



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 08:40 PM UTC

PDB ID : 6S8N / pdb_00006s8n
EMDB ID : EMD-10125
Title : Cryo-EM structure of LptB2FGC in complex with lipopolysaccharide
Authors : Tang, X.D.; Chang, S.H.; Luo, Q.H.; Zhang, Z.Y.; Qiao, W.; Xu, C.H.; Zhang, C.B.; Niu, Y.; Yang, W.X.; Wang, T.; Zhang, Z.B.; Zhu, X.F.; Dong, C.J.; Zhang, X.; Dong, H.H.
Deposited on : 2019-07-10
Resolution : 3.10 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

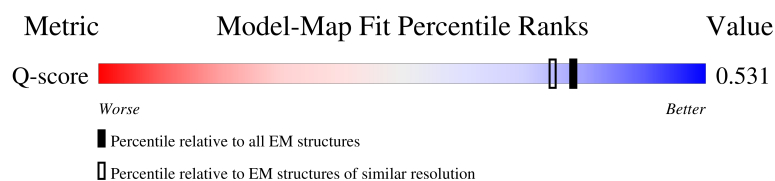
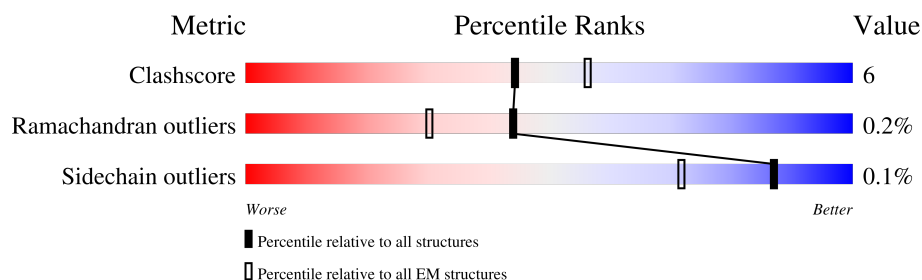
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	14724 (2.60 - 3.60)

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	241	 87% 12%
1	B	241	 83% 15%
2	C	191	 10% 87%
3	F	366	 60% 6% 35%

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Mol	Chain	Length	Quality of chain
4	G	360	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DCQ	B	301	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7831 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 Lipopolysaccharide ABC transporter, ATP-binding protein LptB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	239	Total	C	N	O	S	0	0
			1868	1168	342	353	5		
1	B	238	Total	C	N	O	S	0	0
			1857	1162	338	352	5		

- Molecule 2 is a protein called Lipopolysaccharide export system protein LptC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	24	Total	C	N	O	S	0	0
			187	124	33	27	3		

- Molecule 3 is a protein called Lipopolysaccharide export system permease protein LptF.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	239	Total	C	N	O	S	0	0
			1864	1233	303	313	15		

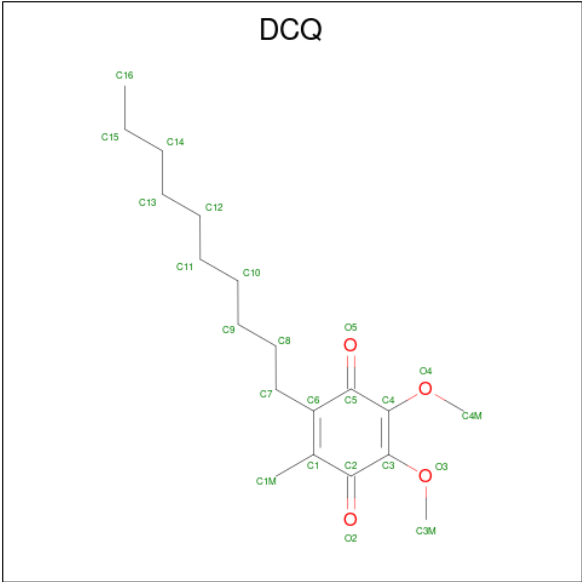
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	274	VAL	PHE	conflict	UNP P0AFA1

- Molecule 4 is a protein called Inner membrane protein yjgQ.

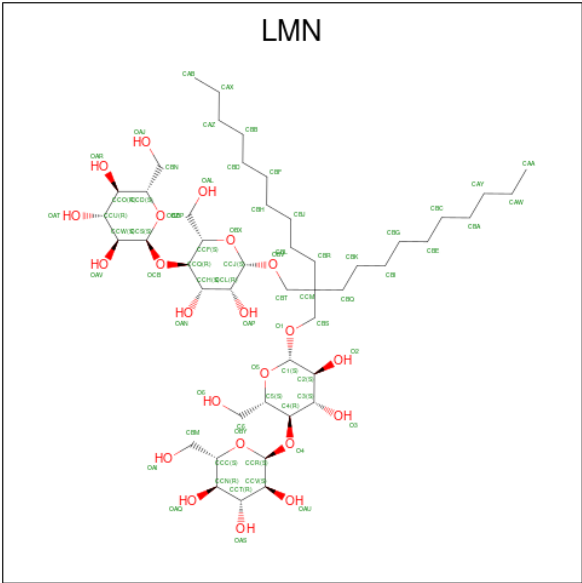
Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	230	Total	C	N	O	S	0	0
			1778	1183	283	295	17		

- Molecule 5 is 2-decyl-5,6-dimethoxy-3-methylcyclohexa-2,5-diene-1,4-dione (CCD ID: DCQ) (formula: C₁₉H₃₀O₄).



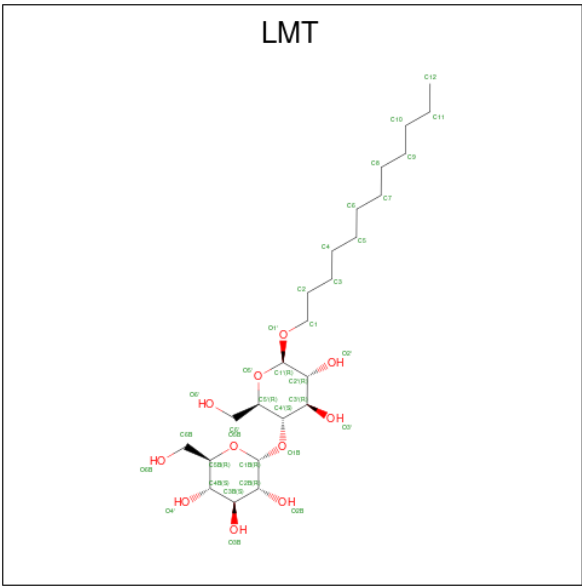
Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	C	O	0
			23	19	4	
5	G	1	Total	C	O	0
			23	19	4	

- Molecule 6 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: C₄₇H₈₈O₂₂).



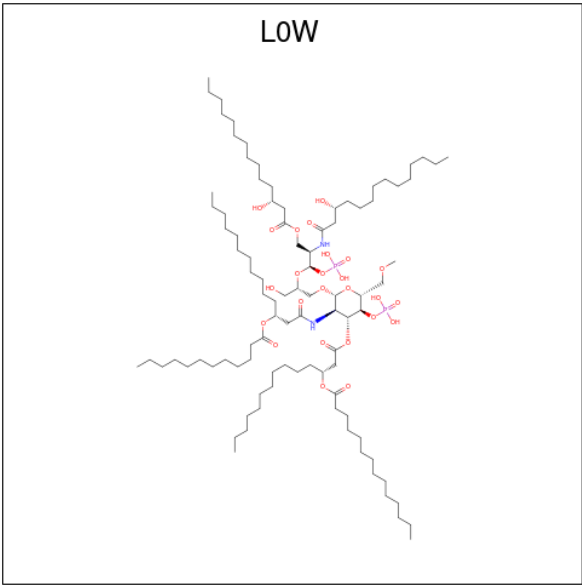
Mol	Chain	Residues	Atoms			AltConf
6	F	1	Total	C	O	0
			34	29	5	
6	G	1	Total	C	O	0
			35	29	6	

- Molecule 7 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



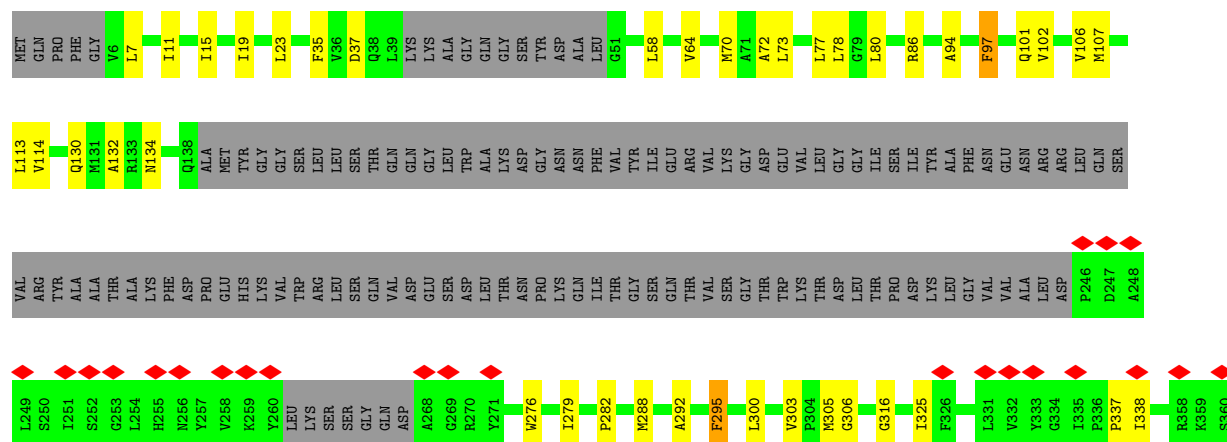
Mol	Chain	Residues	Atoms			AltConf
7	F	1	Total	C	O	0
			14	13	1	
7	G	1	Total	C	O	0
			24	18	6	

- Molecule 8 is lipopolysaccharide fragment (CCD ID: LOW) (formula: C₉₅H₁₈₂N₂O₂₅P₂).



Mol	Chain	Residues	Atoms					AltConf
8	G	1	Total	C	N	O	P	0
			124	95	2	25	2	

- Molecule 4: Inner membrane protein yjgQ



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	546301	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	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	0.199	Depositor
Minimum map value	-0.114	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	243.36002, 243.36002, 243.36002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.014, 1.014, 1.014	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: L0W, LMT, LMN, DCQ

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	0.24	0/1895	0.65	1/2562 (0.0%)
1	B	0.50	2/1884 (0.1%)	0.79	5/2548 (0.2%)
2	C	0.22	0/188	0.51	0/252
3	F	0.24	0/1899	0.58	0/2588
4	G	0.24	0/1816	0.63	2/2456 (0.1%)
All	All	0.32	2/7682 (0.0%)	0.66	8/10406 (0.1%)

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	A	0	1
1	B	0	3
4	G	0	2
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	136	GLN	CB-CG	12.78	1.90	1.52
1	B	136	GLN	CG-CD	12.38	1.82	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	GLN	CB-CG-CD	19.94	146.50	112.60
4	G	97	PHE	N-CA-C	5.91	119.39	110.64
1	B	135	GLY	CA-C-N	5.69	132.41	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	GLY	C-N-CA	5.69	132.41	121.54
1	B	62	ILE	CA-C-N	5.59	132.21	121.54
1	B	62	ILE	C-N-CA	5.59	132.21	121.54
1	A	198	ARG	N-CA-C	-5.29	108.58	114.62
4	G	35	PHE	N-CA-C	-5.03	107.64	112.97

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	ILE	Peptide
1	B	136	GLN	Peptide
1	B	156	PRO	Peptide
1	B	39	GLY	Peptide
4	G	295	PHE	Peptide
4	G	37	ASP	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	1868	0	1888	18	0
1	B	1857	0	1875	40	0
2	C	187	0	220	3	0
3	F	1864	0	2002	12	0
4	G	1778	0	1882	24	0
5	B	23	0	25	17	0
5	G	23	0	30	0	0
6	F	34	0	47	3	0
6	G	35	0	51	2	0
7	F	14	0	25	1	0
7	G	24	0	35	0	0
8	G	124	0	0	6	0
All	All	7831	0	8080	101	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 6.

All (101) 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:G:401:L0W:CAR	8:G:401:L0W:CAT	1.78	1.61
8:G:401:L0W:CAR	8:G:401:L0W:CAP	1.79	1.58
1:B:136:GLN:CB	5:B:301:DCQ:C3	1.83	1.56
1:B:136:GLN:CD	1:B:136:GLN:CG	1.83	1.48
1:B:136:GLN:CB	1:B:136:GLN:CG	1.90	1.47
1:B:136:GLN:HB3	5:B:301:DCQ:C3	1.57	1.19
8:G:401:L0W:CAR	8:G:401:L0W:CAN	2.25	1.14
8:G:401:L0W:CAR	8:G:401:L0W:OAU	1.99	1.09
1:B:136:GLN:HB3	5:B:301:DCQ:C4	1.82	1.08
1:B:136:GLN:CD	5:B:301:DCQ:C3	2.27	1.07
1:B:136:GLN:CB	5:B:301:DCQ:C2	2.44	0.94
1:B:136:GLN:CD	5:B:301:DCQ:O3	2.10	0.93
1:B:2:ALA:N	1:B:28:SER:HG	1.80	0.79
1:B:136:GLN:CB	5:B:301:DCQ:O3	2.32	0.78
8:G:401:L0W:CAR	8:G:401:L0W:CAL	2.72	0.68
1:A:40:ALA:HB1	1:A:212:GLN:H	1.59	0.67
1:B:136:GLN:CD	5:B:301:DCQ:C2	2.69	0.66
1:B:91:ARG:HA	5:B:301:DCQ:H4MB	1.76	0.65
8:G:401:L0W:CAR	8:G:401:L0W:OAQ	2.46	0.64
1:B:60:ILE:H	1:B:68:SER:HB3	1.66	0.61
3:F:32:VAL:HG13	4:G:325:ILE:HD11	1.83	0.60
4:G:78:LEU:HD12	4:G:305:MET:HE2	1.85	0.58
1:A:161:LEU:HB3	1:A:164:PRO:HG3	1.85	0.58
1:B:136:GLN:HB2	5:B:301:DCQ:C2	2.33	0.58
1:A:125:PHE:O	1:A:145:ARG:NH2	2.37	0.57
1:B:89:ILE:O	1:B:91:ARG:NH1	2.38	0.57
1:B:163:GLU:HA	1:B:194:ASP:HB3	1.86	0.57
1:A:91:ARG:HG3	4:G:86:ARG:HD3	1.85	0.57
1:B:136:GLN:OE1	5:B:301:DCQ:C3	2.53	0.56
1:B:136:GLN:CG	1:B:136:GLN:NE2	2.63	0.56
4:G:337:PRO:HB2	4:G:338:ILE:HD12	1.88	0.56
1:A:12:ALA:HB2	1:A:17:ARG:HG3	1.88	0.55
1:B:5:THR:HG23	1:B:25:THR:HG22	1.88	0.55
2:C:10:ILE:HA	6:F:401:LMN:HBFA	1.87	0.55
1:B:91:ARG:HE	5:B:301:DCQ:H7A	1.70	0.55
1:B:18:VAL:HG23	1:B:19:VAL:HG12	1.89	0.55
4:G:58:LEU:HB2	4:G:132:ALA:HB2	1.89	0.55
3:F:8:VAL:HG13	3:F:105:LEU:HD13	1.89	0.54
4:G:15:ILE:HD11	4:G:80:LEU:HG	1.88	0.54
1:A:9:LEU:HD23	1:A:58:GLY:HA3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ALA:HB1	4:G:7:LEU:HD22	1.90	0.53
1:B:88:SER:O	1:B:150:ARG:NH2	2.43	0.52
4:G:19:ILE:HD12	4:G:72:ALA:HA	1.91	0.51
1:B:208:TYR:HB3	1:B:215:LEU:HD11	1.92	0.51
4:G:70:MET:HE3	4:G:316:GLY:HA3	1.92	0.51
1:B:136:GLN:HB3	5:B:301:DCQ:C2	2.31	0.50
1:A:35:LEU:HB2	1:A:209:ILE:HD13	1.94	0.48
4:G:130:GLN:NE2	4:G:134:ASN:OD1	2.45	0.48
3:F:12:LEU:HD13	3:F:105:LEU:HD11	1.94	0.48
1:A:209:ILE:HG21	1:A:230:VAL:HG13	1.95	0.47
1:B:200:THR:HA	1:B:203:VAL:HG12	1.95	0.47
1:B:201:LEU:HD22	1:B:221:PRO:HB3	1.95	0.47
3:F:254:LEU:HD12	3:F:256:ASN:H	1.79	0.47
1:B:91:ARG:HD3	5:B:301:DCQ:H4MB	1.96	0.47
1:B:197:VAL:HG11	1:B:235:LEU:HD21	1.95	0.47
4:G:106:VAL:HG23	4:G:107:MET:HE2	1.95	0.47
4:G:276:TRP:HA	4:G:279:ILE:HG22	1.97	0.46
1:B:3:THR:H	1:B:63:ASP:HB3	1.81	0.46
3:F:60:ALA:HA	3:F:63:ILE:HG12	1.97	0.46
2:C:12:LEU:HD21	3:F:305:LEU:HD13	1.97	0.46
1:A:65:ASP:OD2	1:A:65:ASP:N	2.48	0.46
4:G:305:MET:HB3	6:G:402:LMN:HCJ	1.97	0.46
6:F:401:LMN:HBLA	6:F:401:LMN:HBQ	1.64	0.45
1:A:9:LEU:HD21	1:A:60:ILE:HD11	1.99	0.45
4:G:19:ILE:HG21	4:G:113:LEU:HD21	1.98	0.45
4:G:23:LEU:HD21	4:G:64:VAL:HG13	1.98	0.45
1:A:194:ASP:OD2	1:A:195:HIS:N	2.50	0.45
5:B:301:DCQ:H13	5:B:301:DCQ:H10A	1.66	0.45
4:G:73:LEU:HD12	4:G:292:ALA:HB2	1.99	0.45
4:G:97:PHE:HA	4:G:101:GLN:HE21	1.82	0.44
1:A:195:HIS:CE1	1:B:167:GLY:HA2	2.53	0.44
1:B:89:ILE:HA	1:B:150:ARG:HH21	1.83	0.44
1:A:14:LYS:HE2	1:A:14:LYS:HB2	1.87	0.44
3:F:268:TRP:HA	3:F:271:THR:HG22	2.00	0.44
1:A:72:LEU:HD21	4:G:94:ALA:HB2	2.00	0.43
1:B:4:LEU:HD13	1:B:80:ILE:HD11	2.00	0.43
1:B:135:GLY:HA3	5:B:301:DCQ:H4M	2.01	0.43
1:B:91:ARG:NE	5:B:301:DCQ:H7A	2.33	0.43
6:F:401:LMN:HBR	6:F:401:LMN:HBKA	1.77	0.43
4:G:77:LEU:HD11	4:G:295:PHE:HE2	1.83	0.43
1:B:111:ALA:HA	1:B:114:ARG:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2:SER:HB2	2:C:5:ARG:HB3	2.01	0.42
1:A:18:VAL:HG23	1:A:19:VAL:HG23	1.99	0.42
1:B:163:GLU:HG2	1:B:194:ASP:HA	2.01	0.42
1:B:90:PHE:HD2	1:B:98:ASN:HB2	1.84	0.42
4:G:73:LEU:HB2	4:G:288:MET:HB3	2.02	0.42
3:F:284:VAL:HG23	3:F:285:PRO:HD3	2.00	0.42
4:G:11:ILE:HD13	4:G:102:VAL:HG23	2.01	0.42
4:G:114:VAL:HG13	4:G:282:PRO:HB2	2.01	0.42
1:B:2:ALA:N	1:B:28:SER:OG	2.48	0.41
1:B:65:ASP:N	1:B:65:ASP:OD1	2.52	0.41
3:F:350:THR:OG1	3:F:351:VAL:N	2.53	0.41
3:F:35:LEU:O	3:F:39:VAL:N	2.53	0.41
1:A:96:TYR:HD1	1:A:122:MET:HE1	1.85	0.41
7:F:402:LMT:H71	7:F:402:LMT:H102	1.85	0.41
1:B:44:THR:HG22	1:B:48:MET:HE3	2.02	0.41
3:F:263:ARG:HG3	3:F:321:GLY:HA2	2.02	0.41
4:G:306:GLY:HA2	6:G:402:LMN:HBKA	2.02	0.41
4:G:300:LEU:HD22	4:G:303:VAL:HG21	2.03	0.41
1:A:198:ARG:HD3	1:A:198:ARG:HA	1.83	0.40
3:F:253:THR:HB	3:F:257:THR:HG23	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	237/241 (98%)	208 (88%)	27 (11%)	2 (1%)	16	47
1	B	236/241 (98%)	210 (89%)	26 (11%)	0	100	100
2	C	22/191 (12%)	21 (96%)	1 (4%)	0	100	100
3	F	235/366 (64%)	221 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	G	222/360 (62%)	207 (93%)	15 (7%)	0	100	100
All	All	952/1399 (68%)	867 (91%)	83 (9%)	2 (0%)	44	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	LEU
1	A	213	GLY

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	A	200/202 (99%)	199 (100%)	1 (0%)	81	85
1	B	199/202 (98%)	199 (100%)	0	100	100
2	C	21/173 (12%)	21 (100%)	0	100	100
3	F	206/307 (67%)	206 (100%)	0	100	100
4	G	193/300 (64%)	193 (100%)	0	100	100
All	All	819/1184 (69%)	818 (100%)	1 (0%)	87	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	59	ASN
1	A	98	ASN
1	A	195	HIS

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Mol	Chain	Res	Type
1	B	8	ASN
1	B	27	ASN
1	B	73	HIS
1	B	98	ASN
1	B	113	GLN
1	B	129	HIS
1	B	155	ASN
1	B	182	HIS
1	B	226	GLN
3	F	127	HIS
3	F	267	ASN
3	F	290	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	LMT	F	402	-	13,13,36	0.36	0	12,12,47	1.00	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	LMN	F	401	-	34,34,72	0.92	2 (5%)	40,41,98	2.36	13 (32%)
8	L0W	G	401	-	122,124,124	1.77	15 (12%)	137,148,148	2.81	36 (26%)
5	DCQ	G	404	-	23,23,23	1.80	7 (30%)	27,29,29	2.12	8 (29%)
6	LMN	G	402	-	35,35,72	1.20	2 (5%)	42,43,98	2.17	9 (21%)
5	DCQ	B	301	-	23,23,23	3.21	7 (30%)	27,29,29	4.06	14 (51%)
7	LMT	G	403	-	24,24,36	1.35	2 (8%)	29,29,47	1.72	2 (6%)

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	LMT	F	402	-	-	1/11/11/61	-
6	LMN	F	401	-	-	1/30/46/130	0/1/1/4
8	L0W	G	401	-	-	21/135/157/157	0/1/1/1
5	DCQ	G	404	-	-	4/14/38/38	0/1/1/1
6	LMN	G	402	-	-	4/30/50/130	0/1/1/4
5	DCQ	B	301	-	-	4/14/38/38	0/1/1/1
7	LMT	G	403	-	-	2/15/35/61	0/1/1/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	401	L0W	CAR-CAT	11.44	1.78	1.51
5	B	301	DCQ	O3-C3	9.67	1.60	1.36
8	G	401	L0W	CAP-CAN	-8.74	1.36	1.51
5	B	301	DCQ	O3-C3M	7.60	1.62	1.45
8	G	401	L0W	OAU-CAT	-6.90	1.35	1.44
7	G	403	LMT	O1'-C1'	5.75	1.49	1.40
6	G	402	LMN	OBV-CCJ	5.41	1.49	1.40
8	G	401	L0W	PHC-O4	4.90	1.68	1.59
5	B	301	DCQ	C3-C2	4.90	1.63	1.48
5	G	404	DCQ	C1M-C1	-4.85	1.40	1.50
5	B	301	DCQ	C1M-C1	-4.05	1.42	1.50
5	G	404	DCQ	C7-C6	-3.90	1.41	1.51
5	B	301	DCQ	C4-C3	3.87	1.50	1.36
8	G	401	L0W	C3-C4	3.19	1.58	1.52
5	G	404	DCQ	C6-C1	3.15	1.40	1.35
8	G	401	L0W	CFN-CFM	2.97	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	301	DCQ	C6-C1	2.70	1.40	1.35
8	G	401	L0W	O1-C1	2.70	1.44	1.40
6	F	401	LMN	OBV-CCJ	2.70	1.49	1.40
8	G	401	L0W	CAV-CAT	2.64	1.59	1.50
5	B	301	DCQ	C7-C6	-2.55	1.44	1.51
8	G	401	L0W	O4-C4	2.50	1.52	1.44
5	G	404	DCQ	C3-C2	-2.46	1.41	1.48
5	G	404	DCQ	C4-C5	-2.40	1.41	1.48
8	G	401	L0W	OAU-CAL	2.37	1.48	1.41
5	G	404	DCQ	C1-C2	-2.19	1.39	1.47
5	G	404	DCQ	C6-C5	-2.17	1.40	1.46
6	G	402	LMN	OBX-CCJ	2.11	1.47	1.41
6	F	401	LMN	CCL-CCJ	2.08	1.56	1.50
7	G	403	LMT	O5'-C1'	2.08	1.47	1.41
8	G	401	L0W	CFL-CFK	2.08	1.54	1.50
8	G	401	L0W	PHC-OHF	-2.04	1.47	1.54
8	G	401	L0W	PHG-OHJ	-2.02	1.47	1.54
8	G	401	L0W	PHG-OHI	-2.02	1.47	1.54
8	G	401	L0W	PHC-OHE	-2.01	1.47	1.54

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	401	L0W	OAQ-CAP-CAN	13.39	131.58	108.33
8	G	401	L0W	CAV-CAT-CAR	11.98	139.45	111.80
8	G	401	L0W	CEW-OFJ-CGB	10.06	141.86	117.80
6	G	402	LMN	CBK-CBQ-CCM	9.95	129.16	116.66
5	B	301	DCQ	C3M-O3-C3	9.22	148.86	116.47
8	G	401	L0W	CAV-O1-C1	8.89	132.85	113.80
5	B	301	DCQ	C4M-O4-C4	8.62	146.76	116.47
8	G	401	L0W	CAL-OAU-CAT	7.92	130.54	114.84
5	B	301	DCQ	C4-C3-C2	-7.86	106.26	120.69
7	G	403	LMT	C1-O1'-C1'	7.62	126.69	113.68
6	F	401	LMN	CBL-CBR-CCM	-7.52	107.21	116.66
5	B	301	DCQ	C6-C1-C2	7.13	124.80	119.17
8	G	401	L0W	C8-C7-N2	-6.75	107.04	116.25
5	B	301	DCQ	O3-C3-C2	6.72	139.32	116.64
8	G	401	L0W	C2-N2-C7	6.36	132.27	122.90
6	F	401	LMN	OBX-CCJ-OBV	5.78	122.01	109.40
8	G	401	L0W	CFM-OFZ-CGN	-5.70	104.15	117.80
8	G	401	L0W	C1-C2-N2	-5.51	101.67	110.92
8	G	401	L0W	PHC-O4-C4	5.04	136.89	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	404	DCQ	C4M-O4-C4	4.93	133.79	116.47
5	G	404	DCQ	C3M-O3-C3	4.85	133.51	116.47
8	G	401	L0W	OFZ-CFM-CFN	4.82	120.56	107.26
6	F	401	LMN	CBR-CCM-CBQ	-4.55	98.71	108.54
8	G	401	L0W	CEY-CEX-CEW	-4.49	99.07	114.66
5	B	301	DCQ	C3-C4-C5	4.44	128.85	120.69
6	G	402	LMN	CBS-CCM-CBQ	4.11	117.63	110.54
6	F	401	LMN	CBQ-CBK-CBI	-4.08	101.04	113.19
6	F	401	LMN	CBS-CCM-CBQ	-4.08	103.50	110.54
5	B	301	DCQ	C1M-C1-C6	-4.05	117.79	124.45
8	G	401	L0W	OFZ-CFM-CFL	4.03	115.34	106.72
6	G	402	LMN	CBT-OBV-CCJ	-3.93	103.34	113.31
5	B	301	DCQ	O2-C2-C1	-3.92	109.78	120.73
5	B	301	DCQ	C8-C7-C6	3.86	124.19	113.10
6	F	401	LMN	CBT-OBV-CCJ	3.81	122.97	113.31
8	G	401	L0W	OFZ-CGN-CGP	3.70	119.49	111.48
8	G	401	L0W	C3-O3-CFK	-3.62	111.70	117.59
5	B	301	DCQ	O4-C4-C3	-3.61	109.96	123.64
5	B	301	DCQ	O2-C2-C3	3.57	128.60	121.03
8	G	401	L0W	CDS-CDR-CDQ	-3.56	104.87	114.68
8	G	401	L0W	O1-CAV-CAT	-3.44	102.45	110.82
6	F	401	LMN	OBX-CCF-CBP	3.35	114.75	106.44
5	G	404	DCQ	O4-C4-C3	-3.16	111.69	123.64
6	F	401	LMN	CBR-CCM-CBT	3.15	117.83	109.57
5	G	404	DCQ	O4-C4-C5	3.12	127.15	116.64
5	G	404	DCQ	O3-C3-C2	3.11	127.14	116.64
8	G	401	L0W	O3-C3-C4	3.09	114.39	108.25
5	G	404	DCQ	O3-C3-C4	-3.08	111.97	123.64
8	G	401	L0W	CFT-CFS-CFR	3.08	129.94	114.37
6	G	402	LMN	CBR-CBL-CBJ	3.06	122.29	113.19
8	G	401	L0W	CFR-CFQ-CFP	-3.04	99.02	114.37
8	G	401	L0W	CDP-CDO-NAO	-2.92	112.26	116.25
8	G	401	L0W	CGR-CGQ-CGP	-2.79	102.88	113.13
5	G	404	DCQ	C6-C1-C2	2.75	121.34	119.17
6	G	402	LMN	OBX-CCF-CBP	2.72	113.19	106.44
8	G	401	L0W	CFC-CFB-CFA	-2.70	100.74	114.37
6	F	401	LMN	CBR-CBL-CBJ	2.69	121.20	113.19
6	G	402	LMN	CBQ-CCM-CBT	-2.68	102.55	109.57
6	F	401	LMN	CBI-CBG-CBE	-2.68	100.84	114.37
6	G	402	LMN	CBS-CCM-CBR	-2.67	105.92	110.54
8	G	401	L0W	CFE-CFD-CFC	-2.57	101.37	114.37
8	G	401	L0W	OAM-PHG-OHH	-2.57	100.18	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	401	L0W	O7-C7-N2	2.56	127.29	122.95
8	G	401	L0W	CFP-CFO-CFN	-2.52	104.12	113.62
5	B	301	DCQ	O3-C3-C4	-2.51	114.14	123.64
8	G	401	L0W	OAU-CAL-CAN	-2.49	101.30	109.01
6	G	402	LMN	CBL-CBR-CCM	2.49	119.79	116.66
8	G	401	L0W	C1-C2-C3	-2.48	105.42	109.92
8	G	401	L0W	CGT-CGS-CGR	-2.48	101.82	114.37
7	G	403	LMT	C6-C5-C4	-2.46	101.91	114.37
7	F	402	LMT	C7-C6-C5	-2.30	102.73	114.37
5	B	301	DCQ	C9-C8-C7	-2.29	104.72	113.13
8	G	401	L0W	O5-C5-C6	2.25	111.16	106.69
8	G	401	L0W	OEC-CDO-NAO	2.24	126.75	122.95
8	G	401	L0W	CGV-CGU-CGT	-2.23	103.07	114.37
6	G	402	LMN	OBV-CCJ-CCL	2.23	111.66	108.27
8	G	401	L0W	CEI-CEH-CEG	-2.18	108.66	114.68
8	G	401	L0W	O7-C7-C8	2.16	124.69	121.54
5	G	404	DCQ	O5-C5-C6	-2.16	117.61	121.79
6	F	401	LMN	CBL-CBJ-CBH	-2.14	103.57	114.37
6	F	401	LMN	CBE-CBC-CBA	-2.08	103.86	114.37
8	G	401	L0W	CFA-CEZ-CEY	-2.06	103.95	114.37
5	B	301	DCQ	O5-C5-C6	-2.05	117.83	121.79
6	F	401	LMN	OBV-CCJ-CCL	-2.03	106.81	109.02

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	402	LMN	OBX-CCJ-OBV-CBT
8	G	401	L0W	C5-C4-O4-PHC
8	G	401	L0W	C1-C2-N2-C7
8	G	401	L0W	C2-C1-O1-CAV
8	G	401	L0W	OAM-CAL-OAU-CAT
8	G	401	L0W	CAP-CAN-NAO-CDO
8	G	401	L0W	OAS-CAR-CAT-OAU
8	G	401	L0W	OFY-CFK-O3-C3
8	G	401	L0W	CFL-CFK-O3-C3
8	G	401	L0W	C8-CEW-OFJ-CGB
5	B	301	DCQ	C3-C4-O4-C4M
5	G	404	DCQ	C4-C3-O3-C3M
5	G	404	DCQ	C3-C4-O4-C4M
5	G	404	DCQ	C2-C3-O3-C3M
5	G	404	DCQ	C5-C4-O4-C4M

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Mol	Chain	Res	Type	Atoms
8	G	401	L0W	OFZ-CFM-CFN-CFO
6	F	401	LMN	CCL-CCJ-OBV-CBT
7	G	403	LMT	C2-C1-O1'-C1'
8	G	401	L0W	CEX-CEW-OFJ-CGB
6	G	402	LMN	CBJ-CBL-CBR-CCM
5	B	301	DCQ	C5-C4-O4-C4M
7	G	403	LMT	O5'-C5'-C6'-O6'
8	G	401	L0W	CAN-CAP-OAQ-CEE
6	G	402	LMN	CBI-CBK-CBQ-CCM
6	G	402	LMN	CCL-CCJ-OBV-CBT
8	G	401	L0W	OAU-CAT-CAV-O1
7	F	402	LMT	C2-C1-O1'-C1'
8	G	401	L0W	CAV-CAT-OAU-CAL
8	G	401	L0W	OFZ-CGN-CGP-CGQ
8	G	401	L0W	C5-C6-O6-CBA
5	B	301	DCQ	C2-C3-O3-C3M
8	G	401	L0W	OGO-CGN-OFZ-CFM
5	B	301	DCQ	C7-C8-C9-C10
8	G	401	L0W	C3-C2-N2-C7
8	G	401	L0W	C4-O4-PHC-OHF
8	G	401	L0W	O5-C1-O1-CAV
8	G	401	L0W	CFQ-CFR-CFS-CFT

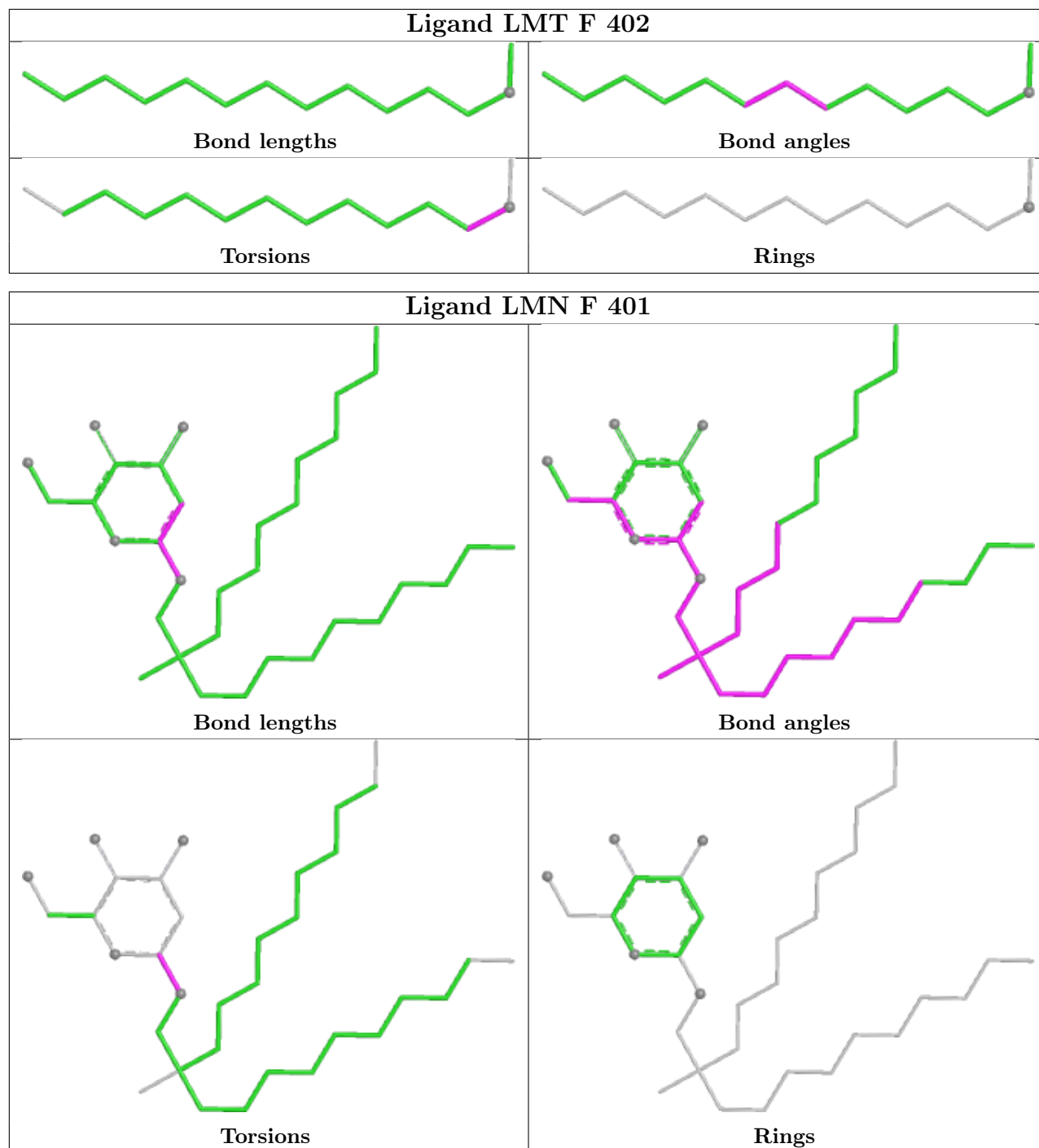
There are no ring outliers.

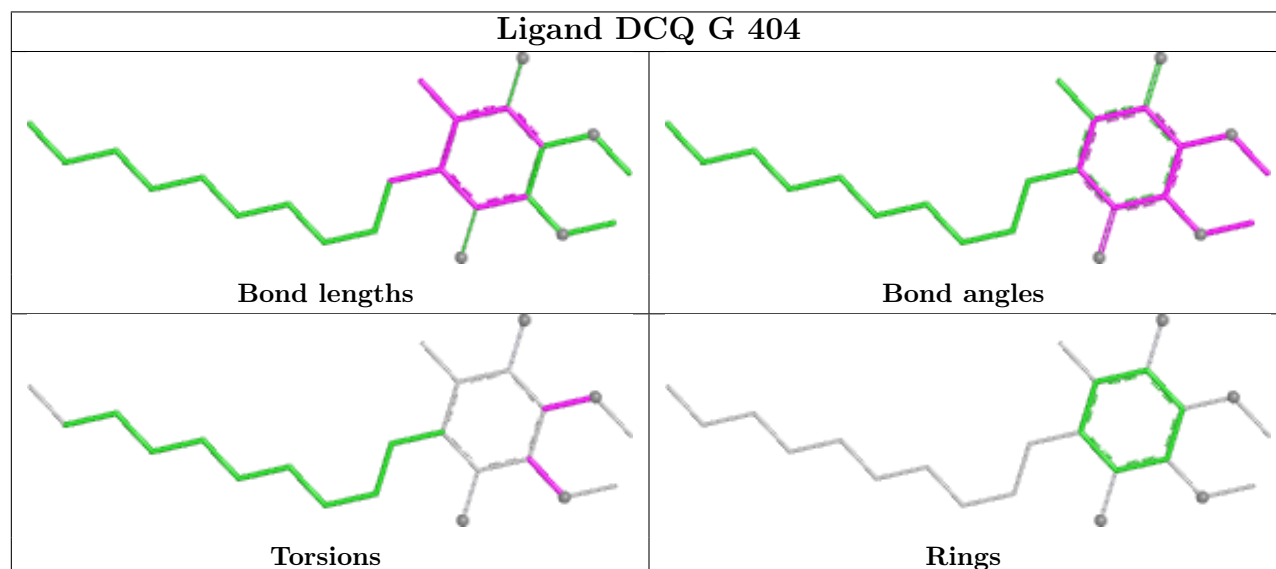
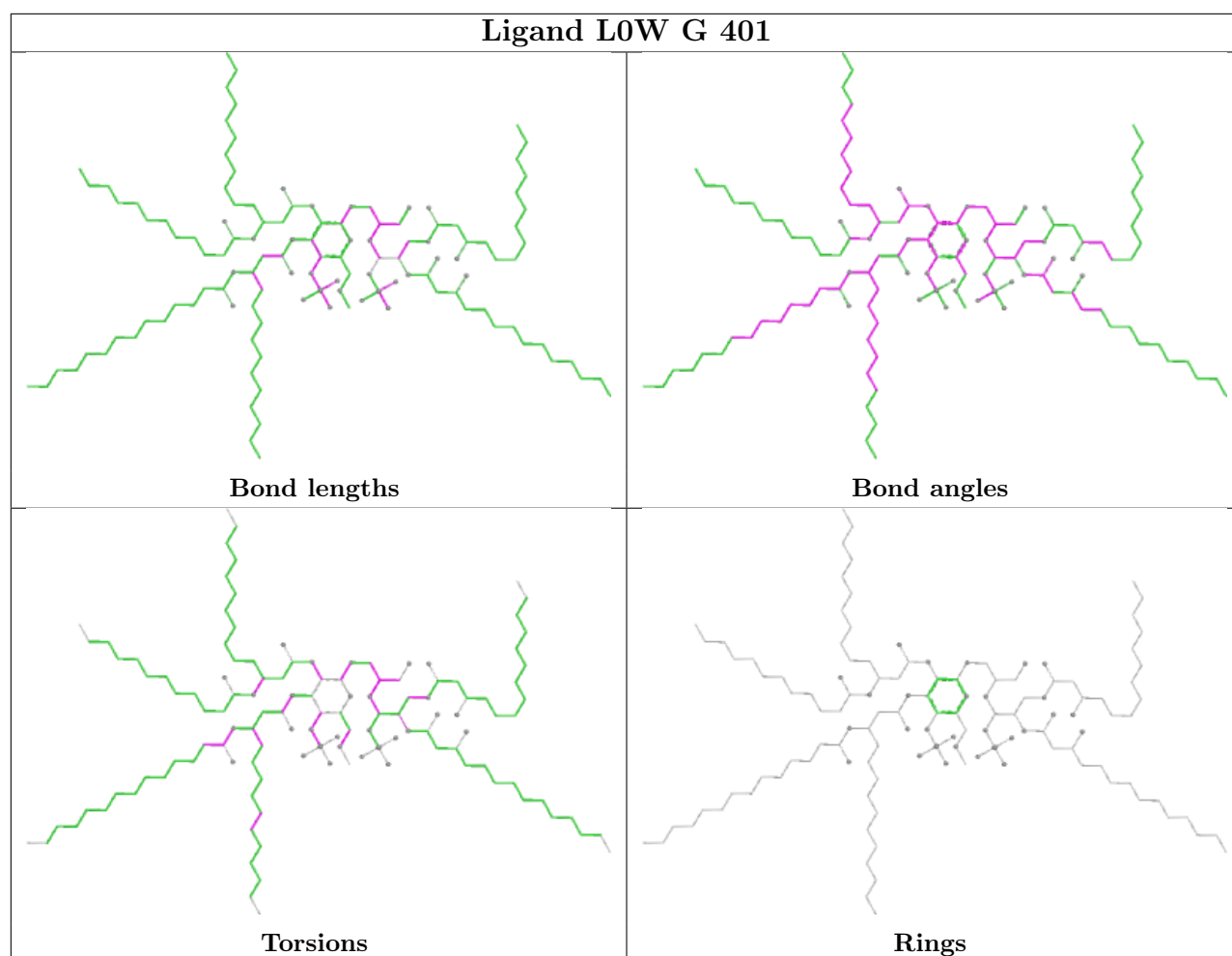
5 monomers are involved in 29 short contacts:

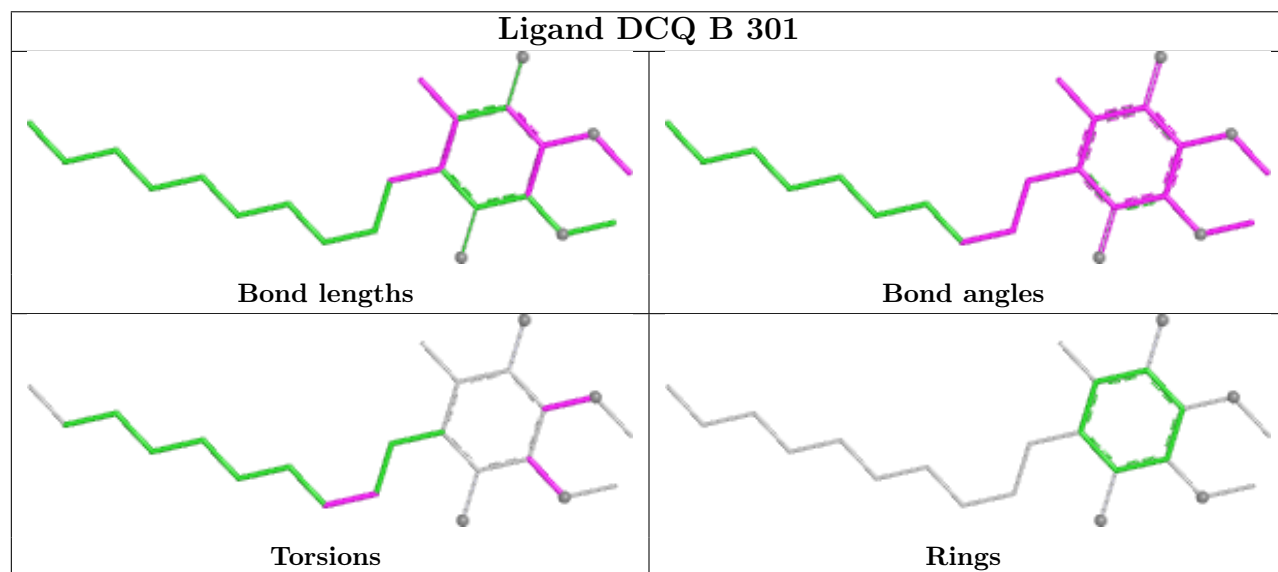
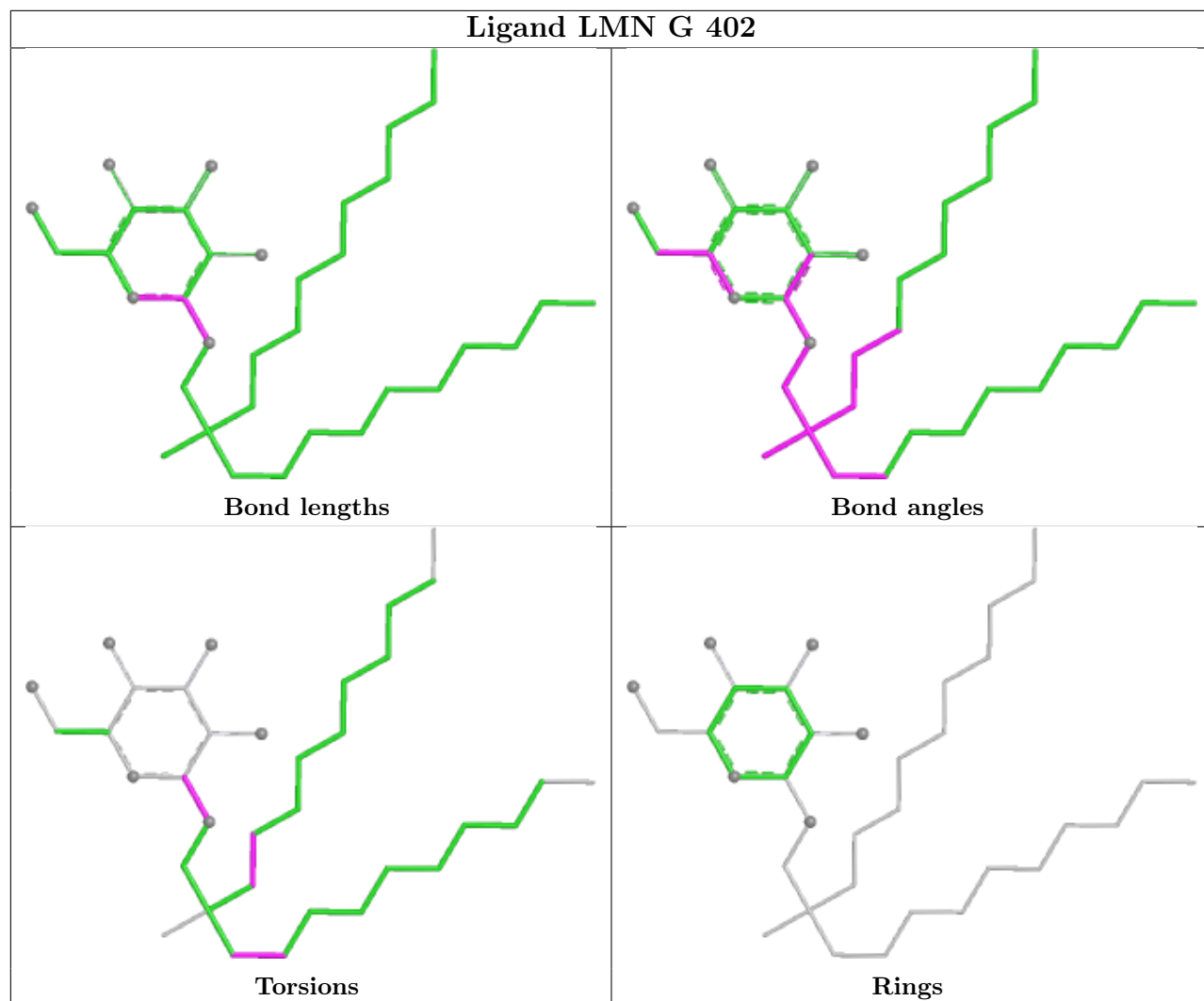
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	402	LMT	1	0
6	F	401	LMN	3	0
8	G	401	L0W	6	0
6	G	402	LMN	2	0
5	B	301	DCQ	17	0

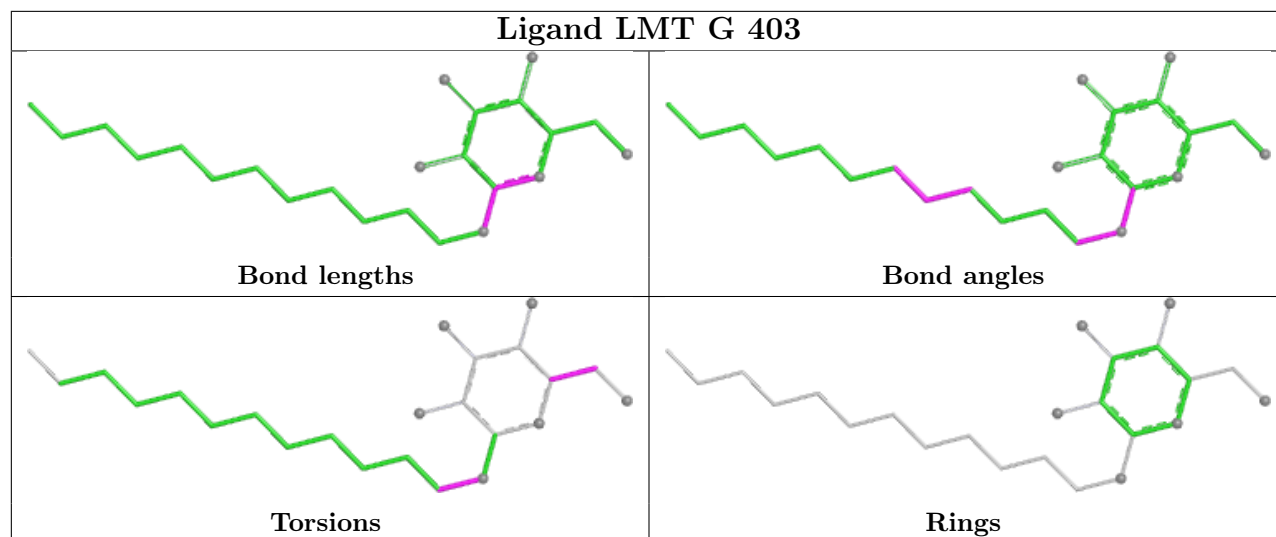
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

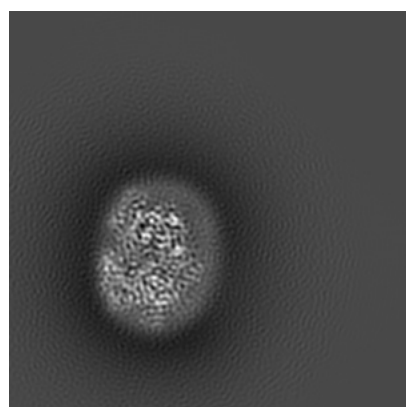
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10125. These allow visual inspection of the internal detail of the map and identification of artifacts.

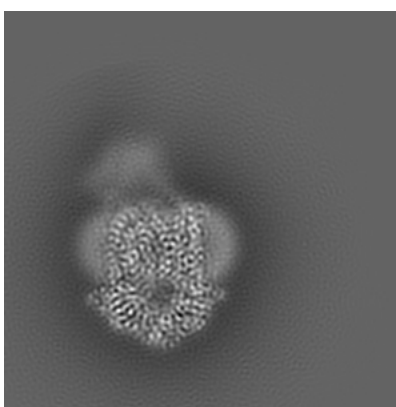
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

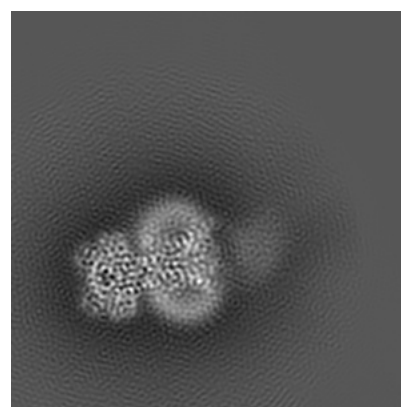
6.1.1 Primary map



X



Y

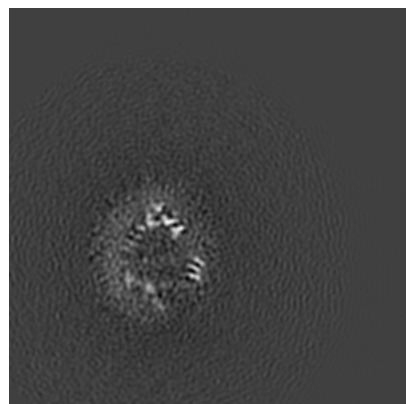


Z

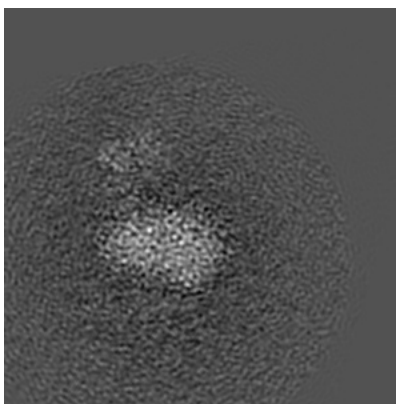
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

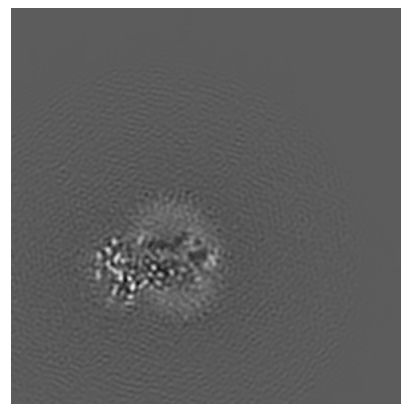
6.2.1 Primary map



X Index: 120



Y Index: 120

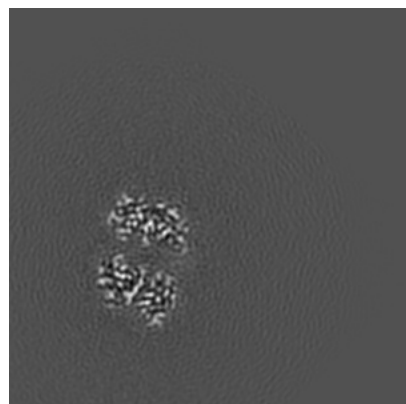


Z Index: 120

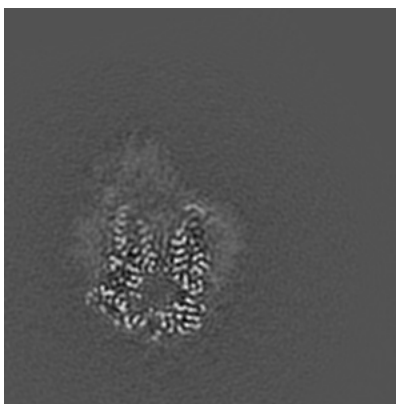
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

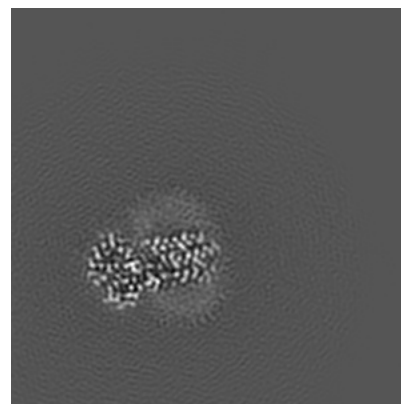
6.3.1 Primary map



X Index: 64



Y Index: 84

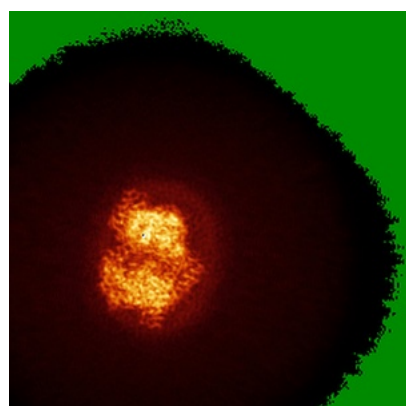


Z Index: 113

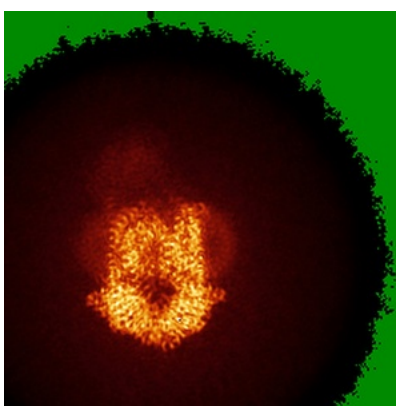
The images above show the largest variance slices of the map in three orthogonal directions.

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

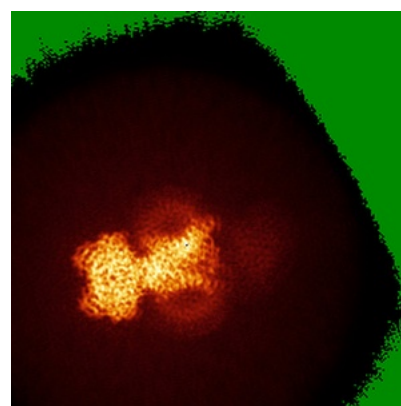
6.4.1 Primary map



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

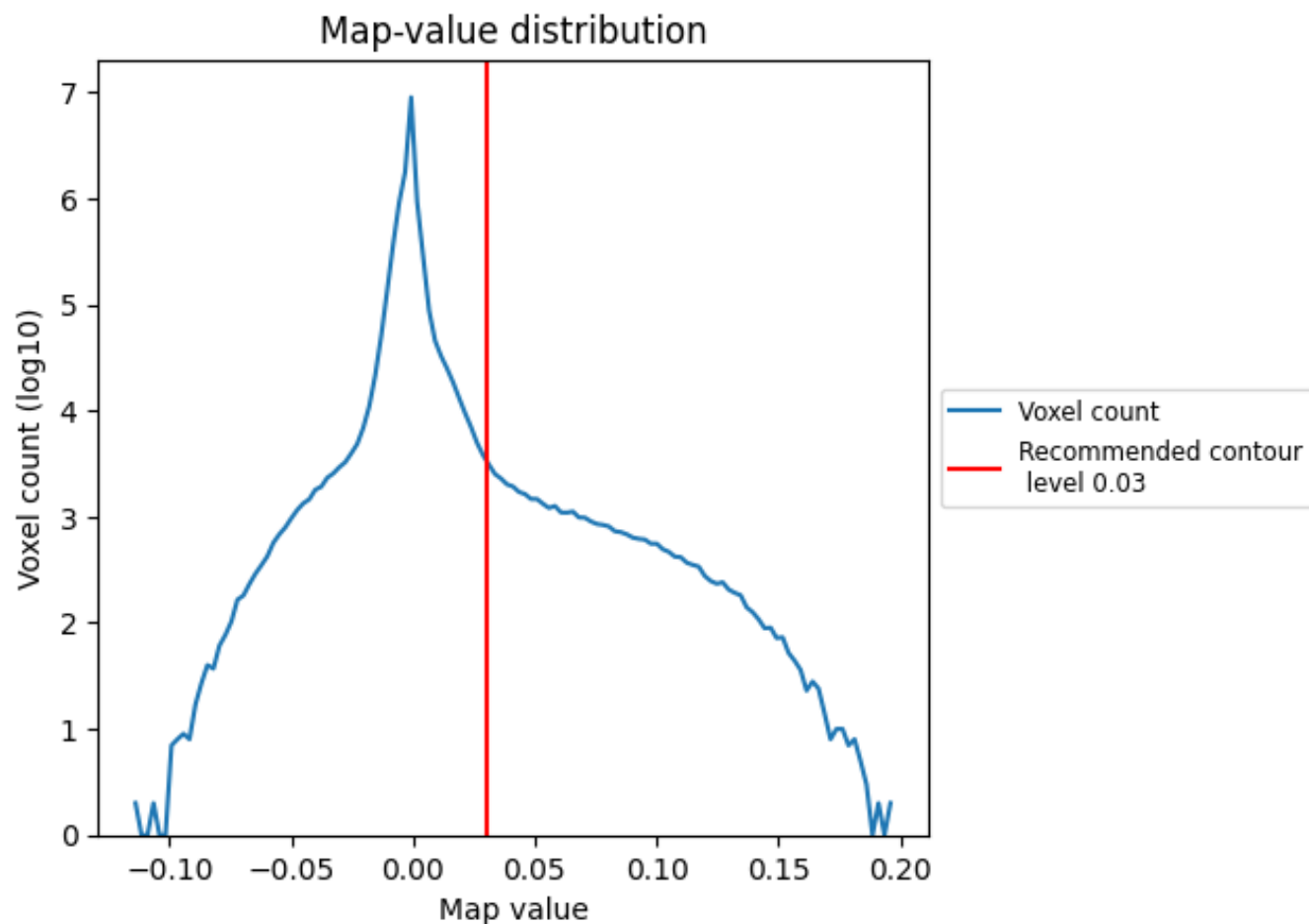
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

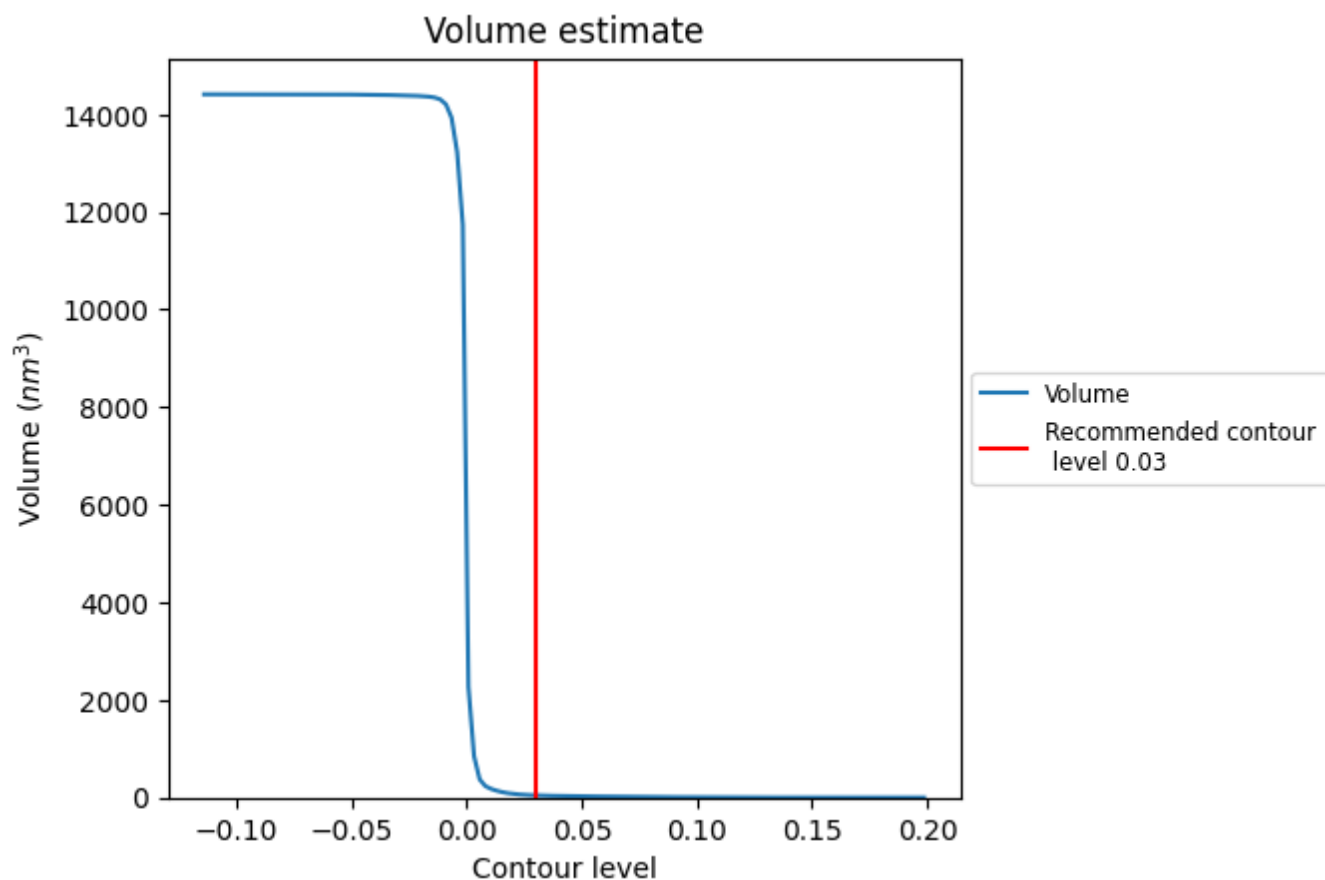
This section contains the results of statistical analysis of the map.

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.

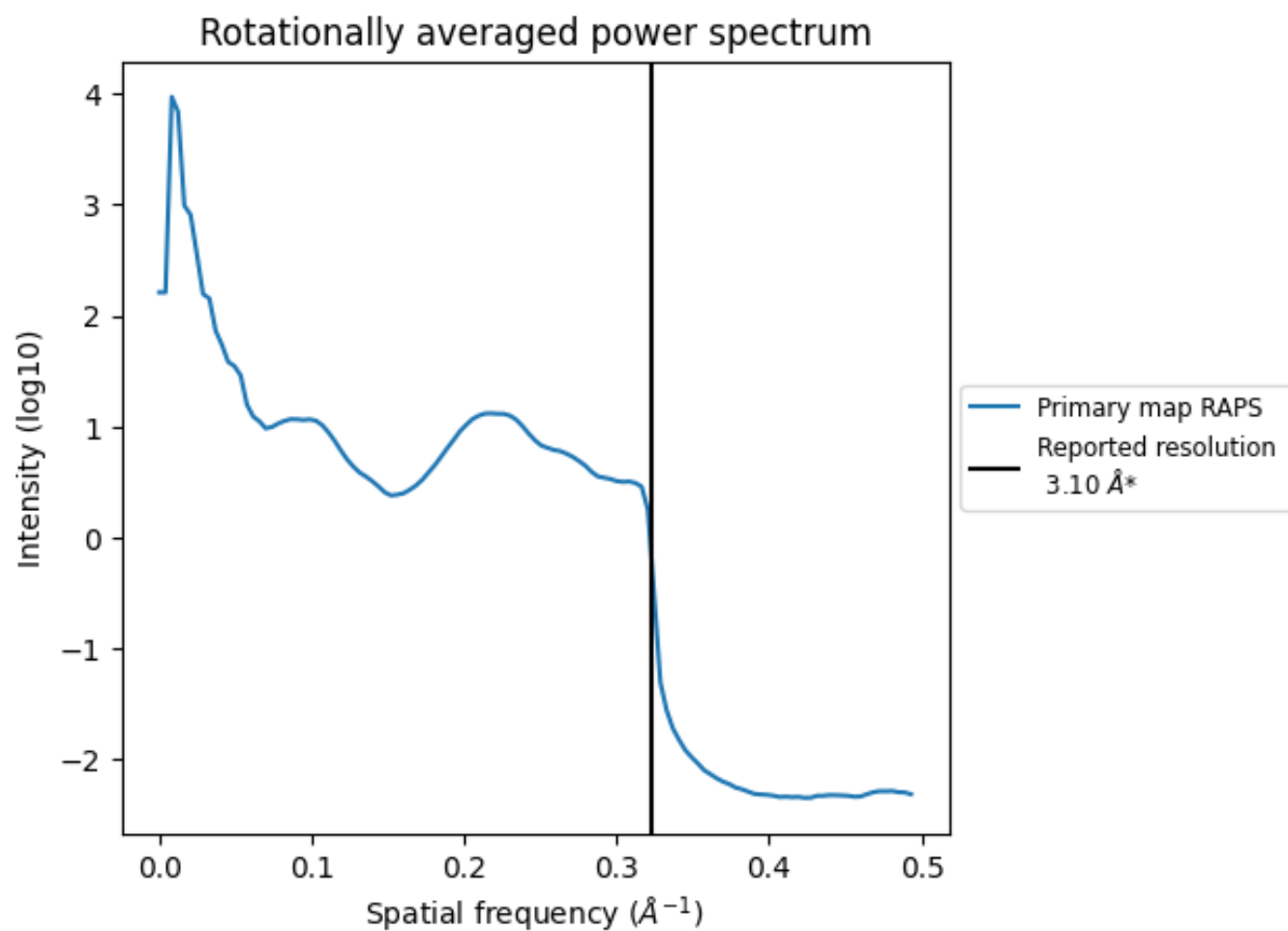
7.2 Volume estimate [i](#)



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

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

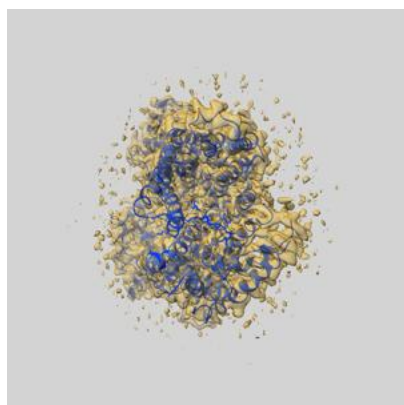
8 Fourier-Shell correlation

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

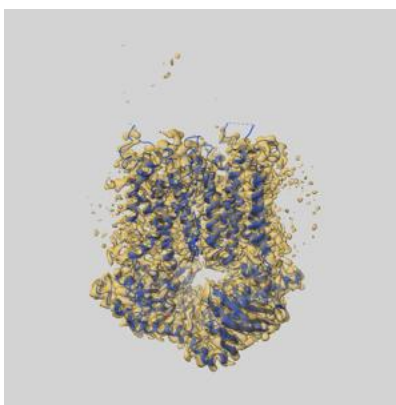
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10125 and PDB model 6S8N. Per-residue inclusion information can be found in section [3](#) on page [7](#).

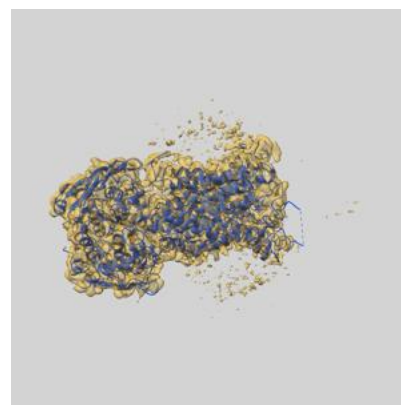
9.1 Map-model overlay [i](#)



X



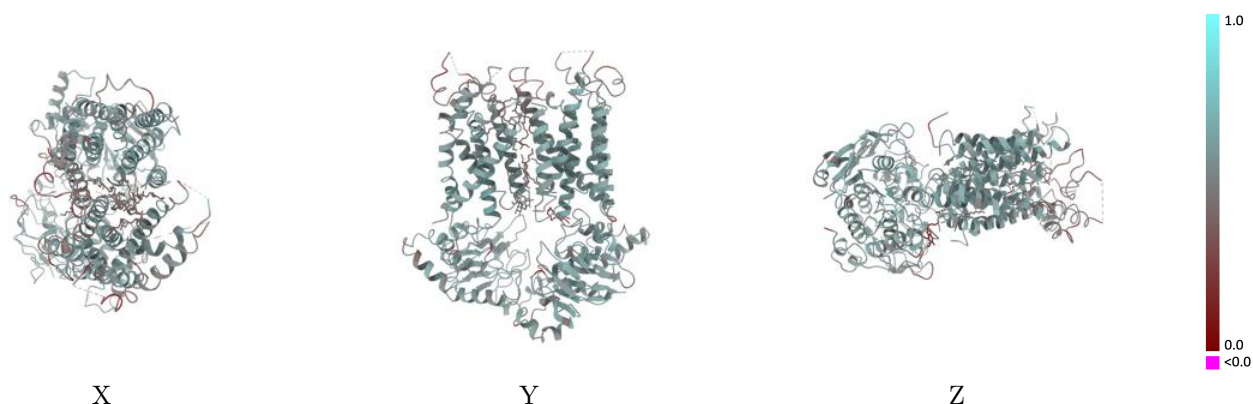
Y



Z

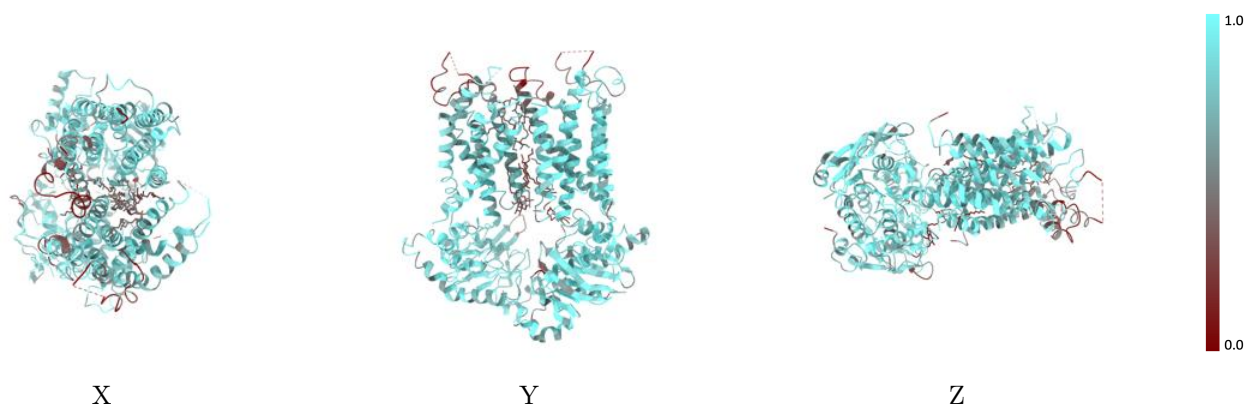
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



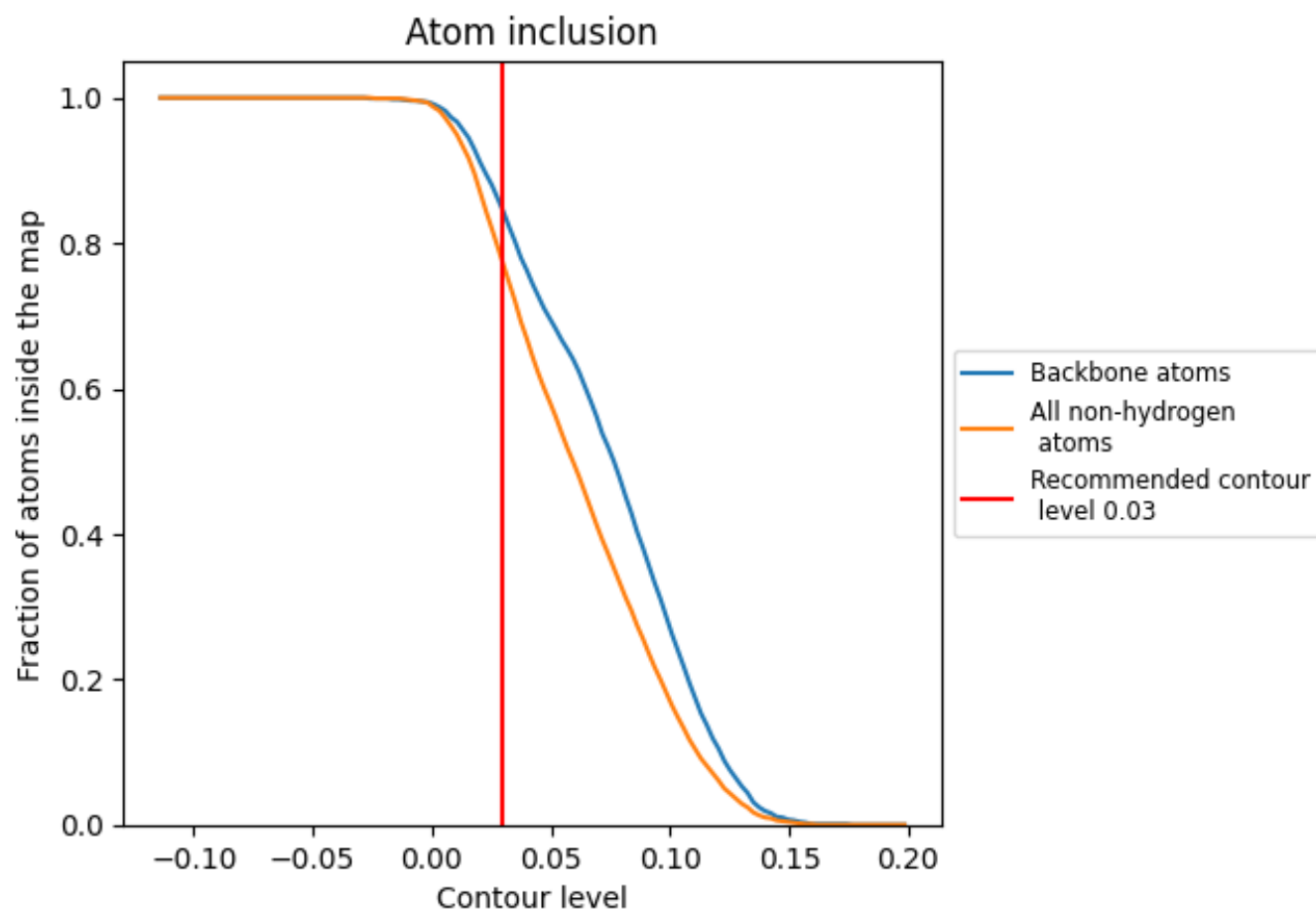
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 77% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7720	0.5310
A	0.8200	0.5420
B	0.8090	0.5390
C	0.8300	0.5620
F	0.7540	0.5310
G	0.7040	0.5090

