



Full wwPDB EM Validation Report ⓘ

May 27, 2024 – 10:11 AM JST

PDB ID : 7DNZ
EMDB ID : EMD-30791
Title : Cryo-EM structure of the human ABCB6 (Hemin and GSH-bound)
Authors : Kim, S.; Lee, S.S.; Park, J.G.; Kim, J.W.; Kim, S.; Kim, N.J.; Hong, S.; Kang, J.Y.; Jin, M.S.
Deposited on : 2020-12-11
Resolution : 3.60 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.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

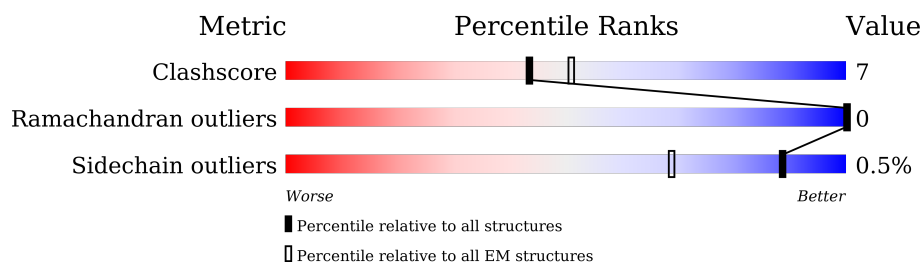
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	842	<div> <div>19%</div> <div>57%</div> <div>13%</div> <div>30%</div> </div>
1	B	842	<div> <div>19%</div> <div>59%</div> <div>11%</div> <div>30%</div> </div>

2 Entry composition [i](#)

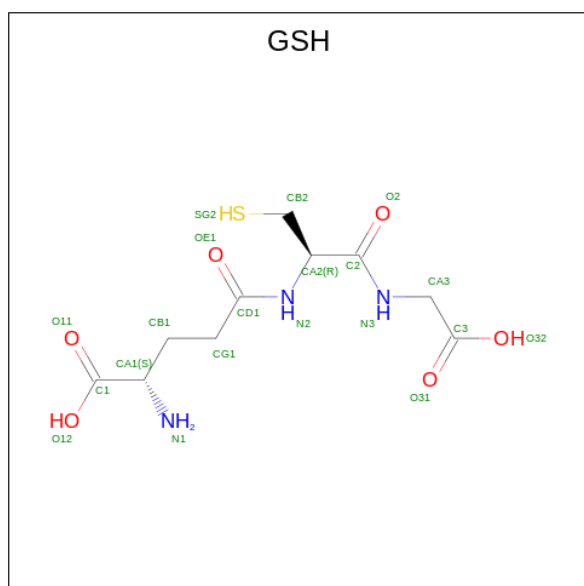
There are 4 unique types of molecules in this entry. The entry contains 9671 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-binding cassette sub-family B member 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	591	Total	C	N	O	S	0	0
			4669	2998	809	845	17		
1	B	591	Total	C	N	O	S	0	0
			4669	2998	809	845	17		

- Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: C₁₀H₁₇N₃O₆S).

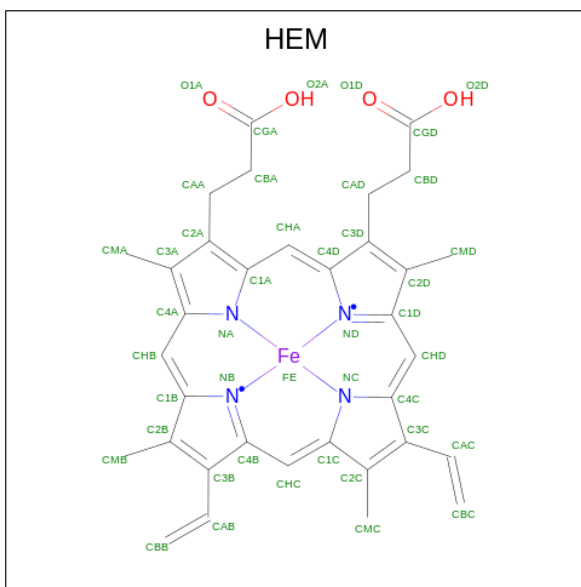


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			20	10	3	6	1	
2	A	1	Total	C	N	O	S	0
			20	10	3	6	1	
2	B	1	Total	C	N	O	S	0
			20	10	3	6	1	
2	B	1	Total	C	N	O	S	0
			20	10	3	6	1	

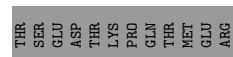
- Molecule 3 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄).



- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	283866	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.223	Depositor
Minimum map value	-0.849	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.306	Depositor
Map size (\AA)	232.4, 232.4, 232.4	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, GSH, HEM

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	0.47	0/4760	0.62	0/6456
1	B	0.47	0/4760	0.61	0/6456
All	All	0.47	0/9520	0.61	0/12912

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	4669	0	4726	77	0
1	B	4669	0	4726	71	0
2	A	40	0	30	1	0
2	B	40	0	30	0	0
3	A	105	0	147	2	0
3	B	105	0	147	2	0
4	B	43	0	30	0	0
All	All	9671	0	9836	137	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 7.

All (137) 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:B:276:ARG:HH21	1:B:279:ASN:HD22	1.40	0.69
1:A:276:ARG:HH21	1:A:279:ASN:HD22	1.40	0.69
1:A:638:ARG:NH1	1:A:654:ILE:O	2.30	0.64
1:B:638:ARG:NH1	1:B:654:ILE:O	2.30	0.64
1:A:542:MET:CE	1:B:319:GLY:HA3	2.29	0.63
1:A:542:MET:HE1	1:B:319:GLY:HA3	1.82	0.61
1:B:428:THR:OG1	1:B:501:GLN:NE2	2.36	0.58
1:A:428:THR:OG1	1:A:501:GLN:NE2	2.36	0.58
1:A:703:ALA:O	1:A:734:ARG:NH1	2.37	0.58
1:B:703:ALA:O	1:B:734:ARG:NH1	2.37	0.57
1:A:589:ARG:NH2	1:A:612:THR:OG1	2.38	0.57
1:B:589:ARG:NH2	1:B:612:THR:OG1	2.38	0.56
1:B:683:ASN:O	1:B:739:ARG:NH2	2.38	0.56
1:A:673:THR:HG21	1:A:736:ALA:HB2	1.88	0.56
1:B:673:THR:HG21	1:B:736:ALA:HB2	1.88	0.56
1:A:320:THR:HG23	1:A:542:MET:HB3	1.88	0.55
1:A:319:GLY:HA3	1:B:542:MET:CE	2.36	0.55
1:B:763:ARG:HA	1:B:766:GLN:HB2	1.89	0.55
1:A:683:ASN:O	1:A:739:ARG:NH2	2.38	0.55
1:A:625:SER:O	1:A:798:LYS:NZ	2.40	0.54
1:B:625:SER:O	1:B:798:LYS:NZ	2.40	0.54
1:B:648:ARG:HG2	1:B:653:ASP:HA	1.90	0.54
1:A:682:ASP:HA	1:A:685:ARG:HB2	1.90	0.54
1:A:648:ARG:HG2	1:A:653:ASP:HA	1.90	0.53
1:A:763:ARG:HA	1:A:766:GLN:HB2	1.89	0.53
1:A:684:ILE:HG22	1:A:735:VAL:HG13	1.91	0.53
1:B:279:ASN:OD1	1:B:539:GLN:NE2	2.42	0.52
1:A:279:ASN:OD1	1:A:539:GLN:NE2	2.43	0.52
1:B:595:VAL:HG21	1:B:647:ILE:HG13	1.91	0.52
1:A:693:ASN:OD1	1:A:694:ASP:N	2.42	0.52
1:B:682:ASP:HA	1:B:685:ARG:HB2	1.90	0.52
1:A:595:VAL:HG21	1:A:647:ILE:HG13	1.91	0.52
1:B:693:ASN:OD1	1:B:694:ASP:N	2.42	0.52
1:B:684:ILE:HG22	1:B:735:VAL:HG13	1.91	0.52
1:A:332:PHE:HB2	1:B:495:VAL:HG21	1.92	0.51
1:A:495:VAL:HG21	1:B:332:PHE:HB2	1.94	0.50
1:A:808:HIS:ND1	1:A:818:TYR:OH	2.30	0.50
1:B:675:LEU:HD11	1:B:683:ASN:HB3	1.94	0.50
1:B:576:ASP:N	1:B:576:ASP:OD1	2.45	0.50
1:A:576:ASP:N	1:A:576:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:SER:HA	1:B:789:VAL:HG22	1.94	0.49
1:A:675:LEU:HD11	1:A:683:ASN:HB3	1.94	0.49
1:A:786:SER:HA	1:A:789:VAL:HG22	1.95	0.49
1:B:357:SER:OG	1:B:358:LEU:N	2.46	0.48
1:A:357:SER:OG	1:A:358:LEU:N	2.46	0.48
1:A:319:GLY:HA3	1:B:542:MET:HE1	1.97	0.47
1:A:589:ARG:N	1:A:650:ASP:OD1	2.39	0.47
1:B:663:ARG:HA	1:B:666:ILE:HG22	1.96	0.47
1:A:314:PHE:HD2	1:A:315:LEU:HD12	1.80	0.47
1:A:546:TRP:HH2	1:B:320:THR:HG21	1.80	0.47
1:B:589:ARG:N	1:B:650:ASP:OD1	2.39	0.47
3:A:904:Y01:HAO1	3:A:904:Y01:HAP1	1.58	0.46
1:A:375:ARG:HB3	1:A:560:ASP:OD2	2.15	0.46
1:B:375:ARG:HB3	1:B:560:ASP:OD2	2.15	0.46
1:A:663:ARG:HA	1:A:666:ILE:HG22	1.97	0.46
1:A:694:ASP:N	1:A:694:ASP:OD1	2.49	0.46
1:A:293:LEU:HD11	1:B:520:VAL:HG13	1.98	0.45
1:A:685:ARG:NH1	1:A:691:ALA:O	2.49	0.45
1:B:694:ASP:N	1:B:694:ASP:OD1	2.49	0.45
1:A:375:ARG:O	1:A:379:SER:HB3	2.16	0.45
1:B:685:ARG:NH1	1:B:691:ALA:O	2.49	0.45
1:A:480:ILE:O	1:A:484:GLN:HG2	2.17	0.45
1:A:520:VAL:HG13	1:B:293:LEU:HD11	1.99	0.45
3:B:905:Y01:HAO1	3:B:905:Y01:HAP1	1.60	0.45
1:A:614:MET:H	1:A:617:GLN:HG3	1.82	0.44
1:A:505:ILE:HG13	1:A:541:TYR:CD1	2.53	0.44
1:A:637:PHE:CE2	1:A:663:ARG:HG3	2.52	0.44
1:B:375:ARG:O	1:B:379:SER:HB3	2.17	0.44
1:B:505:ILE:HG13	1:B:541:TYR:CD1	2.53	0.44
1:B:637:PHE:CE2	1:B:663:ARG:HG3	2.53	0.44
1:B:413:PHE:HE1	1:B:515:LEU:HD22	1.83	0.44
1:B:604:GLU:OE2	1:B:607:GLN:NE2	2.51	0.44
1:B:614:MET:H	1:B:617:GLN:HG3	1.82	0.44
1:A:413:PHE:HE1	1:A:515:LEU:HD22	1.83	0.44
1:B:480:ILE:O	1:B:484:GLN:HG2	2.17	0.44
1:A:439:ARG:HE	1:A:439:ARG:HB2	1.64	0.44
1:A:737:ILE:HA	1:A:740:THR:HG22	2.00	0.44
1:A:572:THR:HG22	1:A:574:VAL:HG13	2.00	0.43
1:A:604:GLU:OE2	1:A:607:GLN:NE2	2.51	0.43
1:A:624:PRO:HB2	1:A:798:LYS:HD3	1.99	0.43
1:A:661:SER:O	1:A:665:HIS:ND1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ILE:HD13	1:A:481:ILE:HA	1.90	0.43
1:A:542:MET:HE3	1:B:319:GLY:HA3	1.98	0.43
1:B:769:LEU:HA	1:B:772:VAL:HG12	1.99	0.43
1:A:464:LYS:HD2	1:A:464:LYS:HA	1.89	0.43
1:A:769:LEU:HA	1:A:772:VAL:HG12	2.00	0.43
1:B:624:PRO:HB2	1:B:798:LYS:HD3	1.99	0.43
1:B:671:GLN:NE2	1:B:671:GLN:HA	2.34	0.43
1:B:737:ILE:HA	1:B:740:THR:HG22	2.00	0.43
1:A:671:GLN:NE2	1:A:671:GLN:HA	2.34	0.42
1:B:245:LYS:H	1:B:245:LYS:HG3	1.68	0.42
1:A:293:LEU:HD21	1:B:520:VAL:HG11	2.01	0.42
1:A:293:LEU:HD12	1:A:293:LEU:HA	1.84	0.42
1:A:413:PHE:CE1	1:A:515:LEU:HD22	2.54	0.42
1:A:520:VAL:HG11	1:B:293:LEU:HD21	2.01	0.42
1:B:538:ILE:HD13	1:B:538:ILE:HA	1.91	0.42
1:B:577:LEU:HD23	1:B:577:LEU:HA	1.95	0.42
1:B:661:SER:O	1:B:665:HIS:ND1	2.51	0.42
1:A:514:LEU:HD23	1:A:514:LEU:HA	1.92	0.42
1:A:540:LEU:HA	1:A:540:LEU:HD23	1.82	0.41
1:B:413:PHE:CE1	1:B:515:LEU:HD22	2.54	0.41
1:B:762:GLU:OE1	1:B:763:ARG:NH2	2.54	0.41
1:A:524:LYS:HE2	1:A:524:LYS:HB3	1.92	0.41
1:B:693:ASN:HA	1:B:696:VAL:HG12	2.02	0.41
1:B:439:ARG:HE	1:B:439:ARG:HB2	1.64	0.41
1:B:572:THR:HG22	1:B:574:VAL:HG13	2.00	0.41
1:A:279:ASN:ND2	1:A:397:ASP:OD1	2.53	0.41
1:A:319:GLY:HA3	1:B:542:MET:HE3	2.03	0.41
1:B:255:PRO:HG2	1:B:261:LEU:HB3	2.02	0.41
1:B:462:THR:HA	1:B:465:TYR:HD1	1.86	0.41
1:A:762:GLU:OE1	1:A:763:ARG:NH2	2.54	0.41
1:B:412:TRP:CD2	3:B:905:Y01:HAI	2.55	0.41
1:B:705:ILE:HG13	1:B:734:ARG:HD3	2.02	0.41
1:A:586:GLN:HG2	1:A:587:LYS:HD3	2.03	0.41
2:A:902:GSH:HN2	1:B:450:ARG:HG3	1.85	0.41
1:B:616:GLY:H	1:B:777:THR:HG22	1.86	0.41
1:A:577:LEU:HD23	1:A:577:LEU:HA	1.95	0.41
1:A:596:HIS:HA	1:A:606:LEU:HB3	2.03	0.41
1:B:450:ARG:HD3	1:B:450:ARG:HA	1.87	0.41
1:B:464:LYS:HA	1:B:464:LYS:HD2	1.89	0.41
1:B:596:HIS:HA	1:B:606:LEU:HB3	2.03	0.41
1:B:789:VAL:HG12	1:B:808:HIS:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:TRP:NE1	1:A:570:GLU:OE2	2.44	0.41
1:A:462:THR:HA	1:A:465:TYR:HD1	1.86	0.41
1:B:279:ASN:ND2	1:B:397:ASP:OD1	2.53	0.41
1:B:425:LEU:HA	1:B:425:LEU:HD23	1.88	0.41
1:B:583:LEU:HD22	1:B:665:HIS:CG	2.56	0.41
1:B:802:ILE:HD11	1:B:805:ARG:HD2	2.03	0.41
1:A:693:ASN:HA	1:A:696:VAL:HG12	2.02	0.40
1:A:643:SER:OG	1:A:644:SER:N	2.54	0.40
1:A:583:LEU:HD22	1:A:665:HIS:CG	2.56	0.40
1:A:255:PRO:HG2	1:A:261:LEU:HB3	2.02	0.40
1:A:412:TRP:CE2	3:A:904:Y01:HAI	2.57	0.40
1:A:554:ILE:O	1:A:558:PHE:HB2	2.22	0.40
1:A:616:GLY:H	1:A:777:THR:HG22	1.86	0.40
1:A:705:ILE:HG13	1:A:734:ARG:HD3	2.02	0.40
1:A:802:ILE:HD11	1:A:805:ARG:HD2	2.03	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	589/842 (70%)	563 (96%)	26 (4%)	0	100	100
1	B	589/842 (70%)	561 (95%)	28 (5%)	0	100	100
All	All	1178/1684 (70%)	1124 (95%)	54 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	498/701 (71%)	496 (100%)	2 (0%)	91	97
1	B	498/701 (71%)	495 (99%)	3 (1%)	86	94
All	All	996/1402 (71%)	991 (100%)	5 (0%)	89	95

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

Mol	Chain	Res	Type
1	A	316	GLN
1	A	455	ASP
1	B	316	GLN
1	B	320	THR
1	B	455	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	279	ASN
1	A	316	GLN
1	A	328	ASN
1	A	539	GLN
1	B	279	ASN
1	B	328	ASN
1	B	539	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 monosaccharides in this entry.

5.6 Ligand geometry

11 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	$\# Z > 2$
3	Y01	A	905	-	38,38,38	0.44	0	57,57,57	0.64	1 (1%)
3	Y01	A	903	-	38,38,38	0.47	0	57,57,57	0.66	0
2	GSH	A	901	-	18,19,19	0.69	0	23,24,24	0.71	0
3	Y01	B	906	-	38,38,38	0.47	0	57,57,57	0.67	0
3	Y01	B	904	-	38,38,38	0.46	0	57,57,57	0.66	0
2	GSH	B	903	-	18,19,19	0.69	0	23,24,24	0.69	0
3	Y01	B	905	-	38,38,38	0.49	0	57,57,57	0.68	1 (1%)
4	HEM	B	901	-	41,50,50	1.34	7 (17%)	45,82,82	1.83	8 (17%)
3	Y01	A	904	-	38,38,38	0.49	0	57,57,57	0.66	1 (1%)
2	GSH	B	902	-	18,19,19	0.70	0	23,24,24	0.72	0
2	GSH	A	902	-	18,19,19	0.70	0	23,24,24	0.71	0

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
3	Y01	A	905	-	-	10/19/77/77	0/4/4/4
3	Y01	A	903	-	-	4/19/77/77	0/4/4/4
2	GSH	A	901	-	-	13/24/24/24	-
3	Y01	B	906	-	-	2/19/77/77	0/4/4/4
3	Y01	B	904	-	-	8/19/77/77	0/4/4/4
2	GSH	B	903	-	-	4/24/24/24	-
3	Y01	B	905	-	-	6/19/77/77	0/4/4/4
4	HEM	B	901	-	-	2/12/54/54	-
3	Y01	A	904	-	-	6/19/77/77	0/4/4/4
2	GSH	B	902	-	-	15/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GSH	A	902	-	-	3/24/24/24	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	901	HEM	C4D-ND	-3.59	1.34	1.40
4	B	901	HEM	C1B-NB	-3.46	1.34	1.40
4	B	901	HEM	FE-NB	2.79	2.10	1.96
4	B	901	HEM	CHB-C1B	2.30	1.40	1.35
4	B	901	HEM	C1D-ND	-2.13	1.34	1.38
4	B	901	HEM	FE-ND	-2.09	1.86	1.96
4	B	901	HEM	C4B-NB	-2.04	1.34	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	901	HEM	CHC-C4B-NB	5.37	130.27	124.43
4	B	901	HEM	C1B-NB-C4B	4.42	109.64	105.07
4	B	901	HEM	CHD-C1D-ND	4.13	128.92	124.43
4	B	901	HEM	CHA-C4D-ND	3.40	128.59	124.38
4	B	901	HEM	CHB-C1B-NB	3.02	128.11	124.38
4	B	901	HEM	C4D-ND-C1D	2.86	108.03	105.07
4	B	901	HEM	CHD-C1D-C2D	-2.34	121.33	124.98
3	A	904	Y01	CAP-CAQ-CBG	-2.09	100.98	105.13
3	B	905	Y01	CAP-CAQ-CBG	-2.09	100.99	105.13
4	B	901	HEM	CMA-C3A-C4A	-2.07	125.29	128.46
3	A	905	Y01	OAW-CBC-CAR	2.01	113.19	108.33

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	GSH	O11-C1-CA1-N1
2	A	901	GSH	CG1-CD1-N2-CA2
2	A	902	GSH	O11-C1-CA1-N1
2	B	902	GSH	O11-C1-CA1-N1
2	B	903	GSH	O11-C1-CA1-N1
3	A	903	Y01	OAG-CAY-OAW-CBC
3	A	903	Y01	CAM-CAY-OAW-CBC
3	A	905	Y01	CAV-CBC-OAW-CAY
3	B	904	Y01	OAG-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
3	B	904	Y01	CAM-CAY-OAW-CBC
4	B	901	HEM	C2B-C3B-CAB-CBB
3	B	904	Y01	CAC-CBB-CBE-CAP
3	B	904	Y01	CAC-CBB-CBE-CBI
2	A	901	GSH	OE1-CD1-N2-CA2
3	B	904	Y01	CAO-CBB-CBE-CBI
3	B	904	Y01	CAO-CBB-CBE-CAP
2	B	902	GSH	OE1-CD1-N2-CA2
2	B	902	GSH	CG1-CD1-N2-CA2
2	B	902	GSH	O12-C1-CA1-N1
2	A	901	GSH	O12-C1-CA1-N1
2	B	903	GSH	O31-C3-CA3-N3
2	B	903	GSH	O32-C3-CA3-N3
2	B	903	GSH	O12-C1-CA1-N1
3	A	905	Y01	CAM-CAY-OAW-CBC
2	A	902	GSH	O12-C1-CA1-N1
3	B	905	Y01	CAO-CBB-CBE-CBI
3	A	905	Y01	OAG-CAY-OAW-CBC
3	B	905	Y01	CAC-CBB-CBE-CAP
3	A	904	Y01	CAO-CBB-CBE-CBI
4	B	901	HEM	C4B-C3B-CAB-CBB
3	B	905	Y01	CAO-CBB-CBE-CAP
3	A	904	Y01	CAO-CBB-CBE-CAP
3	A	904	Y01	CAC-CBB-CBE-CAP
2	A	901	GSH	O2-C2-CA2-N2
3	A	904	Y01	CAL-CAM-CAY-OAW
3	A	904	Y01	CAC-CBB-CBE-CBI
3	B	905	Y01	CAC-CBB-CBE-CBI
2	A	901	GSH	N3-C2-CA2-N2
3	B	905	Y01	CAL-CAM-CAY-OAW
2	B	902	GSH	O2-C2-CA2-N2
2	B	902	GSH	N3-C2-CA2-N2
3	A	905	Y01	CAL-CAM-CAY-OAW
2	A	901	GSH	N2-CD1-CG1-CB1
2	A	901	GSH	OE1-CD1-CG1-CB1
2	B	902	GSH	OE1-CD1-CG1-CB1
2	A	901	GSH	O11-C1-CA1-CB1
2	A	901	GSH	O12-C1-CA1-CB1
2	B	902	GSH	O11-C1-CA1-CB1
2	B	902	GSH	N1-CA1-CB1-CG1
2	B	902	GSH	O12-C1-CA1-CB1
2	B	902	GSH	N2-CD1-CG1-CB1

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Mol	Chain	Res	Type	Atoms
2	B	902	GSH	O2-C2-N3-CA3
3	B	904	Y01	CAM-CAL-CAX-OAF
3	A	905	Y01	CAC-CBB-CBE-CBI
3	A	903	Y01	CAM-CAL-CAX-OAF
2	A	901	GSH	C2-CA2-CB2-SG2
2	B	902	GSH	C2-CA2-CB2-SG2
3	A	903	Y01	CAM-CAL-CAX-OAH
3	B	904	Y01	CAM-CAL-CAX-OAH
3	A	904	Y01	CAL-CAM-CAY-OAG
3	A	905	Y01	CAO-CBB-CBE-CBI
3	A	905	Y01	CAM-CAL-CAX-OAH
2	A	902	GSH	O2-C2-CA2-N2
3	B	905	Y01	CAL-CAM-CAY-OAG
3	B	906	Y01	CAM-CAL-CAX-OAH
3	A	905	Y01	CAM-CAL-CAX-OAF
3	A	905	Y01	CAL-CAM-CAY-OAG
3	B	906	Y01	CAM-CAL-CAX-OAF
2	A	901	GSH	C1-CA1-CB1-CG1
2	B	902	GSH	C1-CA1-CB1-CG1
3	A	905	Y01	CAO-CBB-CBE-CAP
2	B	902	GSH	CA2-C2-N3-CA3
2	A	901	GSH	N1-CA1-CB1-CG1

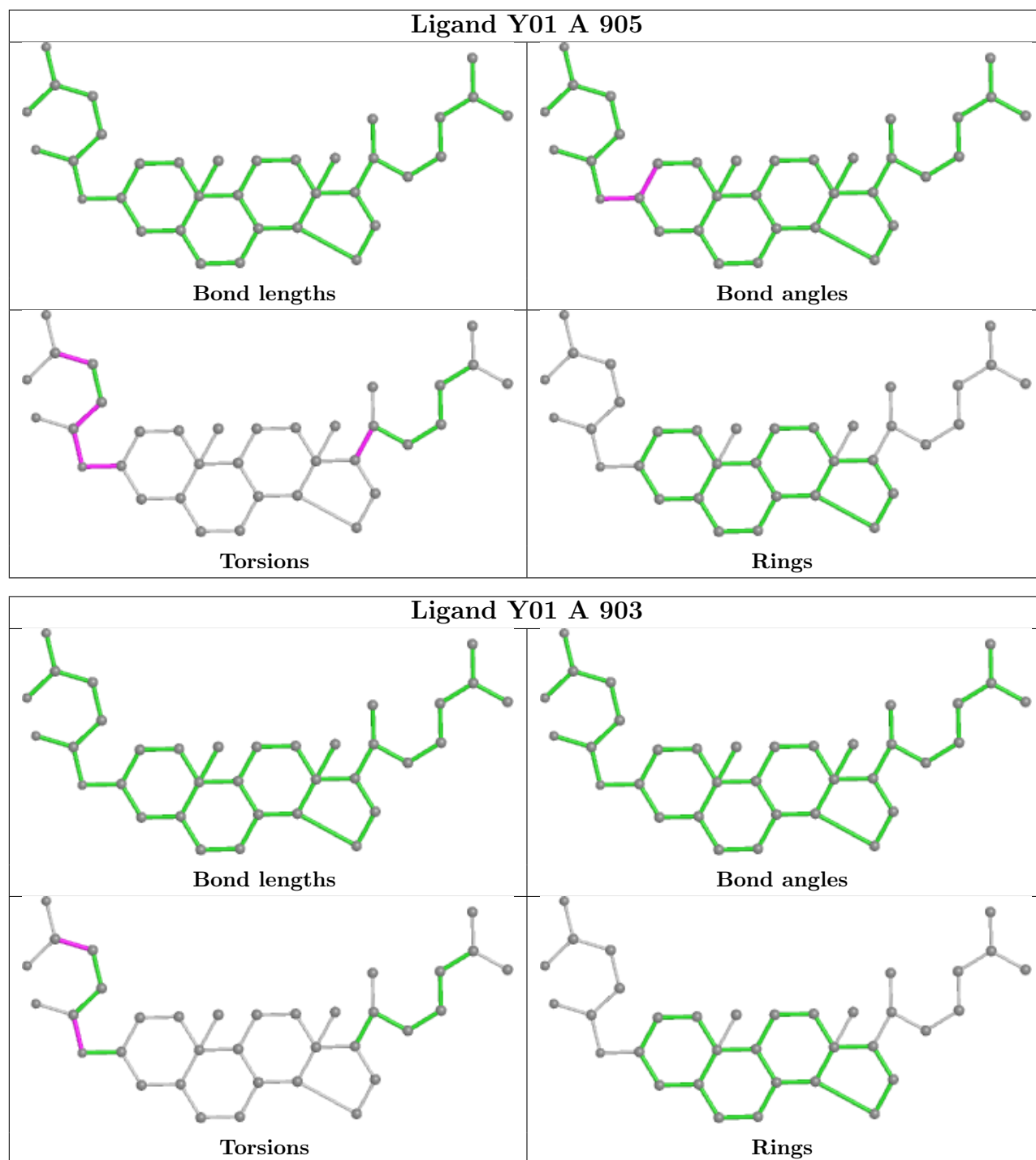
There are no ring outliers.

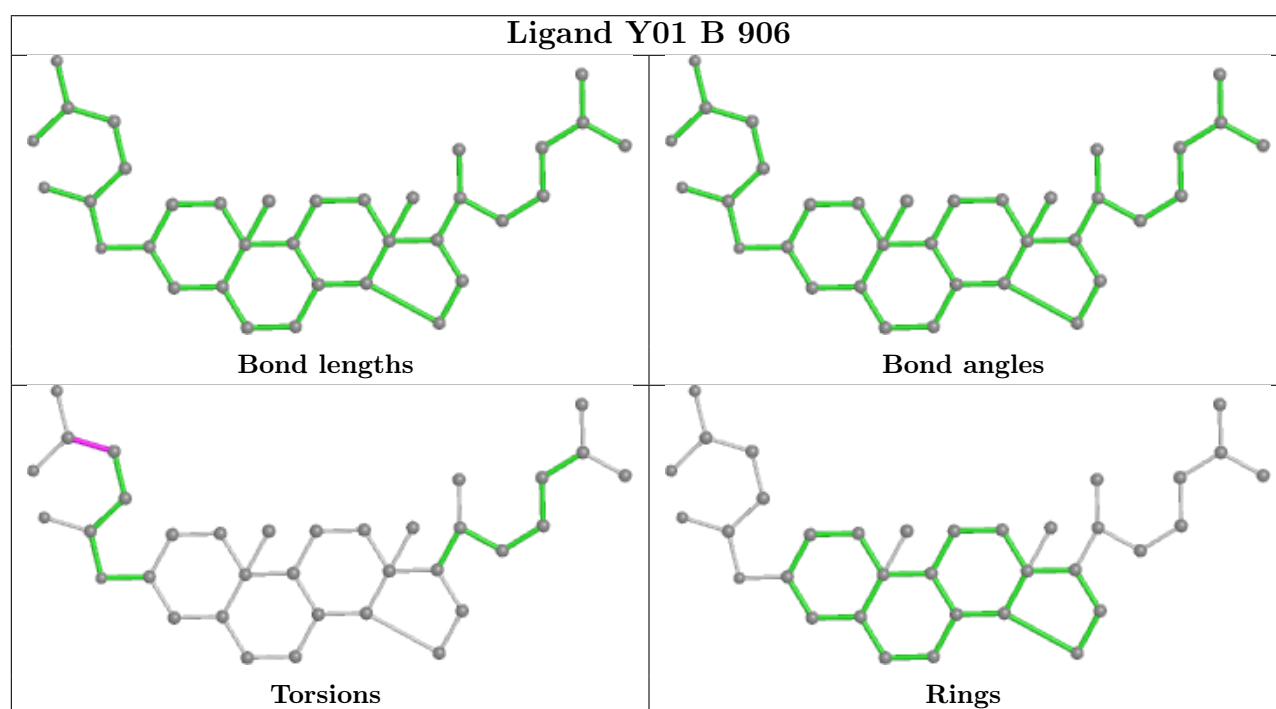
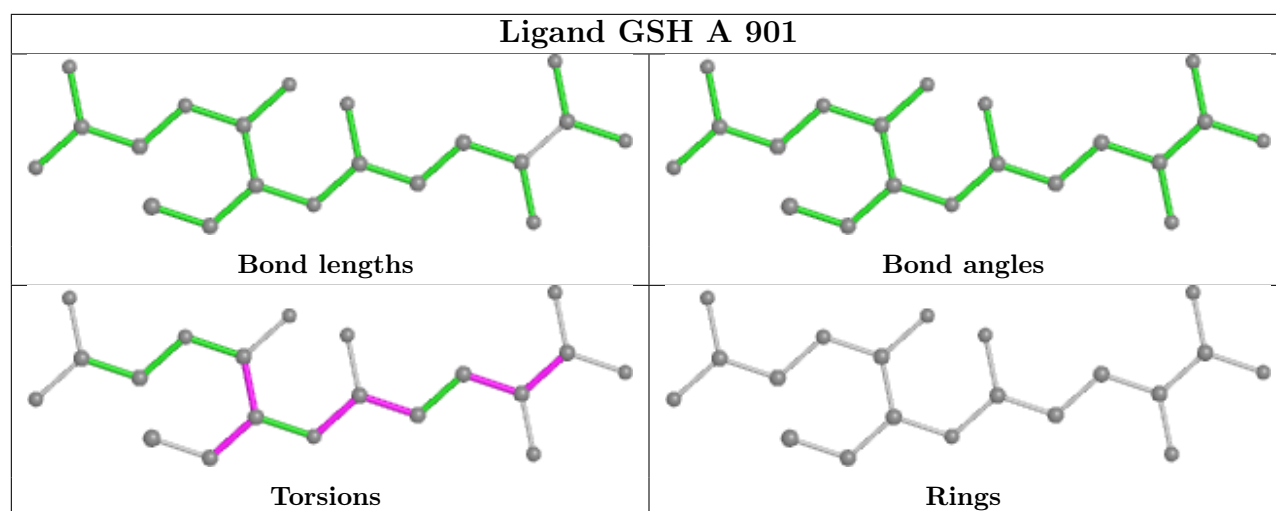
3 monomers are involved in 5 short contacts:

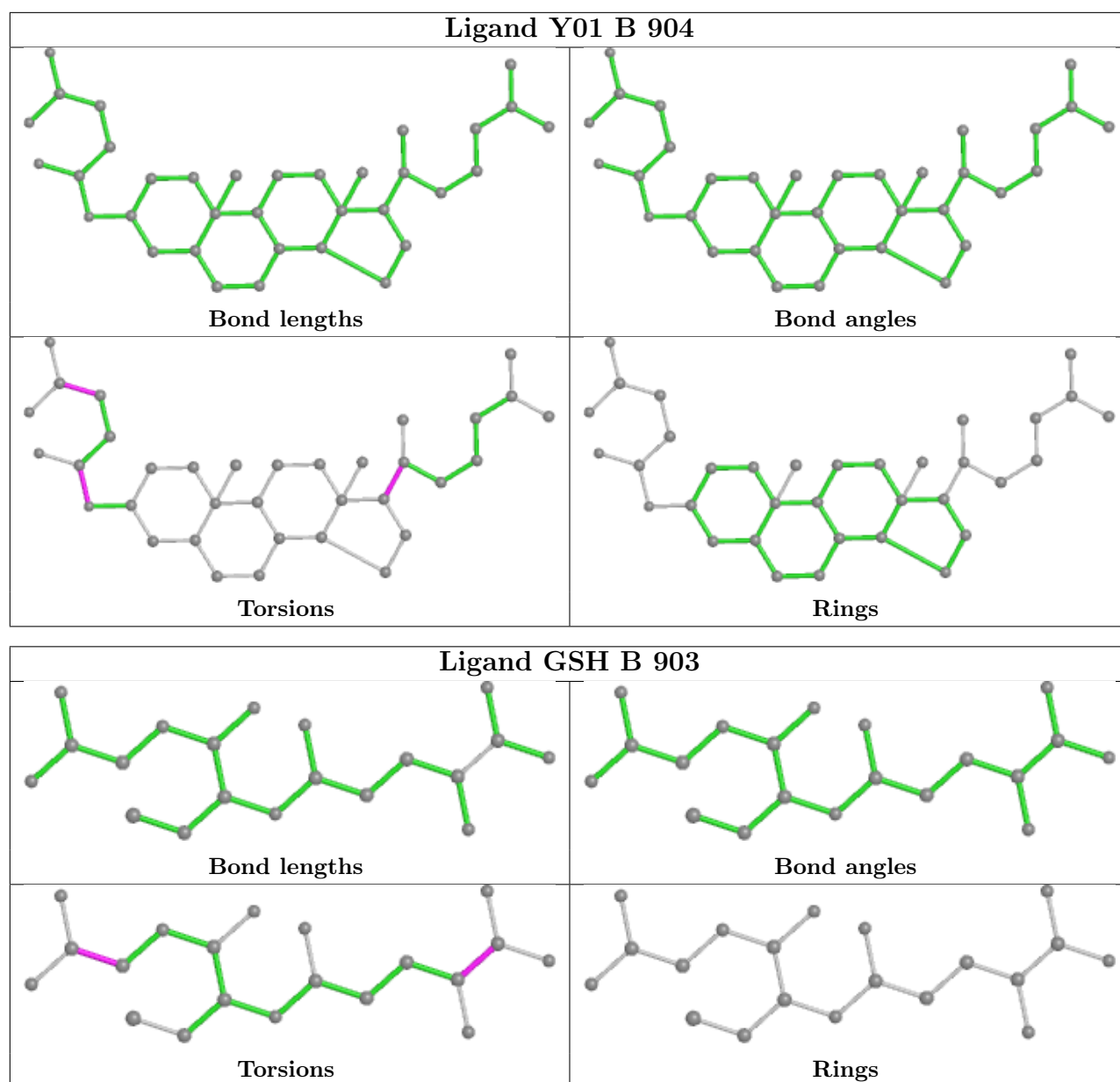
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	905	Y01	2	0
3	A	904	Y01	2	0
2	A	902	GSH	1	0

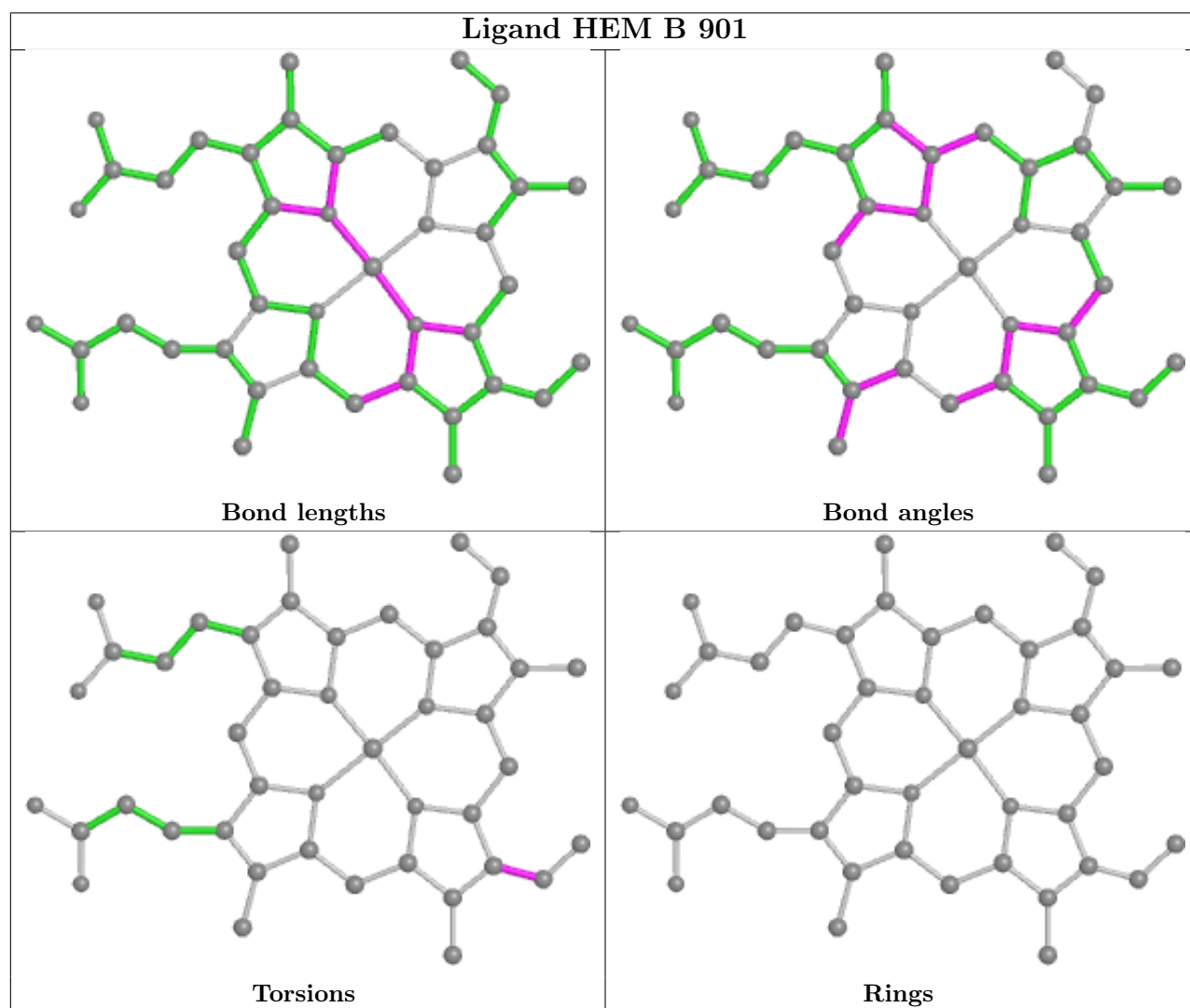
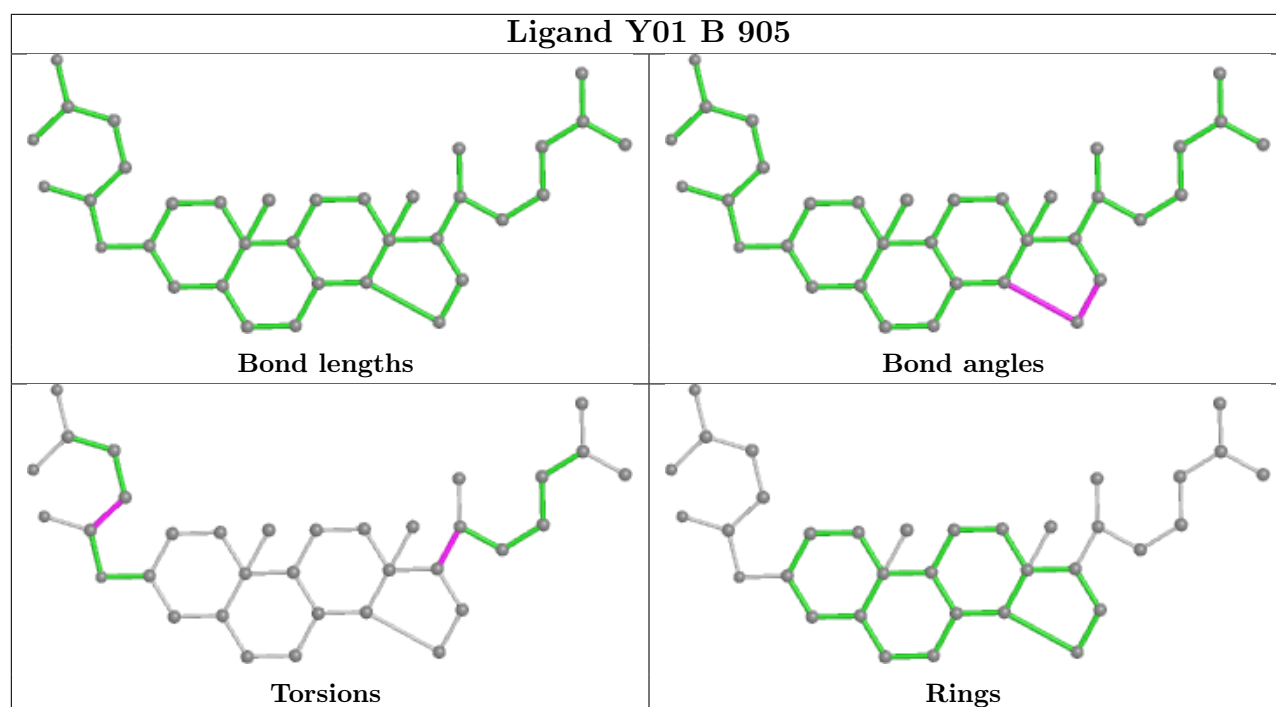
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

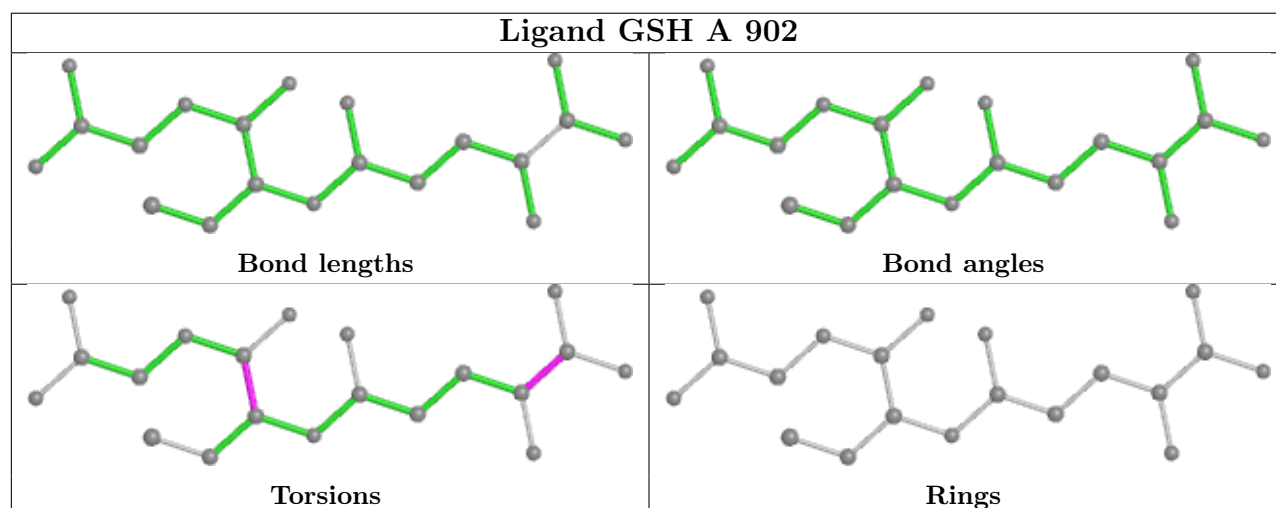
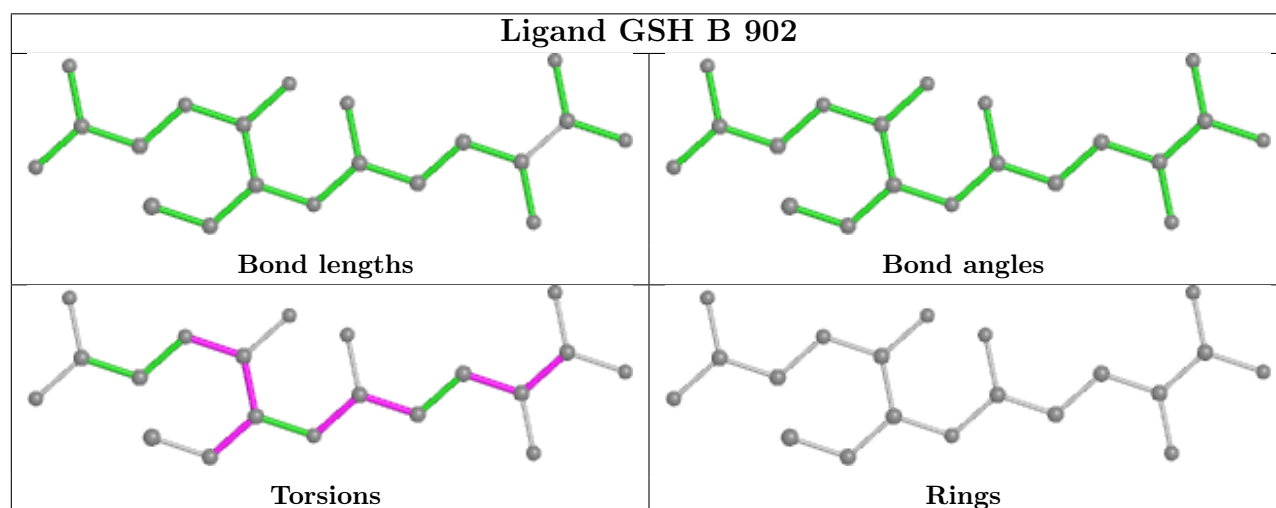
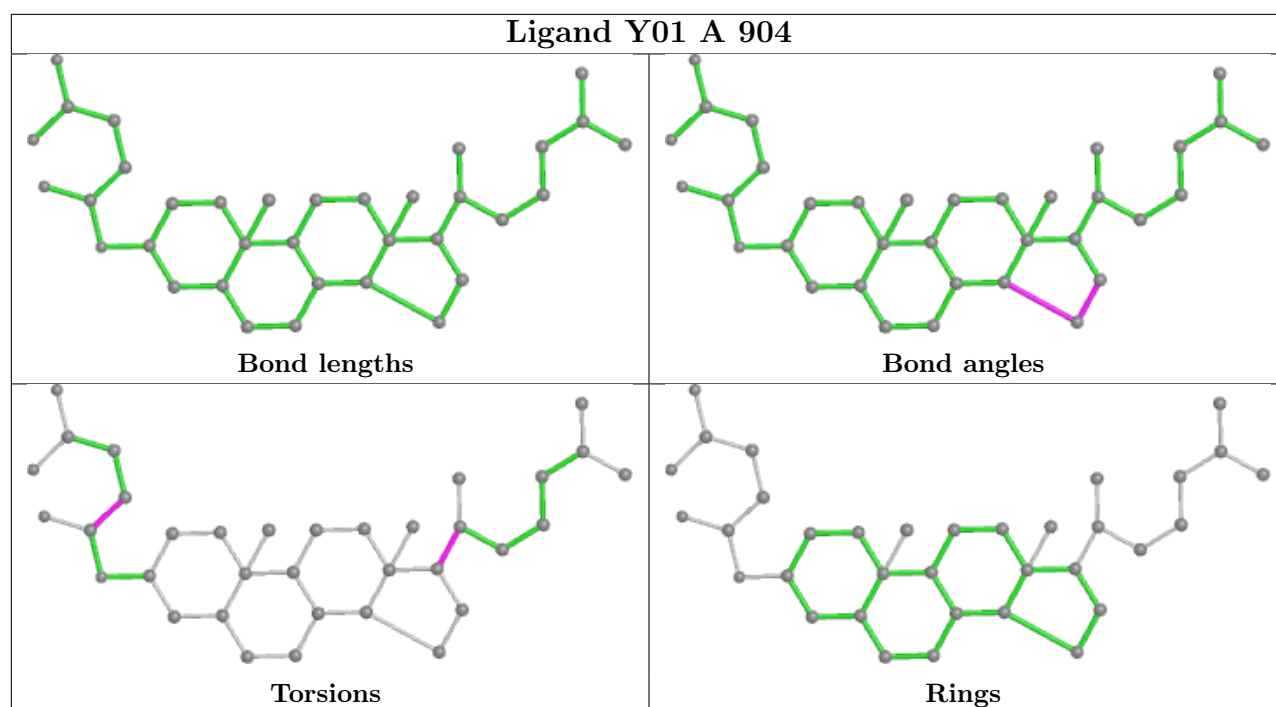
equivalents in the CSD to analyse the geometry.











5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

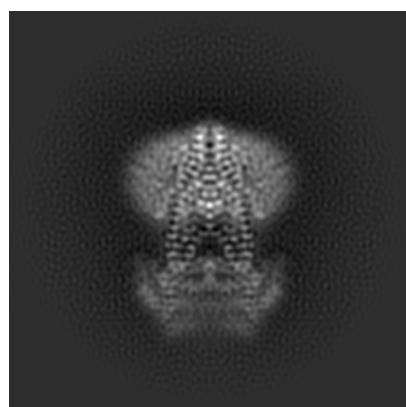
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30791. These allow visual inspection of the internal detail of the map and identification of artifacts.

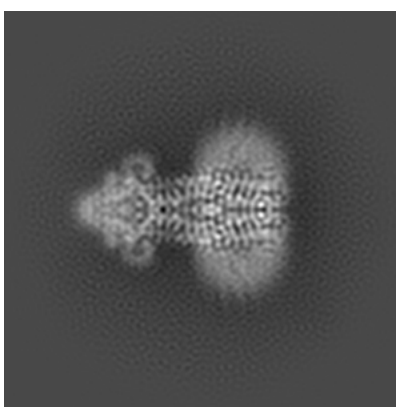
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

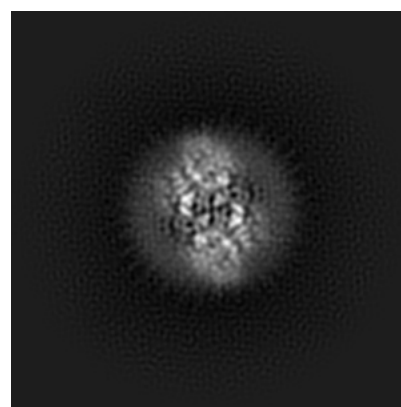
6.1.1 Primary map



X



Y



Z

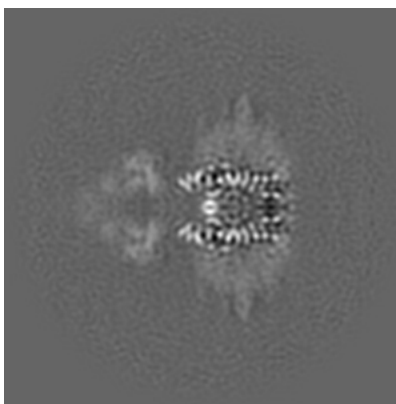
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

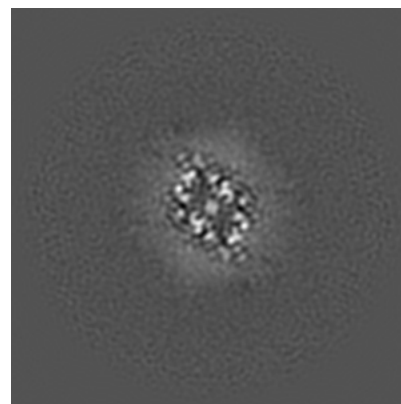
6.2.1 Primary map



X Index: 140



Y Index: 140

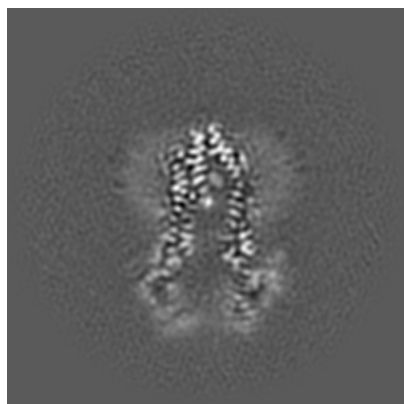


Z Index: 140

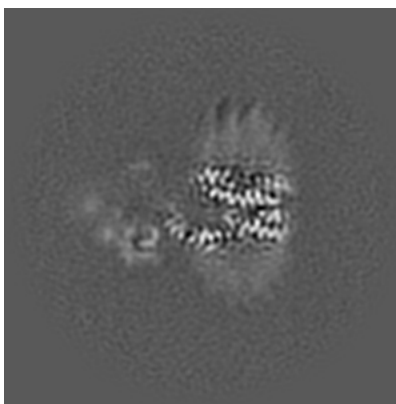
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

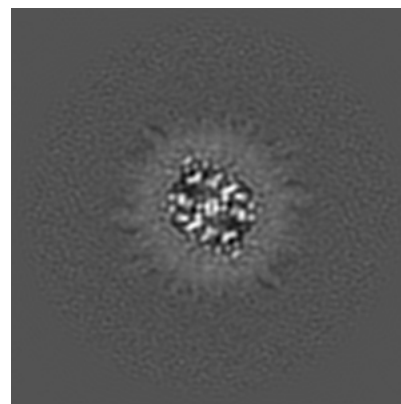
6.3.1 Primary map



X Index: 136



Y Index: 147

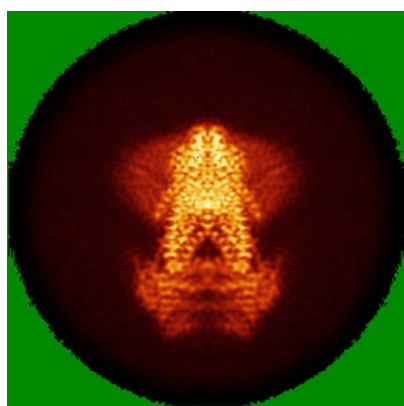


Z Index: 145

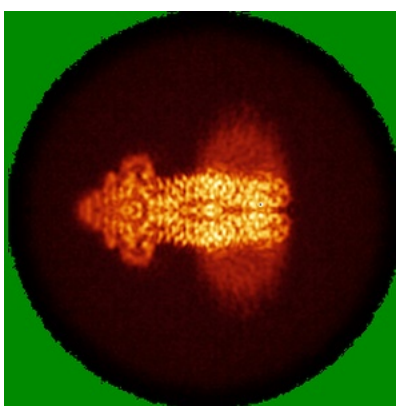
The images above show the largest variance slices of the map in three orthogonal directions.

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

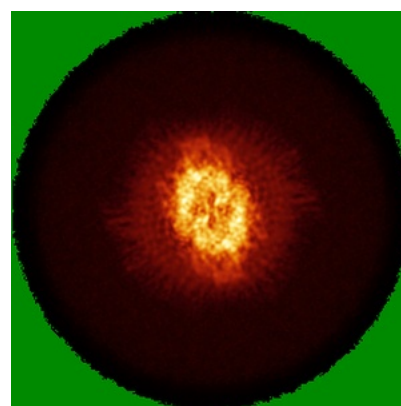
6.4.1 Primary map



X



Y

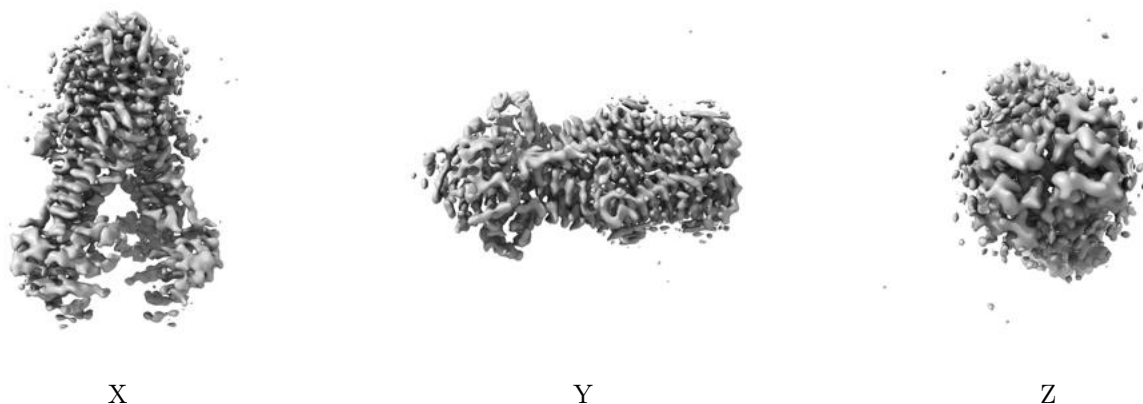


Z

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

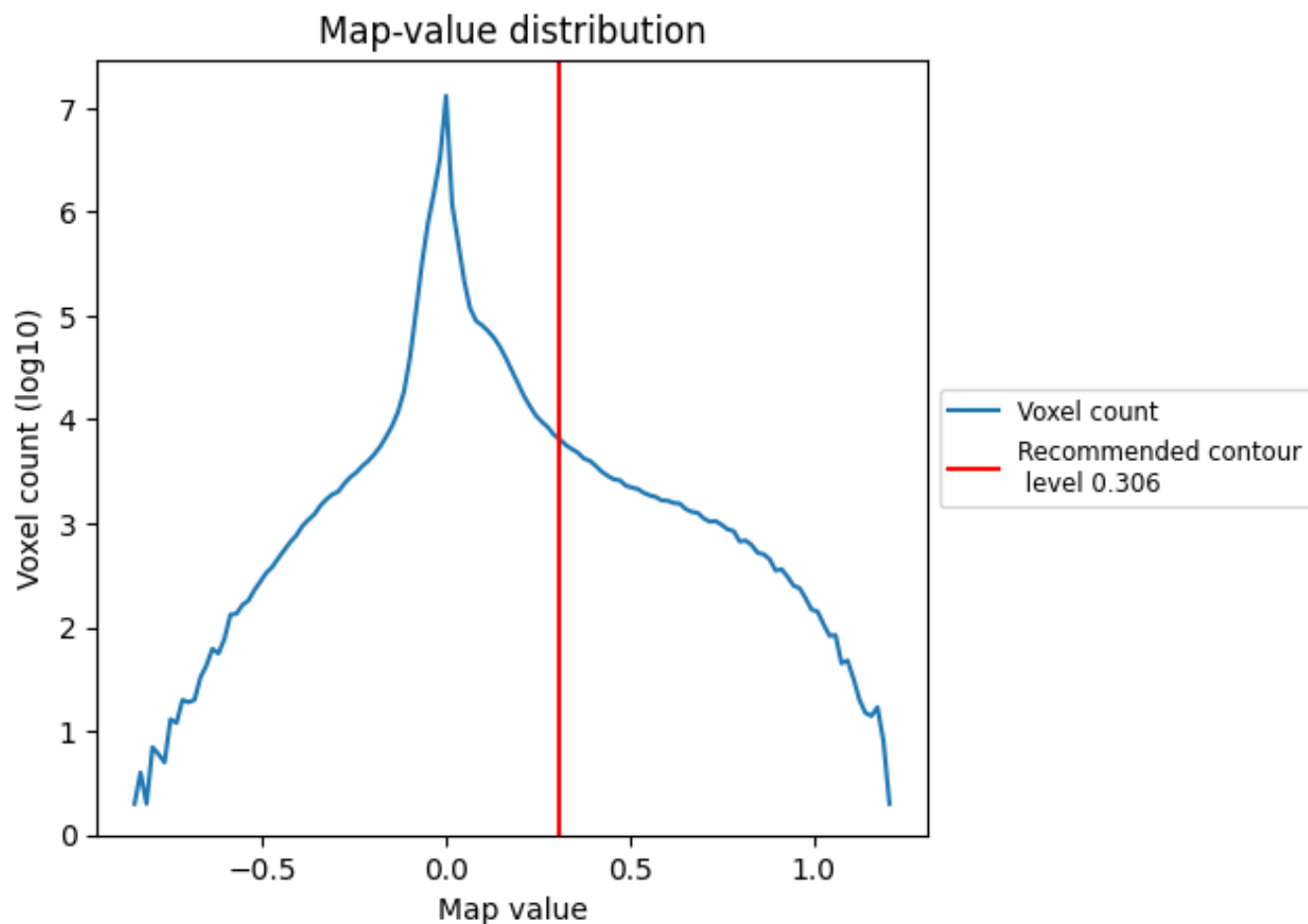
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

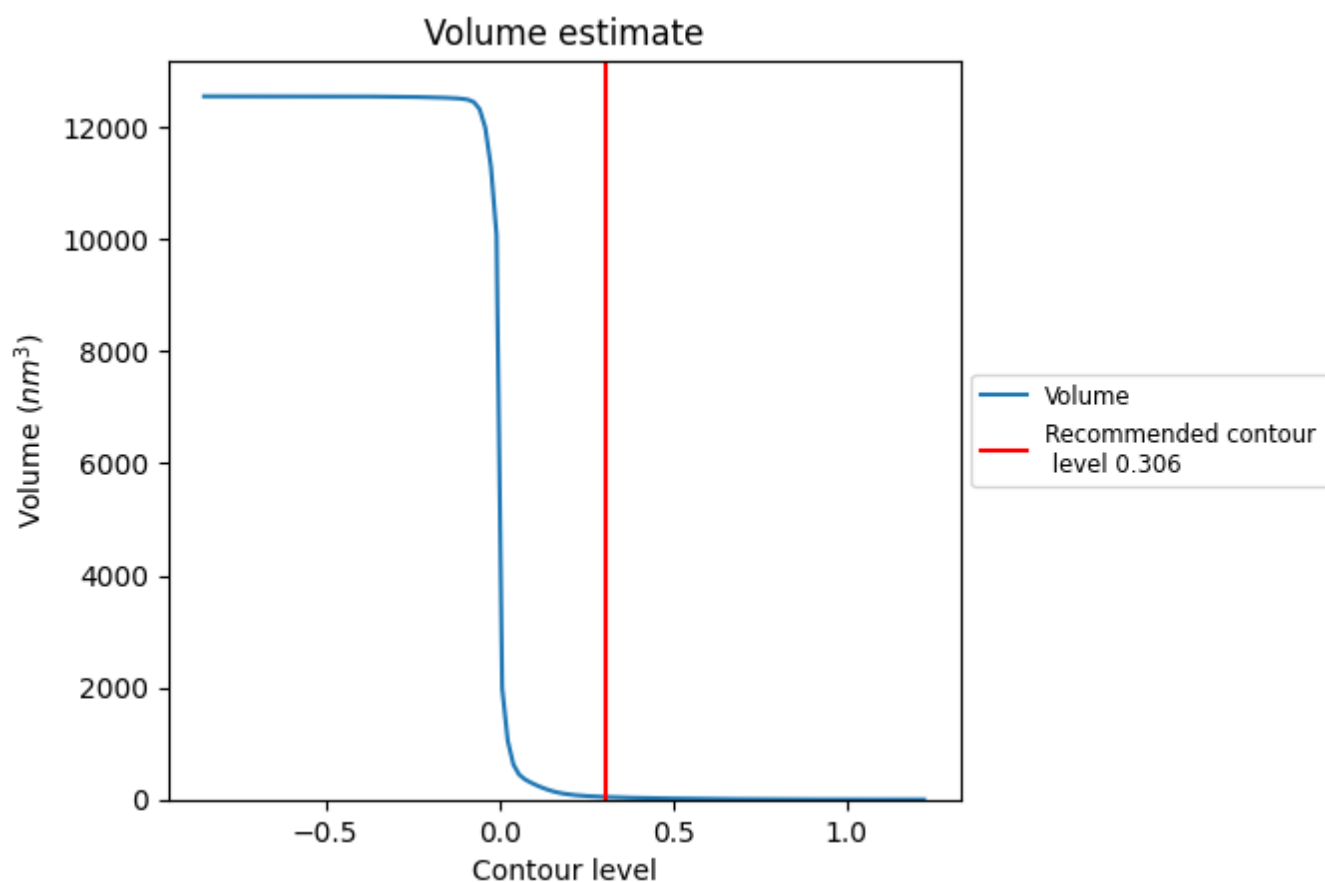
This section contains the results of statistical analysis of the map.

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.

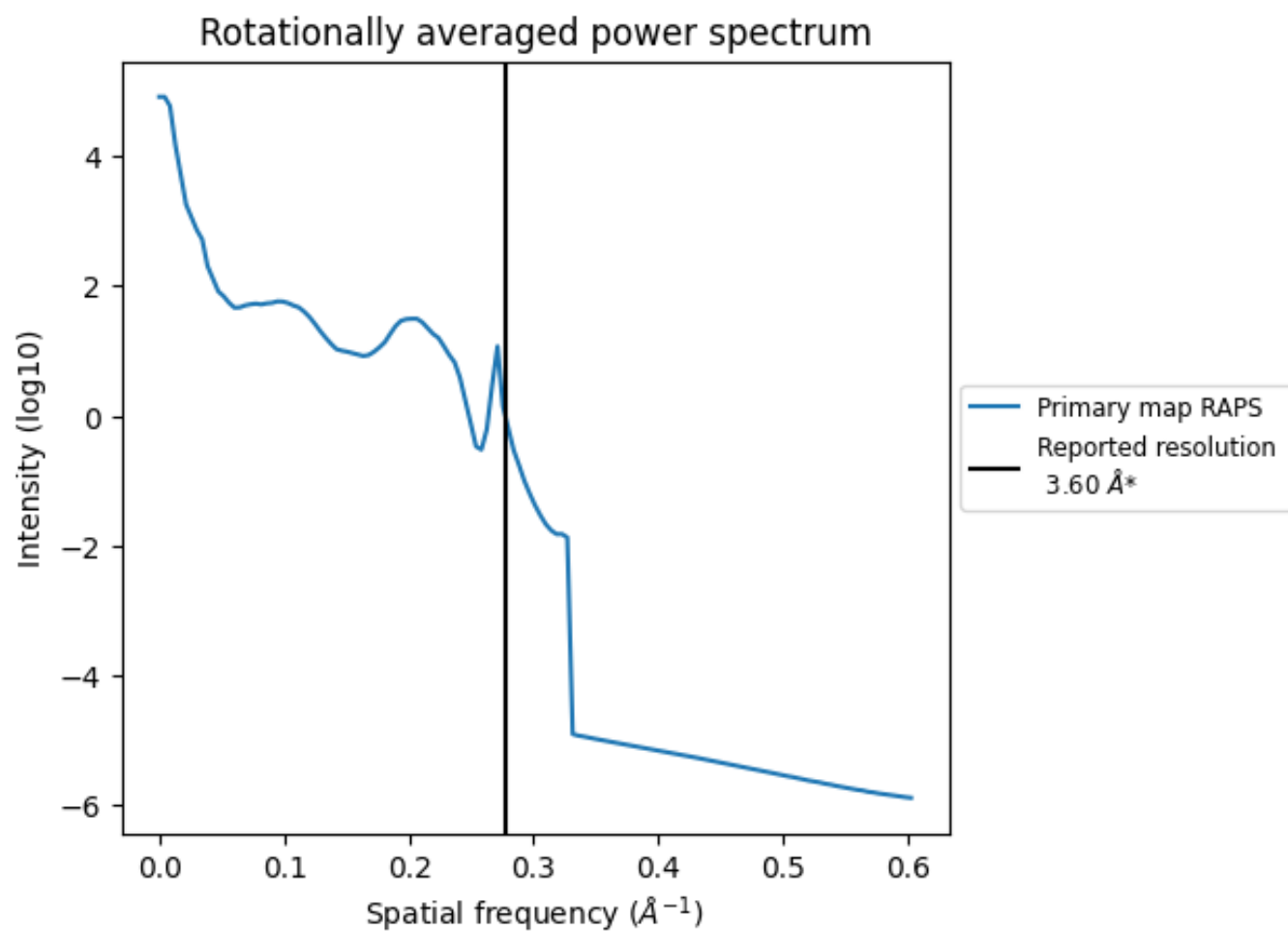
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46 nm³; this corresponds to an approximate mass of 42 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 0.278 Å⁻¹

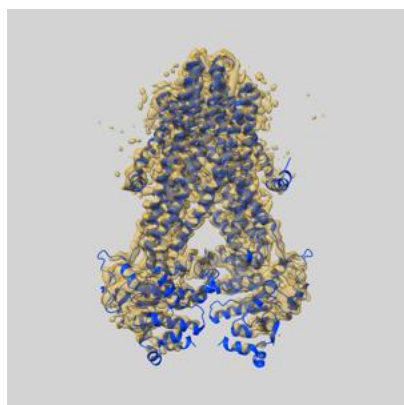
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

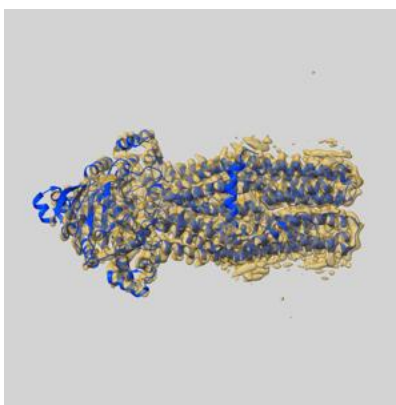
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30791 and PDB model 7DNZ. Per-residue inclusion information can be found in section 3 on page 6.

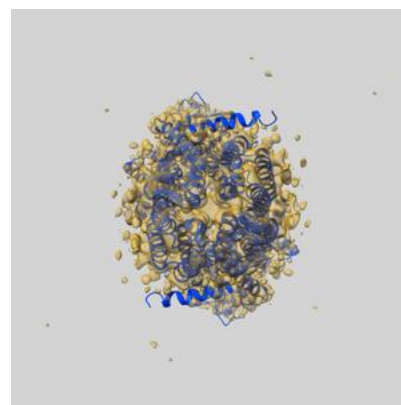
9.1 Map-model overlay [i](#)



X



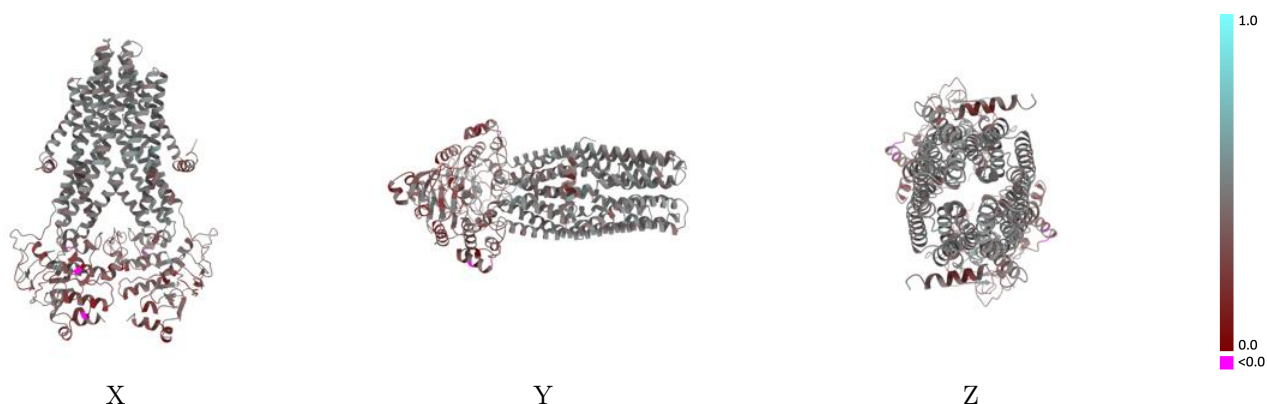
Y



Z

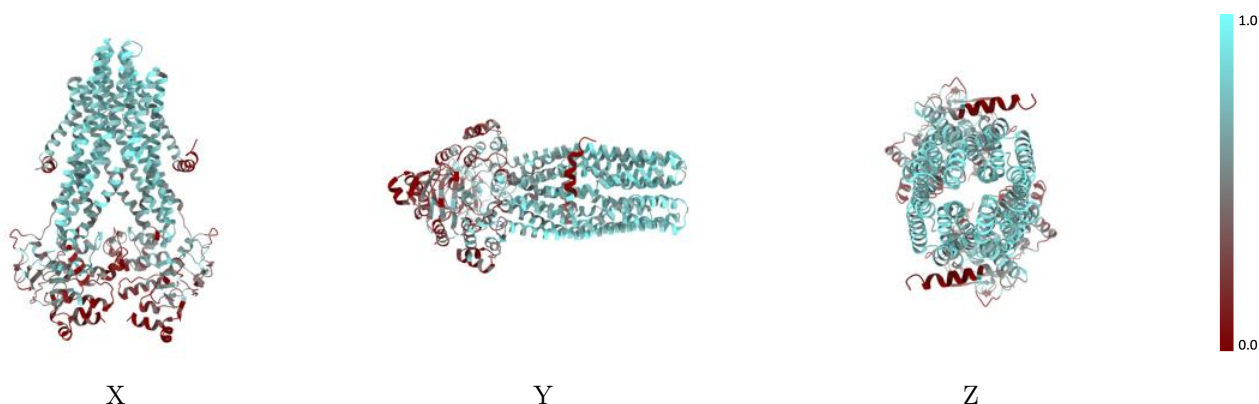
The images above show the 3D surface view of the map at the recommended contour level 0.306 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



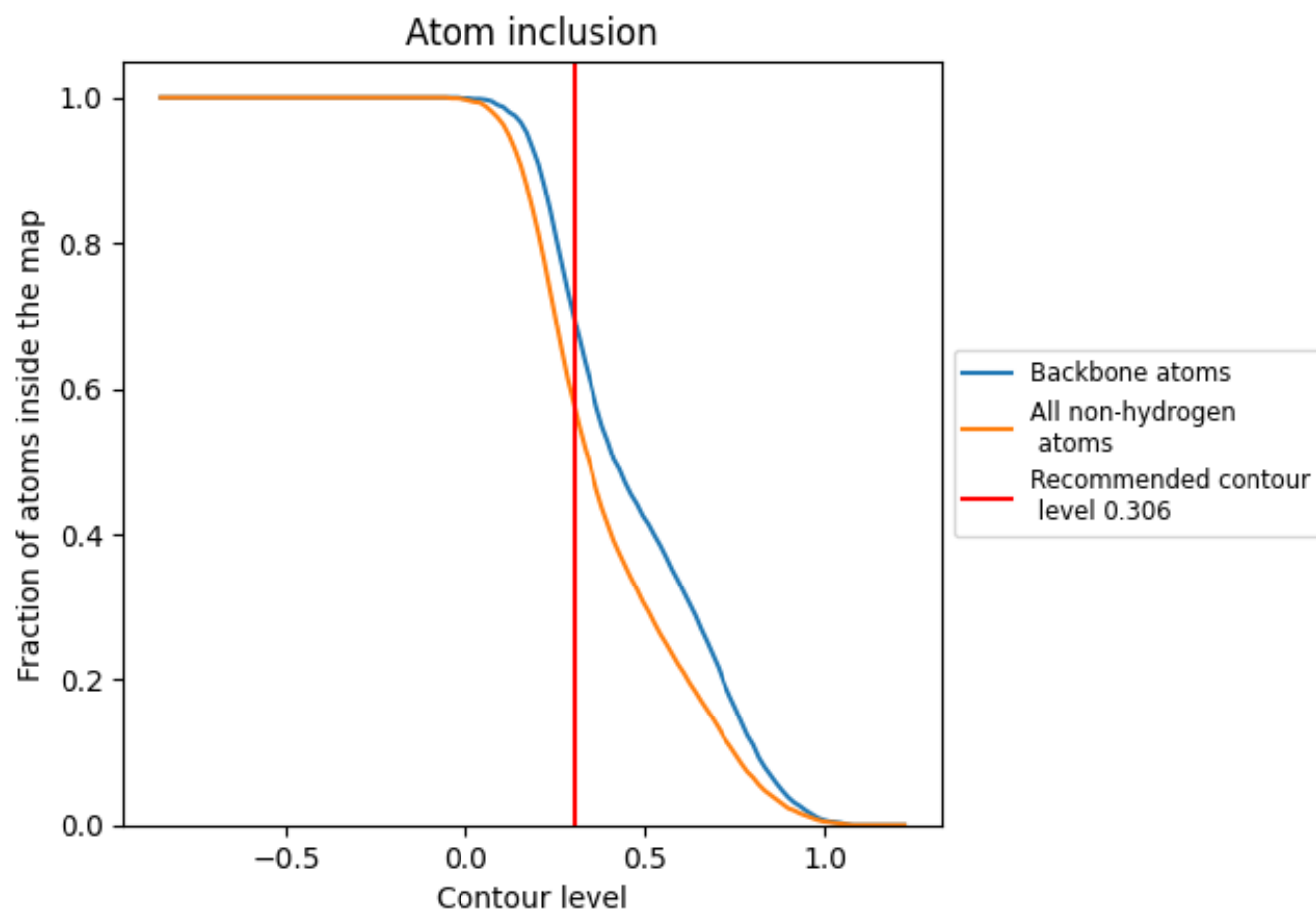
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.306).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 57% 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 (0.306) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5690	<div></div> 0.4150
A	<div></div> 0.5670	<div></div> 0.4170
B	<div></div> 0.5700	<div></div> 0.4140

