



Full wwPDB EM Validation Report ⓘ

Nov 2, 2024 – 08:59 pm GMT

PDB ID : 6SMQ
EMDB ID : EMD-10245
Title : Structure of the RagAB peptide importer in the 'open-closed' state
Authors : White, J.B.R.; Ranson, N.A.; van den Berg, B.
Deposited on : 2019-08-22
Resolution : 3.30 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

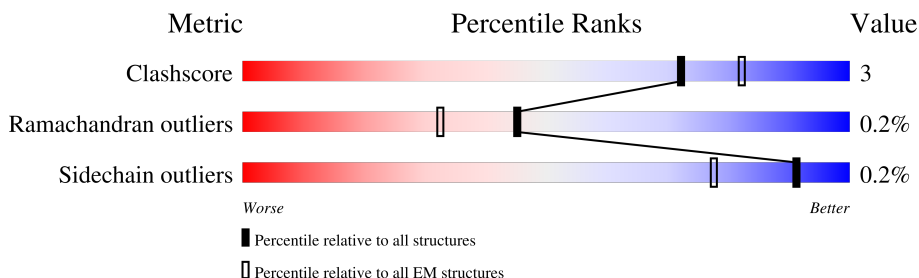
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	482	
1	D	482	
2	B	903	
3	C	13	
4	E	915	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 22136 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 Lipoprotein RagB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	482	Total	C	N	O	S	0	0
			3843	2440	656	738	9		
1	D	482	Total	C	N	O	S	0	0
			3843	2440	656	738	9		

- Molecule 2 is a protein called RagA protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	903	Total	C	N	O	S	1	0
			7076	4484	1183	1377	32		

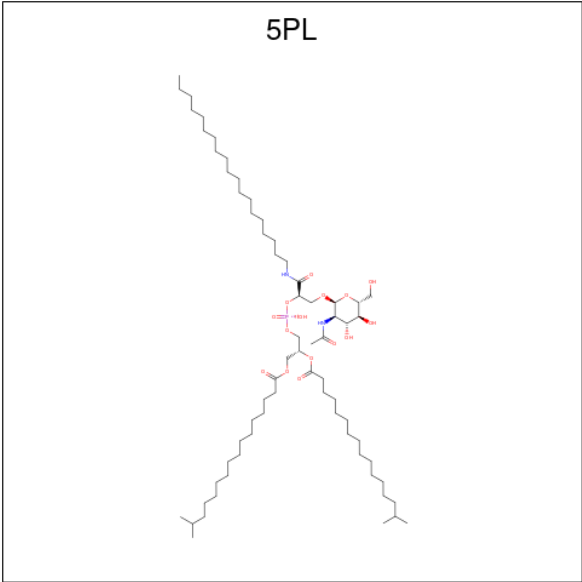
- Molecule 3 is a protein called SER-GLY-ALA-THR-THR-ALA-THR-THR-THR-THR-SER-ASN-SER.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	13	Total	C	N	O	0	0
			82	45	14	23		

- Molecule 4 is a protein called RagA protein.

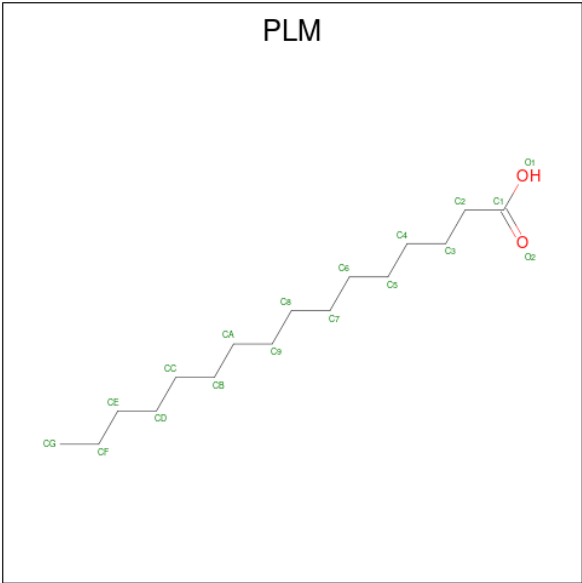
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	911	Total	C	N	O	S	1	0
			7138	4527	1193	1386	32		

- Molecule 5 is (1R,4S,6R)-6-({[2-(ACETYLAMINO)-2-DEOXY-ALPHA-D-GLUCOPYRANOSYL]OXY}METHYL)-4-HYDROXY-1-{[(15-METHYLHEXADECANOYL)OXY]METHYL}-4-OXIDO-7-OXO-3,5-DIOXA-8-AZA-4-PHOSPHAHEPTACOS-1-YL 15-METHYLHEXADECANOATE (three-letter code: 5PL) (formula: C₆₇H₁₂₉N₂O₁₅P).



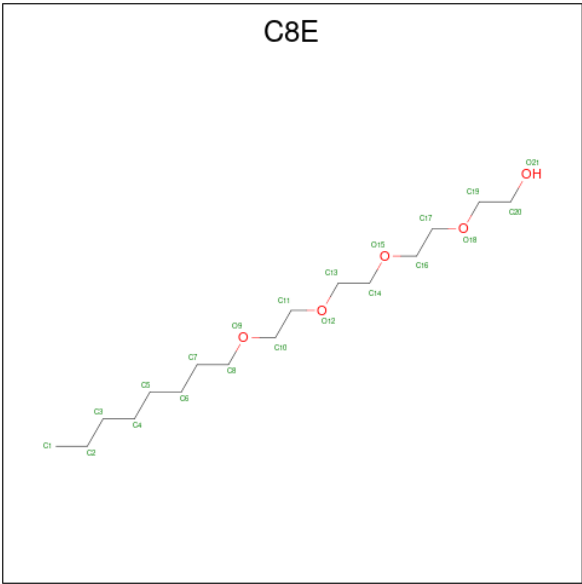
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			27	23	4	
5	D	1	Total	C	O	0
			26	22	4	

- Molecule 6 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			12	11	1	
6	D	1	Total	C	O	0
			8	7	1	

- Molecule 7 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			AltConf
7	B	1	Total	C	O	0
			16	11	5	
7	B	1	Total	C	O	0
			16	11	5	
7	B	1	Total	C	O	0
			21	16	5	
7	E	1	Total	C	O	0
			14	12	2	
7	E	1	Total	C	O	0
			14	12	2	

3 Residue-property plots [i](#)


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

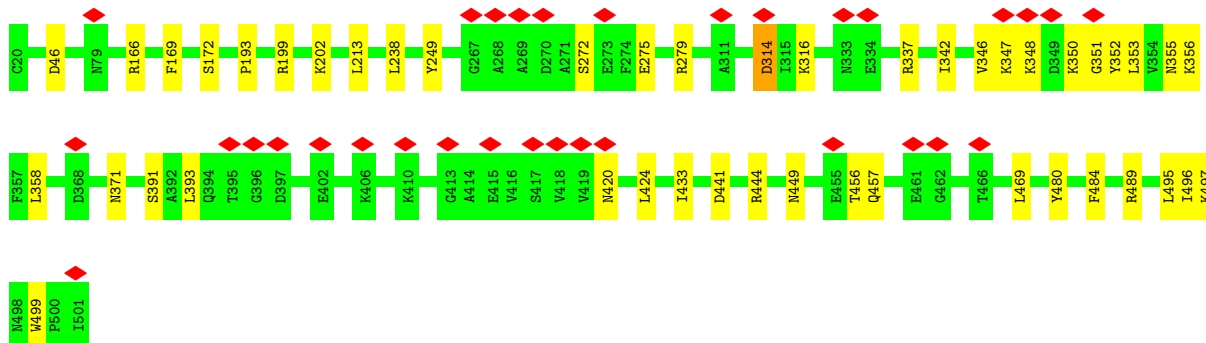
- Molecule 1: Lipoprotein RagB

Chain A:  95% 5%



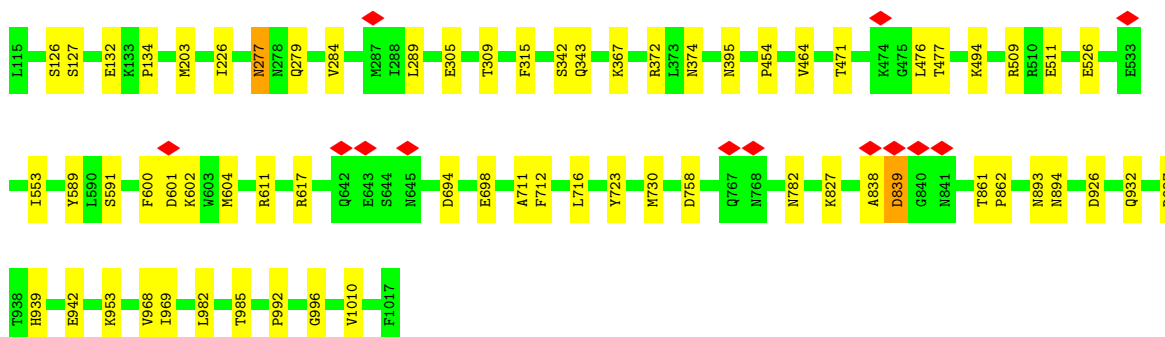
- Molecule 1: Lipoprotein RagB

Chain D:  7% 90% 9%




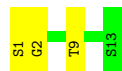
- Molecule 2: RagA protein

Chain B:  93% 7%



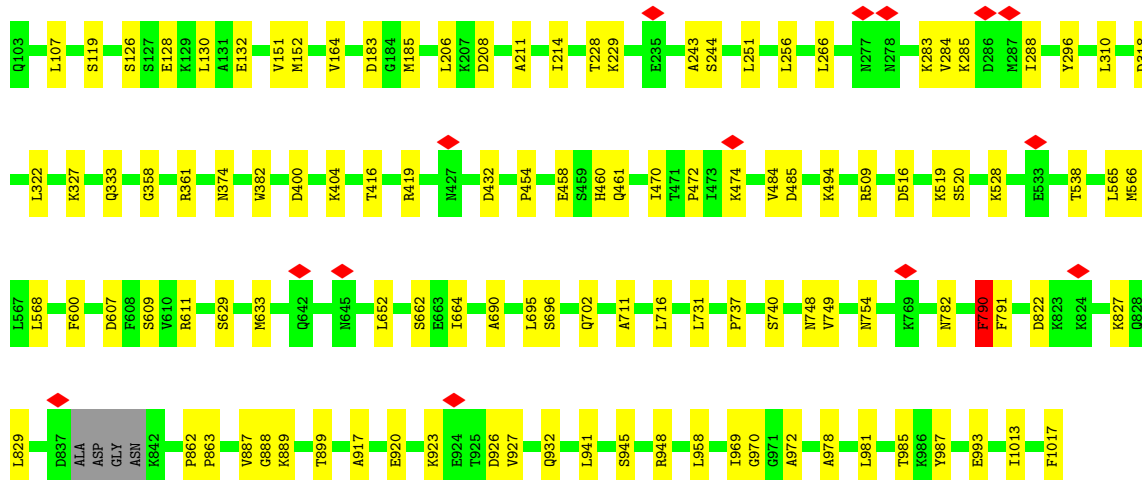
- Molecule 3: SER-GLY-ALA-THR-THR-ALA-THR-THR-THR-THR-SER-ASN-SER

Chain C:  77% 23%



- Molecule 4: RagA protein

Chain E:  87% 12%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	213143	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	77.88	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.536	Depositor
Minimum map value	-0.383	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	231.12001, 231.12001, 231.12001	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C8E, 5PL, PLM

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	0.52	0/3929	0.56	0/5331
1	D	0.44	0/3929	0.54	0/5331
2	B	0.53	0/7244	0.61	1/9799 (0.0%)
3	C	0.39	0/81	0.72	0/111
4	E	0.51	0/7306	0.63	5/9881 (0.1%)
All	All	0.51	0/22489	0.60	6/30453 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
2	B	0	3
4	E	0	3
All	All	0	8

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	432	ASP	CB-CG-OD1	9.08	126.47	118.30
4	E	107	LEU	CA-CB-CG	7.53	132.61	115.30
2	B	996	GLY	C-N-CA	5.41	135.22	121.70
4	E	652	LEU	CA-CB-CG	5.24	127.35	115.30
4	E	474	LYS	CA-CB-CG	5.10	124.62	113.40
4	E	130	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	601	ASP	Peptide
2	B	838	ALA	Peptide
2	B	839	ASP	Peptide
1	D	348	LYS	Peptide
1	D	350	LYS	Peptide
4	E	132	GLU	Peptide
4	E	600	PHE	Peptide
4	E	790	PHE	Peptide

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	3843	0	3739	17	0
1	D	3843	0	3739	25	0
2	B	7076	0	6815	37	0
3	C	82	0	78	2	0
4	E	7138	0	6888	62	0
5	A	27	0	35	0	0
5	D	26	0	33	0	0
6	A	12	0	18	0	0
6	D	8	0	10	0	0
7	B	53	0	76	2	0
7	E	28	0	46	1	0
All	All	22136	0	21477	140	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 3.

All (140) 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)
4:E:214:ILE:O	4:E:611:ARG:NH1	2.30	0.65
4:E:985:THR:HG22	4:E:987:TYR:H	1.63	0.64
4:E:244:SER:HB3	4:E:333:GLN:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:591:SER:OG	2:B:611:ARG:NH2	2.35	0.60
4:E:516:ASP:N	4:E:516:ASP:OD1	2.34	0.60
2:B:342:SER:OG	2:B:343:GLN:N	2.35	0.59
4:E:754:ASN:HD22	4:E:782:ASN:HD21	1.49	0.59
1:A:166:ARG:NH2	1:A:480:TYR:O	2.34	0.59
2:B:711:ALA:HB3	2:B:716:LEU:HB3	1.85	0.58
4:E:206:LEU:HD23	4:E:211:ALA:HB1	1.86	0.58
1:D:314:ASP:OD2	1:D:314:ASP:N	2.36	0.57
1:A:121:ASN:OD1	1:A:156:GLN:NE2	2.38	0.57
1:D:193:PRO:HG3	4:E:690:ALA:HB1	1.86	0.57
1:D:441:ASP:OD1	1:D:444:ARG:NH2	2.36	0.57
2:B:894:ASN:HD21	3:C:9:THR:H	1.53	0.56
1:D:484:PHE:O	1:D:489:ARG:NH1	2.38	0.56
4:E:528:LYS:HB3	4:E:538:THR:HG23	1.88	0.56
1:A:349:ASP:N	1:A:349:ASP:OD1	2.39	0.56
2:B:476:LEU:HA	2:B:526:GLU:O	2.07	0.55
4:E:454:PRO:HD2	4:E:494:LYS:HB3	1.87	0.55
4:E:382:TRP:HD1	4:E:470:ILE:HG23	1.72	0.55
4:E:470:ILE:HG22	4:E:472:PRO:HD3	1.89	0.55
3:C:1:SER:OG	3:C:2:GLY:N	2.40	0.54
2:B:372:ARG:HH11	2:B:374:ASN:HD21	1.55	0.54
4:E:970:GLY:H	4:E:1017:PHE:HA	1.73	0.54
4:E:119:SER:HB3	4:E:633:MET:HB2	1.89	0.53
2:B:132:GLU:OE2	2:B:953:LYS:NZ	2.41	0.53
4:E:509:ARG:NH1	4:E:566:MET:O	2.39	0.53
2:B:723:TYR:OH	2:B:782:ASN:ND2	2.37	0.53
2:B:277:ASN:N	2:B:277:ASN:OD1	2.42	0.53
2:B:367:LYS:HE3	2:B:395:ASN:HD22	1.73	0.52
2:B:134:PRO:HB3	2:B:1010:VAL:HG21	1.92	0.52
2:B:589:TYR:OH	2:B:617:ARG:NH1	2.42	0.52
1:D:166:ARG:NH2	1:D:480:TYR:O	2.41	0.52
2:B:758:ASP:OD1	2:B:758:ASP:N	2.41	0.52
2:B:698:GLU:HG3	2:B:730:MET:HA	1.92	0.52
4:E:400:ASP:O	4:E:404:LYS:NZ	2.43	0.52
4:E:400:ASP:OD1	4:E:400:ASP:N	2.36	0.51
4:E:458:GLU:OE2	4:E:460:HIS:NE2	2.36	0.51
4:E:711:ALA:HB3	4:E:716:LEU:HB3	1.92	0.51
2:B:553:ILE:HD11	4:E:568:LEU:HD22	1.92	0.50
2:B:926:ASP:OD2	2:B:926:ASP:N	2.42	0.50
2:B:937:ASP:OD1	2:B:939:HIS:ND1	2.40	0.50
2:B:279:GLN:OE1	2:B:284:VAL:CG2	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:GLU:OE1	2:B:309:THR:OG1	2.29	0.50
4:E:256:LEU:HD21	4:E:322:LEU:HD22	1.94	0.50
1:D:355:ASN:HD21	1:D:358:LEU:HD22	1.77	0.49
1:D:393:LEU:HD12	1:D:424:LEU:HD13	1.94	0.49
4:E:327:LYS:HB3	4:E:361:ARG:HE	1.76	0.49
4:E:662:SER:O	4:E:662:SER:OG	2.27	0.49
4:E:917:ALA:HA	4:E:927:VAL:HG23	1.95	0.49
1:D:449:ASN:HD22	1:D:469:LEU:HD11	1.78	0.48
2:B:968:VAL:HG23	2:B:969:ILE:HG13	1.95	0.48
1:D:199:ARG:NH1	1:D:496:ILE:O	2.44	0.48
4:E:461:GLN:NE2	4:E:485:ASP:OD1	2.47	0.48
2:B:126:SER:OG	2:B:127:SER:N	2.47	0.48
4:E:607:ASP:N	4:E:607:ASP:OD1	2.46	0.48
4:E:958:LEU:HD12	4:E:972:ALA:HB3	1.94	0.48
1:A:294:SER:O	1:A:299:SER:OG	2.27	0.48
4:E:737:PRO:O	4:E:740:SER:OG	2.26	0.48
4:E:185:MET:HE3	4:E:520:SER:HB3	1.95	0.48
2:B:694:ASP:OD1	2:B:694:ASP:N	2.42	0.47
4:E:318:ASP:OD1	4:E:318:ASP:N	2.44	0.47
4:E:822:ASP:HB2	4:E:829:LEU:HD11	1.96	0.47
1:A:244:LEU:HD22	1:A:387:ILE:HG12	1.96	0.47
4:E:152:MET:HG2	4:E:993:GLU:HG3	1.96	0.47
4:E:920:GLU:O	4:E:923:LYS:NZ	2.47	0.47
1:A:314:ASP:N	1:A:314:ASP:OD1	2.48	0.47
4:E:208:ASP:OD1	4:E:702:GLN:NE2	2.48	0.47
4:E:484:VAL:HG12	4:E:519:LYS:HG2	1.96	0.47
1:A:346:VAL:HG22	1:A:353:LEU:HD23	1.97	0.46
2:B:827:LYS:HA	2:B:932:GLN:HE22	1.79	0.46
1:D:249:TYR:O	1:D:391:SER:OG	2.33	0.46
4:E:978:ALA:HB1	4:E:981:LEU:HD13	1.97	0.46
1:D:272:SER:HA	1:D:275:GLU:HG2	1.97	0.45
4:E:827:LYS:HA	4:E:932:GLN:HE22	1.81	0.45
1:A:165:ASP:OD2	1:A:440:ARG:NH1	2.49	0.45
1:D:489:ARG:HB3	1:D:495:LEU:HD23	1.97	0.45
4:E:266:LEU:HD21	4:E:285:LYS:HB3	1.98	0.45
4:E:284:VAL:HG23	4:E:288:ILE:HD11	1.98	0.45
4:E:863:PRO:HD2	4:E:888:GLY:HA3	1.98	0.45
1:D:352:TYR:HB2	1:D:457:GLN:HE22	1.82	0.45
1:D:172:SER:O	1:D:172:SER:OG	2.35	0.45
4:E:126:SER:OG	4:E:128:GLU:OE1	2.32	0.44
2:B:454:PRO:HD2	2:B:494:LYS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:PHE:O	1:D:202:LYS:NZ	2.40	0.44
1:D:213:LEU:HD21	1:D:238:LEU:HD23	1.99	0.44
1:D:347:LYS:HA	1:D:347:LYS:HD2	1.82	0.44
4:E:609:SER:HB2	4:E:629:SER:HB3	2.00	0.44
2:B:985:THR:HG21	2:B:992:PRO:HG3	1.98	0.44
4:E:862:PRO:HB3	4:E:889:LYS:HB2	2.00	0.44
1:A:405:LEU:HD23	1:A:419:VAL:HG22	1.99	0.44
2:B:289:LEU:HD12	2:B:315:PHE:HZ	1.83	0.44
2:B:861:THR:HA	2:B:862:PRO:HD3	1.89	0.44
1:D:346:VAL:HB	1:D:353:LEU:HD23	1.99	0.44
4:E:887:VAL:HG12	4:E:945:SER:HB3	2.00	0.44
1:A:421:MET:HA	1:A:424:LEU:HB3	1.99	0.44
4:E:664:ILE:HG22	4:E:731:LEU:HD22	1.99	0.44
1:A:421:MET:HG3	1:A:424:LEU:HD23	1.99	0.43
4:E:251:LEU:HD11	4:E:948:ARG:HH12	1.83	0.43
4:E:318:ASP:HB2	4:E:419:ARG:HB3	1.99	0.43
1:A:488:ASP:HB3	1:A:495:LEU:HD13	1.99	0.43
4:E:969:ILE:HA	4:E:1017:PHE:HB2	2.01	0.43
1:A:28:GLY:HA2	4:E:565:LEU:HA	2.01	0.43
1:D:456:THR:OG1	1:D:457:GLN:N	2.51	0.43
1:A:199:ARG:NH1	1:A:496:ILE:O	2.48	0.43
7:B:1101:C8E:H171	7:E:1101:C8E:H82	2.00	0.43
1:D:497:LYS:NZ	1:D:499:TRP:O	2.52	0.43
1:A:294:SER:OG	1:A:295:ALA:N	2.52	0.43
1:D:316:LYS:HB3	1:D:316:LYS:HE3	1.84	0.43
4:E:151:VAL:HG22	4:E:164:VAL:HG22	2.00	0.43
4:E:229:LYS:O	4:E:374:ASN:ND2	2.52	0.42
1:D:279:ARG:NH1	1:D:356:LYS:O	2.52	0.42
4:E:327:LYS:NZ	4:E:358:GLY:O	2.52	0.42
4:E:696:SER:H	4:E:748:ASN:HD21	1.67	0.42
1:A:186:ILE:HD11	1:A:495:LEU:HD12	2.00	0.42
4:E:283:LYS:HB3	4:E:283:LYS:HE2	1.77	0.42
2:B:893:ASN:ND2	2:B:942:GLU:OE2	2.53	0.42
2:B:839:ASP:N	2:B:839:ASP:OD1	2.53	0.42
2:B:203:MET:HE2	2:B:226:ILE:HG12	2.01	0.42
2:B:982:LEU:HD23	2:B:982:LEU:HA	1.92	0.42
4:E:695:LEU:HD23	4:E:695:LEU:HA	1.93	0.42
1:A:99:ASP:N	1:A:99:ASP:OD1	2.52	0.42
2:B:471:THR:HG22	2:B:477:THR:HG23	2.02	0.42
4:E:296:TYR:HE2	4:E:310:LEU:HD23	1.84	0.42
4:E:416:THR:HG22	4:E:899:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:PHE:HB3	2:B:604:MET:HB3	2.01	0.41
4:E:243:ALA:HB3	4:E:1013:ILE:HG22	2.01	0.41
2:B:553:ILE:HD12	2:B:553:ILE:HA	1.90	0.41
2:B:509:ARG:NE	2:B:511:GLU:OE2	2.41	0.41
2:B:464:VAL:HG11	7:B:1103:C8E:H72	2.02	0.41
4:E:696:SER:H	4:E:748:ASN:ND2	2.19	0.41
1:D:342:ILE:HD11	1:D:433:ILE:HD13	2.03	0.41
4:E:926:ASP:OD1	4:E:926:ASP:N	2.52	0.41
2:B:279:GLN:OE1	2:B:284:VAL:HG22	2.21	0.40
4:E:749:VAL:HG21	4:E:790:PHE:HB3	2.04	0.40
1:D:371:ASN:OD1	1:D:371:ASN:N	2.55	0.40
1:D:420:ASN:N	1:D:420:ASN:OD1	2.55	0.40
4:E:941:LEU:HD23	4:E:941:LEU:HA	1.97	0.40
4:E:183:ASP:OD2	4:E:228:THR:OG1	2.27	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	480/482 (100%)	446 (93%)	34 (7%)	0	100	100
1	D	480/482 (100%)	446 (93%)	33 (7%)	1 (0%)	44	71
2	B	902/903 (100%)	834 (92%)	66 (7%)	2 (0%)	44	71
3	C	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
4	E	908/915 (99%)	834 (92%)	72 (8%)	2 (0%)	44	71
All	All	2781/2795 (100%)	2570 (92%)	206 (7%)	5 (0%)	45	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	791	PHE
2	B	602	LYS
4	E	790	PHE
2	B	712	PHE
1	D	351	GLY

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	402/402 (100%)	401 (100%)	1 (0%)	92	95
1	D	402/402 (100%)	399 (99%)	3 (1%)	81	88
2	B	755/754 (100%)	754 (100%)	1 (0%)	92	96
3	C	10/10 (100%)	10 (100%)	0	100	100
4	E	762/763 (100%)	762 (100%)	0	100	100
All	All	2331/2331 (100%)	2326 (100%)	5 (0%)	91	95

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

Mol	Chain	Res	Type
1	A	349	ASP
2	B	277	ASN
1	D	46	ASP
1	D	314	ASP
1	D	337	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	125	ASN
1	A	156	GLN
2	B	150	GLN
2	B	374	ASN

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Mol	Chain	Res	Type
2	B	395	ASN
2	B	638	ASN
2	B	702	GLN
2	B	713	ASN
2	B	748	ASN
2	B	754	ASN
2	B	782	ASN
2	B	835	GLN
2	B	894	ASN
2	B	935	GLN
1	D	86	ASN
1	D	449	ASN
1	D	457	GLN
1	D	490	GLN
4	E	103	GLN
4	E	269	GLN
4	E	278	ASN
4	E	465	ASN
4	E	481	GLN
4	E	597	ASN
4	E	704	ASN
4	E	748	ASN
4	E	754	ASN
4	E	800	ASN
4	E	828	GLN
4	E	932	GLN
4	E	980	ASN

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	C8E	E	1101	-	13,13,20	0.34	0	12,12,19	0.67	0
7	C8E	E	1102	-	13,13,20	0.32	0	12,12,19	0.44	0
7	C8E	B	1101	-	15,15,20	0.42	0	14,14,19	0.46	0
7	C8E	B	1103	-	20,20,20	0.38	0	19,19,19	0.39	0
7	C8E	B	1102	-	15,15,20	0.40	0	14,14,19	0.39	0
6	PLM	A	602	1	11,11,17	0.54	0	10,10,17	0.55	0
6	PLM	D	602	1	7,7,17	0.65	0	6,6,17	0.66	0
5	5PL	D	601	1	25,25,85	1.42	3 (12%)	27,27,101	1.57	3 (11%)
5	5PL	A	601	1	26,26,85	1.42	3 (11%)	28,28,101	1.34	3 (10%)

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	C8E	E	1101	-	-	8/11/11/18	-
7	C8E	E	1102	-	-	9/11/11/18	-
7	C8E	B	1101	-	-	10/13/13/18	-
7	C8E	B	1103	-	-	13/18/18/18	-
7	C8E	B	1102	-	-	9/13/13/18	-
6	PLM	A	602	1	-	4/8/9/15	-
6	PLM	D	602	1	-	1/4/5/15	-
5	5PL	D	601	1	-	8/26/26/107	-
5	5PL	A	601	1	-	6/27/27/107	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	5PL	OCK-CBH	-4.58	1.39	1.47
5	D	601	5PL	OCK-CBH	-4.53	1.39	1.47
5	D	601	5PL	OCL-CBL	2.66	1.41	1.33
5	A	601	5PL	OCL-CBL	2.58	1.40	1.33
5	A	601	5PL	OCK-CBU	2.54	1.41	1.34
5	D	601	5PL	OCK-CBU	2.44	1.41	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	601	5PL	OCK-CBU-CBV	4.45	121.09	111.50
5	A	601	5PL	OCK-CBU-CBV	3.97	120.05	111.50
5	D	601	5PL	CBH-OCK-CBU	-3.79	113.00	117.88
5	D	601	5PL	OCL-CBL-CBM	2.82	120.77	111.91
5	A	601	5PL	OCL-CBL-CBM	2.37	119.36	111.91
5	A	601	5PL	CBH-OCK-CBU	-2.36	114.84	117.88

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	5PL	CBV-CBU-OCK-CBH
5	D	601	5PL	CAW-CBH-CBI-OCL
5	D	601	5PL	OCK-CBH-CBI-OCL
5	D	601	5PL	CBM-CBL-OCL-CBI
5	A	601	5PL	OCN-CBU-OCK-CBH
7	B	1101	C8E	O18-C19-C20-O21
5	D	601	5PL	OCO-CBL-OCL-CBI
7	B	1103	C8E	O12-C13-C14-O15
7	E	1101	C8E	O9-C10-C11-O12
7	B	1102	C8E	O9-C10-C11-O12
7	B	1101	C8E	O12-C13-C14-O15
7	B	1102	C8E	O12-C13-C14-O15
7	B	1102	C8E	O18-C19-C20-O21
7	B	1103	C8E	O18-C19-C20-O21
7	B	1103	C8E	C6-C7-C8-O9
7	E	1101	C8E	C6-C7-C8-O9
7	B	1102	C8E	C6-C7-C8-O9
7	E	1101	C8E	C2-C3-C4-C5
7	B	1103	C8E	C4-C5-C6-C7
5	D	601	5PL	CBV-CBU-OCK-CBH
7	B	1101	C8E	O9-C10-C11-O12

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Mol	Chain	Res	Type	Atoms
5	D	601	5PL	OCN-CBU-OCK-CBH
7	E	1102	C8E	C2-C3-C4-C5
7	B	1101	C8E	O15-C16-C17-O18
7	E	1101	C8E	C5-C6-C7-C8
7	B	1103	C8E	C3-C4-C5-C6
5	D	601	5PL	CBR-CAA-CBP-CBO
7	B	1101	C8E	C6-C7-C8-O9
6	A	602	PLM	C7-C8-C9-CA
7	E	1102	C8E	C1-C2-C3-C4
5	D	601	5PL	CBU-CBV-CBW-CBX
6	D	602	PLM	C2-C3-C4-C5
7	E	1102	C8E	C14-C13-O12-C11
7	E	1102	C8E	C5-C6-C7-C8
7	B	1103	C8E	C16-C17-O18-C19
6	A	602	PLM	C2-C3-C4-C5
7	B	1101	C8E	C20-C19-O18-C17
7	B	1102	C8E	C17-C16-O15-C14
7	B	1102	C8E	C14-C13-O12-C11
7	B	1103	C8E	C10-C11-O12-C13
7	E	1102	C8E	C7-C8-O9-C10
7	B	1103	C8E	C20-C19-O18-C17
7	E	1102	C8E	C3-C4-C5-C6
7	B	1101	C8E	C10-C11-O12-C13
7	B	1102	C8E	C20-C19-O18-C17
7	B	1101	C8E	C7-C8-O9-C10
7	B	1103	C8E	C7-C8-O9-C10
7	B	1103	C8E	C13-C14-O15-C16
7	B	1102	C8E	C13-C14-O15-C16
7	E	1101	C8E	C14-C13-O12-C11
7	B	1103	C8E	C14-C13-O12-C11
7	E	1102	C8E	C4-C5-C6-C7
5	A	601	5PL	CBV-CBW-CBX-CBY
7	B	1103	C8E	C17-C16-O15-C14
7	B	1101	C8E	C16-C17-O18-C19
5	A	601	5PL	CBL-CBM-CBN-CBO
7	B	1101	C8E	C14-C13-O12-C11
7	B	1103	C8E	O15-C16-C17-O18
6	A	602	PLM	C6-C7-C8-C9
5	A	601	5PL	CAA-CBR-CBS-CBT
7	E	1101	C8E	C4-C5-C6-C7
7	E	1101	C8E	C10-C11-O12-C13
5	A	601	5PL	CAF-CAE-CBZ-CBY

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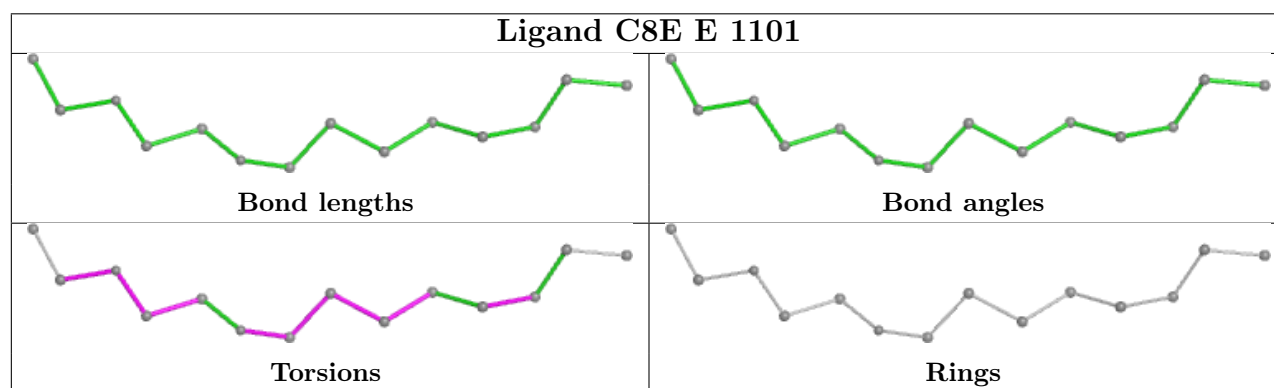
Mol	Chain	Res	Type	Atoms
6	A	602	PLM	C5-C6-C7-C8
7	E	1101	C8E	C7-C8-O9-C10
7	E	1102	C8E	O9-C10-C11-O12
7	E	1102	C8E	C10-C11-O12-C13
7	B	1102	C8E	O15-C16-C17-O18

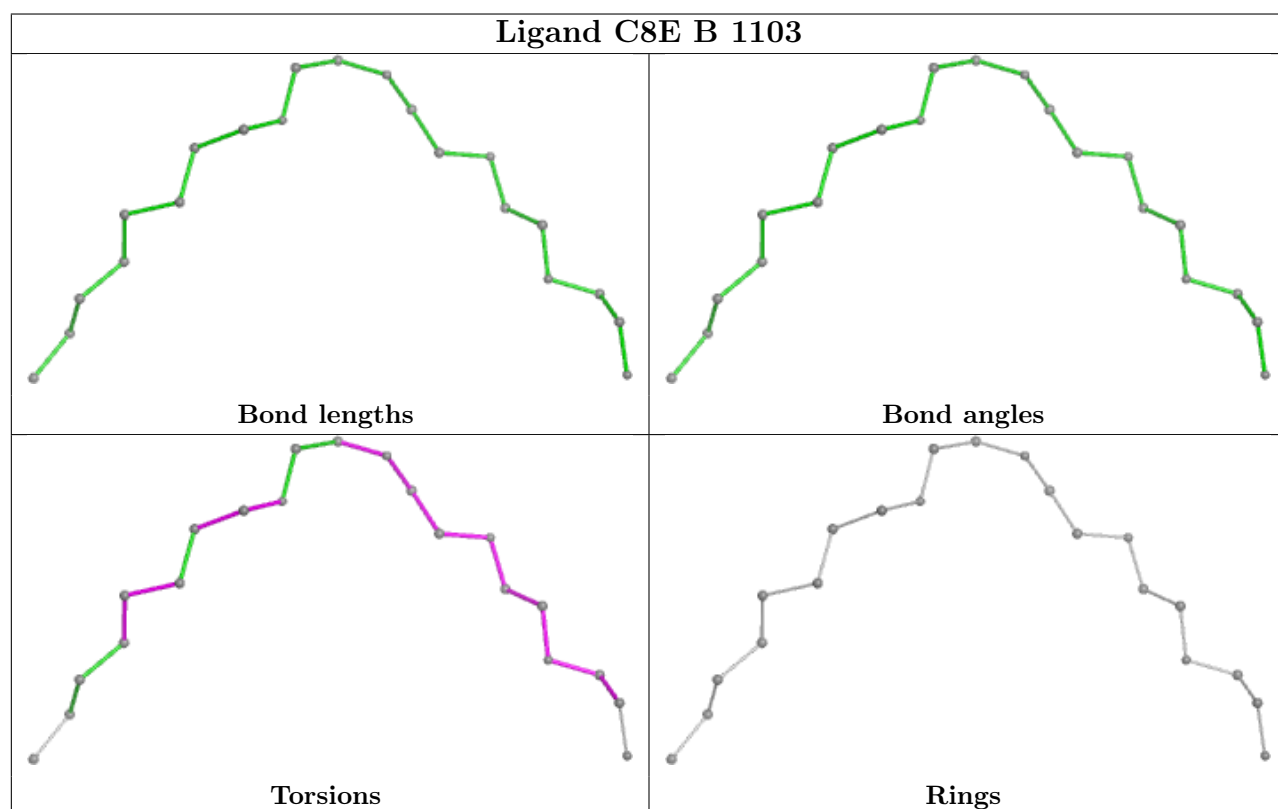
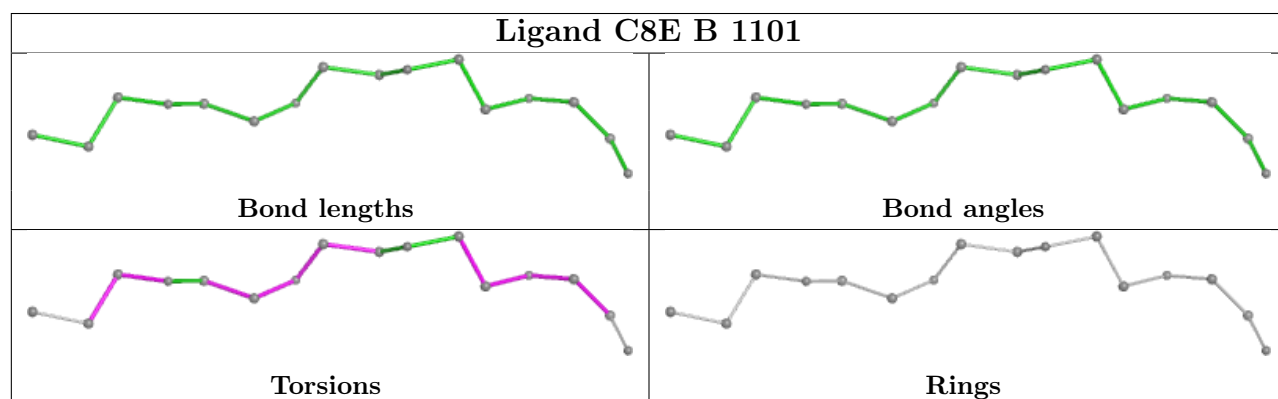
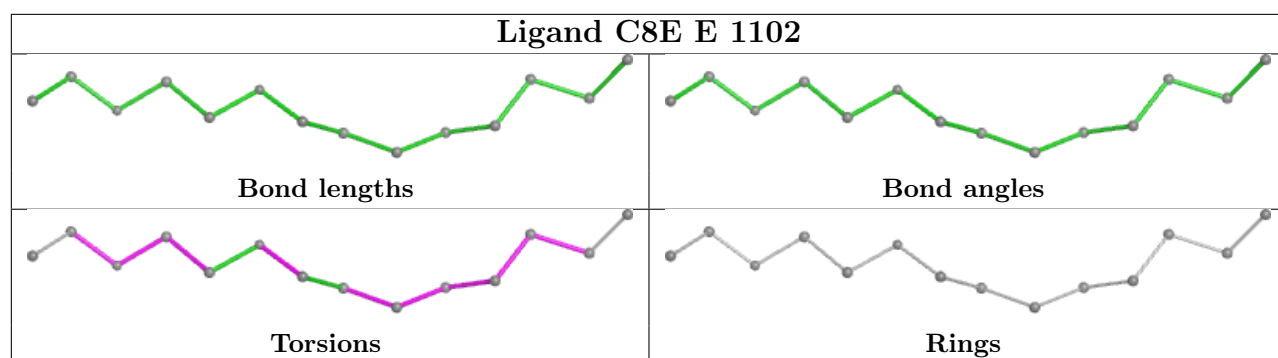
There are no ring outliers.

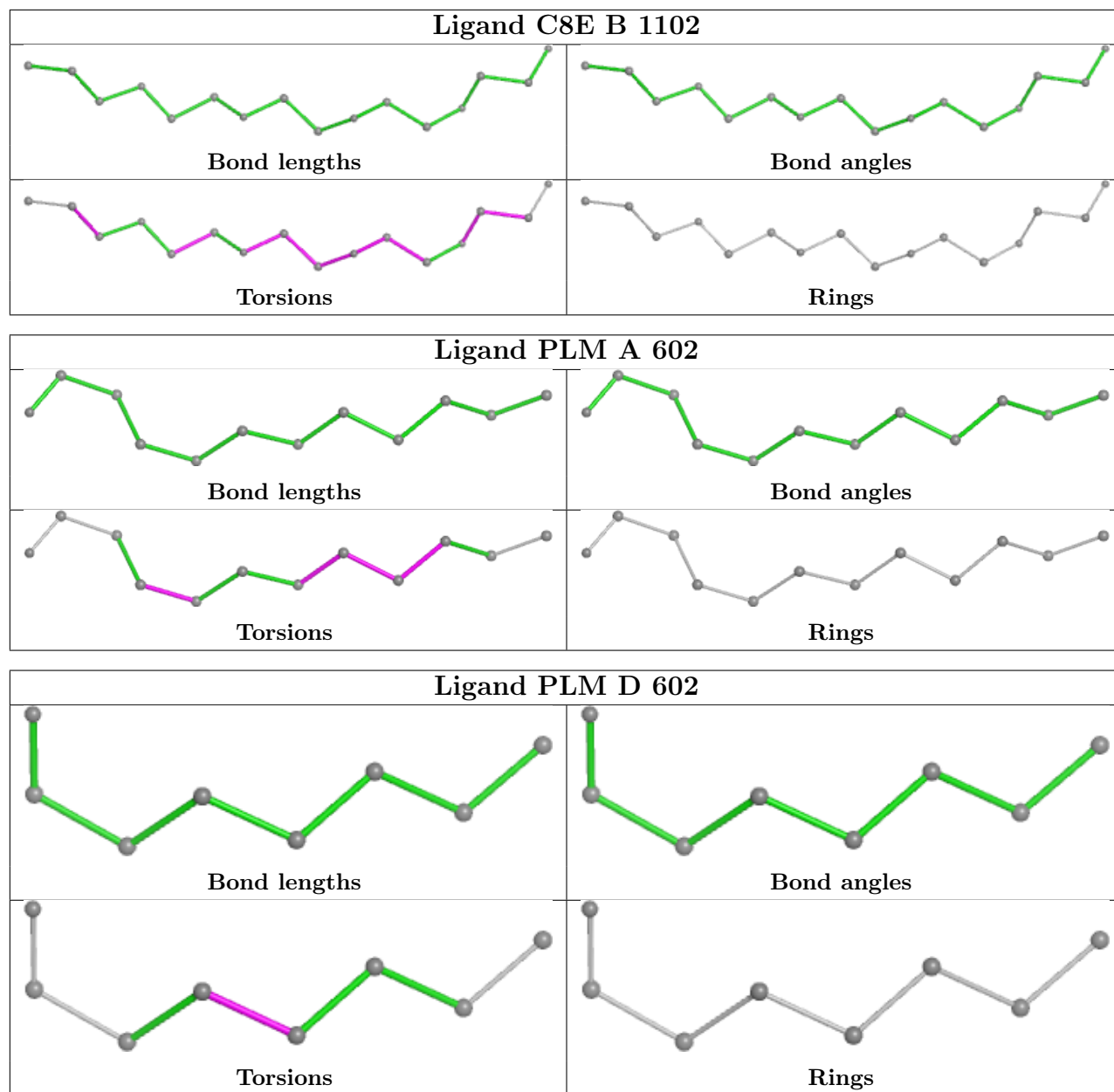
3 monomers are involved in 2 short contacts:

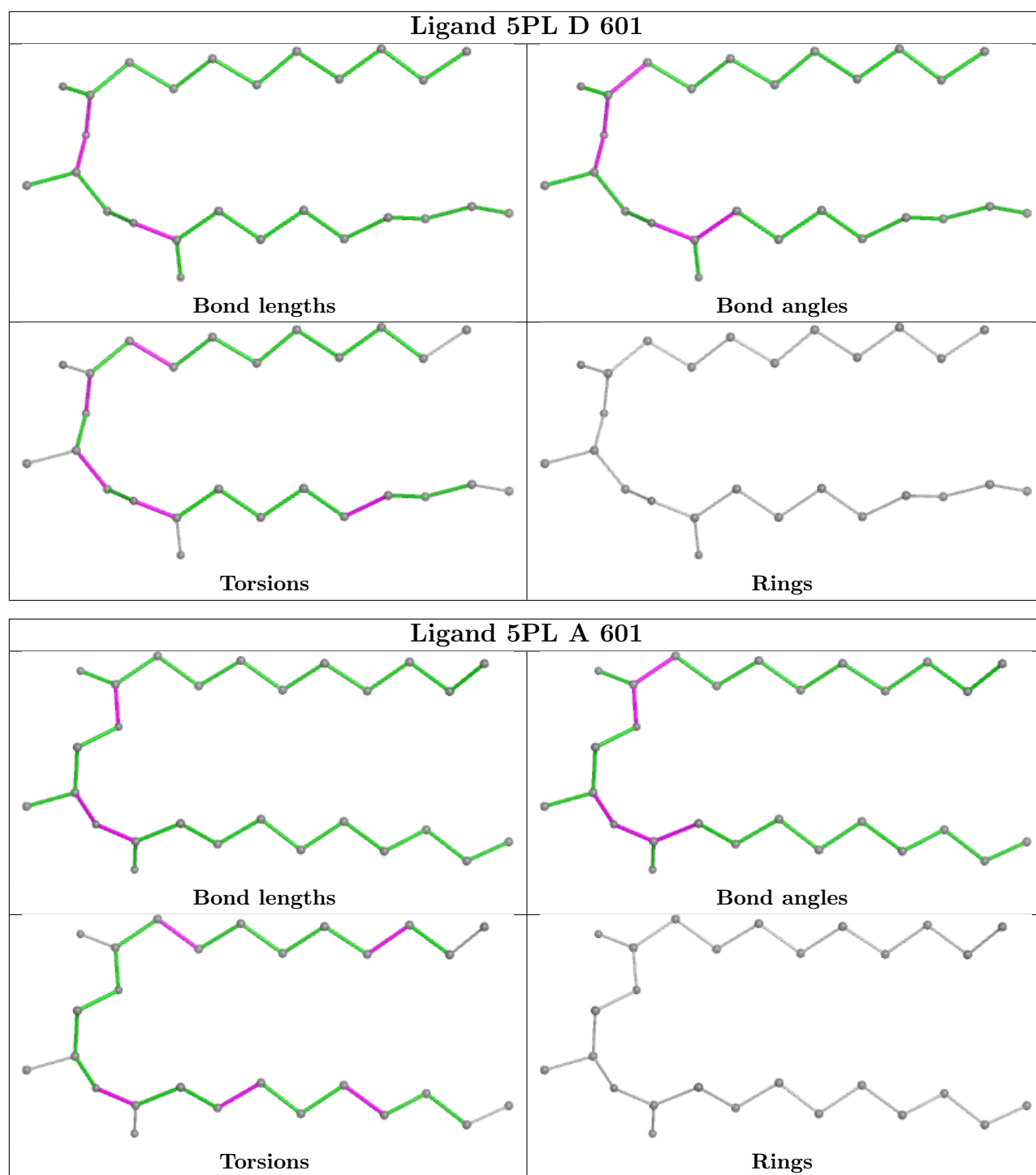
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	1101	C8E	1	0
7	B	1101	C8E	1	0
7	B	1103	C8E	1	0

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

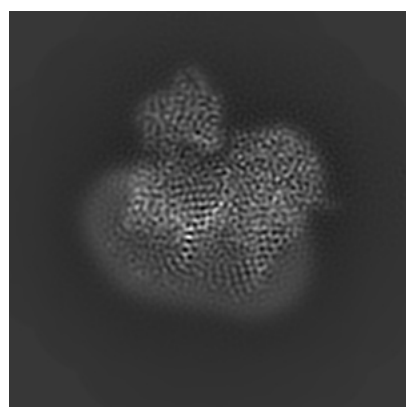
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10245. These allow visual inspection of the internal detail of the map and identification of artifacts.

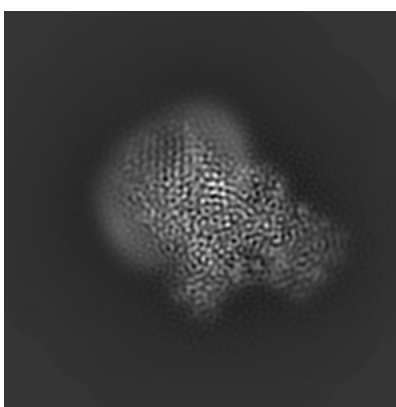
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

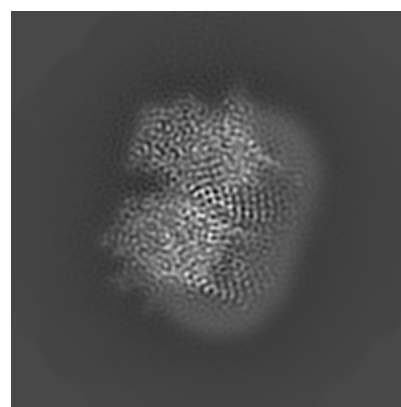
6.1.1 Primary map



X



Y

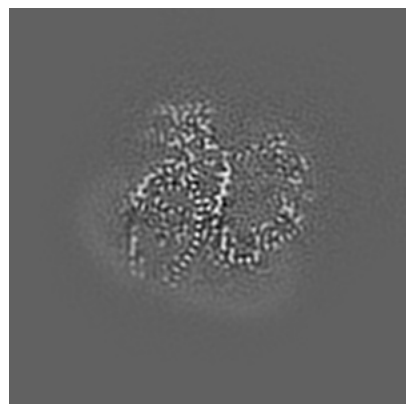


Z

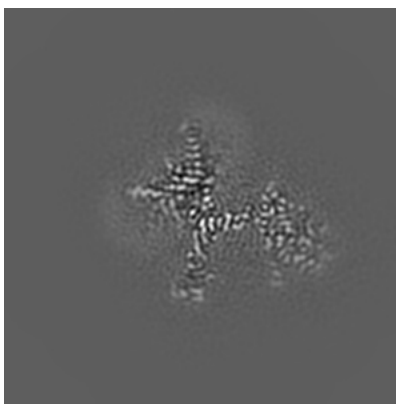
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

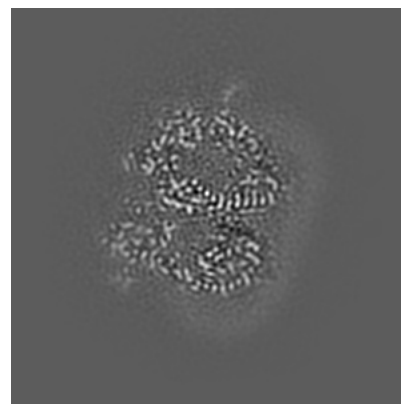
6.2.1 Primary map



X Index: 108



Y Index: 108

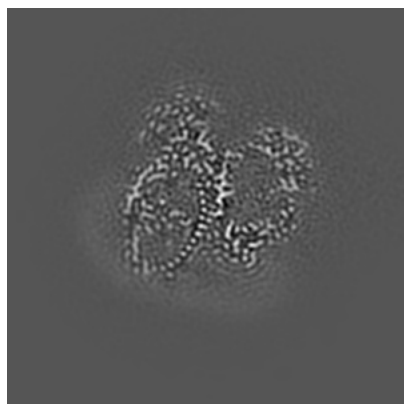


Z Index: 108

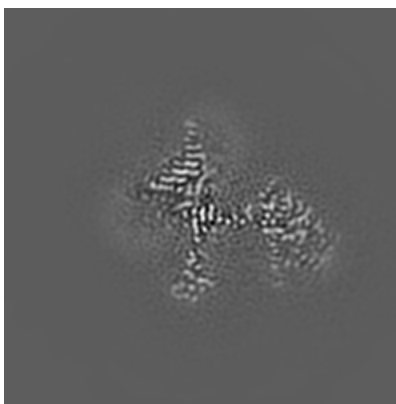
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

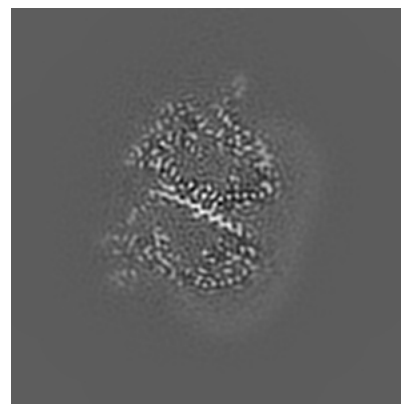
6.3.1 Primary map



X Index: 104



Y Index: 106

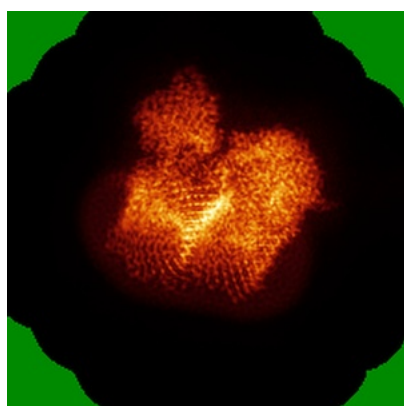


Z Index: 111

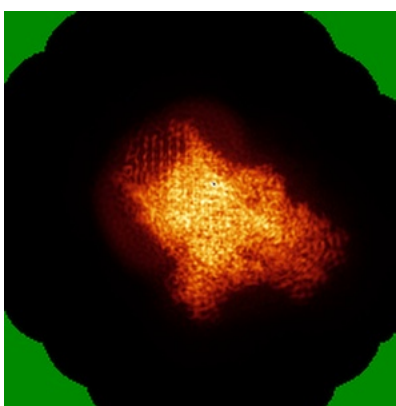
The images above show the largest variance slices of the map in three orthogonal directions.

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

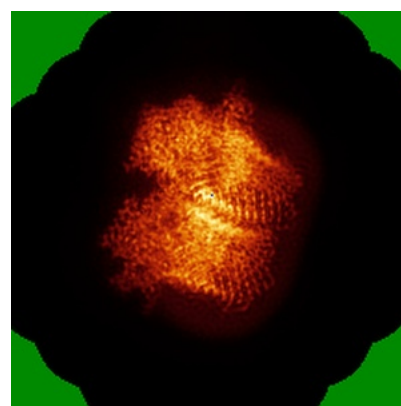
6.4.1 Primary map



X



Y

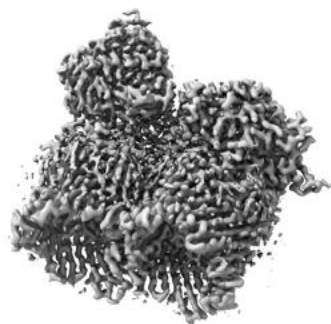


Z

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](#)

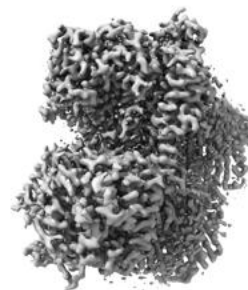
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. 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 shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

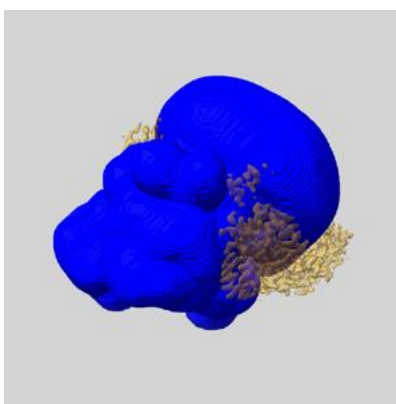
A mask typically either:

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

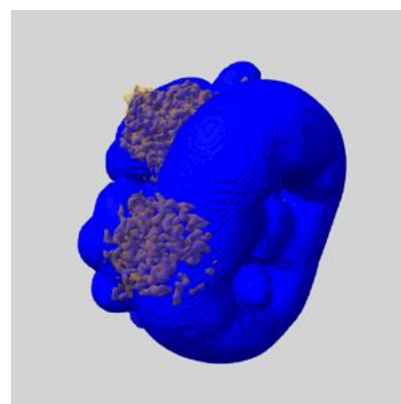
6.6.1 emd_10245_msk_1.map [i](#)



X



Y

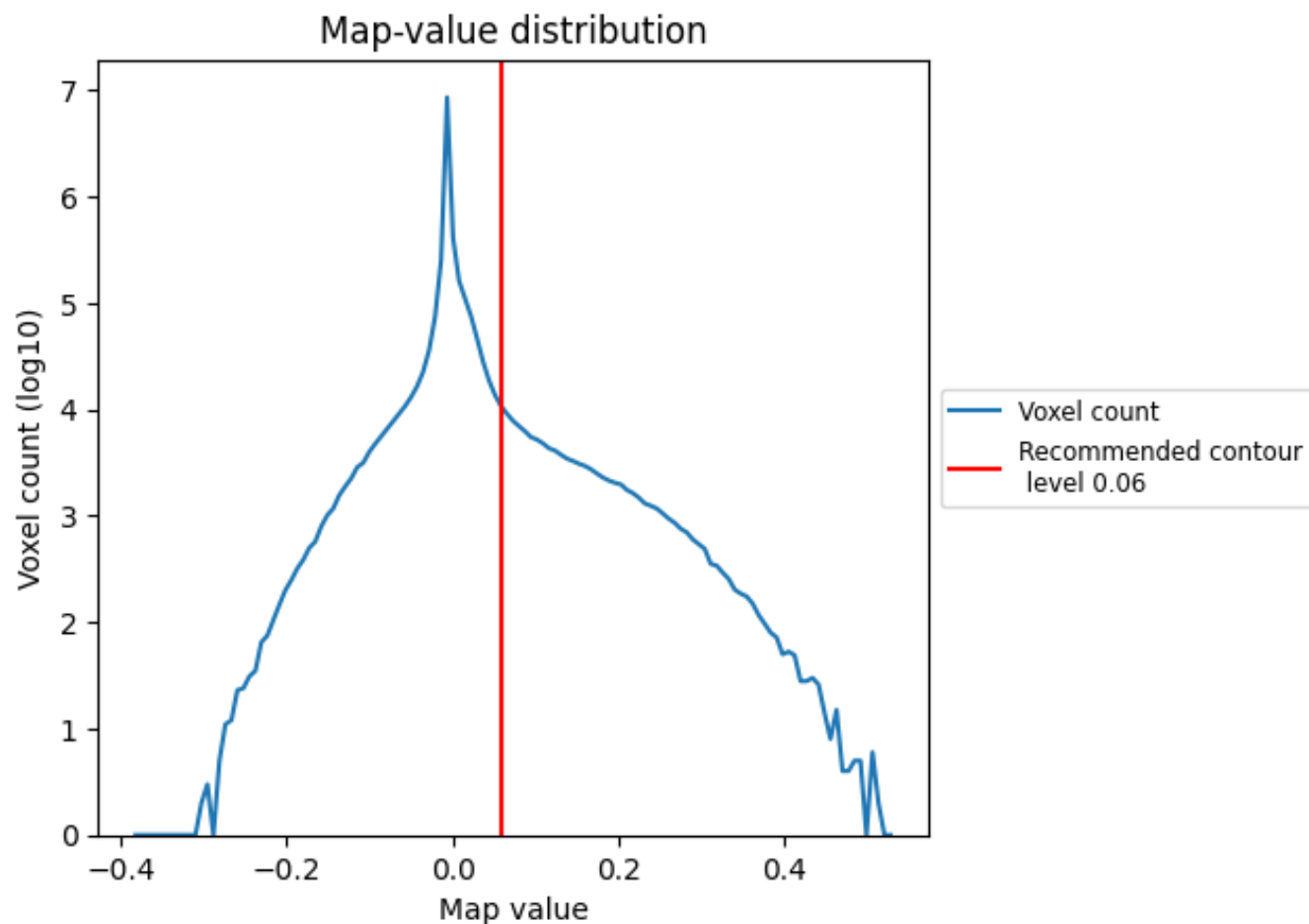


Z

7 Map analysis [i](#)

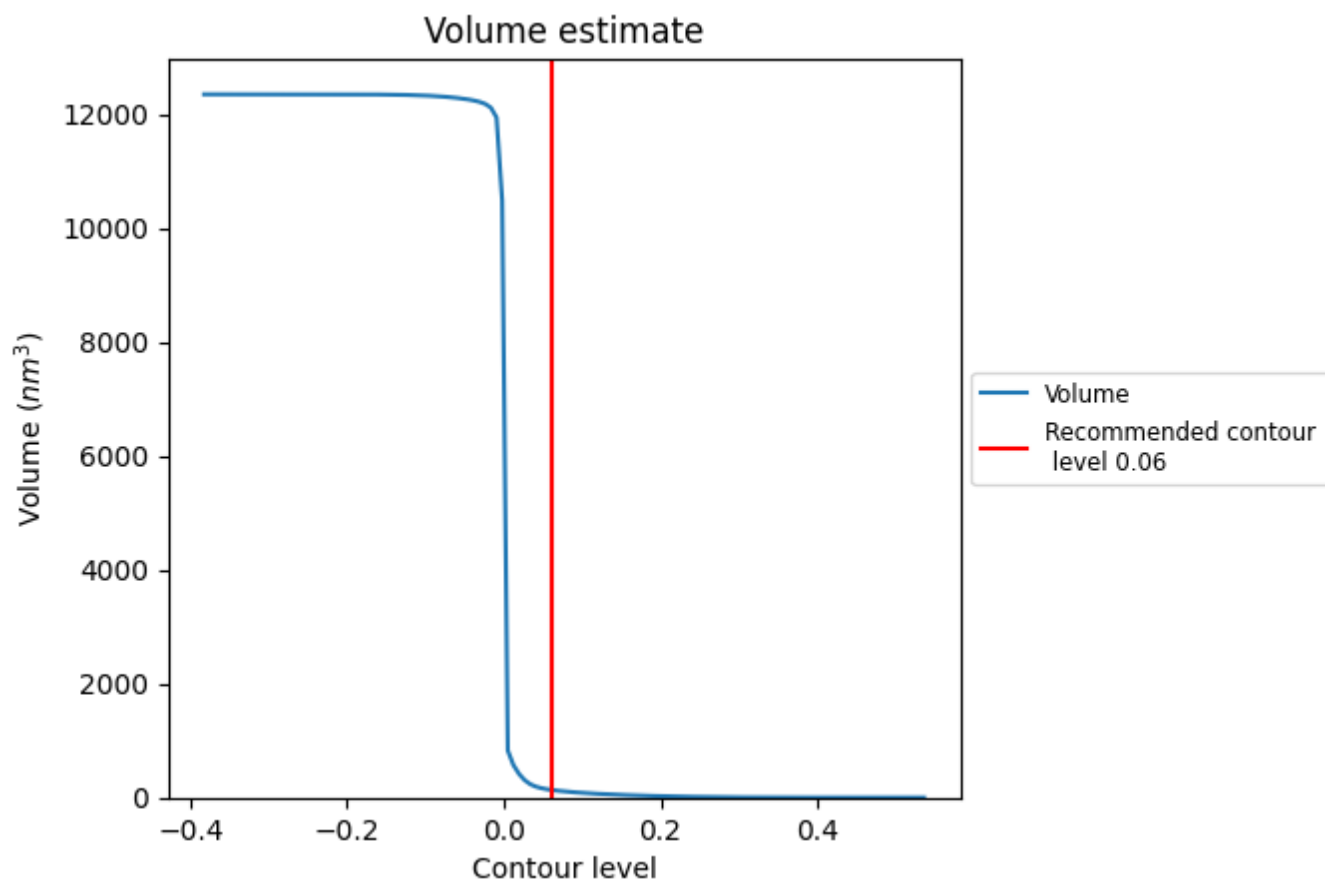
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

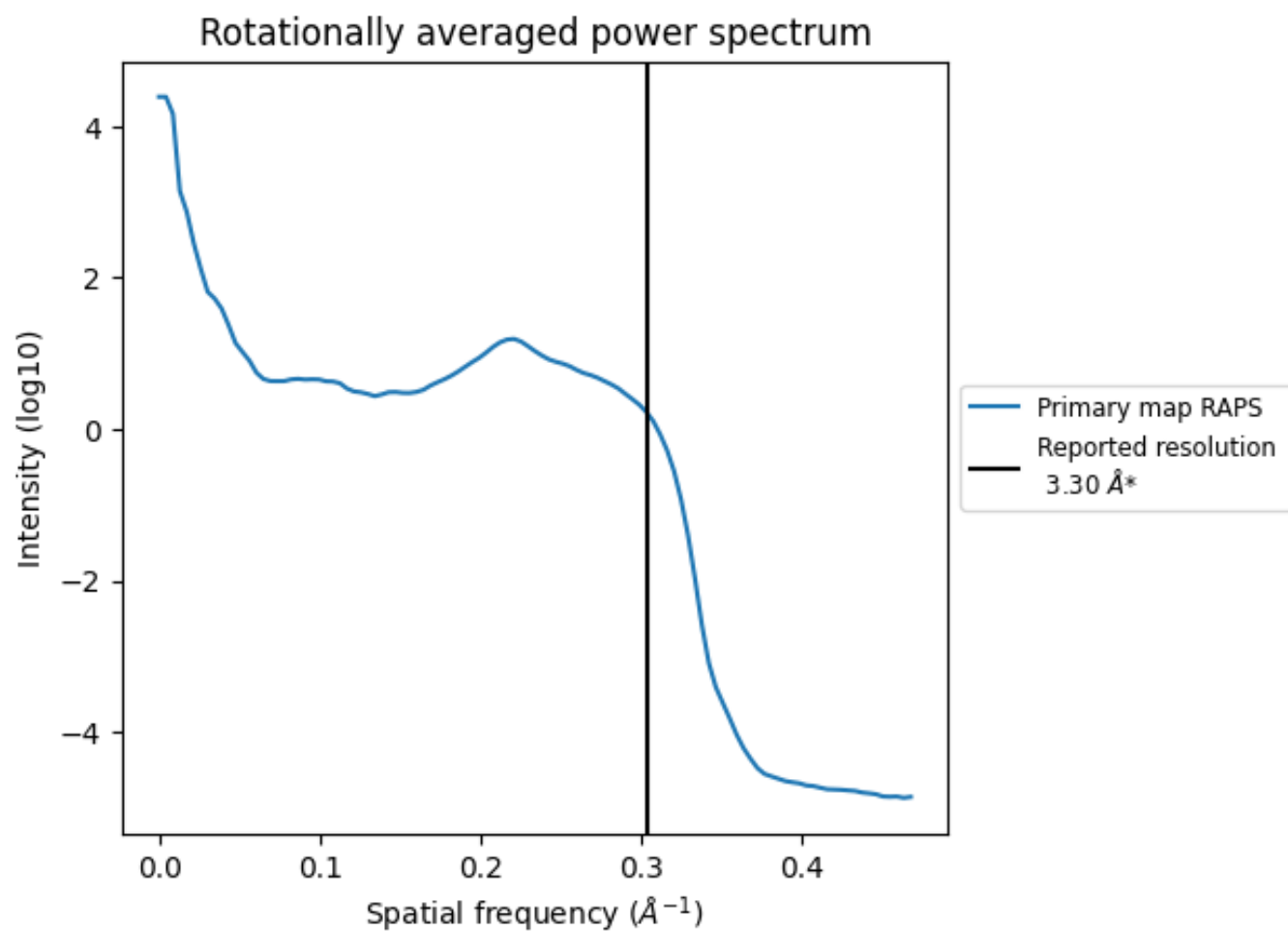
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm³; this corresponds to an approximate mass of 122 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 ⓘ

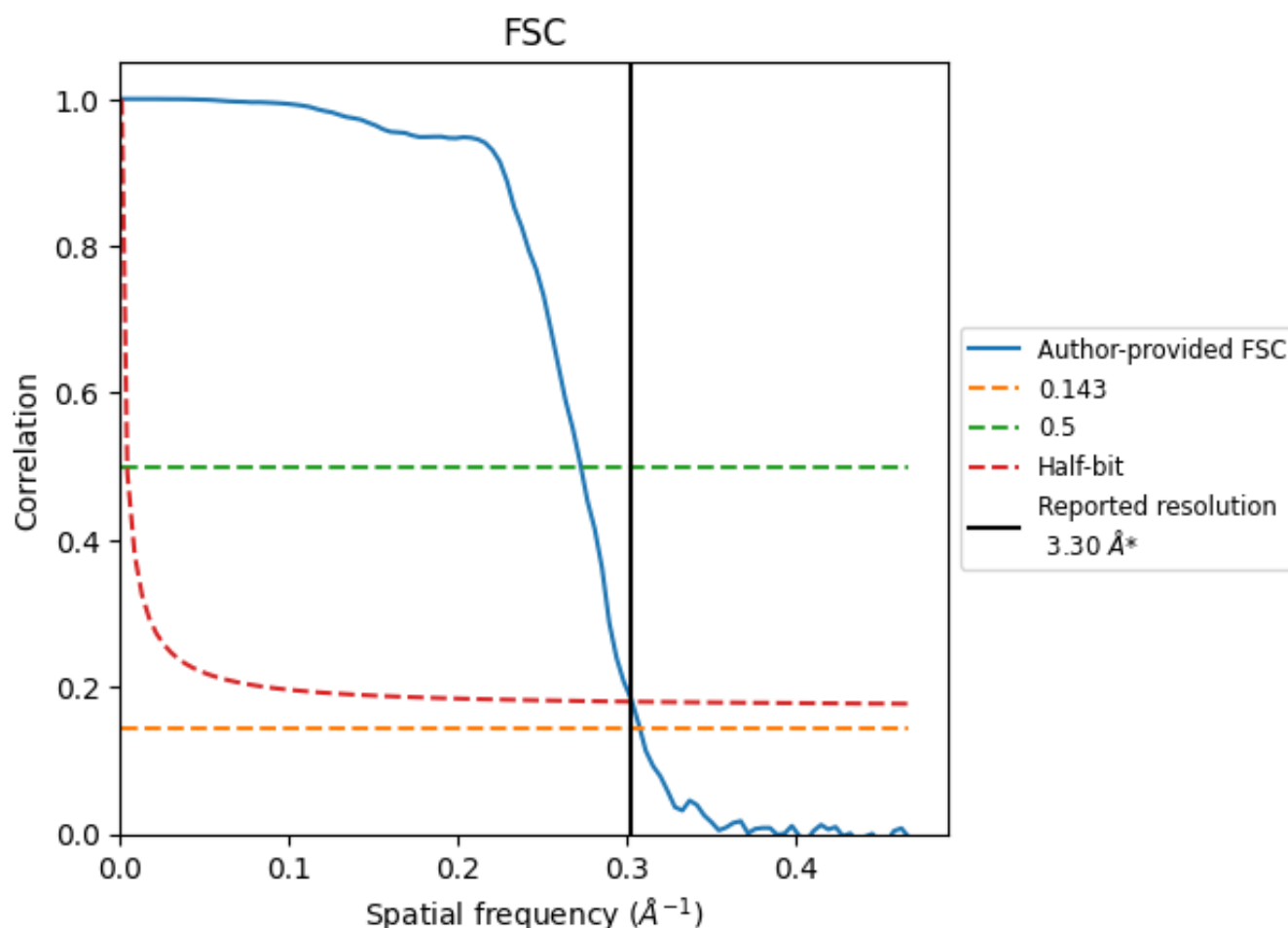


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

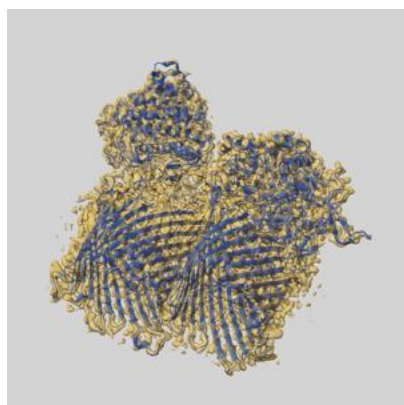
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.25	3.66	3.30
Unmasked-calculated*	-	-	-

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

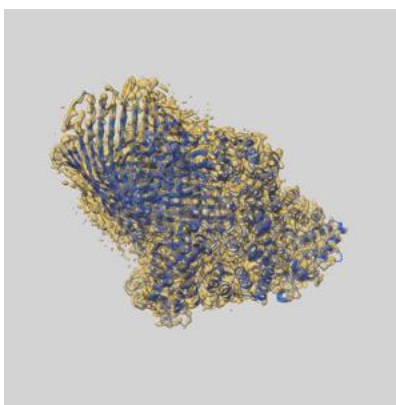
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10245 and PDB model 6SMQ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

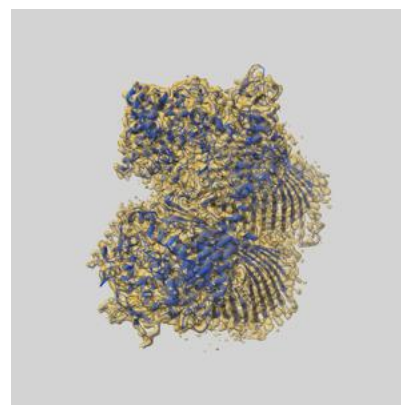
9.1 Map-model overlay [i](#)



X



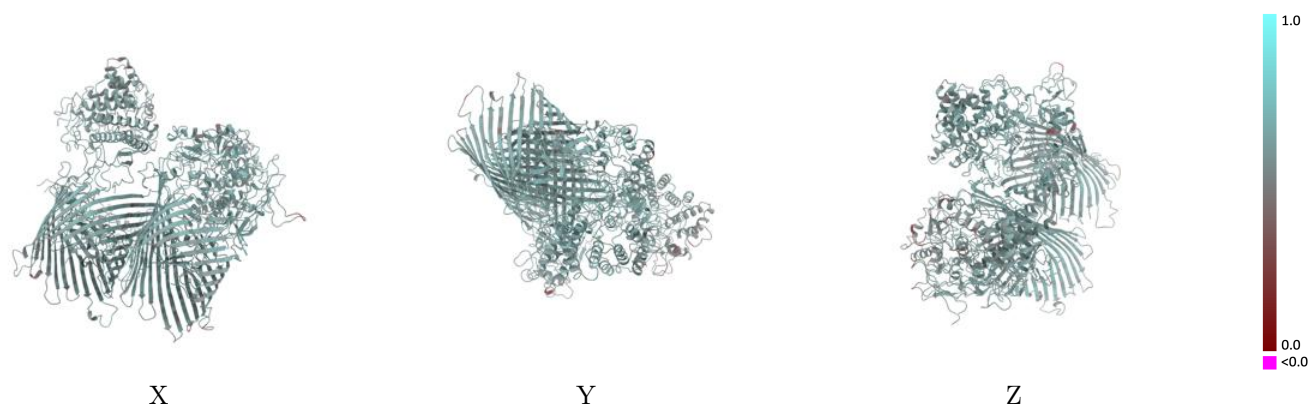
Y



Z

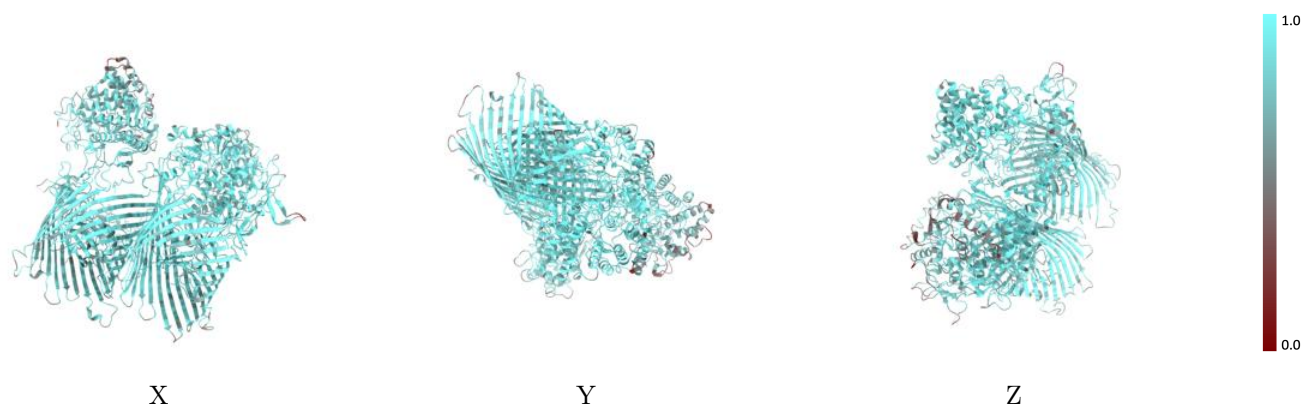
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



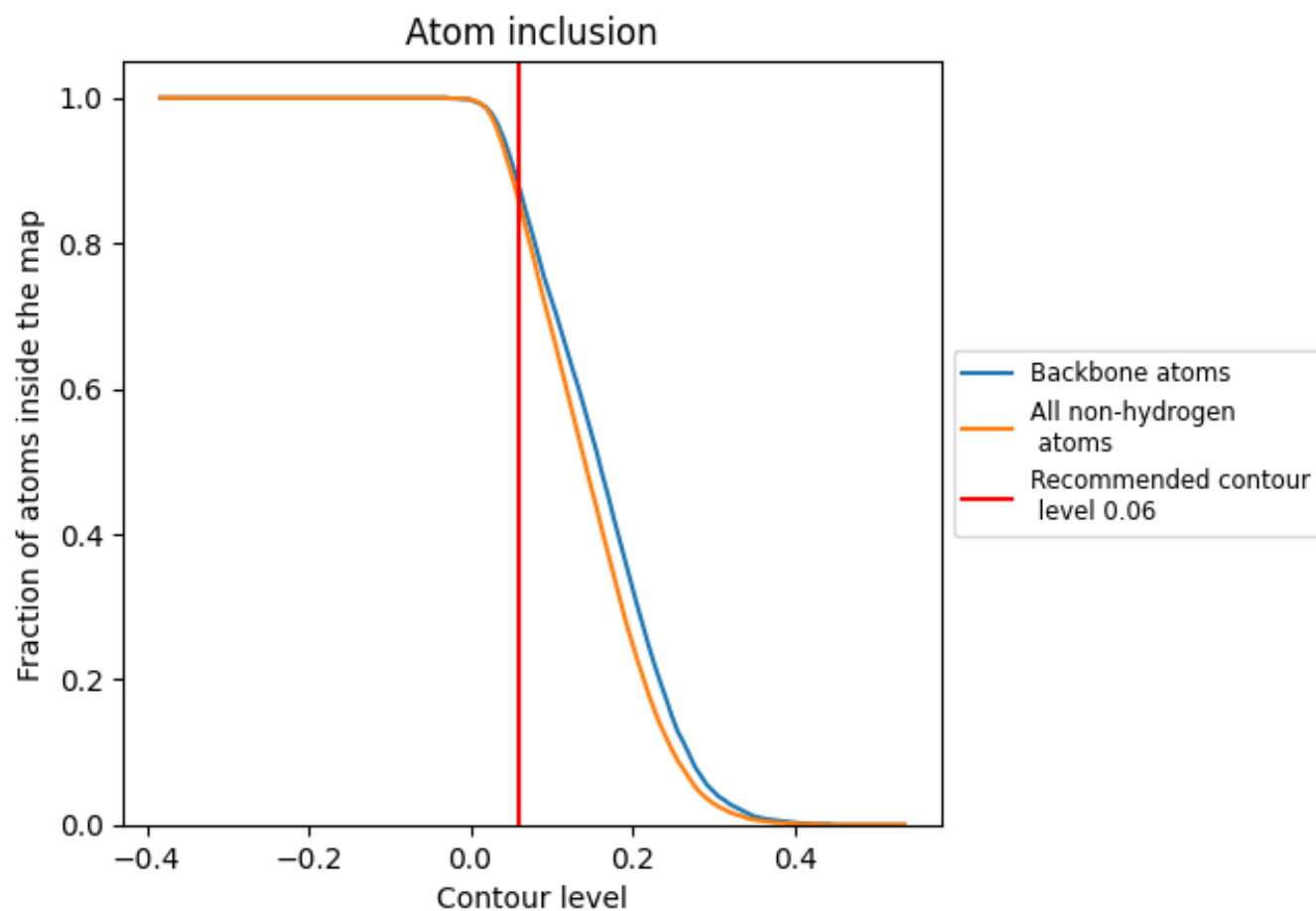
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8580	<div><div></div></div> 0.5870
A	<div><div></div></div> 0.8850	<div><div></div></div> 0.6020
B	<div><div></div></div> 0.8800	<div><div></div></div> 0.5950
C	<div><div></div></div> 0.8420	<div><div></div></div> 0.5390
D	<div><div></div></div> 0.7820	<div><div></div></div> 0.5630
E	<div><div></div></div> 0.8630	<div><div></div></div> 0.5860

