



Full wwPDB EM Validation Report ⓘ

Mar 20, 2025 – 02:29 PM EDT

PDB ID : 9BPG
EMDB ID : EMD-44776
Title : Artemia franciscana ATP synthase FO domain, state 1, pH 7.0
Authors : Mnatsakanyan, N.; Mello, J.F.R.
Deposited on : 2024-05-07
Resolution : 3.30 Å (reported)
Based on initial model : .

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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.41.4

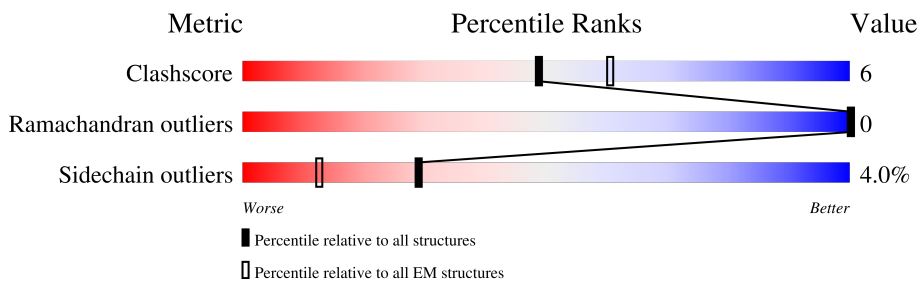
1 Overall quality at a glance i

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	1	128	
1	2	128	
1	3	128	
1	4	128	
1	5	128	
1	6	128	
1	7	128	
1	8	128	

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Mol	Chain	Length	Quality of chain
2	G	290	
3	H	169	
4	I	66	
5	K	265	
6	M	219	
7	N	219	
8	P	44	
9	Q	53	
10	R	119	
11	S	103	
12	T	84	

2 Entry composition i

There are 13 unique types of molecules in this entry. The entry contains 13653 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 synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	75	Total 537	C 355	N 83	O 95	S 4	0	0
1	2	75	Total 537	C 355	N 83	O 95	S 4	0	0
1	3	75	Total 537	C 355	N 83	O 95	S 4	0	0
1	4	75	Total 537	C 355	N 83	O 95	S 4	0	0
1	5	75	Total 537	C 355	N 83	O 95	S 4	0	0
1	6	75	Total 537	C 355	N 83	O 95	S 4	0	0
1	7	75	Total 537	C 355	N 83	O 95	S 4	0	0
1	8	75	Total 537	C 355	N 83	O 95	S 4	0	0

- Molecule 2 is a protein called ATP synthase subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	208	Total 1601	C 1000	N 276	O 313	S 12	0	0

- Molecule 3 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	134	Total 984	C 620	N 161	O 201	S 2	0	0

- Molecule 4 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	37	Total	C	N	O	S	0	0
			304	185	65	52	2		

- Molecule 5 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	132	Total	C	N	O	S	0	0
			1049	683	170	194	2		

- Molecule 6 is a protein called ATP synthase subunit d.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	102	Total	C	N	O	S	0	0
			820	519	137	160	4		

- Molecule 7 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	219	Total	C	N	O	S	0	0
			1716	1157	256	287	16		

- Molecule 8 is a protein called ATP synthase subunit 6.8PL.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	44	Total	C	N	O	0	0
			220	132	44	44		

- Molecule 9 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	46	Total	C	N	O	S	0	0
			390	266	60	60	4		

- Molecule 10 is a protein called ATP synthase subunit f.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	104	Total	C	N	O	S	0	0
			851	555	158	136	2		

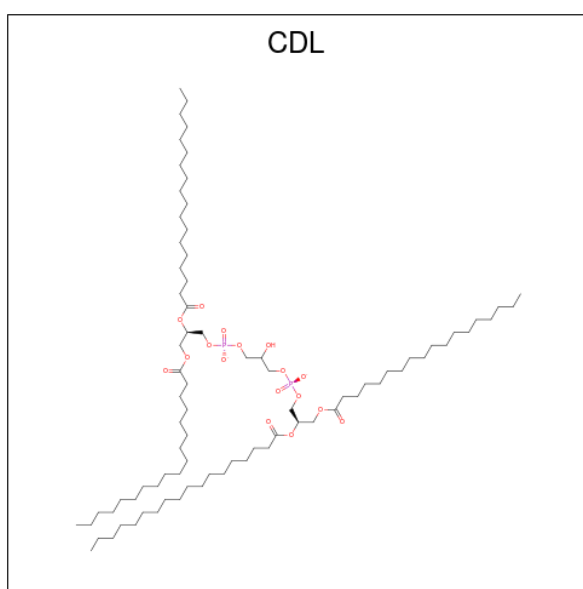
- Molecule 11 is a protein called ATP synthase subunit g.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	S	76	596	392	99	103	2	0	0

- Molecule 12 is a protein called ATP synthase subunit e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	T	82	658	418	122	117	1	0	0

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



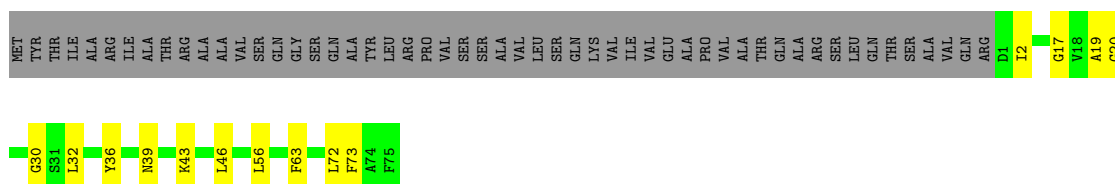
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
13	K	1	91	72	17	2	0
13	S	1	77	58	17	2	0

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.

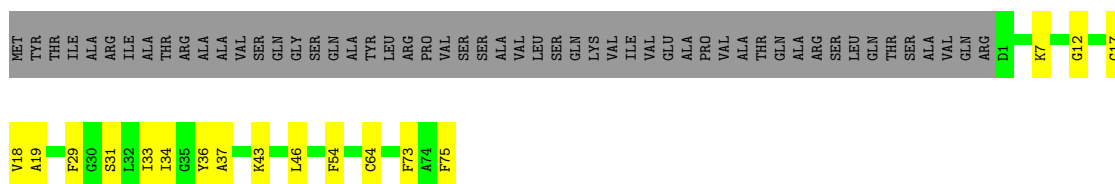
- Molecule 1: ATP synthase subunit c

Chain 1: 



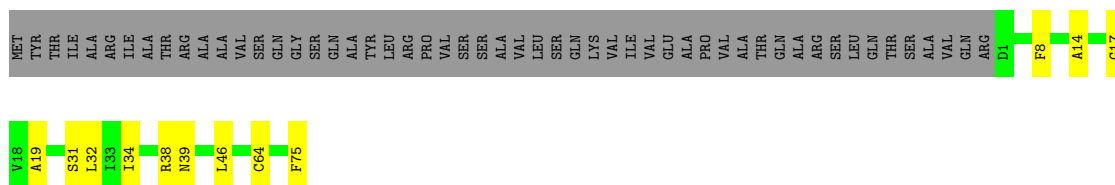
- Molecule 1: ATP synthase subunit c

Chain 2: 



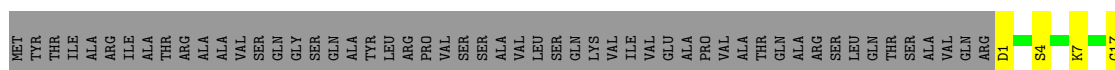
- Molecule 1: ATP synthase subunit c

Chain 3: 



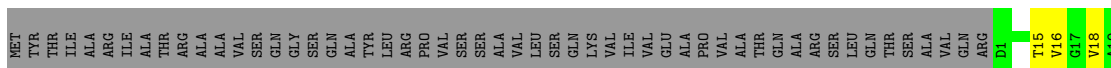
- Molecule 1: ATP synthase subunit c

Chain 4: 

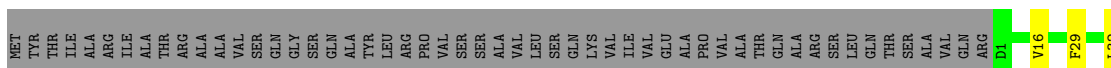




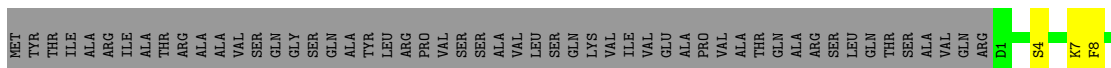
- Molecule 1: ATP synthase subunit c



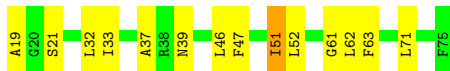
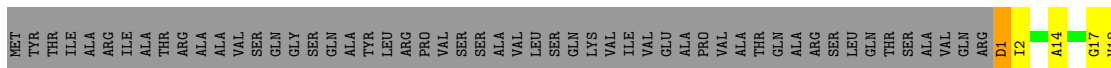
- Molecule 1: ATP synthase subunit c



- Molecule 1: ATP synthase subunit c

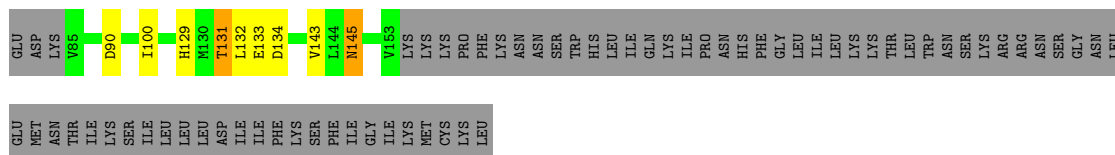


- Molecule 1: ATP synthase subunit c

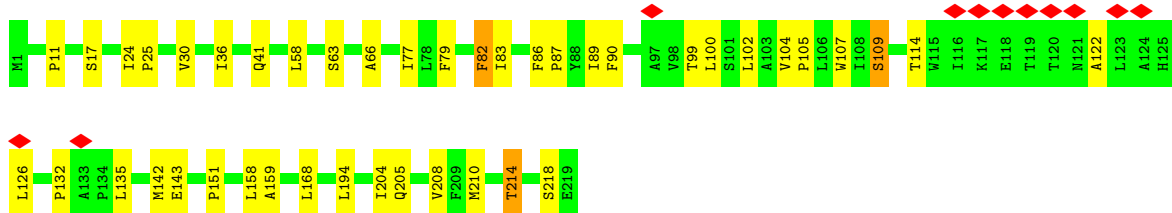
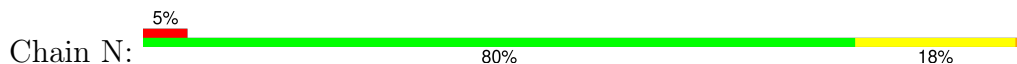


- Molecule 2: ATP synthase subunit gamma

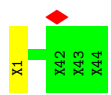




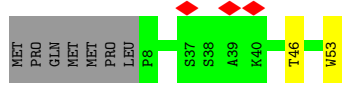
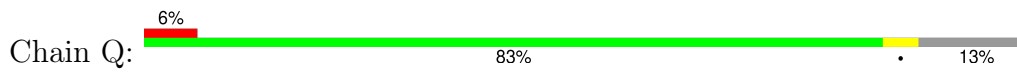
• Molecule 7: ATP synthase subunit a



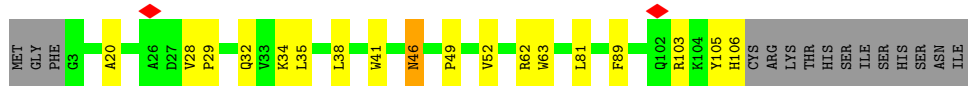
• Molecule 8: ATP synthase subunit 6.8PL



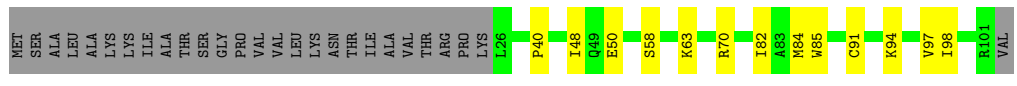
• Molecule 9: ATP synthase protein 8



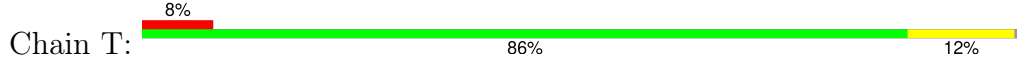
• Molecule 10: ATP synthase subunit f



• Molecule 11: ATP synthase subunit g



• Molecule 12: ATP synthase subunit e





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	673185	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.150	Depositor
Minimum map value	-1.322	Depositor
Average map value	0.043	Depositor
Map value standard deviation	0.150	Depositor
Recommended contour level	0.234	Depositor
Map size (Å)	103.59599, 119.616, 150.588	wwPDB
Map dimensions	141, 112, 97	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

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

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	1	0.30	0/547	0.45	0/734
1	2	0.32	0/547	0.47	0/734
1	3	0.33	0/547	0.46	0/734
1	4	0.33	0/547	0.47	0/734
1	5	0.30	0/547	0.48	0/734
1	6	0.31	0/547	0.49	0/734
1	7	0.33	0/547	0.48	0/734
1	8	0.31	0/547	0.47	0/734
2	G	0.27	0/1622	0.48	0/2184
3	H	0.34	0/998	0.50	0/1359
4	I	0.29	0/308	0.64	0/407
5	K	0.29	0/1074	0.43	0/1447
6	M	0.26	0/837	0.44	0/1123
7	N	0.26	0/1761	0.45	0/2402
9	Q	0.25	0/405	0.42	0/549
10	R	0.31	0/882	0.51	0/1196
11	S	0.26	0/611	0.45	0/829
12	T	0.26	0/670	0.52	0/902
All	All	0.29	0/13544	0.47	0/18270

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	1	537	0	549	11	0
1	2	537	0	549	12	0
1	3	537	0	549	9	0
1	4	537	0	549	9	0
1	5	537	0	549	10	0
1	6	537	0	549	3	0
1	7	537	0	549	10	0
1	8	537	0	549	14	0
2	G	1601	0	1604	12	0
3	H	984	0	974	15	0
4	I	304	0	305	11	0
5	K	1049	0	1045	20	0
6	M	820	0	800	8	0
7	N	1716	0	1811	24	0
8	P	220	0	47	1	0
9	Q	390	0	393	2	0
10	R	851	0	840	11	0
11	S	596	0	617	12	0
12	T	658	0	672	8	0
13	K	91	0	130	6	0
13	S	77	0	101	8	0
All	All	13653	0	13731	152	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 (152) 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)
11:S:70:ARG:NH1	13:S:201:CDL:OA4	1.72	1.23
11:S:70:ARG:HH12	13:S:201:CDL:PA1	1.78	1.07
3:H:96:GLU:HB2	4:I:28:VAL:HG23	1.72	0.72
3:H:86:ASP:N	3:H:86:ASP:OD1	2.28	0.64
10:R:63:TRP:HB2	13:S:201:CDL:H531	1.79	0.64
11:S:70:ARG:CZ	13:S:201:CDL:OA4	2.45	0.64
1:2:19:ALA:HB2	1:3:17:GLY:HA2	1.80	0.63
1:3:19:ALA:HB2	1:4:17:GLY:HA2	1.82	0.62
4:I:13:ARG:NH1	4:I:23:SER:OG	2.32	0.62
5:K:121:GLN:HB3	6:M:100:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:38:ARG:HG3	3:H:43:GLY:HA3	1.82	0.61
1:4:7:LYS:NZ	1:4:75:PHE:O	2.34	0.60
1:7:33:ILE:HG21	1:8:32:LEU:HA	1.83	0.59
3:H:37:ASP:N	3:H:37:ASP:OD1	2.36	0.59
1:1:19:ALA:HB2	1:2:17:GLY:HA2	1.84	0.59
6:M:145:ASN:N	6:M:145:ASN:OD1	2.35	0.58
1:7:31:SER:HA	1:7:34:ILE:HG22	1.86	0.57
1:1:17:GLY:HA2	1:8:19:ALA:HB2	1.87	0.57
1:4:33:ILE:HG21	1:5:32:LEU:HA	1.86	0.57
6:M:131:THR:HG23	6:M:134:ASP:H	1.71	0.56
7:N:99:THR:HG21	7:N:159:ALA:HB2	1.88	0.55
3:H:85:ASN:OD1	3:H:91:GLN:NE2	2.33	0.55
1:1:46:LEU:HD22	1:8:33:ILE:HG23	1.88	0.55
1:4:4:SER:HA	1:4:7:LYS:HD2	1.88	0.55
1:4:40:PRO:HG3	1:5:42:LEU:HD11	1.89	0.55
1:1:30:GLY:O	1:2:31:SER:OG	2.23	0.54
6:M:133:GLU:OE2	8:P:1:UNK:N	2.40	0.54
1:4:1:ASP:OD1	12:T:79:LYS:NZ	2.40	0.54
5:K:5:ARG:NH1	7:N:36:ILE:O	2.34	0.54
2:G:89:LEU:HD13	2:G:112:LEU:HD11	1.89	0.53
7:N:132:PRO:HD2	7:N:135:LEU:HD12	1.90	0.53
2:G:37:GLU:OE1	2:G:214:LYS:NZ	2.41	0.53
5:K:2:ARG:NH2	6:M:129:HIS:O	2.42	0.53
4:I:44:ILE:HG22	4:I:46:ARG:H	1.74	0.52
1:1:39:ASN:ND2	1:8:37:ALA:O	2.42	0.52
5:K:26:TYR:OH	12:T:5:PRO:O	2.27	0.52
1:2:7:LYS:NZ	1:2:75:PHE:O	2.43	0.52
1:2:33:ILE:HG21	1:3:32:LEU:HA	1.92	0.52
5:K:128:LYS:NZ	9:Q:53:TRP:OXT	2.43	0.51
3:H:64:THR:HB	3:H:74:LYS:HG2	1.91	0.51
5:K:110:LEU:HD13	9:Q:46:THR:HG22	1.92	0.51
1:5:33:ILE:HG21	1:6:32:LEU:HA	1.92	0.51
1:7:12:GLY:HA2	1:8:14:ALA:HB2	1.92	0.51
11:S:48:ILE:HG22	12:T:11:PRO:HB2	1.92	0.51
7:N:89:ILE:HG12	10:R:89:PHE:HD2	1.75	0.51
11:S:40:PRO:HG3	12:T:15:ALA:HA	1.93	0.51
1:7:71:LEU:HA	1:7:75:PHE:HB2	1.93	0.50
4:I:30:MET:SD	4:I:30:MET:N	2.84	0.50
7:N:100:LEU:HD12	7:N:104:VAL:HG21	1.93	0.50
10:R:105:TYR:O	10:R:106:HIS:ND1	2.45	0.50
5:K:21:TRP:HA	13:S:201:CDL:H111	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:R:49:PRO:HA	10:R:52:VAL:HG12	1.95	0.49
2:G:69:ILE:HB	2:G:156:ILE:HG23	1.93	0.49
2:G:195:ASP:OD1	4:I:14:ARG:NH1	2.45	0.49
7:N:210:MET:O	7:N:214:THR:OG1	2.31	0.49
1:7:37:ALA:O	1:8:39:ASN:ND2	2.35	0.49
5:K:64:ALA:O	5:K:68:THR:OG1	2.27	0.48
3:H:19:THR:OG1	3:H:30:ASN:OD1	2.32	0.48
1:6:29:PHE:HE2	1:6:54:PHE:HB2	1.78	0.48
1:2:73:PHE:HZ	1:3:75:PHE:HB3	1.78	0.48
7:N:58:LEU:O	7:N:218:SER:OG	2.32	0.48
2:G:109:ARG:HD3	2:G:123:VAL:HB	1.94	0.48
7:N:107:TRP:CD2	7:N:151:PRO:HG3	2.48	0.48
10:R:20:ALA:O	10:R:62:ARG:NH1	2.47	0.47
7:N:105:PRO:O	7:N:109:SER:OG	2.31	0.47
1:8:51:ILE:HG23	7:N:208:VAL:HG23	1.97	0.47
5:K:49:GLU:HG3	5:K:52:VAL:HG22	1.96	0.47
10:R:29:PRO:HG2	10:R:32:GLN:HB2	1.96	0.47
1:5:38:ARG:HA	3:H:52:VAL:HG21	1.97	0.47
2:G:27:SER:O	2:G:31:TYR:N	2.47	0.47
11:S:82:ILE:HD11	12:T:13:ILE:HA	1.96	0.47
5:K:75:GLY:HA2	13:K:301:CDL:H511	1.97	0.47
7:N:63:SER:HB2	7:N:66:ALA:HB3	1.97	0.47
2:G:184:ASP:N	2:G:184:ASP:OD1	2.48	0.47
1:7:19:ALA:HB2	1:8:17:GLY:HA2	1.97	0.46
12:T:46:GLU:O	12:T:50:LYS:HB2	2.15	0.46
3:H:126:MET:HB2	4:I:16:ARG:HD3	1.97	0.46
4:I:39:LEU:O	4:I:43:ALA:CB	2.64	0.46
5:K:56:GLU:HB3	7:N:87:PRO:HB2	1.96	0.46
3:H:126:MET:SD	3:H:126:MET:N	2.81	0.46
1:4:19:ALA:O	1:5:20:GLY:HA3	2.16	0.46
6:M:131:THR:OG1	6:M:132:LEU:N	2.48	0.46
11:S:91:CYS:HB3	11:S:97:VAL:HG12	1.96	0.46
1:2:37:ALA:O	1:3:39:ASN:ND2	2.40	0.46
1:1:56:LEU:HD11	7:N:204:ILE:HG21	1.97	0.45
1:2:12:GLY:HA2	1:3:14:ALA:HB2	1.99	0.45
4:I:35:LEU:HB3	4:I:39:LEU:HB2	1.98	0.45
7:N:77:ILE:HG12	7:N:102:LEU:HD21	1.98	0.45
10:R:103:ARG:NE	11:S:98:ILE:O	2.42	0.45
1:5:16:VAL:HG13	1:6:16:VAL:HB	1.98	0.45
1:8:1:ASP:OD1	1:8:1:ASP:N	2.40	0.45
2:G:228:MET:O	2:G:232:SER:OG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:201:CDL:H332	13:S:201:CDL:H521	1.98	0.45
13:K:301:CDL:H392	13:K:301:CDL:H361	1.71	0.45
1:5:39:ASN:HD21	3:H:48:LEU:HD12	1.82	0.45
4:I:35:LEU:O	4:I:40:ARG:N	2.51	0.44
11:S:91:CYS:HA	11:S:94:LYS:HE2	1.99	0.44
7:N:25:PRO:HG3	7:N:79:PHE:HB3	2.00	0.44
1:3:34:ILE:HG13	1:4:31:SER:HB2	1.99	0.44
7:N:168:LEU:HB3	7:N:194:LEU:HD21	1.98	0.44
10:R:81:LEU:HD23	13:S:201:CDL:H591	1.99	0.44
1:1:2:ILE:HD13	1:8:2:ILE:HG22	2.00	0.44
1:2:34:ILE:HG13	1:3:31:SER:HB3	1.98	0.44
1:7:8:PHE:HB3	1:8:71:LEU:HD21	2.00	0.44
6:M:19:VAL:HB	6:M:24:LYS:HB2	1.99	0.44
1:2:17:GLY:HA3	1:2:64:CYS:SG	2.59	0.43
7:N:24:ILE:HG13	7:N:25:PRO:HD3	2.00	0.43
11:S:85:TRP:CG	12:T:17:ARG:HG3	2.53	0.43
1:1:36:TYR:HE1	1:1:43:LYS:HB2	1.83	0.43
1:4:34:ILE:HG23	1:5:38:ARG:HH22	1.83	0.43
1:5:21:SER:O	1:5:25:ILE:HG12	2.18	0.43
7:N:205:GLN:HA	7:N:208:VAL:HG12	2.00	0.43
11:S:58:SER:HB3	11:S:63:LYS:HB2	1.99	0.43
1:1:32:LEU:HA	1:8:33:ILE:HG21	2.01	0.43
1:7:4:SER:HA	1:7:7:LYS:HE2	1.99	0.43
5:K:2:ARG:NH1	6:M:134:ASP:OD2	2.41	0.43
1:7:66:MET:O	1:7:70:LEU:HB2	2.19	0.43
2:G:177:LYS:HZ2	2:G:198:GLN:HB2	1.84	0.43
5:K:40:GLY:HA3	11:S:84:MET:HB3	2.01	0.43
5:K:29:THR:O	5:K:29:THR:OG1	2.35	0.42
10:R:28:VAL:HB	10:R:41:TRP:HE1	1.83	0.42
5:K:109:THR:HA	5:K:112:GLU:HB2	2.01	0.42
10:R:35:LEU:HA	10:R:38:LEU:HB2	2.00	0.42
2:G:45:GLY:HA3	2:G:211:TYR:CG	2.54	0.42
3:H:18:PHE:HD1	3:H:90:VAL:HB	1.84	0.42
1:1:72:LEU:HD12	1:1:72:LEU:HA	1.91	0.42
1:7:70:LEU:HD12	1:7:70:LEU:HA	1.92	0.42
1:2:36:TYR:HE1	1:2:43:LYS:HB2	1.85	0.42
5:K:67:GLY:HA3	13:K:301:CDL:H342	2.01	0.42
1:1:20:GLY:HA3	1:8:19:ALA:O	2.19	0.41
4:I:39:LEU:O	4:I:43:ALA:HB2	2.20	0.41
3:H:60:PRO:HG2	3:H:138:VAL:HG22	2.01	0.41
1:5:72:LEU:HD12	1:5:72:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:109:ARG:HB2	2:G:123:VAL:HG21	2.03	0.41
2:G:202:GLU:HG3	4:I:20:PHE:HB3	2.01	0.41
7:N:126:LEU:HA	7:N:143:GLU:HG2	2.03	0.41
7:N:30:VAL:HG11	7:N:41:GLN:HA	2.02	0.41
7:N:83:ILE:HA	7:N:86:PHE:HD2	1.85	0.41
1:8:21:SER:HB2	1:8:61:GLY:HA3	2.03	0.41
13:K:301:CDL:H422	13:K:301:CDL:H452	1.75	0.41
12:T:31:ARG:HG2	12:T:35:LEU:HD23	2.03	0.41
3:H:75:TYR:HA	3:H:99:PRO:HA	2.03	0.41
5:K:71:VAL:HG22	13:K:301:CDL:H521	2.02	0.41
7:N:82:PHE:HD1	7:N:82:PHE:HA	1.75	0.41
5:K:97:GLN:HG2	5:K:101:LYS:HE3	2.02	0.40
3:H:63:VAL:N	3:H:75:TYR:O	2.48	0.40
10:R:46:ASN:OD1	10:R:46:ASN:N	2.55	0.40
5:K:21:TRP:HE1	13:S:201:CDL:HA62	1.87	0.40
7:N:114:THR:HG22	7:N:122:ALA:HB2	2.03	0.40
1:2:29:PHE:HE1	1:2:54:PHE:HB2	1.86	0.40
5:K:78:ILE:HD12	13:K:301:CDL:H531	2.02	0.40
7:N:11:PRO:O	7:N:17:SER:OG	2.36	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	1	73/128 (57%)	69 (94%)	4 (6%)	0	100	100
1	2	73/128 (57%)	70 (96%)	3 (4%)	0	100	100
1	3	73/128 (57%)	71 (97%)	2 (3%)	0	100	100
1	4	73/128 (57%)	71 (97%)	2 (3%)	0	100	100
1	5	73/128 (57%)	71 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6	73/128 (57%)	72 (99%)	1 (1%)	0	100	100
1	7	73/128 (57%)	71 (97%)	2 (3%)	0	100	100
1	8	73/128 (57%)	71 (97%)	2 (3%)	0	100	100
2	G	204/290 (70%)	194 (95%)	10 (5%)	0	100	100
3	H	132/169 (78%)	129 (98%)	3 (2%)	0	100	100
4	I	35/66 (53%)	32 (91%)	3 (9%)	0	100	100
5	K	130/265 (49%)	126 (97%)	4 (3%)	0	100	100
6	M	98/219 (45%)	91 (93%)	7 (7%)	0	100	100
7	N	217/219 (99%)	209 (96%)	8 (4%)	0	100	100
9	Q	44/53 (83%)	42 (96%)	2 (4%)	0	100	100
10	R	102/119 (86%)	92 (90%)	10 (10%)	0	100	100
11	S	74/103 (72%)	73 (99%)	1 (1%)	0	100	100
12	T	80/84 (95%)	78 (98%)	2 (2%)	0	100	100
All	All	1700/2611 (65%)	1632 (96%)	68 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	51/93 (55%)	49 (96%)	2 (4%)	27	55
1	2	51/93 (55%)	49 (96%)	2 (4%)	27	55
1	3	51/93 (55%)	48 (94%)	3 (6%)	16	43
1	4	51/93 (55%)	48 (94%)	3 (6%)	16	43
1	5	51/93 (55%)	49 (96%)	2 (4%)	27	55
1	6	51/93 (55%)	49 (96%)	2 (4%)	27	55
1	7	51/93 (55%)	49 (96%)	2 (4%)	27	55
1	8	51/93 (55%)	43 (84%)	8 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	174/244 (71%)	168 (97%)	6 (3%)	32	59
3	H	106/135 (78%)	98 (92%)	8 (8%)	11	34
4	I	31/55 (56%)	30 (97%)	1 (3%)	34	61
5	K	108/225 (48%)	106 (98%)	2 (2%)	52	72
6	M	89/197 (45%)	85 (96%)	4 (4%)	23	52
7	N	194/194 (100%)	188 (97%)	6 (3%)	35	61
9	Q	42/49 (86%)	42 (100%)	0	100	100
10	R	83/97 (86%)	81 (98%)	2 (2%)	44	68
11	S	63/85 (74%)	62 (98%)	1 (2%)	58	76
12	T	67/69 (97%)	67 (100%)	0	100	100
All	All	1365/2094 (65%)	1311 (96%)	54 (4%)	29	55

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	63	PHE
1	1	73	PHE
1	2	18	VAL
1	2	46	LEU
1	3	8	PHE
1	3	46	LEU
1	3	64	CYS
1	4	21	SER
1	4	27	SER
1	4	46	LEU
1	5	15	THR
1	5	18	VAL
1	6	46	LEU
1	6	58	GLU
1	7	34	ILE
1	7	46	LEU
1	8	1	ASP
1	8	18	VAL
1	8	46	LEU
1	8	47	PHE
1	8	51	ILE
1	8	52	LEU
1	8	62	LEU

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Mol	Chain	Res	Type
1	8	63	PHE
2	G	32	THR
2	G	89	LEU
2	G	136	ASP
2	G	174	VAL
2	G	190	ASP
2	G	221	GLN
3	H	24	SER
3	H	37	ASP
3	H	38	VAL
3	H	54	THR
3	H	64	THR
3	H	86	ASP
3	H	105	LEU
3	H	126	MET
4	I	30	MET
5	K	68	THR
5	K	93	PHE
6	M	90	ASP
6	M	131	THR
6	M	143	VAL
6	M	145	ASN
7	N	82	PHE
7	N	90	PHE
7	N	109	SER
7	N	142	MET
7	N	158	LEU
7	N	214	THR
10	R	34	LYS
10	R	46	ASN
11	S	50	GLU

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

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](#)

2 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
13	CDL	S	201	-	76,76,99	0.34	0	82,88,111	0.23	0
13	CDL	K	301	-	89,89,99	0.33	0	95,101,111	0.25	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
13	CDL	S	201	-	-	48/87/87/110	-
13	CDL	K	301	-	-	68/100/100/110	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	K	301	CDL	CA2-OA2-PA1-OA3
13	K	301	CDL	CA2-OA2-PA1-OA5
13	K	301	CDL	CA3-OA5-PA1-OA2
13	K	301	CDL	CA3-OA5-PA1-OA3
13	K	301	CDL	CA3-OA5-PA1-OA4
13	K	301	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
13	S	201	CDL	O1-C1-CB2-OB2
13	S	201	CDL	CA2-OA2-PA1-OA4
13	S	201	CDL	CA2-OA2-PA1-OA5
13	S	201	CDL	CB2-OB2-PB2-OB3
13	S	201	CDL	CB2-OB2-PB2-OB4
13	S	201	CDL	CB2-OB2-PB2-OB5
13	S	201	CDL	OA9-CA7-OA8-CA6
13	S	201	CDL	C31-CA7-OA8-CA6
13	S	201	CDL	OB9-CB7-OB8-CB6
13	S	201	CDL	C71-CB7-OB8-CB6
13	K	301	CDL	OB7-CB5-OB6-CB4
13	K	301	CDL	O1-C1-CA2-OA2
13	K	301	CDL	C11-CA5-OA6-CA4
13	S	201	CDL	C51-CB5-OB6-CB4
13	S	201	CDL	OB7-CB5-OB6-CB4
13	K	301	CDL	OA7-CA5-OA6-CA4
13	K	301	CDL	CB2-C1-CA2-OA2
13	S	201	CDL	CA2-C1-CB2-OB2
13	K	301	CDL	C71-CB7-OB8-CB6
13	K	301	CDL	OA6-CA4-CA6-OA8
13	K	301	CDL	OB9-CB7-OB8-CB6
13	S	201	CDL	CA7-C31-C32-C33
13	S	201	CDL	CB7-C71-C72-C73
13	K	301	CDL	O1-C1-CB2-OB2
13	K	301	CDL	CA2-C1-CB2-OB2
13	S	201	CDL	C39-C40-C41-C42
13	S	201	CDL	C55-C56-C57-C58
13	K	301	CDL	C18-C19-C20-C21
13	K	301	CDL	CA5-C11-C12-C13
13	K	301	CDL	C13-C14-C15-C16
13	S	201	CDL	C37-C38-C39-C40
13	K	301	CDL	C20-C21-C22-C23
13	K	301	CDL	C74-C75-C76-C77
13	K	301	CDL	C11-C12-C13-C14
13	K	301	CDL	C19-C20-C21-C22
13	K	301	CDL	C32-C33-C34-C35
13	S	201	CDL	C53-C54-C55-C56
13	S	201	CDL	C38-C39-C40-C41
13	S	201	CDL	C36-C37-C38-C39
13	S	201	CDL	C12-C13-C14-C15
13	K	301	CDL	C34-C35-C36-C37
13	K	301	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
13	K	301	CDL	C75-C76-C77-C78
13	K	301	CDL	C44-C45-C46-C47
13	S	201	CDL	C13-C14-C15-C16
13	K	301	CDL	C40-C41-C42-C43
13	S	201	CDL	C14-C15-C16-C17
13	K	301	CDL	C36-C37-C38-C39
13	K	301	CDL	C17-C18-C19-C20
13	K	301	CDL	C80-C81-C82-C83
13	K	301	CDL	C16-C17-C18-C19
13	K	301	CDL	C77-C78-C79-C80
13	S	201	CDL	C32-C33-C34-C35
13	S	201	CDL	C17-C18-C19-C20
13	K	301	CDL	OA5-CA3-CA4-CA6
13	K	301	CDL	OB5-CB3-CB4-CB6
13	S	201	CDL	OA5-CA3-CA4-CA6
13	K	301	CDL	C41-C42-C43-C44
13	K	301	CDL	C33-C34-C35-C36
13	K	301	CDL	CB7-C71-C72-C73
13	K	301	CDL	CA3-CA4-CA6-OA8
13	K	301	CDL	C79-C80-C81-C82
13	K	301	CDL	CA3-CA4-OA6-CA5
13	S	201	CDL	OA5-CA3-CA4-OA6
13	S	201	CDL	C16-C17-C18-C19
13	S	201	CDL	C40-C41-C42-C43
13	K	301	CDL	C71-C72-C73-C74
13	S	201	CDL	C43-C44-C45-C46
13	K	301	CDL	C52-C53-C54-C55
13	K	301	CDL	C23-C24-C25-C26
13	K	301	CDL	C55-C56-C57-C58
13	K	301	CDL	C84-C85-C86-C87
13	S	201	CDL	C71-C72-C73-C74
13	K	301	CDL	C22-C23-C24-C25
13	K	301	CDL	OB6-CB4-CB6-OB8
13	S	201	CDL	CA5-C11-C12-C13
13	K	301	CDL	C42-C43-C44-C45
13	S	201	CDL	C20-C21-C22-C23
13	S	201	CDL	OB5-CB3-CB4-OB6
13	K	301	CDL	CB3-CB4-CB6-OB8
13	S	201	CDL	C72-C73-C74-C75
13	S	201	CDL	C34-C35-C36-C37
13	S	201	CDL	OB5-CB3-CB4-CB6
13	K	301	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
13	K	301	CDL	OA5-CA3-CA4-OA6
13	K	301	CDL	OB5-CB3-CB4-OB6
13	K	301	CDL	CA2-OA2-PA1-OA4
13	S	201	CDL	CA2-OA2-PA1-OA3
13	S	201	CDL	C42-C43-C44-C45
13	K	301	CDL	C82-C83-C84-C85
13	K	301	CDL	C78-C79-C80-C81
13	K	301	CDL	C35-C36-C37-C38
13	S	201	CDL	C1-CA2-OA2-PA1
13	S	201	CDL	C57-C58-C59-C60
13	K	301	CDL	C73-C74-C75-C76
13	S	201	CDL	CA4-CA3-OA5-PA1
13	K	301	CDL	C12-C13-C14-C15
13	K	301	CDL	C54-C55-C56-C57
13	S	201	CDL	C44-C45-C46-C47
13	S	201	CDL	C11-C12-C13-C14
13	K	301	CDL	C31-C32-C33-C34
13	K	301	CDL	C37-C38-C39-C40
13	S	201	CDL	C52-C53-C54-C55
13	K	301	CDL	C12-C11-CA5-OA6
13	K	301	CDL	C72-C73-C74-C75
13	K	301	CDL	C39-C40-C41-C42
13	K	301	CDL	CB5-C51-C52-C53
13	K	301	CDL	C12-C11-CA5-OA7
13	S	201	CDL	C33-C34-C35-C36
13	S	201	CDL	C32-C31-CA7-OA8

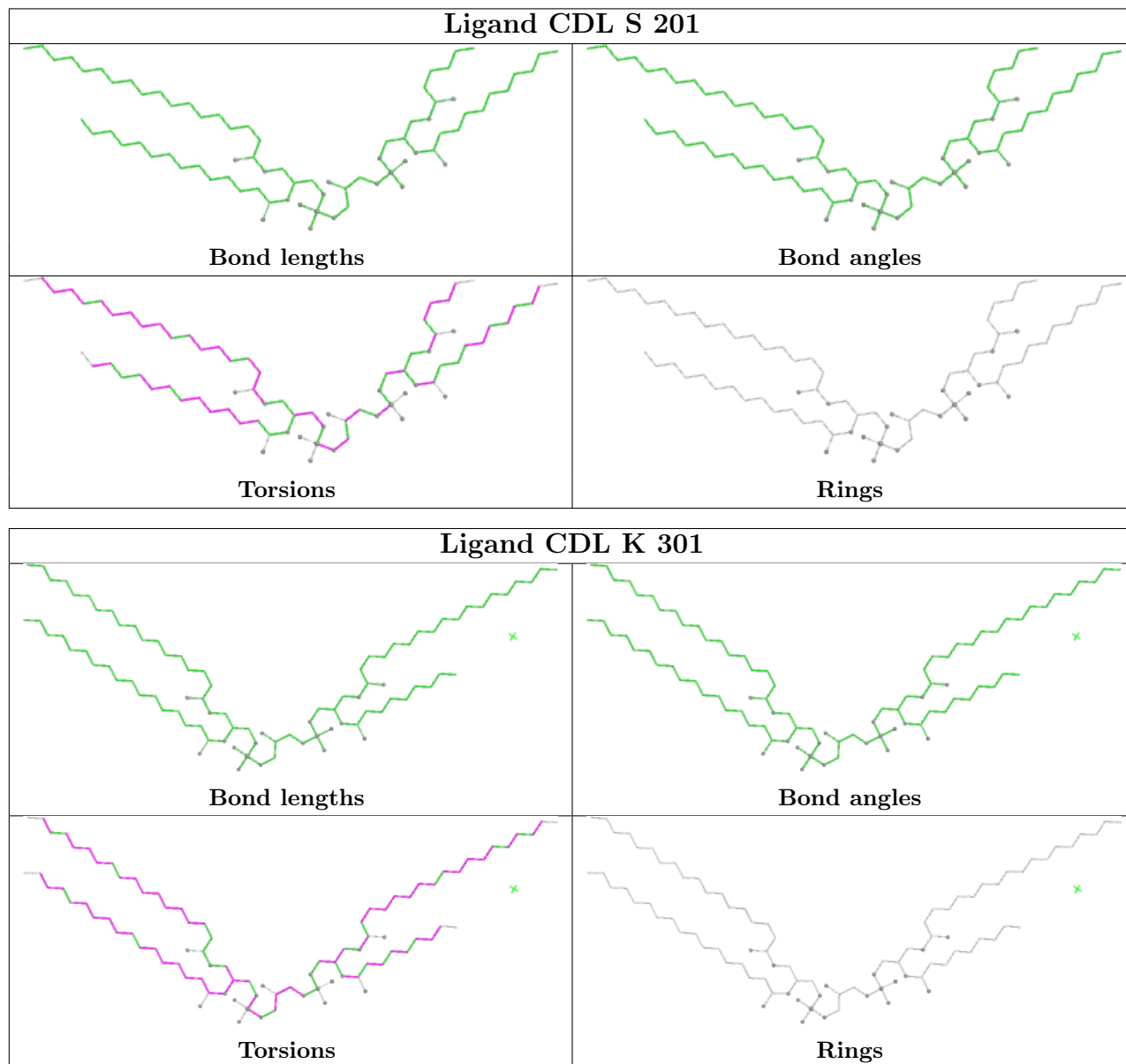
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	S	201	CDL	8	0
13	K	301	CDL	6	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.

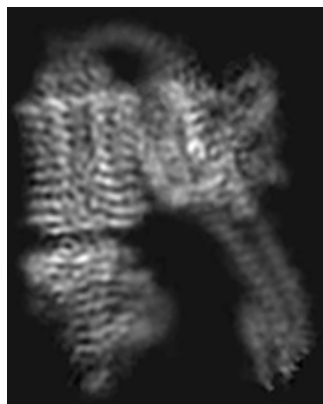
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44776. These allow visual inspection of the internal detail of the map and identification of artifacts.

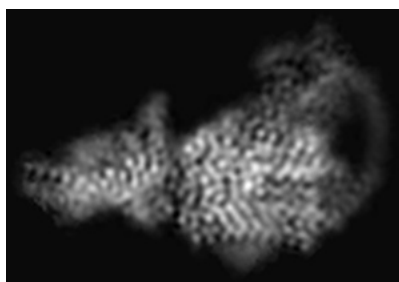
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

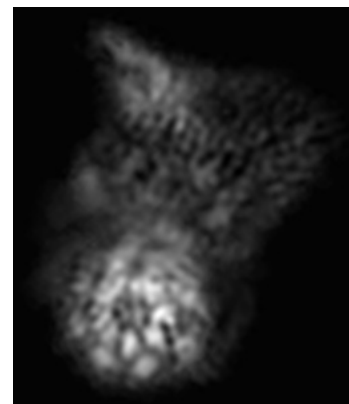
6.1.1 Primary map



X

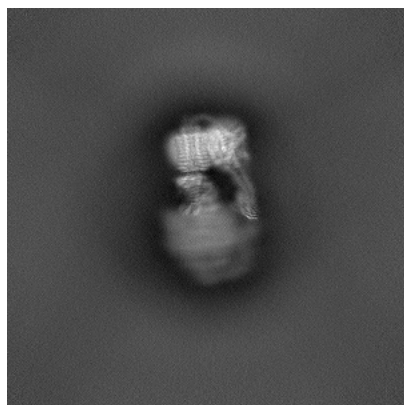


Y

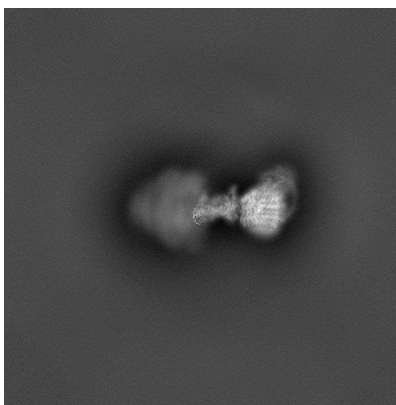


Z

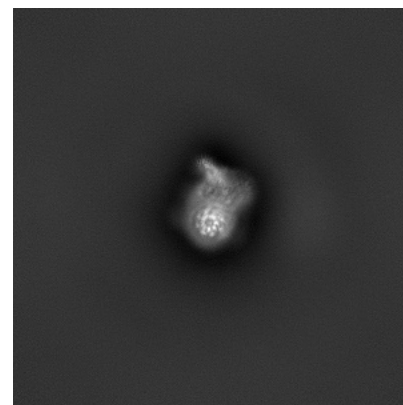
6.1.2 Raw map



X



Y

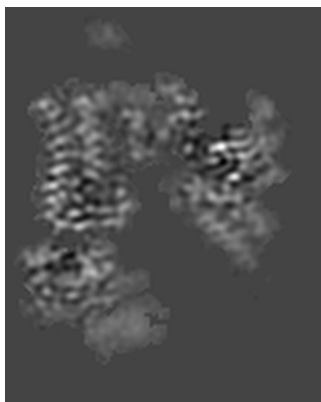


Z

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

6.2 Central slices [i](#)

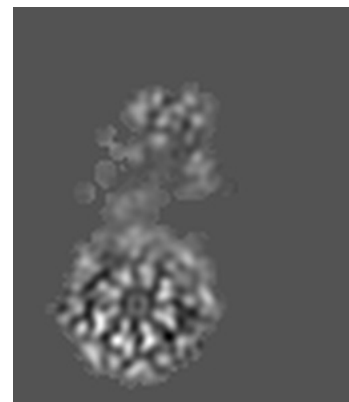
6.2.1 Primary map



X Index: 48

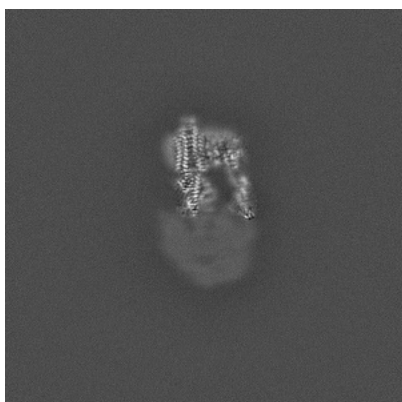


Y Index: 56

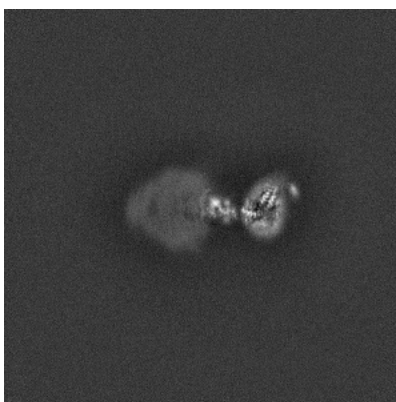


Z Index: 70

6.2.2 Raw map



X Index: 256



Y Index: 256

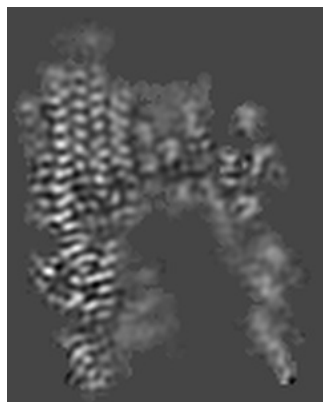


Z Index: 256

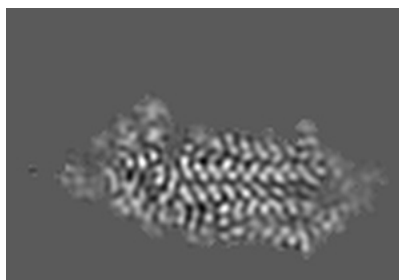
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

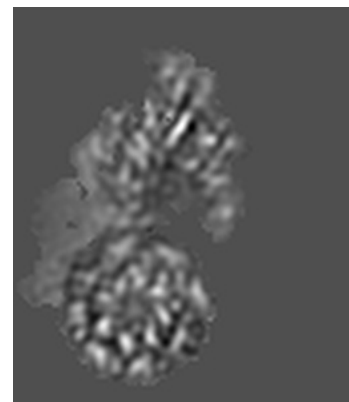
6.3.1 Primary map



X Index: 40

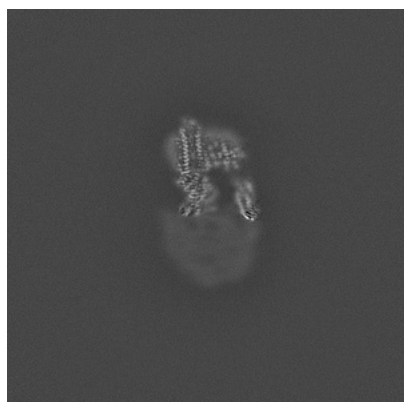


Y Index: 20

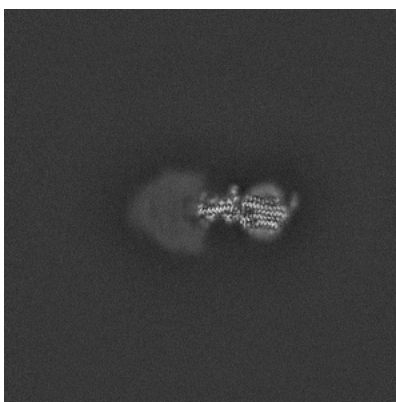


Z Index: 80

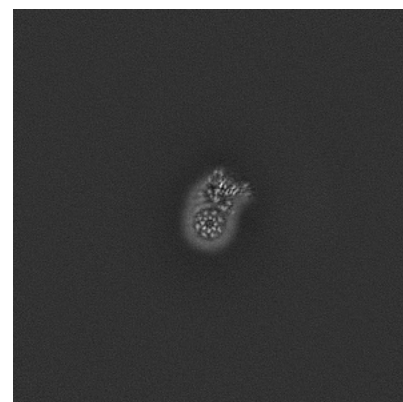
6.3.2 Raw map



X Index: 251



Y Index: 244



Z Index: 332

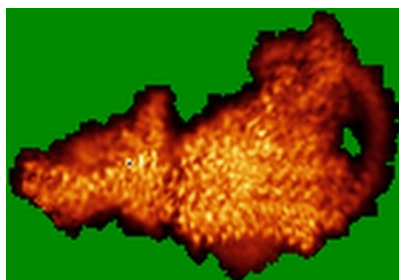
The images above show the largest variance slices of the map in three orthogonal directions.

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

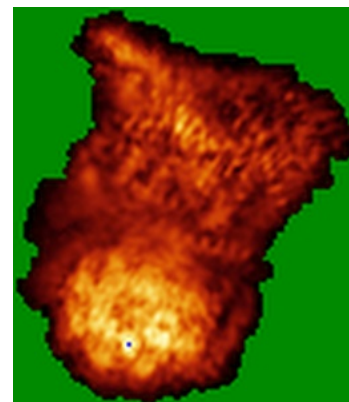
6.4.1 Primary map



X



Y

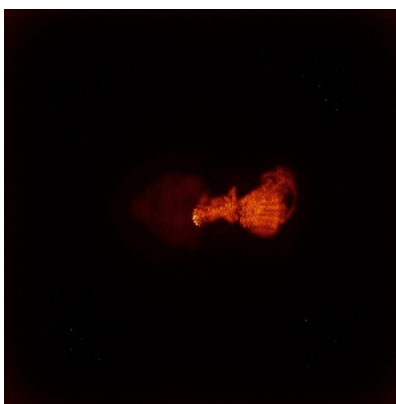


Z

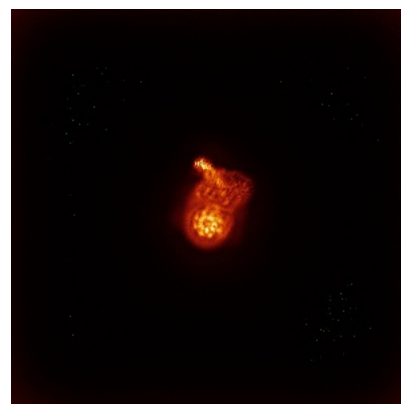
6.4.2 Raw map



X



Y

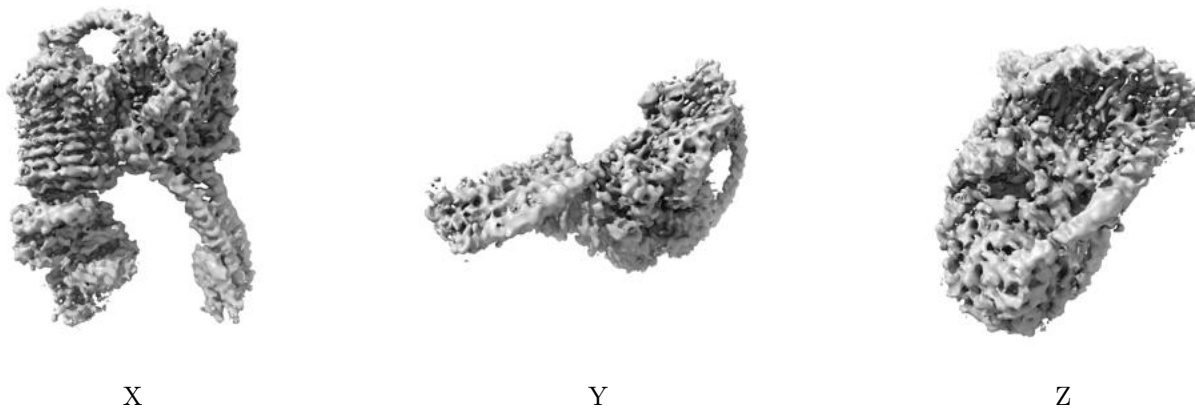


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

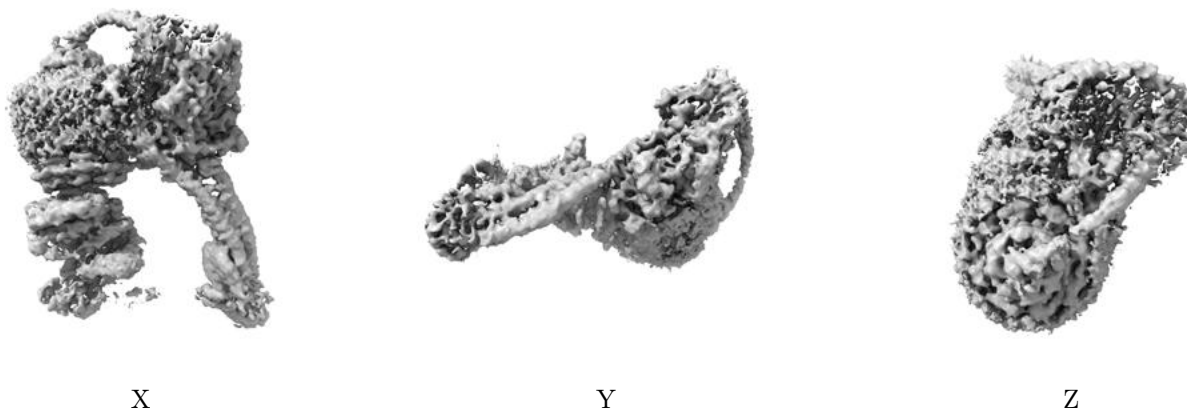
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.234. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

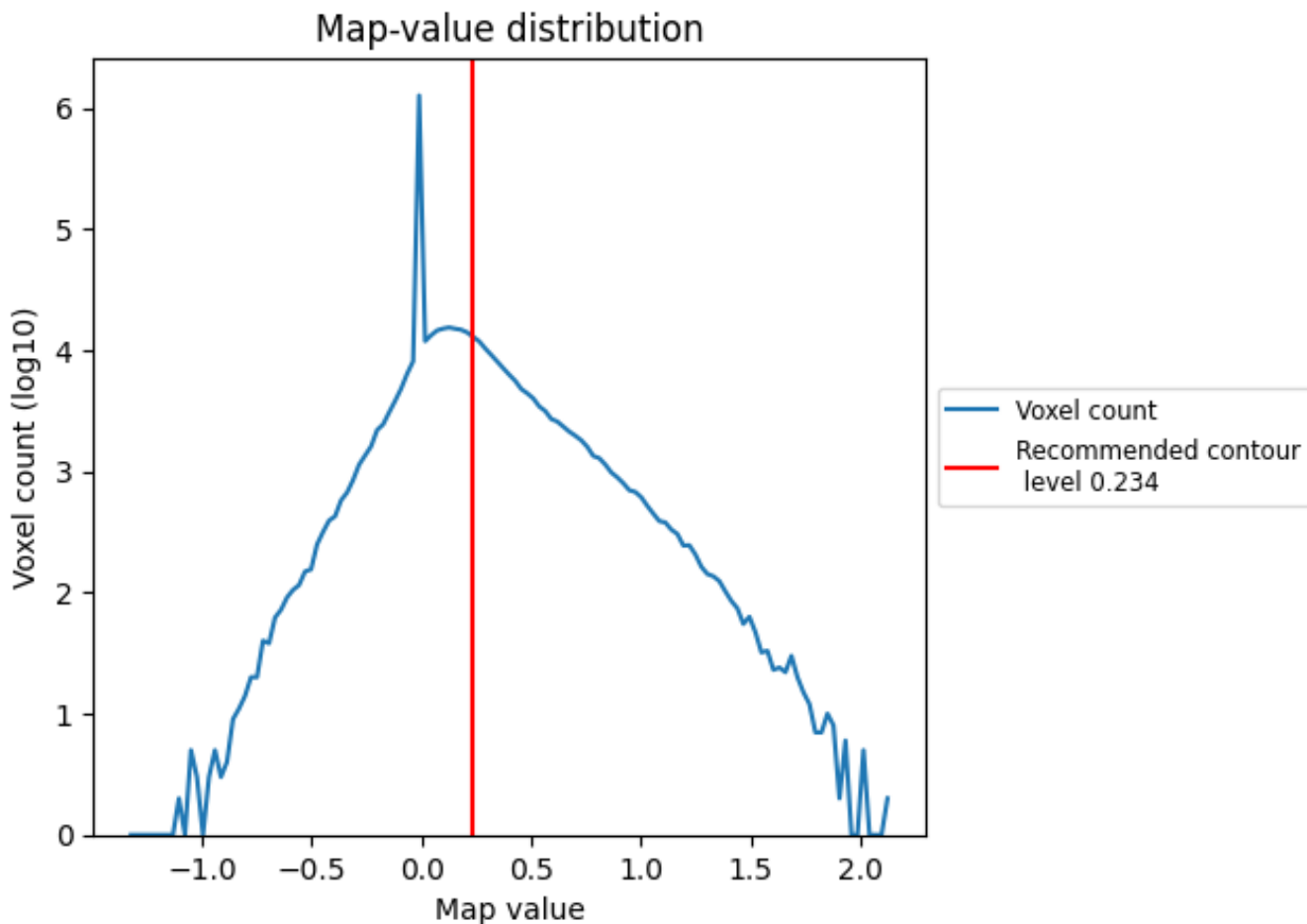
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

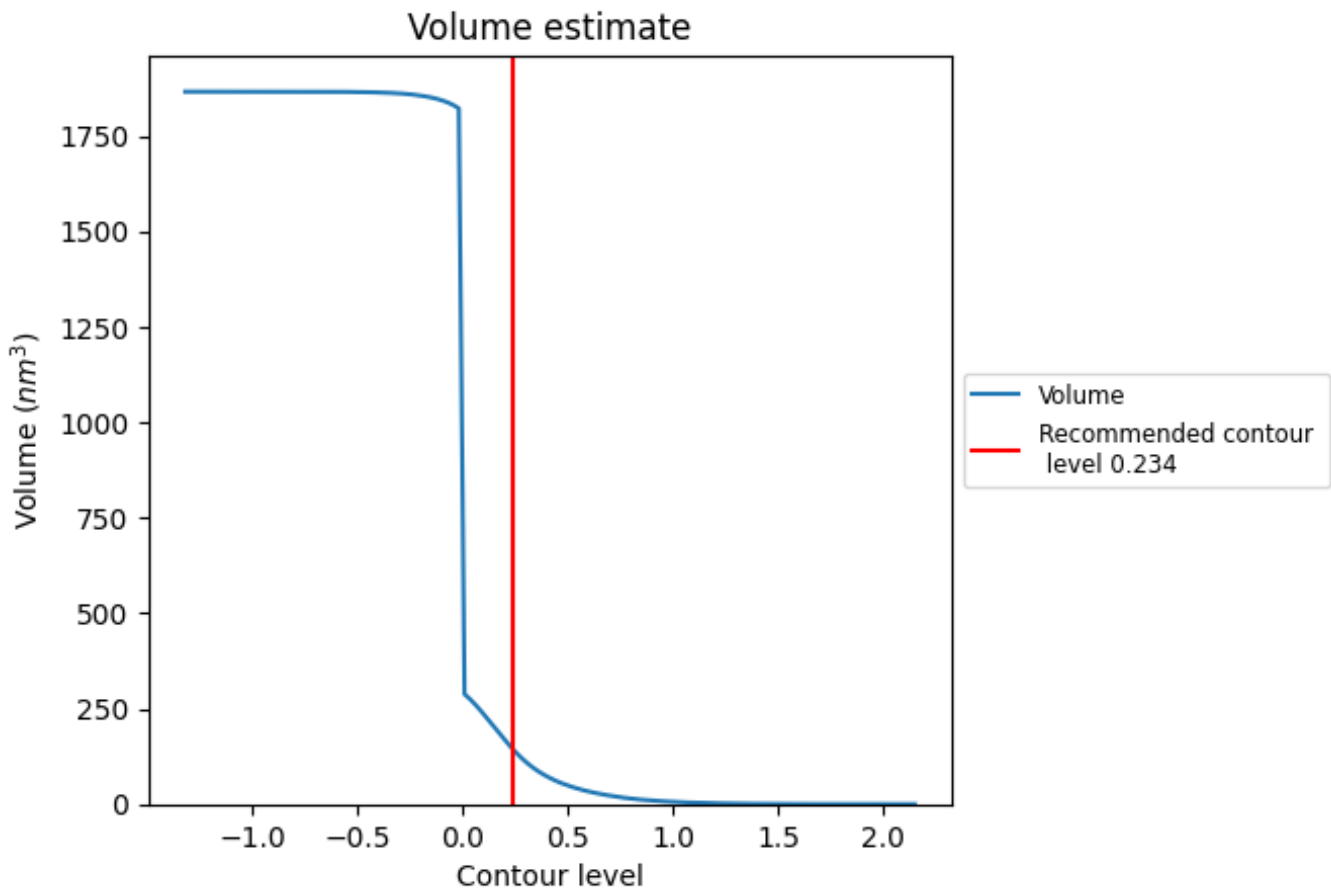
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 146 nm³; this corresponds to an approximate mass of 132 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.

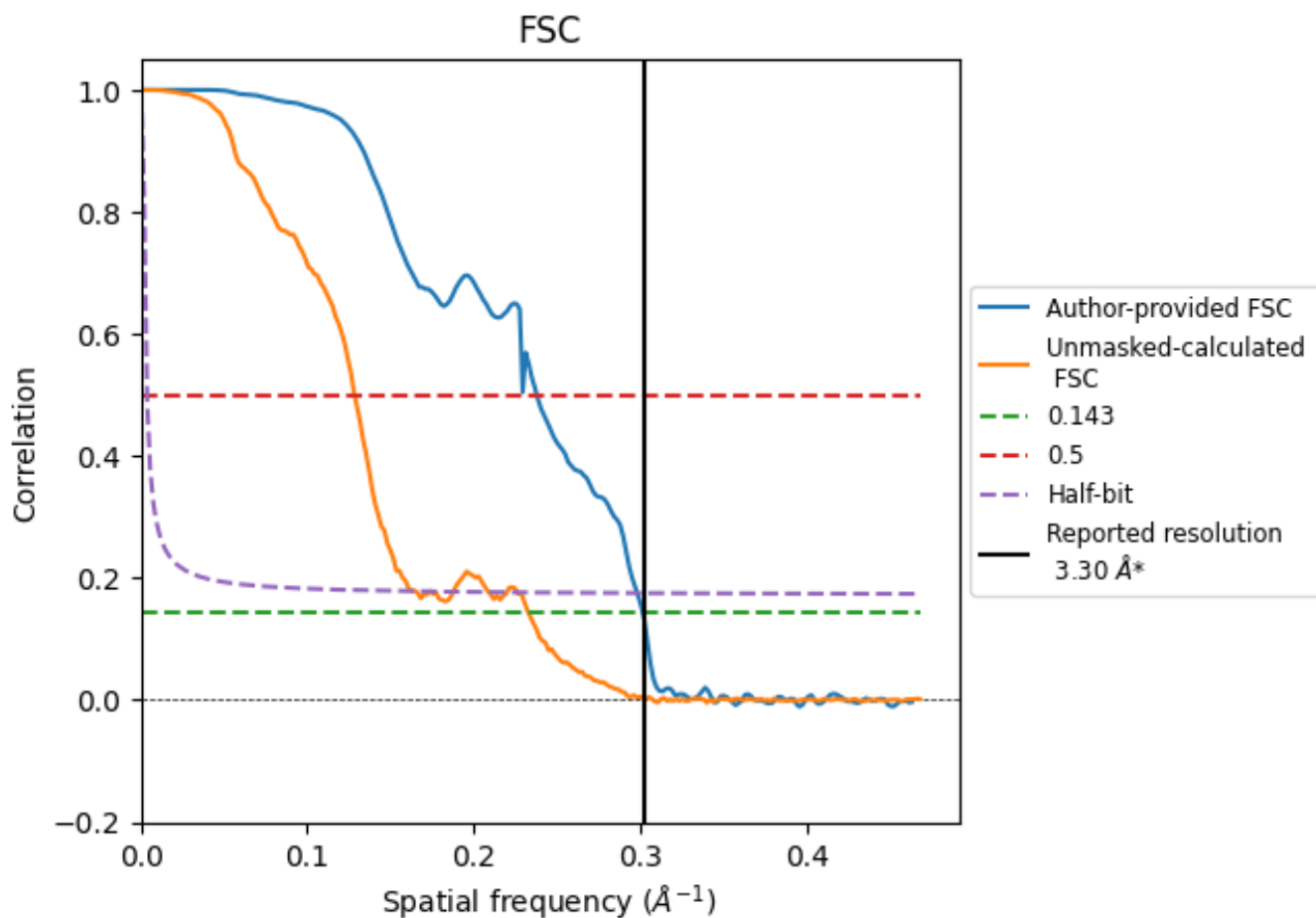
7.3 Rotationally averaged power spectrum [\(i\)](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 Å⁻¹

8.2 Resolution estimates [i](#)

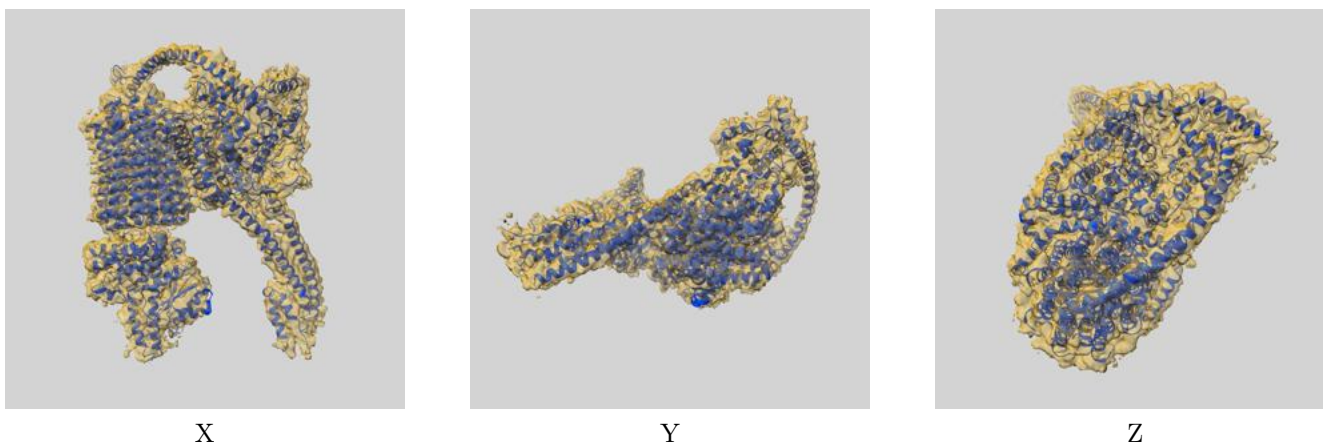
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	4.20	3.35
Unmasked-calculated*	4.29	7.79	6.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.29 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

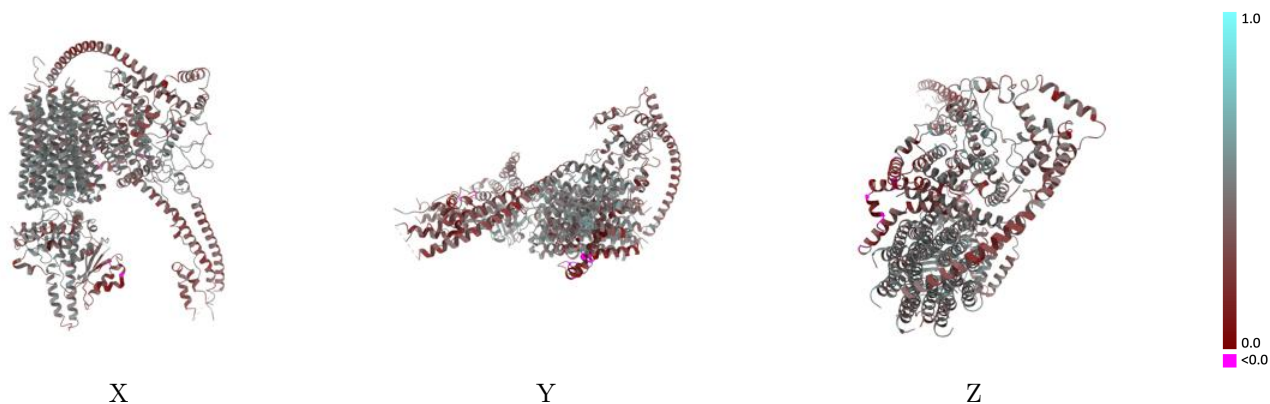
This section contains information regarding the fit between EMDB map EMD-44776 and PDB model 9BPG. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



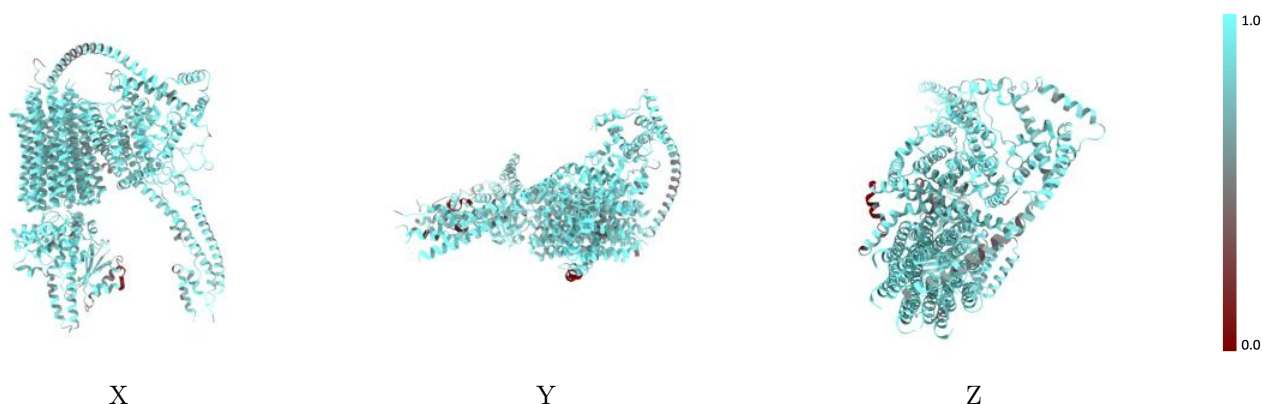
The images above show the 3D surface view of the map at the recommended contour level 0.234 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



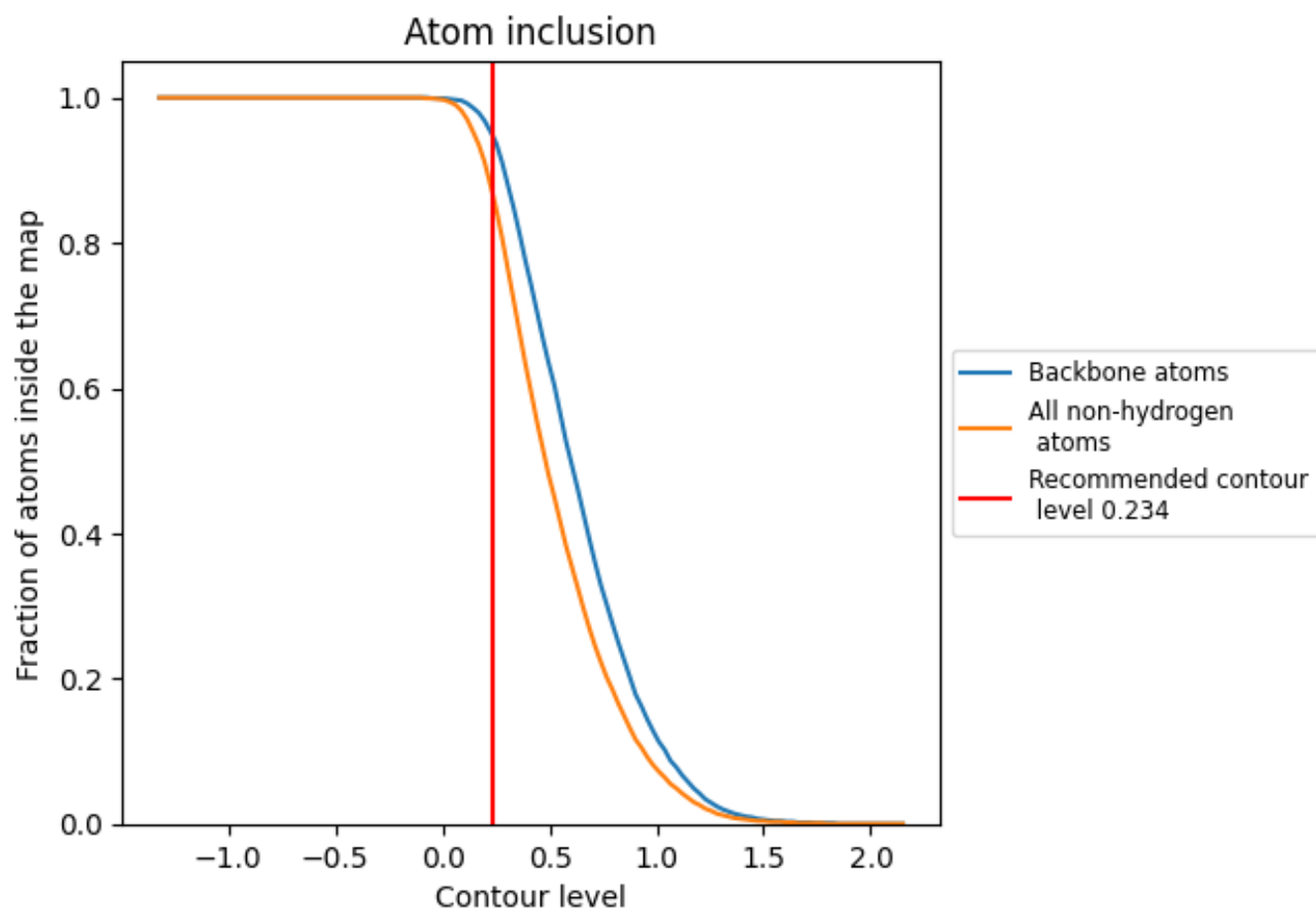
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.234).









































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 87% 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 (0.234) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8680	 0.4100
1	 0.9010	 0.4720
2	 0.9440	 0.4780
3	 0.9250	 0.4840
4	 0.9290	 0.4750
5	 0.9320	 0.4810
6	 0.9510	 0.4820
7	 0.9250	 0.4610
8	 0.9020	 0.4610
G	 0.8160	 0.3830
H	 0.9270	 0.4700
I	 0.8030	 0.3810
K	 0.8510	 0.4060
M	 0.8440	 0.3360
N	 0.8250	 0.3350
P	 0.9640	 0.3130
Q	 0.8320	 0.3790
R	 0.8930	 0.4450
S	 0.8060	 0.3710
T	 0.7320	 0.3160

