2.08	0.83
1:B:326:THR:HG22	1:B:328:TRP:H	1.47	0.78
8:A:605:HEB:HBA2	8:A:605:HEB:CHA	2.12	0.75
8:A:605:HEB:HHA	8:A:605:HEB:CBA	2.14	0.73
2:A:4:ILE:HD12	2:A:471:LEU:HD11	1.70	0.71
2:A:84:TYR:HB2	2:A:462:ALA:HB1	1.73	0.71
2:A:494:PHE:O	2:A:498:ARG:HB2	1.93	0.67
1:B:365:ARG:H	6:B:402:POV:H14A	1.61	0.66
2:A:109:THR:O	10:A:705:HOH:O	2.14	0.65
2:A:382:ARG:NH1	3:H:29:HIS:CG	2.66	0.64
8:A:605:HEB:HMB1	8:A:605:HEB:CBB	2.28	0.64
1:B:262:THR:HG22	1:B:264:ILE:HG22	1.81	0.62
1:B:94:LEU:HD21	2:A:72:THR:HG23	1.81	0.62
2:A:382:ARG:HH12	3:H:29:HIS:CE1	2.17	0.62
2:A:9:ARG:HD3	2:A:459:THR:HG21	1.83	0.61
1:B:28:PHE:HB3	1:B:183:GLN:HG3	1.84	0.60
2:A:252:LYS:NZ	2:A:444:ALA:O	2.35	0.60
2:A:431:PRO:HG2	6:A:601:POV:H35A	1.84	0.59
2:A:382:ARG:NH1	3:H:29:HIS:ND1	2.51	0.59
1:B:235:MET:HE1	1:B:326:THR:HG21	1.83	0.59
1:B:65:ILE:HD13	7:A:603:HDD:HBA2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:360:TYR:OH	2:A:378:ASP:OD2	2.20	0.58
1:B:233:SER:OG	1:B:246:LYS:O	2.15	0.57
2:A:239:ASP:HB2	8:A:605:HEB:C3A	2.34	0.57
2:A:152:GLN:HB3	2:A:249:GLN:HE22	1.70	0.56
2:A:50:ASP:OD2	2:A:508:ARG:NH1	2.39	0.56
2:A:88:VAL:HG11	2:A:453:ILE:HG13	1.87	0.56
1:B:134:ILE:HD12	5:B:401:UQ8:H28	1.87	0.55
1:B:316:PRO:HA	1:B:324:SER:HB3	1.87	0.55
8:A:605:HEB:CBB	8:A:605:HEB:CMB	2.85	0.54
2:A:486:LEU:HD23	3:H:12:THR:HG23	1.89	0.54
1:B:110:ILE:HD11	2:A:491:PHE:HE2	1.73	0.54
2:A:323:LYS:HB3	2:A:347:MET:HE1	1.90	0.53
2:A:99:GLU:OE2	9:A:606:OXY:O2	2.27	0.53
1:B:140:ASN:HD21	1:B:166:ASN:HD21	1.58	0.52
2:A:37:GLU:OE2	2:A:126:HIS:ND1	2.25	0.52
1:B:306:ALA:HB2	5:B:401:UQ8:H11A	1.93	0.51
2:A:322:MET:HG2	2:A:364:VAL:HG12	1.92	0.51
2:A:65:LEU:HD21	2:A:485:PHE:HB3	1.92	0.51
1:B:48:ILE:HD11	1:B:368:LYS:HA	1.93	0.50
2:A:209:LYS:HB2	2:A:211:ARG:HG3	1.93	0.50
2:A:353:TYR:CE2	2:A:455:GLU:HG3	2.47	0.50
2:A:353:TYR:HE2	2:A:455:GLU:HG3	1.78	0.49
2:A:255:ALA:CB	2:A:383:VAL:CG1	2.87	0.49
1:B:71:LEU:HD11	5:B:401:UQ8:H32	1.95	0.48
8:A:604:HEB:HBC1	8:A:604:HEB:HMC1	1.93	0.48
1:B:228:GLY:HA3	1:B:254:ALA:HB3	1.95	0.48
1:B:45:GLU:OE1	1:B:199:ARG:NH2	2.47	0.48
1:B:147:PHE:O	1:B:317:SER:OG	2.31	0.48
1:B:191:ARG:NH1	1:B:364:GLY:O	2.46	0.47
2:A:48:TYR:OH	4:X:25:GLU:OE1	2.25	0.47
1:B:248:VAL:HB	1:B:321:MET:O	2.14	0.47
1:B:343:VAL:HG11	2:A:98:ILE:HG12	1.97	0.47
2:A:382:ARG:NH2	3:H:29:HIS:CD2	2.83	0.47
2:A:382:ARG:HH22	3:H:29:HIS:CD2	2.33	0.47
1:B:110:ILE:HB	1:B:115:TRP:CD1	2.50	0.47
2:A:382:ARG:O	2:A:385:PRO:HD2	2.14	0.47
2:A:430:ILE:O	2:A:433:PRO:HD2	2.15	0.47
1:B:87:TYR:O	1:B:91:ILE:HG12	2.16	0.46
6:A:602:POV:H21A	6:A:602:POV:H39A	1.98	0.46
1:B:103:GLY:O	1:B:107:ARG:HB2	2.16	0.46
1:B:109:LYS:HD2	2:A:496:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:205:TRP:O	2:A:209:LYS:HG2	2.16	0.46
1:B:39:LEU:O	1:B:49:MET:HE1	2.16	0.45
1:B:312:PRO:HB2	1:B:326:THR:HG23	1.97	0.45
1:B:98:PHE:HB3	2:A:485:PHE:HE2	1.82	0.45
2:A:498:ARG:HH11	2:A:498:ARG:HG2	1.82	0.45
2:A:181:GLN:HB3	4:X:3:TYR:HB2	1.97	0.45
1:B:110:ILE:HD11	2:A:491:PHE:CE2	2.50	0.45
1:B:51:ASN:HD21	1:B:379:TYR:H	1.64	0.45
6:A:602:POV:H22A	6:A:602:POV:H25A	1.60	0.44
2:A:99:GLU:OE2	2:A:144:ILE:HB	2.17	0.44
2:A:238:GLY:HA2	2:A:239:ASP:HA	1.68	0.44
2:A:386:LEU:HD11	2:A:447:GLY:HA2	2.00	0.43
1:B:80:ALA:HB1	2:A:82:SER:HB2	1.99	0.43
1:B:138:PHE:HE2	5:B:401:UQ8:H26A	1.84	0.43
8:A:605:HEB:CBC	8:A:605:HEB:CMC	2.97	0.43
1:B:83:PHE:HD1	1:B:90:MET:HG3	1.84	0.43
2:A:49:LYS:HE3	2:A:118:TRP:CE3	2.54	0.43
2:A:18:TYR:OH	2:A:486:LEU:HB2	2.19	0.43
2:A:232:LEU:O	2:A:236:VAL:HG22	2.19	0.43
1:B:246:LYS:HB2	1:B:246:LYS:HE3	1.51	0.42
2:A:77:PHE:O	2:A:85:SER:OG	2.38	0.42
1:B:153:LEU:HD12	2:A:164:MET:HB2	2.01	0.42
2:A:209:LYS:HZ3	6:A:602:POV:H12A	1.84	0.42
1:B:11:TRP:CZ2	1:B:340:MET:HB3	2.55	0.42
1:B:358:CYS:HB3	2:A:113:LEU:HD11	2.02	0.42
2:A:49:LYS:HE2	2:A:53:LYS:HE3	2.02	0.42
2:A:325:TYR:CD2	2:A:364:VAL:HB	2.55	0.42
2:A:181:GLN:HG2	4:X:4:PHE:CZ	2.55	0.42
2:A:325:TYR:O	2:A:329:GLU:HG2	2.20	0.42
2:A:328:LEU:O	2:A:332:ARG:HG3	2.20	0.42
7:A:603:HDD:HAD2	7:A:603:HDD:HMD2	1.77	0.42
1:B:32:VAL:HG22	1:B:188:LEU:HG	2.03	0.41
1:B:296:SER:HA	1:B:299:LEU:HD12	2.01	0.41
2:A:425:ALA:HA	6:A:601:POV:H315	2.02	0.41
1:B:110:ILE:HD12	1:B:115:TRP:CD2	2.55	0.41
5:B:401:UQ8:H42A	5:B:401:UQ8:H46	1.91	0.41
3:H:9:LEU:O	3:H:13:ILE:HG12	2.20	0.41
5:B:401:UQ8:H10	5:B:401:UQ8:H7A	1.74	0.41
2:A:231:VAL:O	2:A:235:ILE:HG12	2.21	0.41
8:A:605:HEB:CMC	8:A:605:HEB:HBC1	2.51	0.41
1:B:215:PHE:CE2	5:B:401:UQ8:H4MA	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:PHE:CE1	6:B:402:POV:H3A	2.57	0.40
2:A:441:TRP:CE2	8:A:604:HEB:HAB2	2.56	0.40
8:A:604:HEB:HBC1	8:A:604:HEB:CMC	2.52	0.40
1:B:376:HIS:CD2	2:A:505:LYS:HG3	2.56	0.40
5:B:401:UQ8:H15	5:B:401:UQ8:H12A	1.72	0.40
2:A:18:TYR:HD1	2:A:69:THR:HG21	1.87	0.40
2:A:65:LEU:HD12	2:A:489:GLU:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	376/379 (99%)	368 (98%)	8 (2%)	0	100	100
2	A	436/522 (84%)	433 (99%)	3 (1%)	0	100	100
3	H	25/29 (86%)	25 (100%)	0	0	100	100
4	X	24/37 (65%)	23 (96%)	1 (4%)	0	100	100
All	All	861/967 (89%)	849 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	312/313 (100%)	312 (100%)	0	100	100
2	A	363/426 (85%)	360 (99%)	3 (1%)	73	87
3	H	22/24 (92%)	22 (100%)	0	100	100
4	X	18/28 (64%)	18 (100%)	0	100	100
All	All	715/791 (90%)	712 (100%)	3 (0%)	81	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	4	ILE
2	A	347	MET
2	A	498	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	51	ASN
1	B	140	ASN
2	A	46	GLN
2	A	249	GLN
2	A	330	GLN
2	A	449	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	$\# Z > 2$
7	HDD	A	603	2	46,52,52	2.41	21 (45%)	62,89,89	2.37	25 (40%)
6	POV	A	602	-	42,42,51	1.21	7 (16%)	48,50,59	1.08	2 (4%)
6	POV	B	403	-	37,37,51	1.20	6 (16%)	40,42,59	1.17	2 (5%)
6	POV	B	402	-	51,51,51	1.11	6 (11%)	57,59,59	1.11	2 (3%)
9	OXY	A	606	-	1,1,1	0.25	0	-		
5	UQ8	B	401	-	53,53,53	2.23	16 (30%)	66,67,67	1.66	17 (25%)
8	HEB	A	604	2	50,50,50	2.80	24 (48%)	66,82,82	2.61	27 (40%)
6	POV	A	601	-	51,51,51	1.11	6 (11%)	57,59,59	1.07	2 (3%)
8	HEB	A	605	2	50,50,50	4.62	29 (58%)	66,82,82	5.40	43 (65%)

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
7	HDD	A	603	2	-	5/9/89/89	0/1/9/9
6	POV	A	602	-	-	17/46/46/55	-
6	POV	B	403	-	-	23/39/39/55	-
6	POV	B	402	-	-	23/55/55/55	-
5	UQ8	B	401	-	-	12/51/75/75	0/1/1/1
8	HEB	A	604	2	1/1/3/8	2/14/54/54	-
6	POV	A	601	-	-	25/55/55/55	-
8	HEB	A	605	2	1/1/3/8	8/14/54/54	-

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	605	HEB	FE-ND	13.58	2.36	1.94
5	B	401	UQ8	C6-C1	10.44	1.53	1.35
8	A	605	HEB	C1C-C2C	-9.33	1.21	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	605	HEB	C1A-C2A	-8.78	1.29	1.45
8	A	605	HEB	C1B-C2B	-8.00	1.28	1.44
8	A	605	HEB	C4A-NA	7.09	1.53	1.39
8	A	605	HEB	FE-NC	7.07	2.18	1.95
8	A	605	HEB	C4D-ND	6.52	1.51	1.38
8	A	605	HEB	FE-NB	6.11	2.13	1.94
8	A	605	HEB	CHA-C4D	6.08	1.53	1.39
8	A	604	HEB	FE-ND	5.95	2.13	1.94
8	A	605	HEB	C1D-C2D	-5.87	1.32	1.44
8	A	605	HEB	C2A-C3A	-5.82	1.24	1.36
8	A	605	HEB	C1C-NC	5.81	1.50	1.39
8	A	604	HEB	FE-NB	5.74	2.12	1.94
8	A	605	HEB	CHC-C1C	5.16	1.51	1.39
8	A	604	HEB	FE-NC	5.14	2.12	1.95
8	A	605	HEB	C3C-C2C	-5.13	1.23	1.41
8	A	605	HEB	FE-NA	5.11	2.12	1.95
8	A	605	HEB	C4B-C3B	-5.00	1.36	1.45
7	A	603	HDD	O1D-CGD	4.96	1.43	1.35
5	B	401	UQ8	C4-C3	4.94	1.54	1.36
8	A	605	HEB	CHB-C4A	4.90	1.48	1.38
8	A	605	HEB	C4A-C3A	-4.88	1.35	1.45
8	A	604	HEB	CHD-C1D	4.86	1.48	1.38
8	A	605	HEB	CHD-C1D	4.82	1.48	1.38
8	A	605	HEB	C3B-C2B	-4.69	1.26	1.36
8	A	604	HEB	C2A-C3A	4.61	1.46	1.36
8	A	604	HEB	CHA-C1A	4.50	1.47	1.38
8	A	605	HEB	C4B-NB	4.49	1.48	1.40
8	A	604	HEB	CHC-C4B	4.49	1.47	1.38
8	A	604	HEB	C3D-C2D	4.48	1.46	1.36
7	A	603	HDD	C3B-C2B	4.41	1.46	1.37
8	A	604	HEB	C3B-C2B	4.41	1.46	1.36
7	A	603	HDD	CHC-C4B	4.40	1.47	1.38
7	A	603	HDD	CHB-C1B	4.36	1.46	1.38
8	A	604	HEB	FE-NA	4.28	2.09	1.95
8	A	605	HEB	CBC-CAC	4.26	1.50	1.30
7	A	603	HDD	C4C-NC	-4.23	1.31	1.39
8	A	604	HEB	CHB-C4A	4.13	1.46	1.38
8	A	605	HEB	CHA-C1A	3.93	1.46	1.38
8	A	604	HEB	C4B-NB	-3.82	1.33	1.40
7	A	603	HDD	C4A-NA	-3.82	1.32	1.39
7	A	603	HDD	O1D-C3D	-3.81	1.40	1.46
7	A	603	HDD	C1A-NA	-3.79	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	603	HDD	C1C-NC	-3.79	1.32	1.39
8	A	604	HEB	CHA-C4D	3.77	1.47	1.39
8	A	605	HEB	C1B-NB	3.72	1.46	1.38
8	A	605	HEB	CHC-C4B	3.63	1.45	1.38
8	A	605	HEB	CHB-C1B	3.58	1.47	1.39
7	A	603	HDD	CHB-C4A	3.49	1.47	1.39
8	A	604	HEB	CHB-C1B	3.29	1.46	1.39
7	A	603	HDD	CHD-C4C	3.28	1.46	1.39
7	A	603	HDD	CHA-C1A	3.18	1.46	1.39
8	A	604	HEB	C1D-ND	-3.15	1.34	1.40
8	A	605	HEB	C4C-NC	3.01	1.45	1.39
7	A	603	HDD	C1B-NB	-2.99	1.34	1.39
8	A	604	HEB	CHD-C4C	2.89	1.45	1.39
7	A	603	HDD	CHC-C1C	2.79	1.45	1.39
8	A	604	HEB	C4A-NA	-2.79	1.34	1.39
8	A	604	HEB	CHC-C1C	2.76	1.45	1.39
8	A	604	HEB	C1A-NA	-2.75	1.34	1.39
8	A	604	HEB	C1C-NC	-2.72	1.34	1.39
6	A	601	POV	O21-C21	2.69	1.41	1.34
7	A	603	HDD	C4D-ND	-2.68	1.33	1.37
6	B	403	POV	P-O12	2.67	1.64	1.54
6	B	402	POV	O21-C21	2.67	1.41	1.34
6	B	403	POV	O21-C21	2.66	1.41	1.34
5	B	401	UQ8	C7-C8	2.64	1.54	1.50
7	A	603	HDD	C2A-C3A	2.63	1.45	1.38
8	A	604	HEB	O2A-CGA	-2.62	1.22	1.30
8	A	605	HEB	C1A-NA	2.61	1.44	1.39
8	A	604	HEB	O2D-CGD	-2.59	1.22	1.30
6	B	403	POV	O31-C31	2.59	1.40	1.33
6	A	602	POV	O31-C31	2.54	1.40	1.33
6	A	602	POV	O21-C21	2.54	1.41	1.34
6	B	403	POV	P-O11	2.53	1.68	1.60
8	A	604	HEB	C4C-NC	-2.53	1.34	1.39
5	B	401	UQ8	C7-C6	2.51	1.56	1.51
5	B	401	UQ8	C6-C5	2.49	1.53	1.46
6	A	601	POV	O31-C31	2.48	1.40	1.33
6	A	601	POV	O21-C2	-2.44	1.40	1.46
6	B	402	POV	O31-C31	2.44	1.40	1.33
7	A	603	HDD	C4A-C3A	2.44	1.48	1.43
6	B	403	POV	O21-C2	-2.44	1.40	1.46
6	A	602	POV	O21-C2	-2.39	1.41	1.46
6	B	402	POV	O31-C3	-2.35	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	603	HDD	C4B-NB	-2.34	1.35	1.39
5	B	401	UQ8	O5-C5	-2.33	1.18	1.23
6	B	402	POV	O21-C2	-2.30	1.41	1.46
6	A	602	POV	P-O11	2.28	1.68	1.59
5	B	401	UQ8	C11-C9	2.27	1.56	1.51
5	B	401	UQ8	C21-C19	2.26	1.56	1.51
7	A	603	HDD	C1C-C2C	2.26	1.48	1.43
6	B	402	POV	P-O11	2.26	1.68	1.59
6	A	602	POV	O31-C3	-2.22	1.40	1.45
6	A	601	POV	P-O11	2.21	1.68	1.59
6	A	601	POV	O31-C3	-2.20	1.40	1.45
7	A	603	HDD	C1D-ND	-2.20	1.34	1.37
5	B	401	UQ8	C36-C34	2.15	1.55	1.51
5	B	401	UQ8	C33-C34	2.15	1.38	1.33
6	B	403	POV	O31-C3	-2.15	1.40	1.45
5	B	401	UQ8	O4-C4M	-2.13	1.40	1.45
8	A	605	HEB	O2D-CGD	-2.13	1.23	1.30
5	B	401	UQ8	C41-C39	2.12	1.55	1.51
6	A	602	POV	C12-N	-2.09	1.45	1.51
6	A	601	POV	C15-N	-2.08	1.44	1.50
6	B	402	POV	C15-N	-2.07	1.44	1.50
5	B	401	UQ8	O3-C3	2.06	1.41	1.36
5	B	401	UQ8	O2-C2	-2.05	1.18	1.23
5	B	401	UQ8	C31-C29	2.05	1.55	1.51
6	A	602	POV	C15-N	-2.05	1.44	1.50
8	A	604	HEB	C3C-C2C	2.05	1.48	1.41
5	B	401	UQ8	O4-C4	2.03	1.41	1.36
7	A	603	HDD	O2A-CGA	-2.00	1.24	1.30

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	605	HEB	C1D-C2D-C3D	15.33	123.11	106.98
8	A	605	HEB	C1B-C2B-C3B	13.05	120.70	106.98
8	A	605	HEB	C2A-C1A-NA	-12.65	98.12	110.32
8	A	605	HEB	C3C-C4C-NC	-11.72	99.93	109.80
8	A	605	HEB	C3C-C2C-C1C	11.42	120.63	107.17
8	A	605	HEB	C1A-C2A-C3A	11.25	121.92	107.11
8	A	605	HEB	C2B-C1B-NB	-10.16	98.16	109.90
8	A	605	HEB	C3B-C4B-NB	-10.10	99.10	110.17
8	A	605	HEB	C2D-C1D-ND	-9.65	98.75	109.84
8	A	605	HEB	C3D-C4D-ND	-9.27	101.39	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	605	HEB	CMB-C2B-C1B	-7.22	113.75	125.03
8	A	605	HEB	C1D-ND-C4D	6.74	113.19	105.21
8	A	604	HEB	C3C-C2C-C1C	-5.99	100.11	107.17
8	A	605	HEB	C3A-C4A-NA	-5.98	98.57	109.64
7	A	603	HDD	C3C-C4C-NC	5.96	114.82	109.80
7	A	603	HDD	C3C-C2C-C1C	-5.93	100.18	107.17
8	A	605	HEB	CMC-C2C-C1C	-5.80	116.58	125.42
8	A	604	HEB	CBA-CAA-C2A	-5.71	96.75	112.53
8	A	604	HEB	C2B-C1B-NB	5.62	116.40	109.90
8	A	605	HEB	CAA-C2A-C3A	-5.60	117.39	127.87
7	A	603	HDD	C2A-C1A-NA	5.55	116.31	110.15
8	A	605	HEB	CHB-C1B-C2B	5.50	133.72	125.03
8	A	604	HEB	C1B-C2B-C3B	-5.17	101.54	106.98
8	A	604	HEB	C3C-C4C-NC	5.11	114.10	109.80
8	A	605	HEB	CHA-C1A-NA	5.07	129.97	124.45
8	A	605	HEB	CHA-C4D-C3D	4.93	131.96	124.77
8	A	605	HEB	C2C-C1C-NC	-4.90	102.28	110.14
8	A	604	HEB	C3D-C4D-ND	4.89	115.07	110.35
8	A	605	HEB	CMD-C2D-C1D	-4.78	117.57	125.03
8	A	605	HEB	C4B-NB-C1B	4.72	110.80	105.21
8	A	605	HEB	CHC-C4B-C3B	4.55	133.62	125.23
8	A	605	HEB	CHB-C4A-C3A	4.52	134.88	125.49
8	A	604	HEB	C3B-C4B-NB	4.47	115.07	110.17
8	A	605	HEB	CHA-C1A-C2A	4.46	131.91	124.86
8	A	605	HEB	CAB-C3B-C4B	-4.43	119.03	124.79
7	A	603	HDD	C3B-C2B-C1B	-4.42	102.86	107.05
8	A	604	HEB	C2D-C1D-ND	4.41	114.91	109.84
6	B	402	POV	O21-C21-C22	4.39	120.97	111.48
8	A	604	HEB	C2C-C1C-NC	4.23	116.93	110.14
6	A	601	POV	O21-C21-C22	4.16	120.48	111.48
8	A	604	HEB	CAD-C3D-C4D	4.04	131.74	124.70
7	A	603	HDD	C3D-O1D-CGD	-3.96	107.45	111.14
5	B	401	UQ8	C7-C8-C9	-3.92	120.08	126.83
6	A	602	POV	O21-C21-C22	3.91	119.94	111.48
8	A	604	HEB	CMB-C2B-C1B	3.85	131.05	125.03
6	B	403	POV	O21-C21-C22	3.79	119.69	111.48
7	A	603	HDD	C2C-C1C-NC	3.73	116.12	110.14
8	A	604	HEB	C2A-C1A-NA	3.54	113.74	110.32
8	A	604	HEB	C4A-C3A-C2A	-3.44	101.87	106.97
5	B	401	UQ8	C32-C33-C34	-3.44	119.76	127.62
8	A	605	HEB	CHB-C1B-NB	3.43	128.12	124.42
7	A	603	HDD	C4A-C3A-C2A	-3.37	102.96	106.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	603	HDD	CMA-C3A-C4A	3.37	130.55	125.42
7	A	603	HDD	C4B-C3B-C2B	-3.32	103.94	106.81
7	A	603	HDD	CAD-CBD-CGD	-3.31	99.56	104.48
8	A	604	HEB	CHA-C4D-ND	-3.27	120.91	124.42
5	B	401	UQ8	C12-C13-C14	-3.22	120.25	127.62
7	A	603	HDD	C1A-C2A-C3A	-3.20	101.92	106.87
8	A	605	HEB	CBA-CAA-C2A	3.20	121.37	112.53
8	A	604	HEB	C3A-C4A-NA	3.19	115.54	109.64
5	B	401	UQ8	C10-C9-C11	3.18	120.75	115.23
7	A	603	HDD	C2D-C1D-CHD	-3.16	119.36	124.27
8	A	605	HEB	C4A-C3A-C2A	3.16	111.66	106.97
5	B	401	UQ8	C25-C24-C26	3.14	120.68	115.23
8	A	604	HEB	C4D-C3D-C2D	-3.13	102.34	106.89
8	A	604	HEB	C1D-C2D-C3D	-3.13	103.69	106.98
7	A	603	HDD	CAB-C3B-C4B	3.09	132.20	124.82
5	B	401	UQ8	C15-C14-C16	3.05	120.52	115.23
8	A	605	HEB	CHD-C4C-NC	3.02	129.33	123.86
7	A	603	HDD	CMC-C2C-C1C	3.01	130.01	125.42
8	A	605	HEB	C4B-C3B-C2B	2.98	111.23	106.89
6	A	602	POV	O31-C31-C32	2.93	120.76	111.83
8	A	604	HEB	CHB-C1B-NB	-2.92	121.28	124.42
8	A	604	HEB	CAB-C3B-C4B	2.90	128.56	124.79
5	B	401	UQ8	C37-C38-C39	-2.89	121.01	127.62
5	B	401	UQ8	C40-C39-C41	2.86	120.19	115.23
8	A	605	HEB	O2D-CGD-O1D	-2.83	116.04	123.33
5	B	401	UQ8	C35-C34-C36	2.83	120.14	115.23
7	A	603	HDD	C2B-C1B-NB	2.83	114.87	109.64
6	A	601	POV	O31-C31-C32	2.72	120.14	111.83
6	B	402	POV	O31-C31-C32	2.71	120.09	111.83
7	A	603	HDD	CHD-C1D-ND	2.68	127.97	124.28
7	A	603	HDD	CHB-C1B-C2B	-2.67	119.93	125.49
5	B	401	UQ8	C1M-C1-C6	-2.67	120.07	124.45
7	A	603	HDD	O1D-CGD-O2D	2.65	123.04	120.81
8	A	605	HEB	C4C-C3C-C2C	2.63	110.58	107.30
6	B	403	POV	O31-C31-C32	2.62	119.83	111.83
8	A	605	HEB	CAA-CBA-CGA	-2.62	106.72	113.67
7	A	603	HDD	C3A-C4A-NA	2.60	114.31	110.14
5	B	401	UQ8	C7-C6-C1	-2.57	120.48	124.89
8	A	605	HEB	CHD-C1D-C2D	2.57	134.26	126.95
5	B	401	UQ8	C17-C18-C19	-2.57	121.74	127.62
5	B	401	UQ8	C20-C19-C21	2.57	119.69	115.23
5	B	401	UQ8	C22-C23-C24	-2.54	121.81	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	605	HEB	CMD-C2D-C3D	-2.52	119.32	126.15
7	A	603	HDD	CHA-C4D-ND	2.52	127.76	124.28
7	A	603	HDD	O1D-C3D-CAD	2.48	107.65	103.06
8	A	604	HEB	CHB-C4A-C3A	-2.48	120.33	125.49
5	B	401	UQ8	C27-C28-C29	-2.47	121.98	127.62
7	A	603	HDD	CBD-CAD-C3D	2.45	107.47	103.98
8	A	605	HEB	C4A-NA-C1A	2.39	109.72	105.82
8	A	604	HEB	CMD-C2D-C1D	2.39	128.76	125.03
7	A	603	HDD	OND-C2D-C3D	2.38	116.04	110.46
8	A	604	HEB	CHC-C4B-NB	-2.36	121.44	124.37
7	A	603	HDD	C4C-C3C-C2C	-2.36	104.37	107.30
8	A	605	HEB	CHC-C4B-NB	2.35	127.27	124.37
8	A	605	HEB	C4D-C3D-C2D	-2.29	103.56	106.89
5	B	401	UQ8	C30-C29-C31	2.24	119.12	115.23
8	A	605	HEB	CHC-C1C-NC	2.21	127.87	123.86
8	A	604	HEB	C1A-C2A-C3A	-2.20	104.20	107.11
8	A	604	HEB	O2D-CGD-CBD	2.19	120.91	114.00
8	A	604	HEB	CMC-C2C-C1C	2.19	128.75	125.42
7	A	603	HDD	CHC-C1C-NC	-2.17	119.92	123.86
5	B	401	UQ8	C46-C44-C45	2.16	119.57	114.59
8	A	605	HEB	CBC-CAC-C3C	-2.13	116.87	127.53
8	A	604	HEB	C4B-C3B-C2B	-2.13	103.79	106.89
8	A	605	HEB	CHD-C1D-ND	2.11	126.98	124.37
8	A	604	HEB	CHC-C1C-C2C	-2.11	121.31	127.43
8	A	605	HEB	CHA-C4D-ND	2.07	126.65	124.42
8	A	605	HEB	CAA-C2A-C1A	-2.06	120.66	124.85

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	604	HEB	NA
8	A	605	HEB	NA

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	402	POV	C11-O12-P-O13
6	B	402	POV	O12-C11-C12-N
6	B	403	POV	C1-O11-P-O12
6	B	403	POV	C1-O11-P-O13
6	B	403	POV	O21-C2-C3-O31
6	A	601	POV	C11-O12-P-O11

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Mol	Chain	Res	Type	Atoms
6	A	601	POV	C11-O12-P-O13
6	A	601	POV	O12-C11-C12-N
6	A	601	POV	C22-C21-O21-C2
6	A	601	POV	O22-C21-O21-C2
6	A	602	POV	C1-O11-P-O12
6	A	602	POV	C1-O11-P-O13
6	A	602	POV	O22-C21-O21-C2
7	A	603	HDD	C2B-C3B-CAB-CBB
7	A	603	HDD	C4B-C3B-CAB-CBB
8	A	605	HEB	C1A-C2A-CAA-CBA
8	A	605	HEB	C3A-C2A-CAA-CBA
6	B	402	POV	O32-C31-O31-C3
8	A	605	HEB	C2B-C3B-CAB-CBB
8	A	605	HEB	C4B-C3B-CAB-CBB
6	B	402	POV	C32-C31-O31-C3
6	B	403	POV	O22-C21-O21-C2
6	B	403	POV	C22-C21-O21-C2
6	A	602	POV	C22-C21-O21-C2
5	B	401	UQ8	C40-C39-C41-C42
5	B	401	UQ8	C12-C11-C9-C10
5	B	401	UQ8	C38-C39-C41-C42
5	B	401	UQ8	C39-C41-C42-C43
5	B	401	UQ8	C24-C26-C27-C28
5	B	401	UQ8	C19-C21-C22-C23
5	B	401	UQ8	C14-C16-C17-C18
6	A	601	POV	C32-C31-O31-C3
6	A	602	POV	C32-C31-O31-C3
6	A	601	POV	O32-C31-O31-C3
6	B	402	POV	C31-C32-C33-C34
6	A	602	POV	C31-C32-C33-C34
6	A	602	POV	O32-C31-O31-C3
5	B	401	UQ8	C12-C11-C9-C8
6	B	403	POV	C31-C32-C33-C34
6	B	402	POV	C24-C25-C26-C27
6	B	402	POV	C311-C312-C313-C314
6	B	403	POV	C311-C312-C313-C314
6	B	403	POV	C23-C24-C25-C26
6	A	602	POV	C34-C35-C36-C37
6	A	601	POV	C35-C36-C37-C38
6	B	402	POV	C34-C35-C36-C37
6	A	602	POV	C210-C211-C212-C213
6	A	601	POV	C214-C215-C216-C217

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Mol	Chain	Res	Type	Atoms
6	B	402	POV	C311-C310-C39-C38
6	A	602	POV	C22-C23-C24-C25
6	A	602	POV	C36-C37-C38-C39
6	B	402	POV	C25-C26-C27-C28
6	A	601	POV	C311-C312-C313-C314
6	A	601	POV	C32-C33-C34-C35
6	B	402	POV	C26-C27-C28-C29
6	B	403	POV	C26-C27-C28-C29
6	A	601	POV	C210-C211-C212-C213
6	B	403	POV	C37-C38-C39-C310
6	B	403	POV	C1-O11-P-O14
6	B	403	POV	C32-C31-O31-C3
6	A	601	POV	C313-C314-C315-C316
6	A	601	POV	C23-C24-C25-C26
6	B	402	POV	C21-C22-C23-C24
6	A	601	POV	C215-C216-C217-C218
6	A	601	POV	C1-C2-C3-O31
6	A	602	POV	C211-C212-C213-C214
6	B	403	POV	O32-C31-O31-C3
6	A	601	POV	C37-C38-C39-C310
6	B	403	POV	C310-C311-C312-C313
6	B	402	POV	C310-C311-C312-C313
6	B	403	POV	O11-C1-C2-O21
6	B	402	POV	C1-C2-C3-O31
6	B	403	POV	C1-C2-C3-O31
6	A	601	POV	C39-C310-C311-C312
6	B	402	POV	O21-C2-C3-O31
6	B	402	POV	C23-C24-C25-C26
6	B	403	POV	C32-C33-C34-C35
6	A	602	POV	O12-C11-C12-N
5	B	401	UQ8	C25-C24-C26-C27
6	B	403	POV	O11-C1-C2-C3
6	A	602	POV	O11-C1-C2-C3
6	A	601	POV	C25-C26-C27-C28
6	A	602	POV	O11-C1-C2-O21
6	A	601	POV	O21-C2-C3-O31
6	A	601	POV	C310-C311-C312-C313
6	B	403	POV	C36-C37-C38-C39
6	B	402	POV	C1-O11-P-O14
6	B	402	POV	C11-O12-P-O11
6	B	402	POV	C11-O12-P-O14
6	B	403	POV	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
5	B	401	UQ8	C5-C4-O4-C4M
6	B	403	POV	C312-C313-C314-C315
6	A	602	POV	C21-C22-C23-C24
6	A	601	POV	C29-C210-C211-C212
6	B	402	POV	C35-C36-C37-C38
7	A	603	HDD	CAA-CBA-CGA-O1A
7	A	603	HDD	C2A-CAA-CBA-CGA
8	A	605	HEB	CAD-CBD-CGD-O1D
8	A	604	HEB	CAD-CBD-CGD-O1D
7	A	603	HDD	CAA-CBA-CGA-O2A
8	A	605	HEB	CAD-CBD-CGD-O2D
5	B	401	UQ8	C3-C4-O4-C4M
6	A	601	POV	C311-C310-C39-C38
6	B	402	POV	C210-C211-C212-C213
5	B	401	UQ8	C23-C24-C26-C27
8	A	604	HEB	CAD-CBD-CGD-O2D
6	A	601	POV	C31-C32-C33-C34
6	A	602	POV	C27-C28-C29-C210
6	B	402	POV	C27-C28-C29-C210
6	B	403	POV	C27-C28-C29-C210
6	A	601	POV	C21-C22-C23-C24
6	B	403	POV	C25-C26-C27-C28
6	B	402	POV	C313-C314-C315-C316
8	A	605	HEB	CAA-CBA-CGA-O1A
8	A	605	HEB	CAA-CBA-CGA-O2A

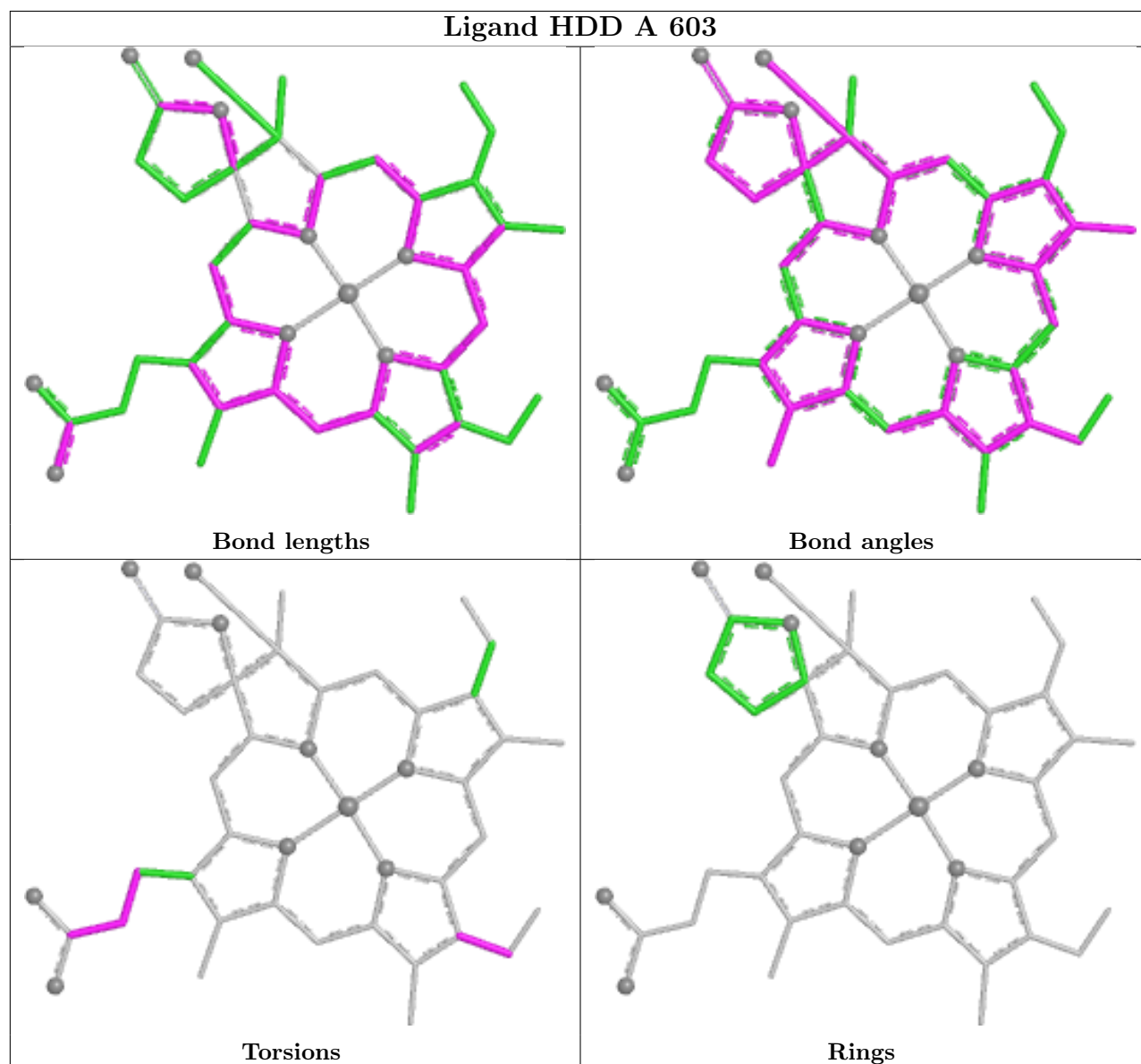
There are no ring outliers.

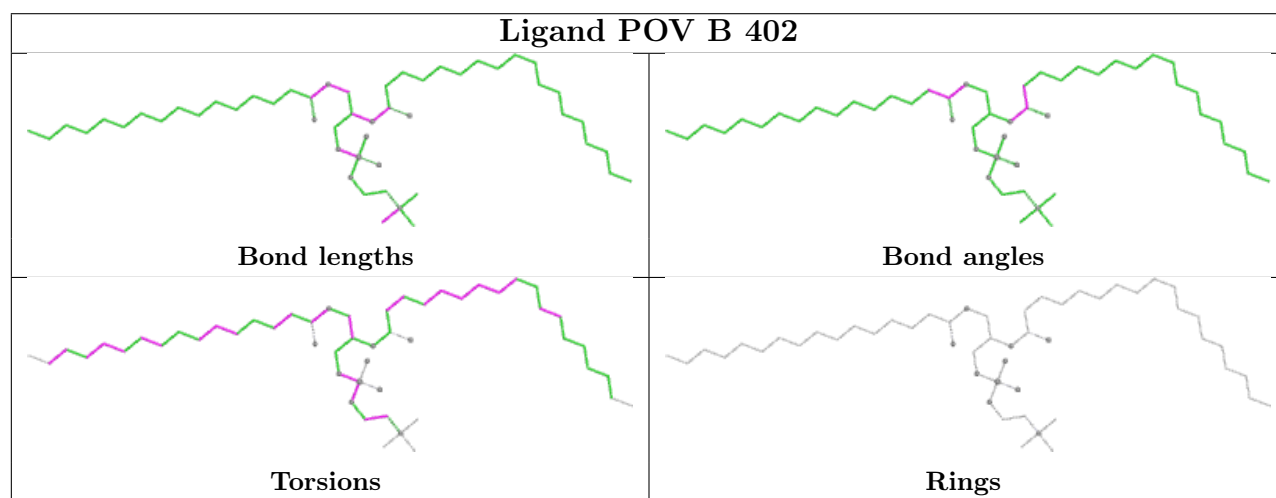
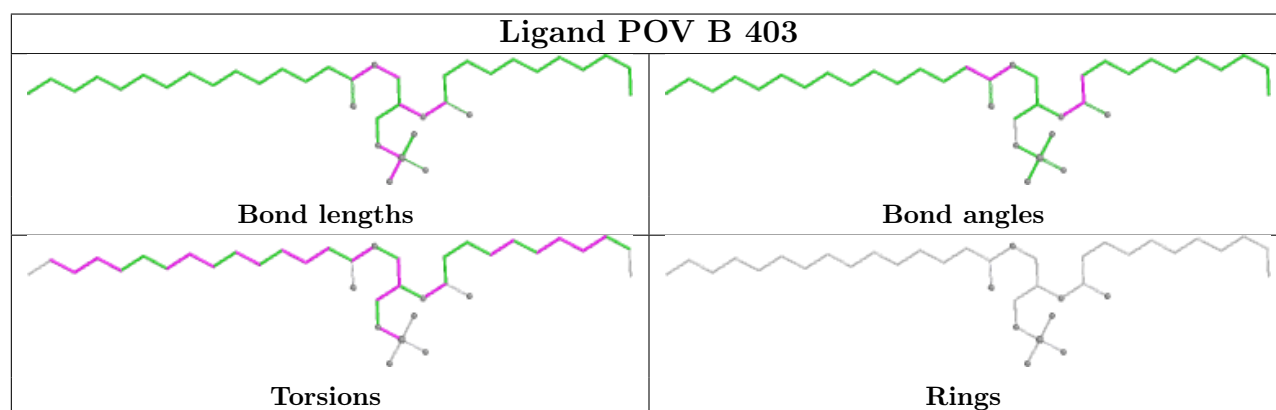
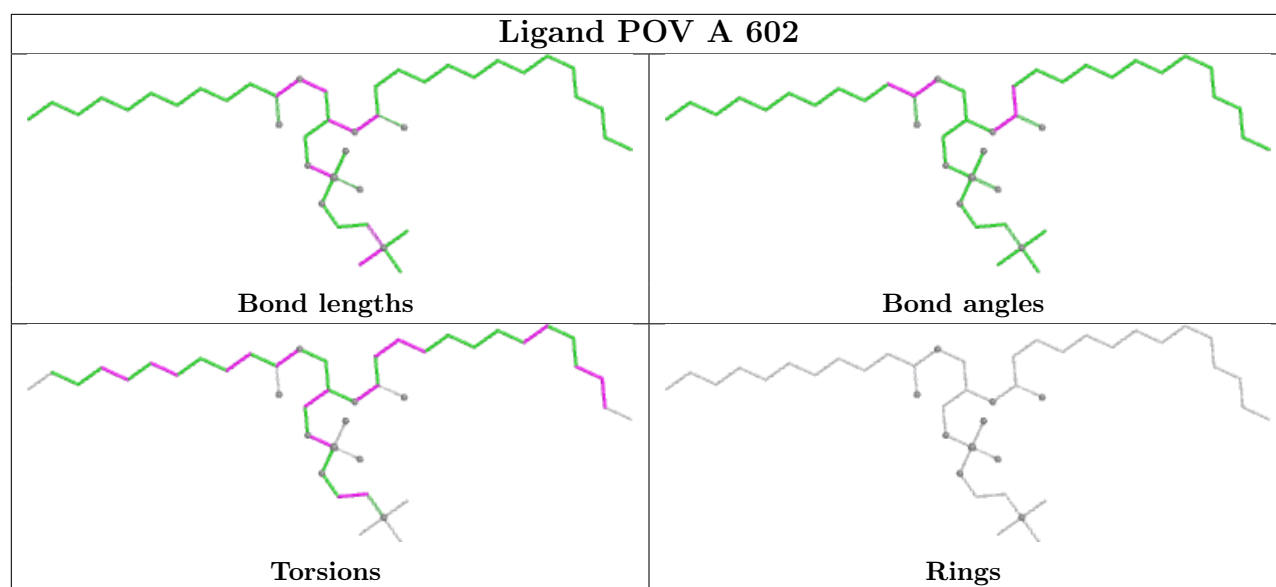
8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	603	HDD	3	0
6	A	602	POV	3	0
6	B	402	POV	2	0
9	A	606	OXY	1	0
5	B	401	UQ8	8	0
8	A	604	HEB	4	0
6	A	601	POV	2	0
8	A	605	HEB	9	0

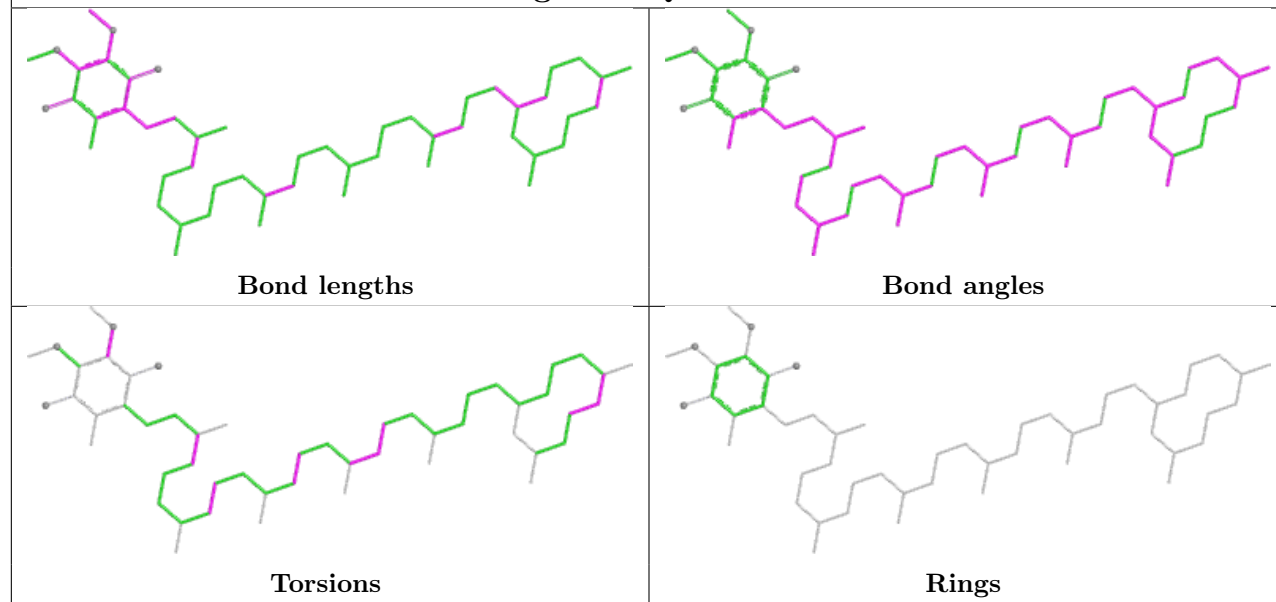
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

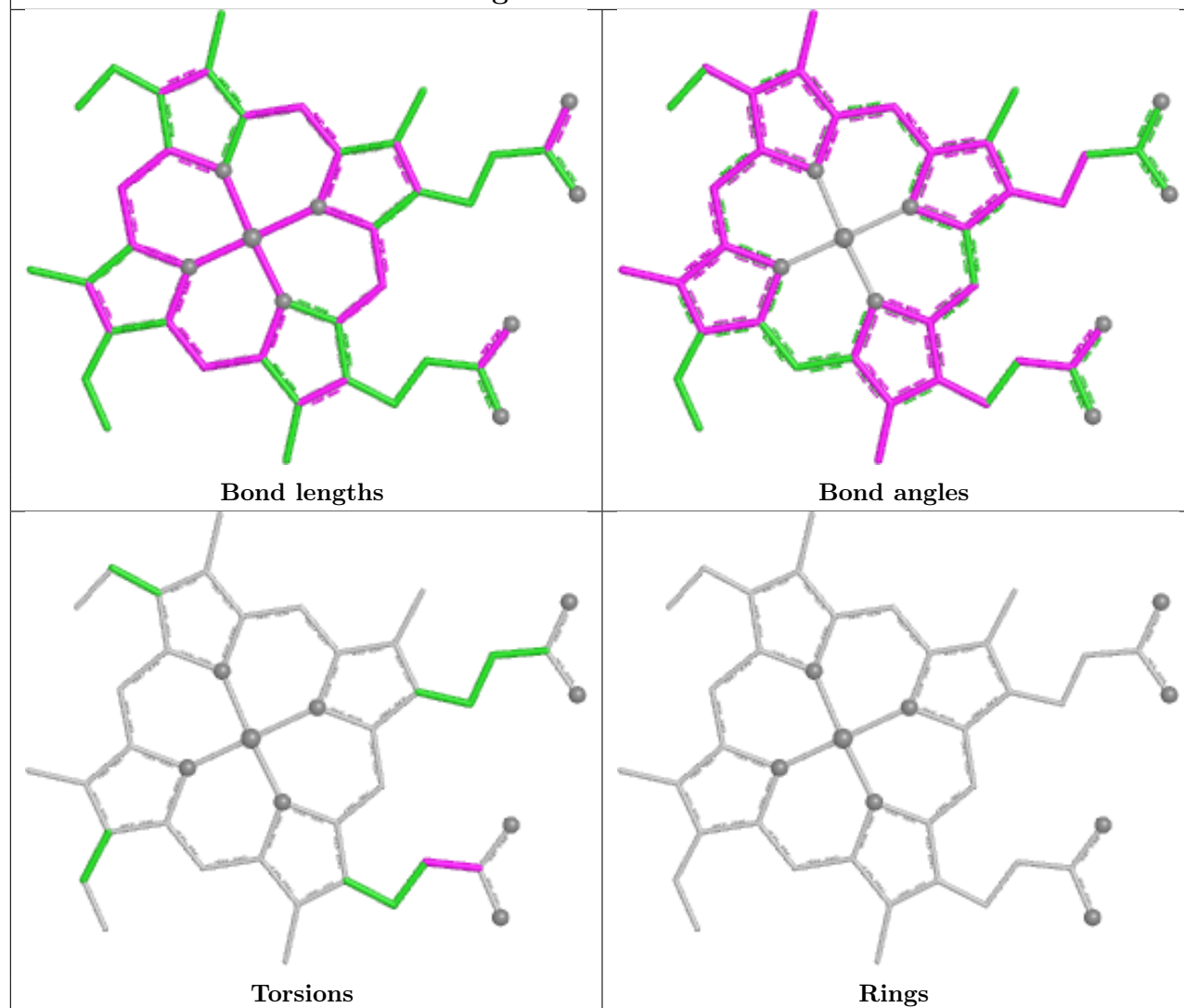


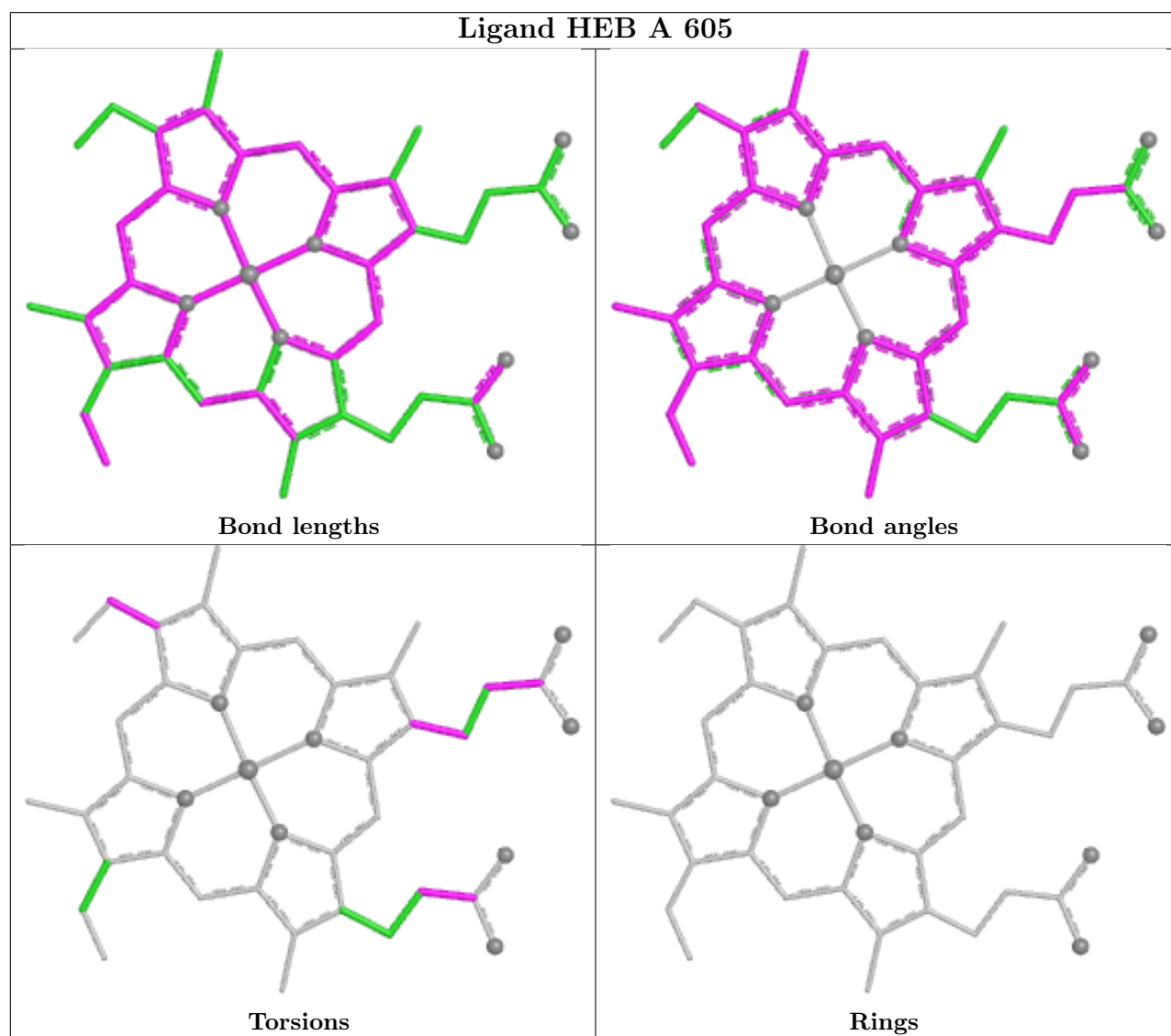
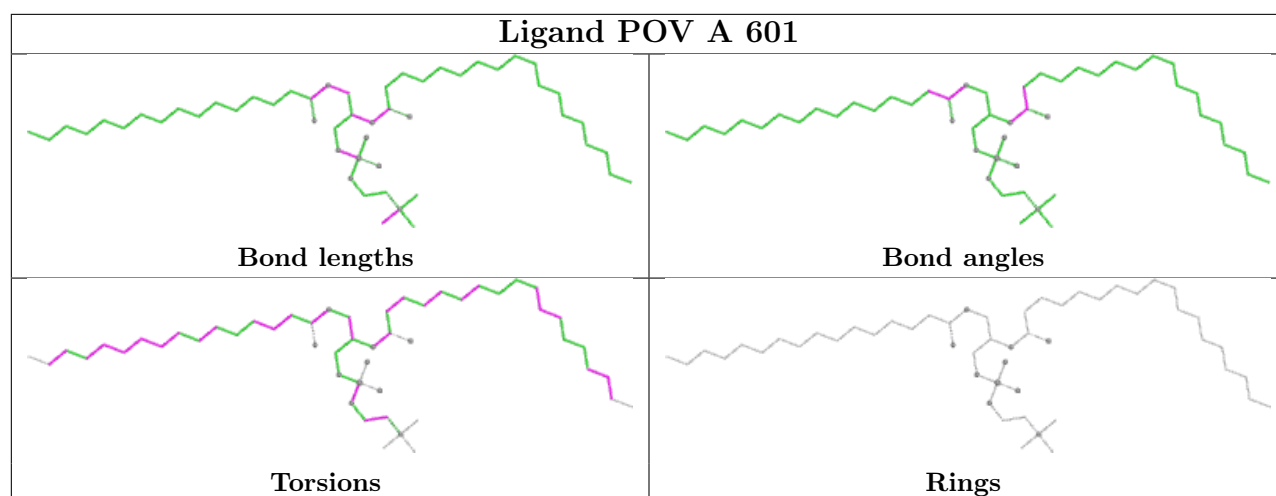


Ligand UQ8 B 401



Ligand HEB A 604





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.

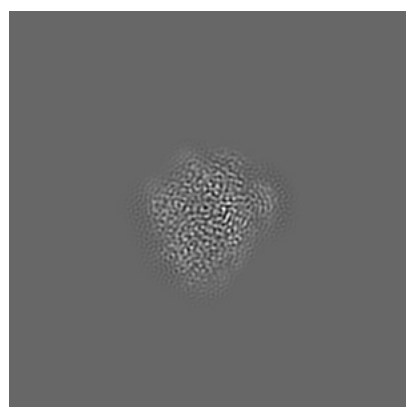
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4908. These allow visual inspection of the internal detail of the map and identification of artifacts.

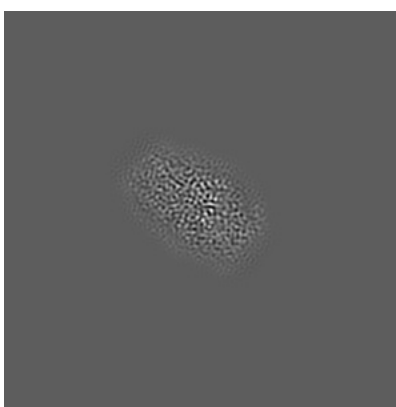
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

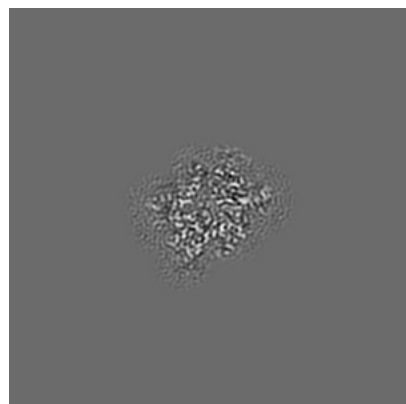


Z

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

6.2 Central slices [i](#)

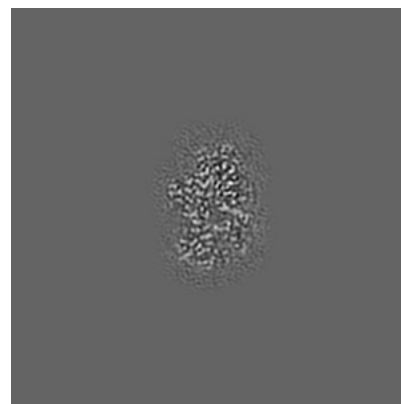
6.2.1 Primary map



X Index: 150



Y Index: 150

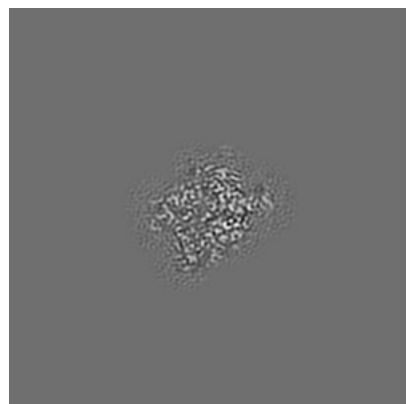


Z Index: 150

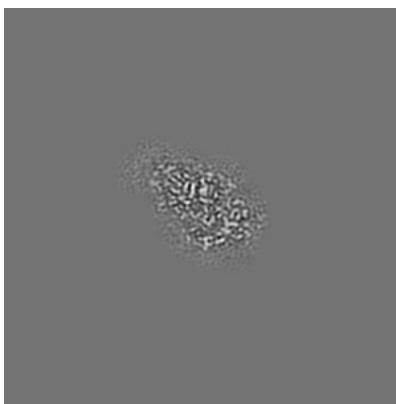
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

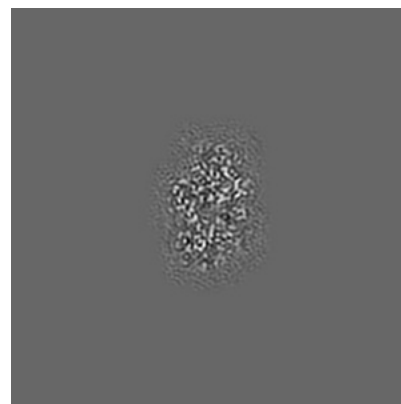
6.3.1 Primary map



X Index: 154



Y Index: 161

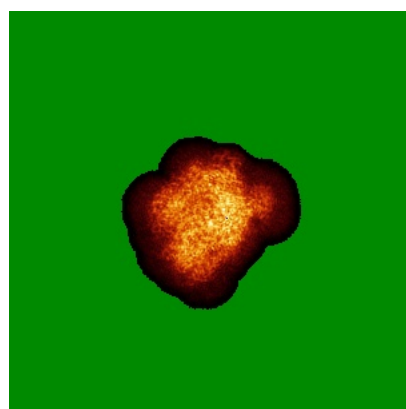


Z Index: 154

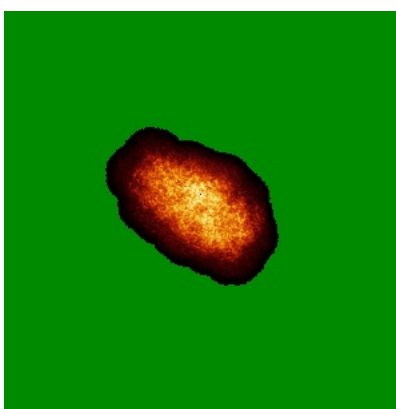
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

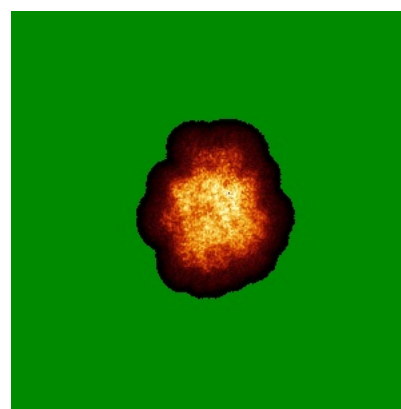
6.4.1 Primary map



X



Y



Z

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 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

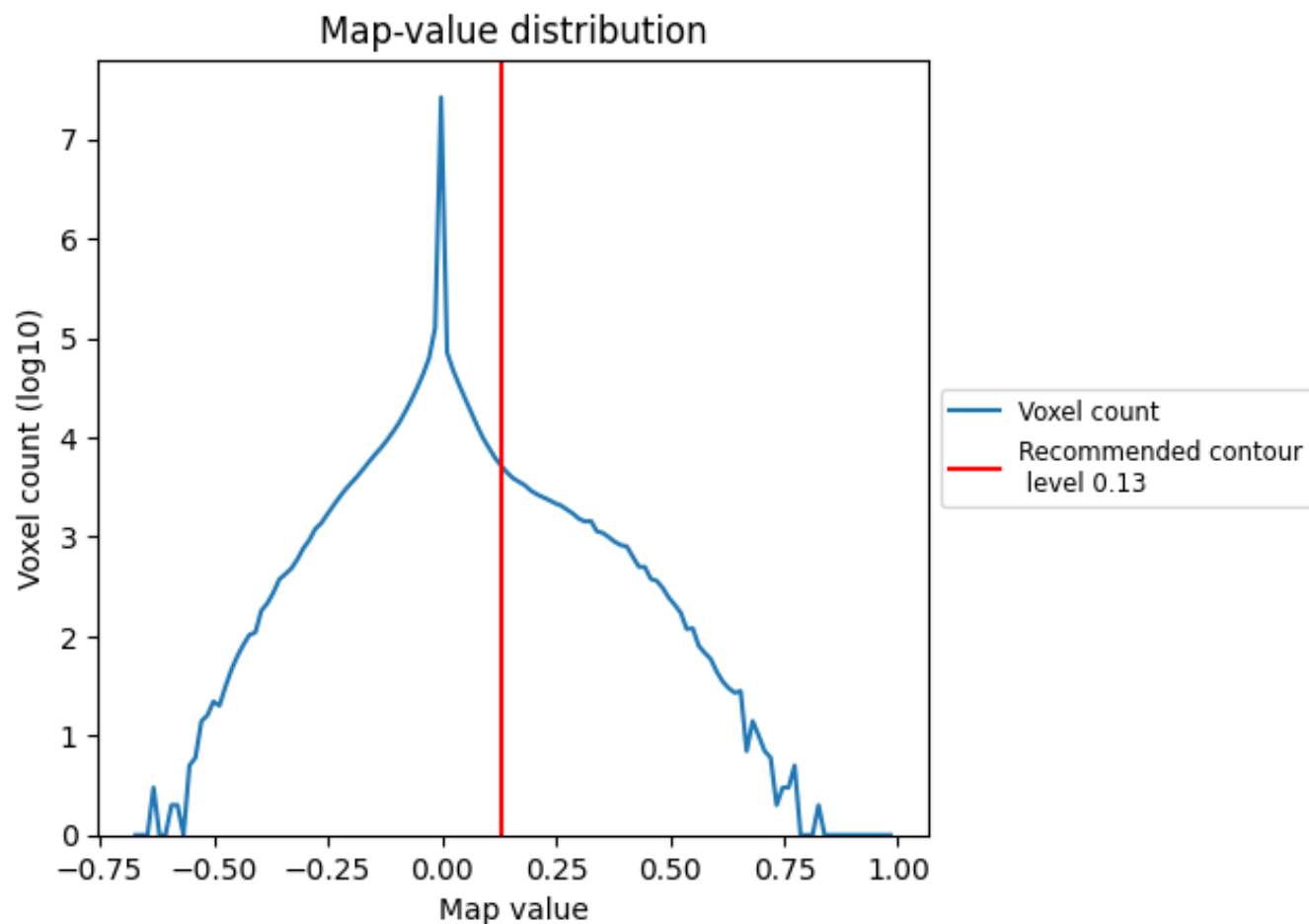
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

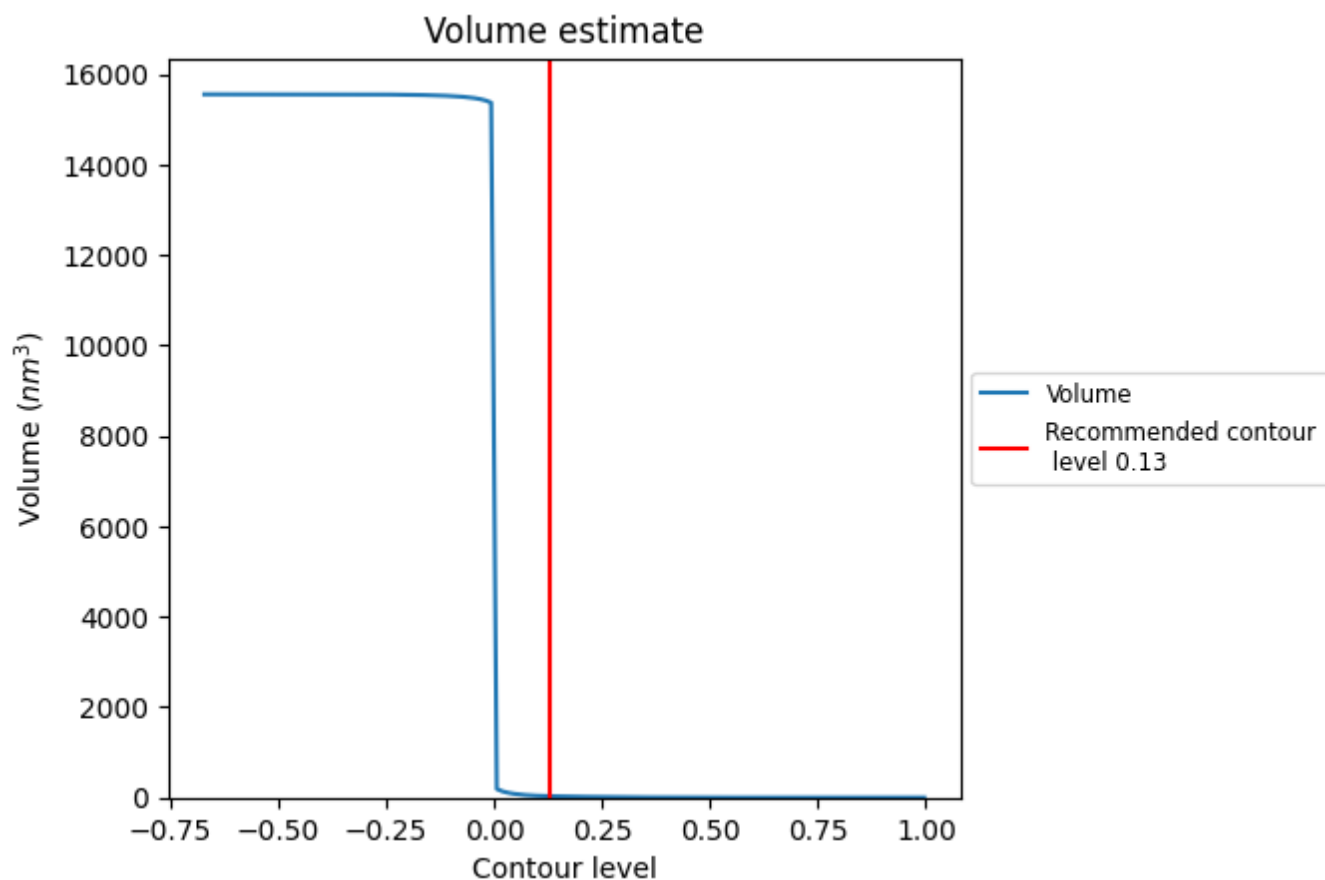
This section contains the results of statistical analysis of the map.

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.

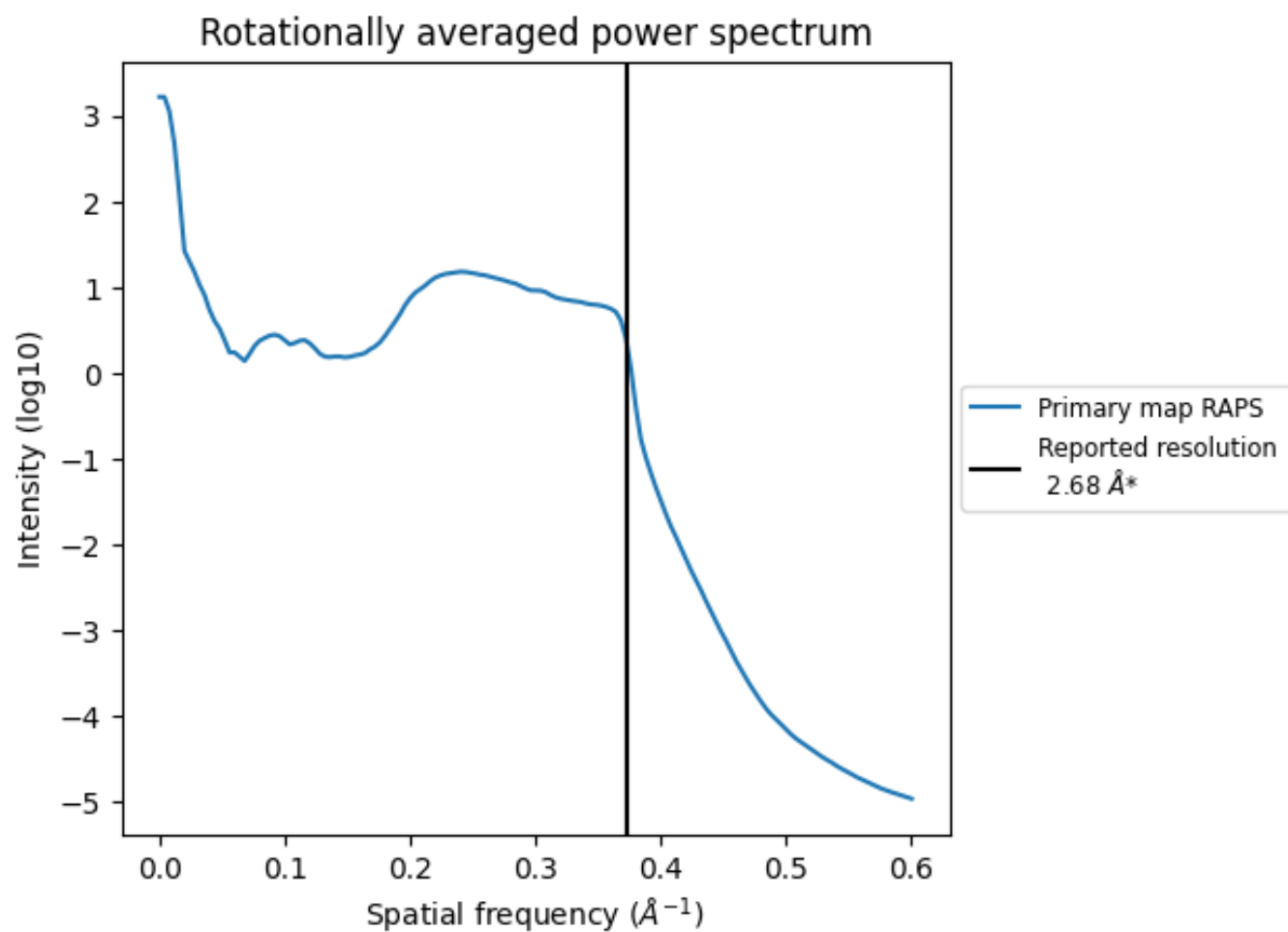
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 30 nm^3 ; this corresponds to an approximate mass of 27 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 ⓘ

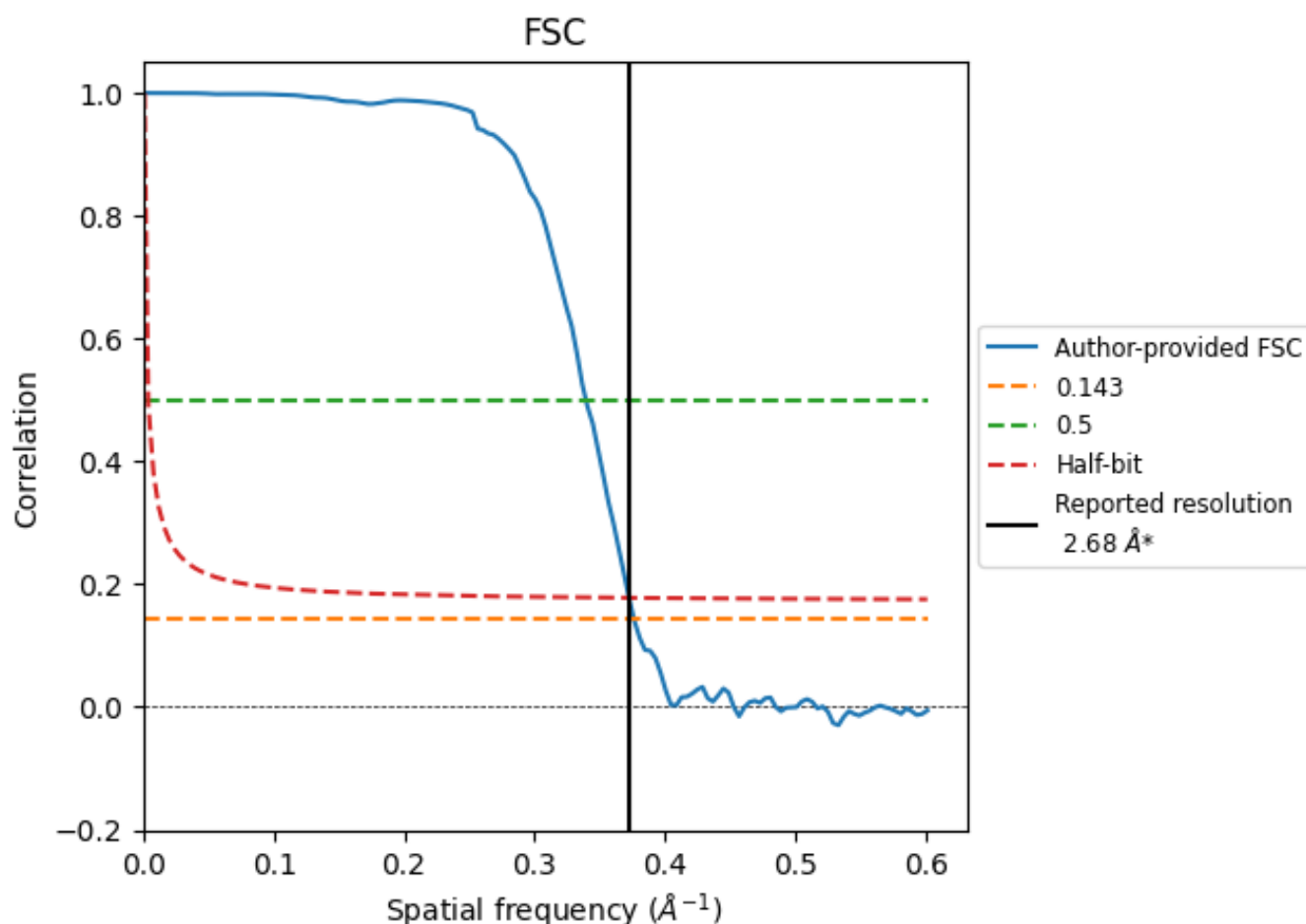


*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

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 0.373 Å⁻¹

8.2 Resolution estimates [i](#)

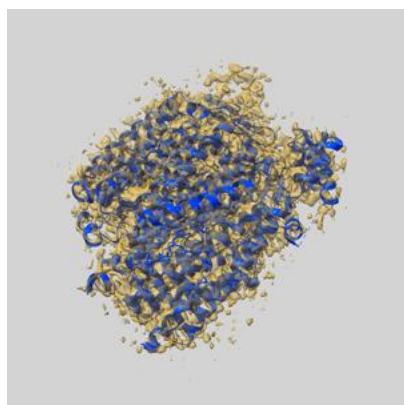
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	2.66	2.95	2.69
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

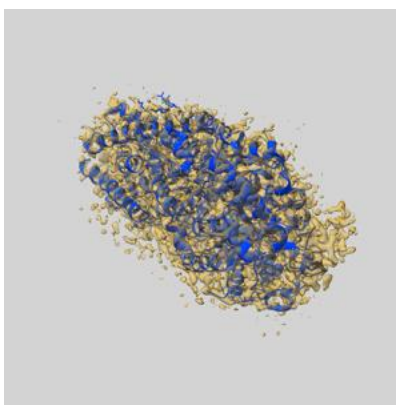
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4908 and PDB model 6RKO. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

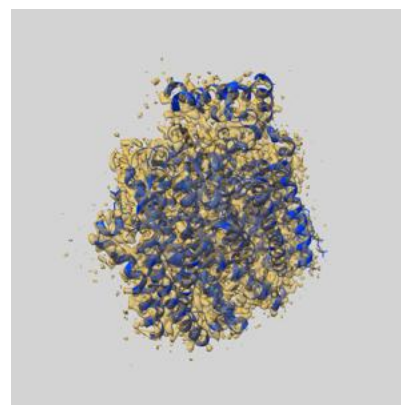
9.1 Map-model overlay [i](#)



X



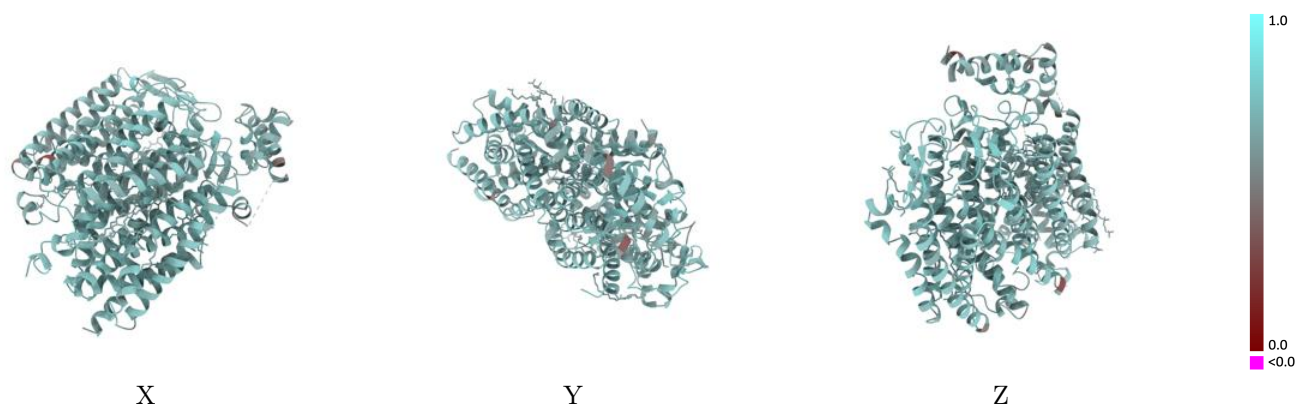
Y



Z

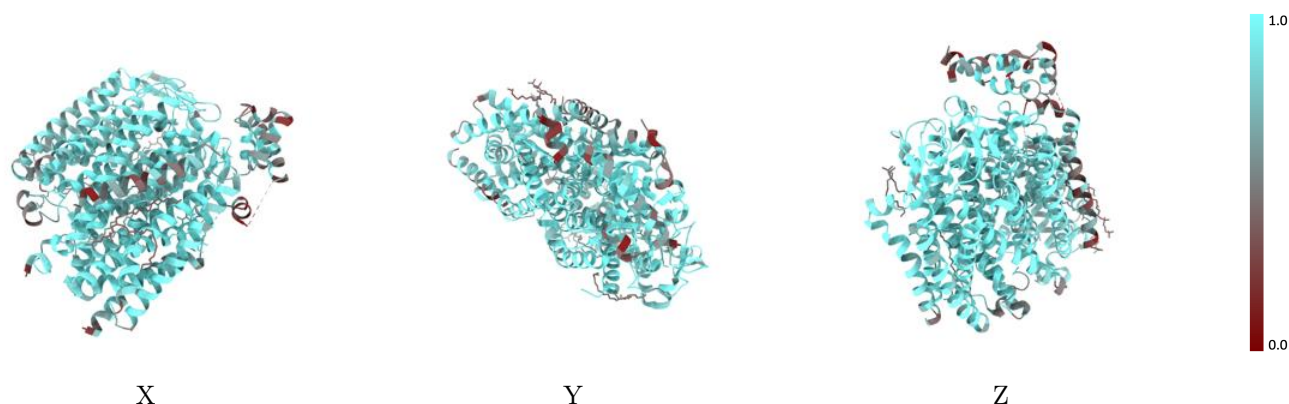
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



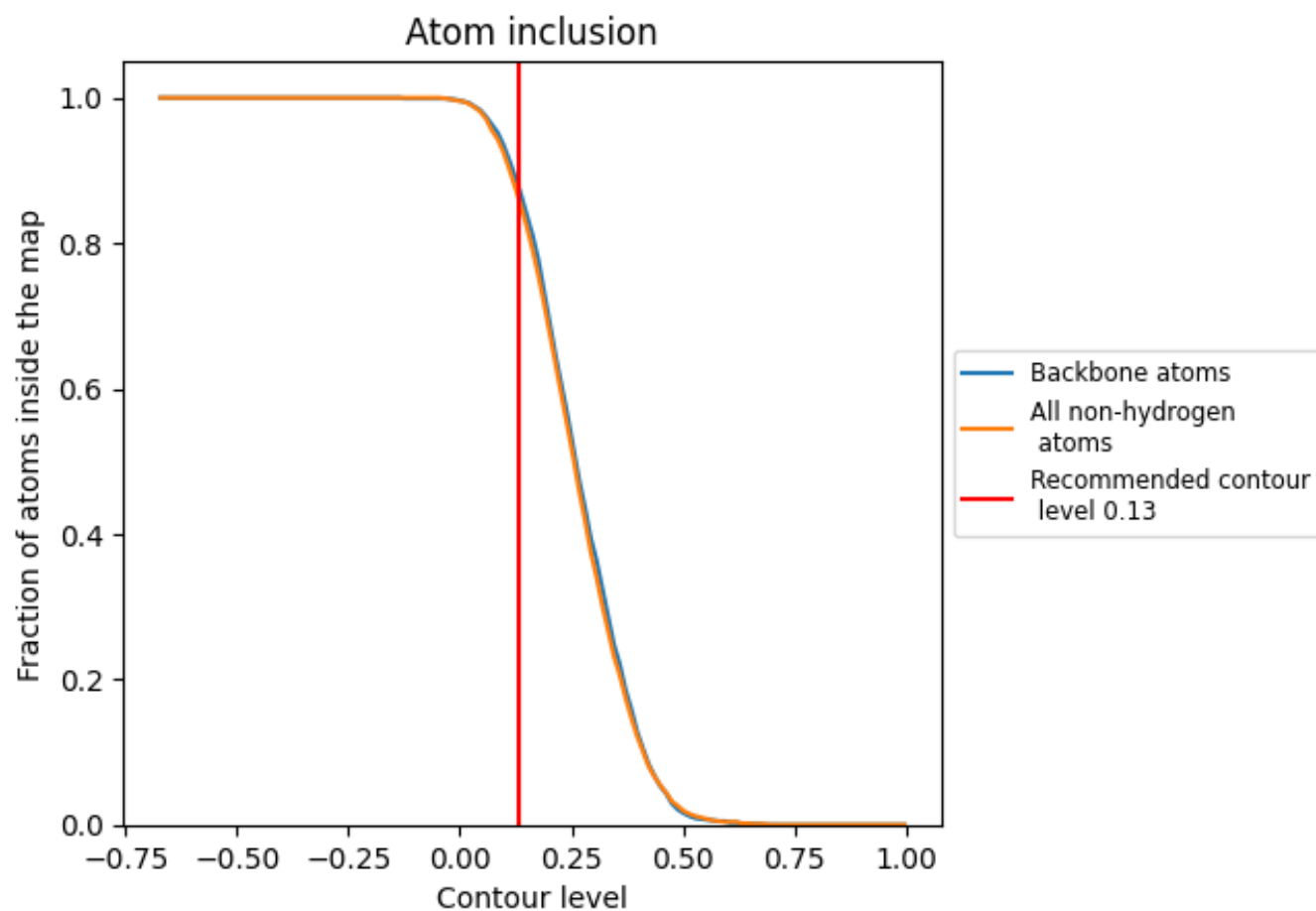
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 86% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8650	0.6650
A	0.8700	0.6660
B	0.8990	0.6690
H	0.4870	0.6320
X	0.6740	0.6370

