



Full wwPDB EM Validation Report ⓘ

Mar 20, 2025 – 03:04 PM EDT

PDB ID : 9B3J
EMDB ID : EMD-44142
Title : Artemia franciscana ATP synthase state 2 (composite structure), pH 8.0
Authors : Mnatsakanyan, N.; Mello, J.F.R.
Deposited on : 2024-03-19
Resolution : 2.73 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

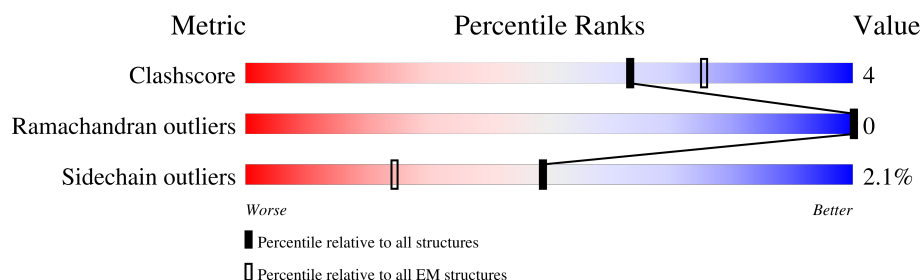
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.73 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.









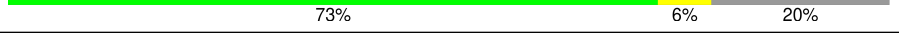
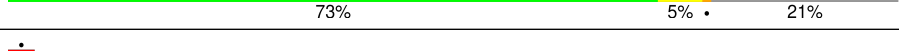
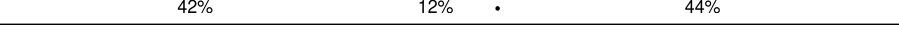
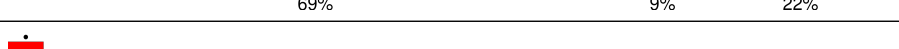
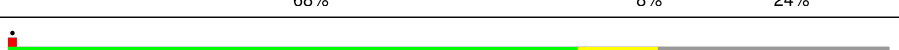

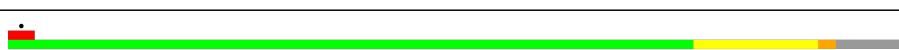
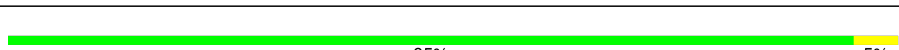
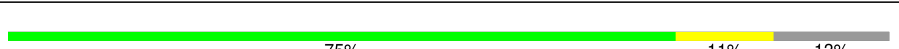




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	551	
2	B	551	
2	C	551	
3	D	524	
3	E	524	
3	F	524	
4	G	290	
5	H	169	
6	I	66	
7	K	265	
8	L	99	
9	M	219	
10	N	219	
11	O	207	
12	P	44	
13	Q	53	
14	R	119	
15	S	103	
16	T	84	

2 Entry composition [i](#)

There are 19 unique types of molecules in this entry. The entry contains 39095 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
1	1	75	Total	C	N	O	S	0	0
			537	355	83	95	4		
1	2	75	Total	C	N	O	S	0	0
			537	355	83	95	4		
1	3	75	Total	C	N	O	S	0	0
			537	355	83	95	4		
1	4	75	Total	C	N	O	S	0	0
			537	355	83	95	4		
1	5	75	Total	C	N	O	S	0	0
			537	355	83	95	4		
1	6	75	Total	C	N	O	S	0	0
			537	355	83	95	4		
1	7	75	Total	C	N	O	S	0	0
			537	355	83	95	4		
1	8	75	Total	C	N	O	S	0	0
			537	355	83	95	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	500	Total	C	N	O	S	0	0
			3815	2401	673	727	14		
2	B	503	Total	C	N	O	S	0	0
			3842	2419	676	733	14		
2	C	501	Total	C	N	O	S	0	0
			3828	2411	674	729	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	465	Total	C	N	O	S	0	0
			3525	2239	597	678	11		
3	E	455	Total	C	N	O	S	0	0
			3454	2192	588	663	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	469	Total	C	N	O	S	0	0
			3554	2255	602	686	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	231	Total	C	N	O	S	0	0
			1792	1125	305	349	13		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	208	Total	C	N	O	S	0	0
			1686	1081	292	306	7		

- Molecule 8 is a protein called ATP synthase coupling factor 6, F6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	75	Total	C	N	O	S	0	0
			594	380	95	117	2		

- Molecule 9 is a protein called ATP synthase subunit d.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	161	Total	C	N	O	S	0	0
			1309	836	222	246	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	216	Total	C	N	O	S	0	0
			1695	1144	253	284	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	191	Total	C	N	O	S	0	0
			1463	935	254	269	5		

- Molecule 12 is a protein called ATP synthase subunit 6.8PL.

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

- Molecule 13 is a protein called ATP synthase protein 8.

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

- Molecule 14 is a protein called ATP synthase subunit f.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	105	Total	C	N	O	S	0	0
			856	558	159	137	2		

- Molecule 15 is a protein called ATP synthase subunit g.

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

- Molecule 16 is a protein called ATP synthase subunit e.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	76	Total	C	N	O	S	0	0
			607	384	114	108	1		

- Molecule 17 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

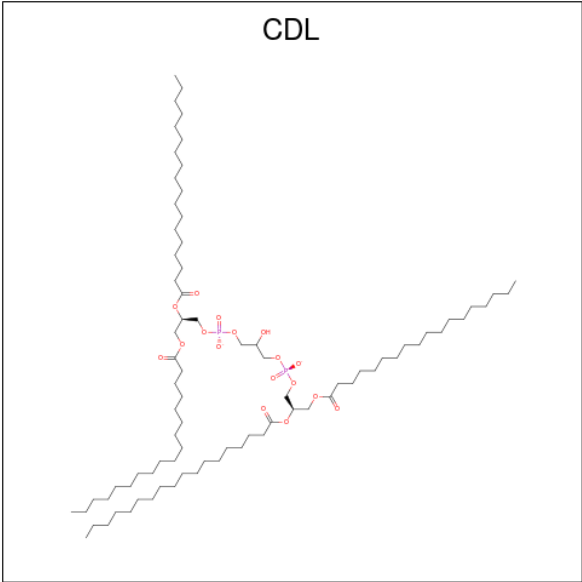


Mol	Chain	Residues	Atoms					AltConf
17	A	1	Total 31	C 10	N 5	O 13	P 3	0
17	B	1	Total 31	C 10	N 5	O 13	P 3	0
17	C	1	Total 31	C 10	N 5	O 13	P 3	0
17	D	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
18	A	1	Total Mg 1 1	0
18	B	1	Total Mg 1 1	0
18	C	1	Total Mg 1 1	0
18	D	1	Total Mg 1 1	0

- Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



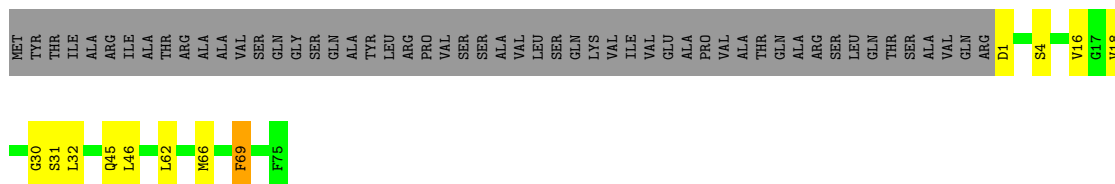
Mol	Chain	Residues	Atoms				AltConf
19	R	1	Total	C	O	P	0
			82	63	17	2	
19	S	1	Total	C	O	P	0
			75	56	17	2	

3 Residue-property plots

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

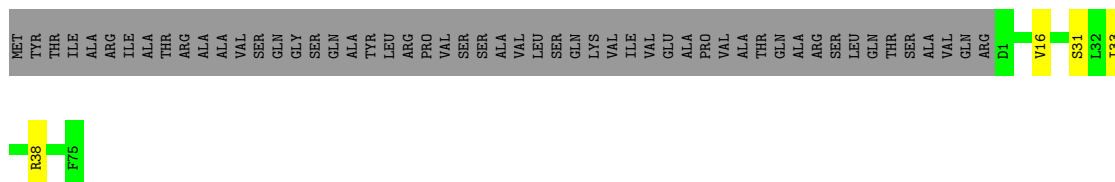
- Molecule 1: ATP synthase subunit c

Chain 1: 



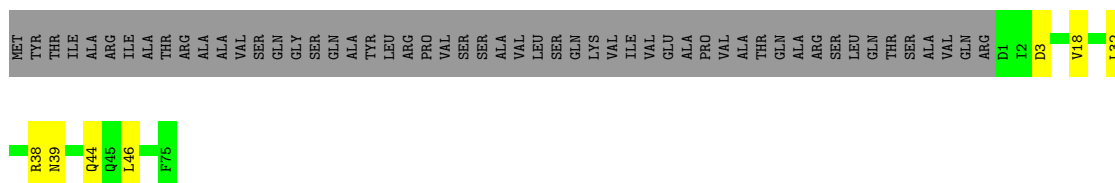
- Molecule 1: ATP synthase subunit c

Chain 2: 



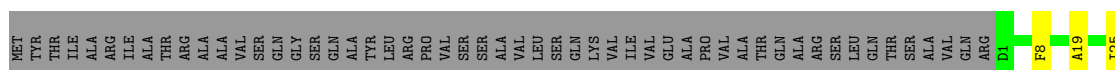
- Molecule 1: ATP synthase subunit c

Chain 3: 



- Molecule 1: ATP synthase subunit c

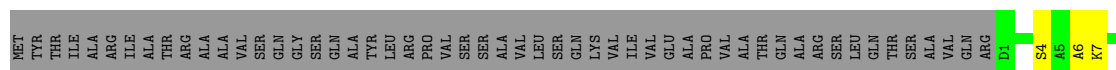
Chain 4: 





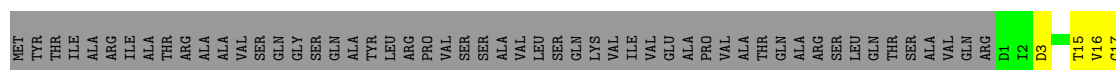
- Molecule 1: ATP synthase subunit c

Chain 5: 48% 9% 41%



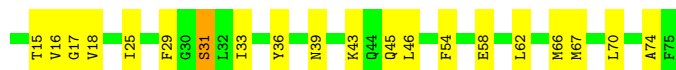
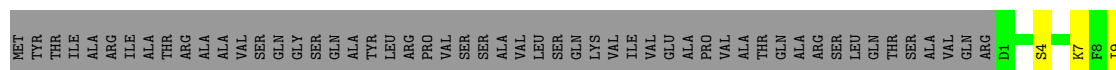
- Molecule 1: ATP synthase subunit c

Chain 6: 47% 11% 41%



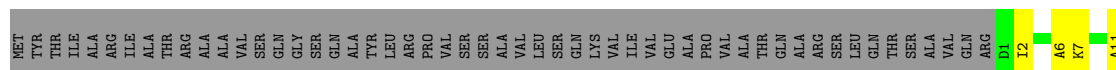
- Molecule 1: ATP synthase subunit c

Chain 7: 41% 17% 41%



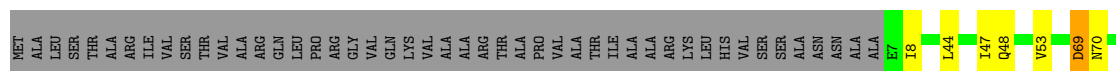
- Molecule 1: ATP synthase subunit c


Chain 8: 43% 15% 41%

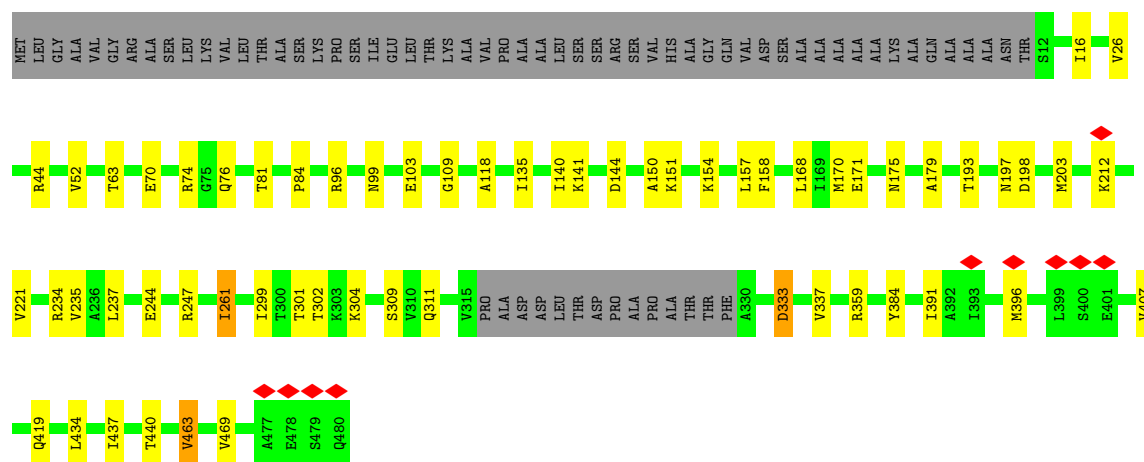


- Molecule 2: ATP synthase subunit alpha


Chain A: 83% 8% 9%

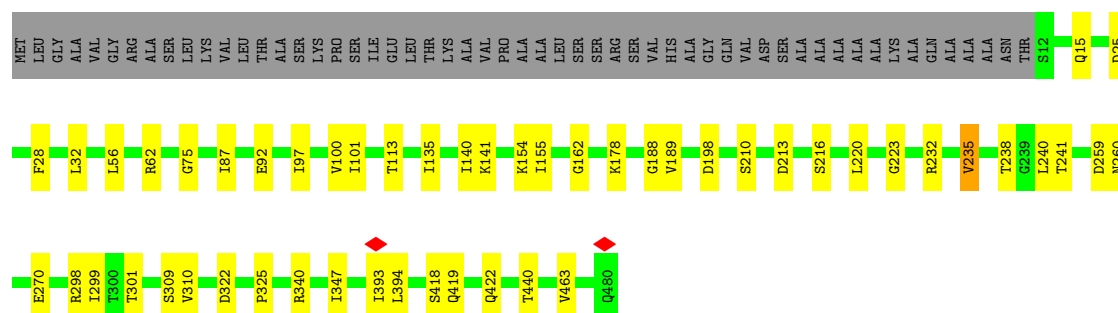


Chain E: 



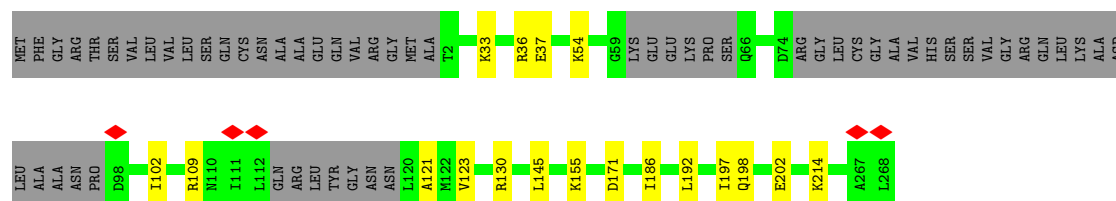
- Molecule 3: ATP synthase subunit beta

Chain F: 



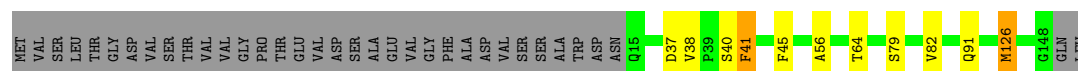
- Molecule 4: ATP synthase subunit gamma

Chain G: 



- Molecule 5: ATP synthase subunit delta

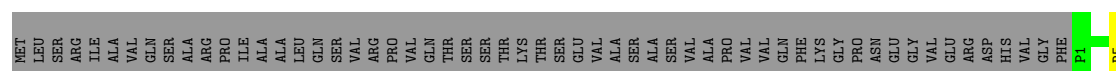
Chain H: 



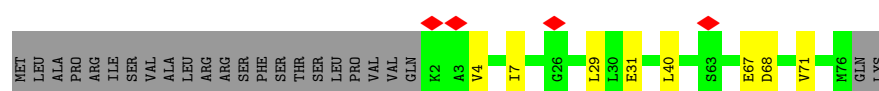
- Molecule 6: ATP synthase subunit epsilon



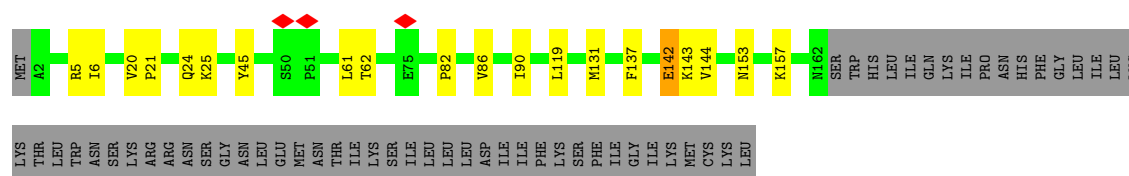
- Molecule 7: ATP synthase subunit b



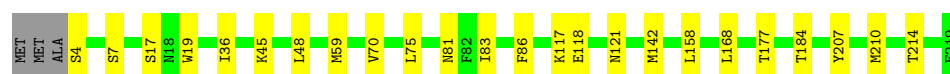
- Molecule 8: ATP synthase coupling factor 6, F6



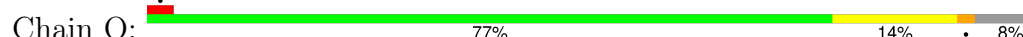
- Molecule 9: ATP synthase subunit d

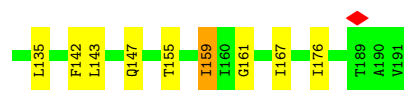


- Molecule 10: ATP synthase subunit a

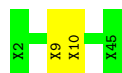


- Molecule 11: ATP synthase subunit OSCP





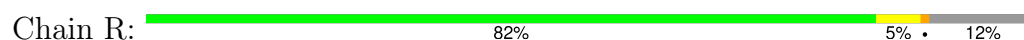
- Molecule 12: ATP synthase subunit 6.8PL



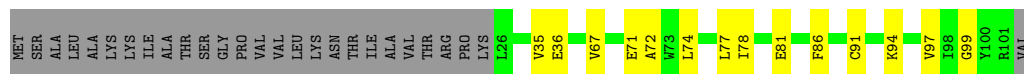
- Molecule 13: ATP synthase protein 8



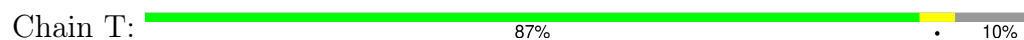
- Molecule 14: ATP synthase subunit f



- Molecule 15: ATP synthase subunit g



- Molecule 16: 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	302409	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	80.276	Depositor
Minimum map value	-62.935	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	1.020	Depositor
Recommended contour level	3.55	Depositor
Map size (Å)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	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: ATP, MG, 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	0.35	0/547	0.46	0/734
1	2	0.35	0/547	0.44	0/734
1	3	0.35	0/547	0.44	0/734
1	4	0.36	0/547	0.43	0/734
1	5	0.37	0/547	0.45	0/734
1	6	0.38	0/547	0.46	0/734
1	7	0.37	0/547	0.47	0/734
1	8	0.34	0/547	0.43	0/734
2	A	0.29	0/3867	0.50	0/5217
2	B	0.29	0/3896	0.50	0/5257
2	C	0.29	0/3882	0.50	0/5238
3	D	0.30	0/3582	0.50	0/4862
3	E	0.28	0/3506	0.49	0/4751
3	F	0.30	0/3611	0.50	0/4901
4	G	0.29	0/1809	0.45	0/2427
5	H	0.35	0/998	0.46	0/1359
6	I	0.31	0/308	0.62	0/407
7	K	0.34	0/1720	0.44	0/2311
8	L	0.26	0/604	0.38	0/809
9	M	0.30	0/1343	0.45	0/1808
10	N	0.33	0/1740	0.48	0/2375
11	O	0.25	0/1478	0.47	0/1986
13	Q	0.35	0/405	0.47	0/549
14	R	0.39	0/887	0.54	0/1203
15	S	0.40	0/611	0.52	0/829
16	T	0.28	0/617	0.50	0/830
All	All	0.31	0/39240	0.49	0/52991

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	5	0
1	3	537	0	549	3	0
1	4	537	0	549	5	0
1	5	537	0	549	12	0
1	6	537	0	549	14	0
1	7	537	0	549	17	0
1	8	537	0	549	15	0
2	A	3815	0	3916	23	0
2	B	3842	0	3945	35	0
2	C	3828	0	3934	22	0
3	D	3525	0	3593	32	0
3	E	3454	0	3528	35	0
3	F	3554	0	3618	30	0
4	G	1792	0	1838	11	0
5	H	984	0	974	8	0
6	I	304	0	305	7	0
7	K	1686	0	1709	27	0
8	L	594	0	599	7	0
9	M	1309	0	1301	10	0
10	N	1695	0	1785	19	0
11	O	1463	0	1581	16	0
12	P	220	0	47	2	0
13	Q	390	0	393	6	0
14	R	856	0	842	5	0
15	S	596	0	617	13	0
16	T	607	0	622	3	0
17	A	31	0	12	0	0
17	B	31	0	12	0	0
17	C	31	0	12	1	0
17	D	31	0	12	0	0
18	A	1	0	0	0	0
18	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	C	1	0	0	0	0
18	D	1	0	0	0	0
19	R	82	0	111	3	0
19	S	75	0	94	0	0
All	All	39095	0	39792	317	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 4.

All (317) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:33:ILE:HG21	1:3:32:LEU:HA	1.76	0.68
7:K:25:PHE:HZ	15:S:77:LEU:HD13	1.59	0.68
1:6:38:ARG:HH21	5:H:45:PHE:HB3	1.62	0.65
1:6:37:ALA:O	1:7:39:ASN:ND2	2.29	0.64
6:I:13:ARG:NH1	6:I:23:SER:OG	2.31	0.64
15:S:86:PHE:HB2	16:T:20:ALA:HB1	1.79	0.63
10:N:17:SER:HB3	10:N:19:TRP:HD1	1.64	0.63
7:K:5:ARG:NH1	10:N:36:ILE:O	2.31	0.62
1:7:4:SER:HA	1:7:7:LYS:HE2	1.82	0.61
7:K:140:TYR:HB2	9:M:82:PRO:HD3	1.81	0.61
7:K:15:GLY:HA3	19:R:201:CDL:H141	1.82	0.61
1:7:33:ILE:HG21	1:8:32:LEU:HA	1.82	0.60
3:D:191:GLU:OE2	3:D:260:ASN:ND2	2.34	0.60
7:K:141:ARG:HB2	9:M:45:TYR:HB3	1.84	0.60
2:A:53:VAL:HG21	2:A:73:ILE:HD13	1.83	0.59
11:O:110:MET:HA	11:O:113:HIS:HB3	1.83	0.59
2:A:258:ARG:NH1	2:A:308:ARG:O	2.36	0.59
2:A:185:ASN:OD1	2:A:188:ARG:NH1	2.36	0.59
3:F:92:GLU:HB2	3:F:113:THR:HG22	1.84	0.59
2:C:258:ARG:NH1	2:C:308:ARG:O	2.36	0.58
15:S:35:VAL:O	16:T:14:ARG:NH2	2.37	0.58
2:B:67:GLU:O	3:E:74:ARG:NH1	2.36	0.58
4:G:155:LYS:HB2	4:G:171:ASP:HB2	1.84	0.58
7:K:168:ILE:HG21	8:L:40:LEU:HD22	1.85	0.58
3:E:44:ARG:NH2	3:E:70:GLU:O	2.36	0.58
10:N:81:ASN:HD21	10:N:158:LEU:HD11	1.69	0.57
3:F:393:ILE:HG13	3:F:394:LEU:HG	1.86	0.57
4:G:37:GLU:OE1	4:G:214:LYS:NZ	2.36	0.57
3:D:161:ALA:O	3:D:340:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:29:HIS:O	6:I:33:ARG:NH1	2.37	0.56
2:B:12:LEU:HD22	11:O:89:LEU:HD21	1.87	0.56
3:F:240:LEU:HD21	3:F:298:ARG:HB2	1.87	0.56
7:K:29:THR:HB	7:K:33:GLY:HA3	1.88	0.56
12:P:9:UNK:O	13:Q:25:THR:OG1	2.23	0.56
1:2:38:ARG:HB2	1:3:38:ARG:HH11	1.69	0.56
11:O:9:ILE:HD11	11:O:109:ILE:HG12	1.87	0.56
2:C:423:ARG:HD2	2:C:461:ILE:HD11	1.86	0.56
3:E:171:GLU:OE2	3:E:175:ASN:ND2	2.39	0.56
2:C:163:GLN:NE2	2:C:165:GLU:OE1	2.39	0.56
1:6:30:GLY:O	1:7:31:SER:OG	2.21	0.56
2:B:164:ARG:NH2	2:B:345:ILE:O	2.39	0.55
1:1:32:LEU:HA	1:8:33:ILE:HG21	1.89	0.55
10:N:177:THR:O	10:N:184:THR:OG1	2.24	0.55
5:H:56:ALA:HB3	5:H:82:VAL:HB	1.89	0.55
7:K:168:ILE:O	7:K:172:ASN:ND2	2.40	0.55
14:R:35:LEU:HA	14:R:38:LEU:HB2	1.89	0.54
1:1:16:VAL:HG13	1:2:16:VAL:HB	1.89	0.54
1:7:36:TYR:OH	1:8:45:GLN:OE1	2.26	0.54
1:5:37:ALA:O	1:6:39:ASN:ND2	2.40	0.54
2:A:179:ALA:HB1	2:A:267:ILE:HD13	1.90	0.54
2:B:186:GLN:O	2:B:190:ASN:ND2	2.41	0.54
3:E:141:LYS:NZ	3:E:463:VAL:O	2.38	0.54
7:K:196:LYS:NZ	8:L:4:VAL:O	2.40	0.54
2:C:53:VAL:HG21	2:C:73:ILE:HD13	1.88	0.54
1:6:19:ALA:HB2	1:7:17:GLY:HA2	1.89	0.54
1:1:30:GLY:O	1:2:31:SER:OG	2.26	0.53
2:A:139:ARG:NH1	3:D:193:THR:OG1	2.41	0.53
1:1:66:MET:HB2	10:N:168:LEU:HD13	1.89	0.53
7:K:179:ARG:NH2	8:L:31:GLU:OE1	2.41	0.53
15:S:67:VAL:HG12	15:S:72:ALA:HB2	1.91	0.53
2:B:51:GLU:OE2	2:B:90:ARG:NH2	2.42	0.53
1:8:7:LYS:NZ	1:8:75:PHE:O	2.42	0.53
2:B:148:THR:HG23	2:B:182:ALA:HB2	1.90	0.53
11:O:110:MET:O	11:O:114:ARG:NE	2.38	0.53
3:F:210:SER:H	3:F:216:SER:HB3	1.72	0.52
3:E:99:ASN:HD21	3:E:103:GLU:HB2	1.74	0.52
2:A:382:ALA:HB2	2:A:488:GLN:HA	1.90	0.52
3:E:157:LEU:HD21	3:E:168:LEU:HD23	1.91	0.52
2:A:8:ILE:HD12	7:K:170:GLN:HE21	1.74	0.52
2:B:423:ARG:HD2	2:B:461:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:247:ARG:NH1	3:D:302:THR:OG1	2.43	0.52
5:H:79:SER:HB2	6:I:24:VAL:HG13	1.90	0.52
3:E:170:MET:HE1	3:E:203:MET:HA	1.91	0.51
1:1:31:SER:OG	1:8:30:GLY:O	2.25	0.51
10:N:45:LYS:HE3	13:Q:31:TYR:HA	1.92	0.51
3:D:301:THR:HG23	3:D:306:SER:HA	1.93	0.51
1:8:11:ALA:O	1:8:15:THR:OG1	2.29	0.51
2:B:258:ARG:NH2	2:B:308:ARG:O	2.39	0.51
3:F:162:GLY:O	3:F:340:ARG:NH1	2.43	0.51
4:G:33:LYS:HG3	4:G:36:ARG:HH21	1.74	0.51
7:K:168:ILE:HG13	8:L:40:LEU:HD13	1.92	0.51
3:D:47:ARG:NH1	3:D:103:GLU:OE2	2.44	0.51
3:D:347:ILE:HG23	3:D:418:SER:HB3	1.93	0.51
3:F:140:ILE:HA	3:F:419:GLN:HE22	1.75	0.51
1:1:1:ASP:N	1:1:4:SER:OG	2.44	0.51
2:A:69:ASP:OD1	2:A:70:ASN:ND2	2.41	0.51
3:F:97:ILE:HG12	3:F:220:LEU:HD12	1.92	0.51
7:K:63:ILE:HD13	10:N:86:PHE:HD1	1.76	0.51
3:E:299:ILE:HG21	3:E:309:SER:HB2	1.93	0.51
2:B:150:MET:HB2	2:B:153:VAL:HG12	1.93	0.51
3:F:347:ILE:HG23	3:F:418:SER:HB3	1.92	0.51
7:K:25:PHE:CZ	15:S:77:LEU:HD13	2.42	0.51
7:K:135:GLN:HE22	8:L:71:VAL:HA	1.75	0.51
1:2:33:ILE:HG23	1:3:46:LEU:HD22	1.92	0.50
2:C:270:ASP:N	2:C:270:ASP:OD1	2.44	0.50
3:E:391:ILE:HG12	3:E:396:MET:HA	1.93	0.50
3:E:234:ARG:HA	3:E:237:LEU:HD23	1.93	0.50
7:K:172:ASN:HD21	8:L:29:LEU:HD22	1.76	0.50
2:B:270:ASP:OD1	2:B:270:ASP:N	2.42	0.50
1:4:8:PHE:HB2	1:5:6:ALA:HB1	1.93	0.50
15:S:36:GLU:HA	16:T:14:ARG:HH21	1.75	0.50
14:R:103:ARG:HG2	15:S:99:GLY:HA3	1.94	0.50
3:D:285:GLN:HG3	3:D:288:LEU:HB2	1.94	0.49
11:O:90:LEU:HD21	11:O:102:VAL:HG21	1.92	0.49
1:6:36:TYR:OH	1:7:45:GLN:NE2	2.45	0.49
2:B:44:LEU:HD13	2:B:47:ILE:HD12	1.94	0.49
2:B:254:GLY:HA3	2:B:266:ILE:HD11	1.94	0.49
4:G:198:GLN:NE2	4:G:202:GLU:OE2	2.40	0.49
1:8:51:ILE:HG21	10:N:207:TYR:HD2	1.78	0.49
3:D:334:ALA:HA	3:D:358:SER:HA	1.94	0.49
2:B:46:ASN:O	2:B:90:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:38:ILE:HD13	2:C:285:LEU:HG	1.95	0.49
3:F:232:ARG:NH2	3:F:270:GLU:OE1	2.45	0.49
1:7:25:ILE:HD11	1:7:58:GLU:HB2	1.93	0.49
2:A:44:LEU:HD13	2:A:47:ILE:HD12	1.95	0.49
2:C:51:GLU:OE2	2:C:90:ARG:NH1	2.45	0.49
3:F:141:LYS:HG2	3:F:440:THR:HG22	1.95	0.49
11:O:111:ALA:O	11:O:116:GLU:N	2.46	0.49
1:4:33:ILE:HG21	1:5:32:LEU:HA	1.95	0.49
2:A:420:ARG:NH1	2:A:449:VAL:O	2.46	0.49
2:B:136:ILE:O	3:E:197:ASN:ND2	2.46	0.49
2:B:483:ILE:HD11	2:B:497:LEU:HD11	1.95	0.49
3:D:255:LEU:HD23	3:D:308:THR:HB	1.95	0.49
2:B:80:LYS:NZ	3:D:35:ILE:O	2.45	0.49
2:B:450:ARG:NH1	2:B:494:ASP:OD2	2.46	0.49
3:E:144:ASP:HB3	3:E:437:ILE:HD13	1.95	0.49
11:O:4:LEU:HG	11:O:6:LYS:H	1.76	0.49
2:B:179:ALA:HB1	2:B:267:ILE:HG12	1.95	0.49
3:F:141:LYS:NZ	3:F:463:VAL:O	2.42	0.49
3:F:178:LYS:NZ	3:F:422:GLN:OE1	2.43	0.49
3:D:247:ARG:NH1	3:D:248:ASP:OD1	2.46	0.49
4:G:192:LEU:HB3	4:G:197:ILE:HD11	1.95	0.49
2:B:90:ARG:HH21	2:B:92:GLY:HA2	1.77	0.48
2:B:94:ILE:HD11	2:B:128:ARG:HD2	1.94	0.48
1:5:7:LYS:HB3	1:5:72:LEU:HD12	1.96	0.48
2:B:163:GLN:NE2	2:B:165:GLU:OE1	2.47	0.48
3:D:44:ARG:NH1	3:D:70:GLU:O	2.39	0.48
3:E:135:ILE:O	3:E:151:LYS:NZ	2.46	0.48
9:M:25:LYS:HD2	13:Q:53:TRP:HE1	1.77	0.48
1:5:30:GLY:O	1:6:31:SER:OG	2.24	0.48
2:C:170:ASP:O	2:C:175:LYS:NZ	2.46	0.48
3:E:135:ILE:HA	3:E:150:ALA:HA	1.96	0.48
7:K:159:LEU:HA	9:M:61:LEU:HD21	1.96	0.48
3:D:16:ILE:HD12	3:D:76:GLN:HB3	1.95	0.48
1:7:43:LYS:HA	1:7:46:LEU:HD12	1.96	0.48
3:E:154:LYS:O	3:E:333:ASP:N	2.46	0.48
4:G:102:ILE:HG12	4:G:121:ALA:HB3	1.95	0.48
11:O:121:VAL:HG21	11:O:135:LEU:HD21	1.96	0.48
5:H:40:SER:OG	5:H:41:PHE:N	2.47	0.48
10:N:4:SER:N	10:N:7:SER:HG	2.12	0.48
4:G:145:LEU:HD13	4:G:202:GLU:HG2	1.96	0.48
10:N:118:GLU:HB3	10:N:121:ASN:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:GLY:H	2:B:322:THR:HB	1.79	0.47
2:C:114:PRO:HG3	2:C:121:ILE:HG23	1.95	0.47
3:D:254:VAL:HB	3:D:307:ILE:HG12	1.95	0.47
3:E:141:LYS:HG2	3:E:440:THR:HG22	1.97	0.47
7:K:129:ARG:HB3	9:M:90:ILE:HG21	1.95	0.47
2:A:195:GLU:HA	2:A:198:LYS:HE2	1.96	0.47
3:E:384:TYR:HE1	3:E:407:VAL:HG13	1.80	0.47
11:O:63:ARG:NH1	11:O:92:GLU:O	2.48	0.47
2:B:457:GLU:OE1	2:B:460:LYS:NZ	2.47	0.47
3:E:16:ILE:HA	3:E:26:VAL:HG12	1.96	0.47
2:C:175:LYS:NZ	17:C:601:ATP:O1B	2.43	0.47
3:E:333:ASP:OD2	3:E:359:ARG:NH2	2.43	0.47
2:C:179:ALA:HB1	2:C:267:ILE:HG12	1.97	0.47
1:7:18:VAL:HG12	1:8:60:MET:HB3	1.97	0.47
3:F:213:ASP:OD1	3:F:213:ASP:N	2.45	0.47
15:S:67:VAL:HG22	15:S:71:GLU:OE2	2.14	0.47
7:K:24:PHE:CE2	15:S:74:LEU:HB2	2.50	0.47
3:E:179:ALA:HB2	3:E:434:LEU:HD21	1.96	0.46
14:R:28:VAL:O	14:R:41:TRP:NE1	2.38	0.46
2:C:151:LYS:HG2	2:C:441:GLN:HG2	1.97	0.46
2:C:426:GLU:HG3	2:C:458:PRO:HB3	1.97	0.46
15:S:91:CYS:HA	15:S:94:LYS:HE2	1.96	0.46
2:A:313:SER:OG	2:A:316:ASN:ND2	2.43	0.46
3:D:156:GLY:HA3	3:D:332:LEU:HD13	1.98	0.46
7:K:137:GLU:OE2	7:K:141:ARG:NH2	2.41	0.46
3:E:96:ARG:NH2	3:E:109:GLY:O	2.48	0.46
3:F:189:VAL:HG22	3:F:235:VAL:HG12	1.97	0.46
2:B:152:ALA:HA	2:B:428:LEU:HD22	1.98	0.46
3:F:299:ILE:HG21	3:F:309:SER:HB2	1.98	0.46
4:G:130:ARG:NH1	6:I:47:GLU:O	2.49	0.46
5:H:38:VAL:HG11	5:H:82:VAL:HG21	1.97	0.46
1:4:30:GLY:O	1:5:31:SER:OG	2.24	0.46
3:F:87:ILE:HD13	3:F:238:THR:HG23	1.99	0.46
15:S:78:ILE:O	15:S:81:GLU:HB3	2.16	0.45
2:C:446:TYR:OH	2:C:494:ASP:OD1	2.33	0.45
3:E:221:VAL:HG12	3:E:235:VAL:HG13	1.97	0.45
2:B:175:LYS:HG3	2:B:352:LEU:HD23	1.99	0.45
2:C:105:GLY:HA2	2:C:226:MET:HG3	1.98	0.45
6:I:13:ARG:NH1	6:I:27:GLU:OE2	2.45	0.45
7:K:137:GLU:O	7:K:141:ARG:HG2	2.16	0.45
8:L:7:ILE:HD11	11:O:176:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:19:ALA:HB2	1:6:17:GLY:HA2	1.99	0.45
15:S:77:LEU:HD23	15:S:77:LEU:HA	1.61	0.45
3:F:223:GLY:HA3	3:F:235:VAL:HG21	1.99	0.45
2:B:34:ILE:HG12	2:B:82:ILE:HB	1.98	0.45
1:5:64:CYS:SG	1:5:65:LEU:N	2.89	0.45
2:C:397:TYR:CG	2:C:421:GLY:HA3	2.52	0.44
3:E:309:SER:OG	3:E:311:GLN:NE2	2.49	0.44
3:D:35:ILE:HG22	3:D:36:LEU:HG	1.98	0.44
10:N:117:LYS:HG2	10:N:118:GLU:HG3	1.98	0.44
1:5:33:ILE:HG21	1:6:32:LEU:HA	1.98	0.44
3:F:28:PHE:HB2	3:F:32:LEU:HD23	1.98	0.44
2:A:472:ILE:HA	2:A:476:HIS:HB2	2.00	0.44
2:A:491:PRO:HA	2:A:494:ASP:HB3	1.98	0.44
2:B:139:ARG:NH1	3:E:193:THR:OG1	2.51	0.44
3:D:52:VAL:HA	3:D:63:THR:HG22	1.98	0.44
12:P:10:UNK:HA	13:Q:25:THR:HG21	1.99	0.44
1:8:71:LEU:HD23	1:8:75:PHE:HD2	1.83	0.44
3:D:262:PHE:HA	3:D:265:THR:HG22	1.97	0.44
1:6:16:VAL:HG13	1:7:16:VAL:HB	1.99	0.44
2:B:74:VAL:HB	2:B:241:PRO:HG3	2.00	0.44
3:F:155:ILE:HD13	3:F:310:VAL:HG22	1.99	0.44
2:C:38:ILE:HD12	2:C:284:LEU:HB2	1.99	0.44
7:K:166:ARG:NH2	9:M:62:THR:OG1	2.50	0.44
10:N:59:MET:HG3	10:N:214:THR:HG23	2.00	0.43
9:M:20:VAL:HA	9:M:21:PRO:HD3	1.85	0.43
11:O:81:ASP:OD1	11:O:81:ASP:N	2.51	0.43
2:A:289:PRO:HB2	2:A:293:ALA:HA	2.01	0.43
3:D:244:GLU:HG2	3:D:247:ARG:HH21	1.83	0.43
10:N:48:LEU:HD21	10:N:75:LEU:HD21	1.99	0.43
10:N:48:LEU:HD12	13:Q:30:LEU:HD23	2.00	0.43
2:B:426:GLU:HG3	2:B:458:PRO:HB3	1.98	0.43
3:D:96:ARG:NH2	3:D:109:GLY:O	2.41	0.43
3:F:141:LYS:H	3:F:419:GLN:HE22	1.66	0.43
3:F:322:ASP:HB3	3:F:325:PRO:HD2	2.01	0.43
4:G:186:ILE:HD12	4:G:186:ILE:HA	1.92	0.43
5:H:126:MET:SD	5:H:126:MET:N	2.79	0.43
2:A:48:GLN:HG2	3:D:73:VAL:HG12	2.01	0.43
2:B:99:VAL:O	2:B:123:SER:OG	2.36	0.43
2:C:23:GLU:OE2	2:C:30:ARG:NE	2.49	0.43
2:A:455:LYS:HD2	2:A:505:LEU:HD13	2.01	0.43
1:5:4:SER:OG	1:6:3:ASP:OD1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:96:ASP:O	2:A:126:ARG:NH2	2.51	0.42
2:A:133:ALA:HB3	3:D:226:ASN:HB2	2.01	0.42
2:B:267:ILE:HG13	2:B:324:LEU:HB2	2.01	0.42
3:E:463:VAL:HG21	3:E:469:VAL:HG22	2.01	0.42
4:G:109:ARG:HD3	4:G:123:VAL:HG21	2.00	0.42
1:5:65:LEU:HD11	1:6:67:MET:HG3	2.02	0.42
5:H:37:ASP:HB2	5:H:64:THR:HB	2.01	0.42
1:7:67:MET:HA	1:7:70:LEU:HB3	2.02	0.42
2:A:397:TYR:CG	2:A:421:GLY:HA3	2.54	0.42
2:B:210:ARG:NH1	3:D:124:PRO:O	2.52	0.42
3:E:52:VAL:HA	3:E:63:THR:HG22	2.00	0.42
3:F:56:LEU:HD11	3:F:62:ARG:HB2	2.01	0.42
7:K:25:PHE:CD1	7:K:34:PRO:HG3	2.54	0.42
11:O:143:LEU:HD13	11:O:147:GLN:HB3	2.01	0.42
9:M:24:GLN:HG2	9:M:25:LYS:HE2	2.02	0.42
9:M:137:PHE:HB3	9:M:143:LYS:HG2	2.00	0.42
2:C:114:PRO:HG2	2:C:120:PRO:HA	2.02	0.42
3:D:33:PRO:HA	3:D:34:PRO:HD3	1.94	0.42
1:1:62:LEU:HB3	10:N:168:LEU:HD21	2.01	0.42
1:7:9:ILE:HG13	1:8:6:ALA:HB1	2.01	0.42
2:A:270:ASP:OD1	2:A:272:SER:OG	2.30	0.42
3:F:87:ILE:HD11	3:F:241:THR:HB	2.02	0.42
4:G:54:LYS:HD3	4:G:54:LYS:HA	1.93	0.42
6:I:20:PHE:O	6:I:24:VAL:HG23	2.20	0.42
11:O:57:LYS:HG2	11:O:97:LYS:HA	2.01	0.42
1:1:69:PHE:HD1	1:1:69:PHE:HA	1.75	0.41
2:C:148:THR:HG23	2:C:182:ALA:HB2	2.01	0.41
2:C:273:LYS:NZ	2:C:328:GLU:OE1	2.47	0.41
3:D:51:GLU:OE2	3:D:120:HIS:NE2	2.38	0.41
3:F:210:SER:OG	3:F:213:ASP:OD1	2.27	0.41
1:1:16:VAL:HB	1:8:16:VAL:HG13	2.03	0.41
1:4:25:ILE:HD11	1:4:58:GLU:HB2	2.01	0.41
2:B:311:LYS:HA	2:B:320:SER:HA	2.02	0.41
3:E:140:ILE:HA	3:E:419:GLN:HE22	1.84	0.41
3:E:212:LYS:HE2	3:E:212:LYS:HB3	1.94	0.41
3:F:100:VAL:HB	3:F:235:VAL:HG23	2.02	0.41
11:O:35:VAL:HG23	11:O:83:THR:HB	2.02	0.41
1:6:15:THR:HG22	1:6:65:LEU:HD12	2.02	0.41
3:D:184:SER:O	3:D:218:VAL:HA	2.20	0.41
3:E:302:THR:HG23	3:E:304:LYS:H	1.85	0.41
10:N:70:VAL:HG12	10:N:210:MET:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:45:GLN:OE1	1:8:36:TYR:OH	2.33	0.41
2:B:44:LEU:HB3	2:B:47:ILE:HB	2.02	0.41
3:D:324:ALA:O	3:D:328:THR:OG1	2.36	0.41
7:K:9:PRO:HG3	14:R:73:GLY:HA2	2.01	0.41
2:A:294:TYR:CZ	2:A:338:ILE:HD11	2.56	0.41
3:D:419:GLN:NE2	3:D:433:LYS:O	2.48	0.41
3:E:261:ILE:HD13	3:E:261:ILE:HA	1.86	0.41
1:1:46:LEU:HD21	1:8:37:ALA:HB2	2.03	0.41
3:F:25:ASP:OD1	3:F:25:ASP:N	2.53	0.41
7:K:78:ILE:HD12	19:R:201:CDL:H511	2.02	0.41
10:N:83:ILE:H	10:N:83:ILE:HG13	1.74	0.41
3:E:244:GLU:HG2	3:E:247:ARG:HH21	1.86	0.41
1:4:19:ALA:HB2	1:5:17:GLY:HA2	2.03	0.41
1:6:33:ILE:HG23	1:7:46:LEU:HD22	2.03	0.41
1:7:62:LEU:O	1:7:66:MET:N	2.51	0.41
2:C:129:VAL:HB	2:C:248:TYR:HB3	2.02	0.41
3:D:16:ILE:HA	3:D:26:VAL:HG12	2.02	0.41
7:K:6:PRO:HG2	14:R:70:PRO:HG3	2.02	0.41
7:K:68:THR:HA	19:R:201:CDL:H312	2.03	0.41
9:M:142:GLU:H	9:M:142:GLU:HG3	1.56	0.41
11:O:159:ILE:O	11:O:161:GLY:N	2.54	0.41
3:E:158:PHE:HB2	3:E:337:VAL:HA	2.02	0.41
10:N:17:SER:HB3	10:N:19:TRP:CD1	2.51	0.41
1:7:29:PHE:O	1:7:33:ILE:HG12	2.21	0.40
2:A:267:ILE:HG12	2:A:324:LEU:HB2	2.03	0.40
3:E:84:PRO:HB2	3:E:118:ALA:HB1	2.04	0.40
3:E:299:ILE:HD13	3:E:309:SER:HB2	2.01	0.40
3:F:100:VAL:HG13	3:F:101:ILE:HG23	2.03	0.40
3:F:259:ASP:HA	3:F:260:ASN:HA	1.66	0.40
15:S:67:VAL:CG1	15:S:72:ALA:HB2	2.52	0.40
1:8:7:LYS:HD2	1:8:71:LEU:HB3	2.02	0.40
1:8:21:SER:HB3	1:8:61:GLY:HA3	2.04	0.40
3:D:165:LYS:HB2	3:D:165:LYS:HE3	1.84	0.40
3:F:188:GLY:O	3:F:223:GLY:N	2.54	0.40
5:H:126:MET:HB2	6:I:16:ARG:HD3	2.04	0.40
11:O:5:VAL:HB	11:O:8:PRO:HG3	2.02	0.40
1:7:70:LEU:HD12	1:7:74:ALA:HB3	2.04	0.40
2:B:26:GLU:HA	2:B:45:LYS:HB2	2.04	0.40
3:D:97:ILE:HG12	3:D:220:LEU:HD13	2.04	0.40
3:E:16:ILE:HD12	3:E:76:GLN:HB3	2.04	0.40
3:F:15:GLN:HB3	3:F:75:GLY:HA2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:45:LYS:HZ1	13:Q:32:GLN:H	1.69	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	1	73/128 (57%)	72 (99%)	1 (1%)	0	100	100
1	2	73/128 (57%)	72 (99%)	1 (1%)	0	100	100
1	3	73/128 (57%)	73 (100%)	0	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
1	6	73/128 (57%)	73 (100%)	0	0	100	100
1	7	73/128 (57%)	73 (100%)	0	0	100	100
1	8	73/128 (57%)	72 (99%)	1 (1%)	0	100	100
2	A	496/551 (90%)	486 (98%)	10 (2%)	0	100	100
2	B	501/551 (91%)	494 (99%)	7 (1%)	0	100	100
2	C	499/551 (91%)	493 (99%)	6 (1%)	0	100	100
3	D	463/524 (88%)	444 (96%)	19 (4%)	0	100	100
3	E	451/524 (86%)	435 (96%)	16 (4%)	0	100	100
3	F	467/524 (89%)	448 (96%)	19 (4%)	0	100	100
4	G	223/290 (77%)	221 (99%)	2 (1%)	0	100	100
5	H	132/169 (78%)	125 (95%)	7 (5%)	0	100	100
6	I	35/66 (53%)	30 (86%)	5 (14%)	0	100	100
7	K	206/265 (78%)	200 (97%)	6 (3%)	0	100	100
8	L	73/99 (74%)	72 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	M	159/219 (73%)	142 (89%)	17 (11%)	0	100	100
10	N	214/219 (98%)	206 (96%)	8 (4%)	0	100	100
11	O	189/207 (91%)	174 (92%)	15 (8%)	0	100	100
13	Q	44/53 (83%)	41 (93%)	3 (7%)	0	100	100
14	R	103/119 (87%)	98 (95%)	5 (5%)	0	100	100
15	S	74/103 (72%)	71 (96%)	3 (4%)	0	100	100
16	T	74/84 (88%)	74 (100%)	0	0	100	100
All	All	4987/6142 (81%)	4831 (97%)	156 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	51/93 (55%)	49 (96%)	2 (4%)	27	47
1	2	51/93 (55%)	51 (100%)	0	100	100
1	3	51/93 (55%)	47 (92%)	4 (8%)	10	19
1	4	51/93 (55%)	51 (100%)	0	100	100
1	5	51/93 (55%)	48 (94%)	3 (6%)	16	29
1	6	51/93 (55%)	50 (98%)	1 (2%)	50	69
1	7	51/93 (55%)	48 (94%)	3 (6%)	16	29
1	8	51/93 (55%)	47 (92%)	4 (8%)	10	19
2	A	407/446 (91%)	404 (99%)	3 (1%)	81	89
2	B	411/446 (92%)	403 (98%)	8 (2%)	52	71
2	C	410/446 (92%)	402 (98%)	8 (2%)	50	69
3	D	379/418 (91%)	372 (98%)	7 (2%)	54	72
3	E	371/418 (89%)	365 (98%)	6 (2%)	58	75
3	F	382/418 (91%)	377 (99%)	5 (1%)	65	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	G	198/244 (81%)	198 (100%)	0	100	100
5	H	106/135 (78%)	103 (97%)	3 (3%)	38	59
6	I	31/55 (56%)	30 (97%)	1 (3%)	34	55
7	K	178/225 (79%)	176 (99%)	2 (1%)	70	83
8	L	65/87 (75%)	63 (97%)	2 (3%)	35	56
9	M	142/197 (72%)	133 (94%)	9 (6%)	15	27
10	N	192/194 (99%)	191 (100%)	1 (0%)	86	92
11	O	158/171 (92%)	150 (95%)	8 (5%)	20	36
13	Q	42/49 (86%)	41 (98%)	1 (2%)	44	64
14	R	83/97 (86%)	82 (99%)	1 (1%)	67	82
15	S	63/85 (74%)	62 (98%)	1 (2%)	58	75
16	T	61/69 (88%)	60 (98%)	1 (2%)	58	75
All	All	4087/4944 (83%)	4003 (98%)	84 (2%)	49	69

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	18	VAL
1	1	69	PHE
1	3	3	ASP
1	3	18	VAL
1	3	39	ASN
1	3	44	GLN
1	5	18	VAL
1	5	31	SER
1	5	64	CYS
1	6	31	SER
1	7	15	THR
1	7	31	SER
1	7	54	PHE
1	8	2	ILE
1	8	15	THR
1	8	18	VAL
1	8	63	PHE
2	A	69	ASP
2	A	91	THR
2	A	244	TYR
2	B	95	VAL

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Mol	Chain	Res	Type
2	B	146	MET
2	B	164	ARG
2	B	197	LYS
2	B	223	THR
2	B	244	TYR
2	B	322	THR
2	B	481	ASP
2	C	91	THR
2	C	146	MET
2	C	154	ASP
2	C	157	VAL
2	C	164	ARG
2	C	298	VAL
2	C	301	LEU
2	C	455	LYS
3	D	37	ASN
3	D	87	ILE
3	D	138	THR
3	D	220	LEU
3	D	302	THR
3	D	328	THR
3	D	333	ASP
3	E	81	THR
3	E	198	ASP
3	E	261	ILE
3	E	301	THR
3	E	333	ASP
3	E	463	VAL
3	F	135	ILE
3	F	154	LYS
3	F	198	ASP
3	F	235	VAL
3	F	301	THR
5	H	41	PHE
5	H	91	GLN
5	H	126	MET
6	I	16	ARG
7	K	29	THR
7	K	144	LEU
8	L	67	GLU
8	L	68	ASP
9	M	5	ARG

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Mol	Chain	Res	Type
9	M	6	ILE
9	M	86	VAL
9	M	119	LEU
9	M	131	MET
9	M	142	GLU
9	M	144	VAL
9	M	153	ASN
9	M	157	LYS
10	N	142	MET
11	O	4	LEU
11	O	5	VAL
11	O	37	LYS
11	O	102	VAL
11	O	142	PHE
11	O	155	THR
11	O	159	ILE
11	O	167	ILE
13	Q	36	VAL
14	R	35	LEU
15	S	97	VAL
16	T	46	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	6	44	GLN
3	D	27	GLN
3	D	54	GLN
3	D	77	ASN
3	D	132	GLN
3	D	133	GLN
3	D	226	ASN
3	D	249	GLN
3	D	252	GLN
3	D	331	HIS
3	D	388	GLN
3	E	31	GLN
3	E	54	GLN
3	E	132	GLN
3	E	311	GLN
3	E	370	HIS
3	E	419	GLN

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Mol	Chain	Res	Type
3	F	54	GLN
3	F	175	ASN
3	F	311	GLN
3	F	382	GLN
3	F	414	GLN
3	F	419	GLN
5	H	67	GLN
5	H	85	ASN
5	H	91	GLN
7	K	121	GLN
7	K	135	GLN
7	K	148	ASN
7	K	170	GLN
7	K	172	ASN
9	M	48	GLN
10	N	52	ASN
10	N	67	ASN
10	N	147	ASN
16	T	40	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](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
17	ATP	B	601	18	28,33,33	0.80	0	34,52,52	0.75	1 (2%)
17	ATP	D	601	18	28,33,33	0.77	0	34,52,52	0.79	1 (2%)
17	ATP	C	601	18	28,33,33	0.79	0	34,52,52	0.81	1 (2%)
19	CDL	S	201	-	74,74,99	0.37	0	80,86,111	0.26	0
17	ATP	A	601	18	28,33,33	0.78	0	34,52,52	0.85	2 (5%)
19	CDL	R	201	-	81,81,99	0.35	0	87,93,111	0.26	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
17	ATP	B	601	18	-	4/18/38/38	0/3/3/3
17	ATP	D	601	18	-	5/18/38/38	0/3/3/3
17	ATP	C	601	18	-	0/18/38/38	0/3/3/3
19	CDL	S	201	-	-	37/85/85/110	-
17	ATP	A	601	18	-	0/18/38/38	0/3/3/3
19	CDL	R	201	-	-	42/92/92/110	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	601	ATP	C5-C6-N6	2.27	123.76	120.31
17	A	601	ATP	C5-C6-N6	2.26	123.76	120.31
17	D	601	ATP	C5-C6-N6	2.22	123.70	120.31
17	C	601	ATP	C5-C6-N6	2.22	123.70	120.31
17	A	601	ATP	O3G-PG-O2G	2.07	115.55	107.80

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	B	601	ATP	PB-O3B-PG-O2G
19	R	201	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
19	R	201	CDL	C11-CA5-OA6-CA4
19	R	201	CDL	CB2-OB2-PB2-OB3
19	R	201	CDL	CB2-OB2-PB2-OB5
19	R	201	CDL	CB3-OB5-PB2-OB3
19	R	201	CDL	CB3-OB5-PB2-OB4
19	S	201	CDL	O1-C1-CB2-OB2
19	S	201	CDL	CA2-OA2-PA1-OA3
19	S	201	CDL	CA2-OA2-PA1-OA4
19	S	201	CDL	CA2-OA2-PA1-OA5
19	S	201	CDL	CB3-OB5-PB2-OB2
19	S	201	CDL	CB3-OB5-PB2-OB3
19	S	201	CDL	C51-CB5-OB6-CB4
19	S	201	CDL	OB9-CB7-OB8-CB6
19	S	201	CDL	OA9-CA7-OA8-CA6
19	S	201	CDL	C31-CA7-OA8-CA6
19	R	201	CDL	OA7-CA5-OA6-CA4
19	S	201	CDL	OB7-CB5-OB6-CB4
19	S	201	CDL	C71-CB7-OB8-CB6
19	R	201	CDL	O1-C1-CB2-OB2
19	S	201	CDL	O1-C1-CA2-OA2
19	S	201	CDL	CB2-C1-CA2-OA2
19	R	201	CDL	C31-CA7-OA8-CA6
19	S	201	CDL	CA7-C31-C32-C33
19	R	201	CDL	OA9-CA7-OA8-CA6
19	R	201	CDL	CB7-C71-C72-C73
19	S	201	CDL	C11-CA5-OA6-CA4
19	S	201	CDL	OA7-CA5-OA6-CA4
19	S	201	CDL	CA2-C1-CB2-OB2
19	R	201	CDL	CA7-C31-C32-C33
19	R	201	CDL	C51-C52-C53-C54
19	S	201	CDL	C13-C14-C15-C16
19	R	201	CDL	C32-C33-C34-C35
19	R	201	CDL	CA5-C11-C12-C13
19	S	201	CDL	CA5-C11-C12-C13
19	R	201	CDL	C54-C55-C56-C57
19	R	201	CDL	O1-C1-CA2-OA2
19	S	201	CDL	C71-C72-C73-C74
19	S	201	CDL	C51-C52-C53-C54
19	R	201	CDL	C12-C13-C14-C15
19	S	201	CDL	C77-C78-C79-C80
17	B	601	ATP	PA-O3A-PB-O1B
17	D	601	ATP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
19	R	201	CDL	C61-C62-C63-C64
19	R	201	CDL	C56-C57-C58-C59
19	S	201	CDL	C1-CA2-OA2-PA1
19	R	201	CDL	C71-C72-C73-C74
19	R	201	CDL	C15-C16-C17-C18
17	D	601	ATP	C3'-C4'-C5'-O5'
19	R	201	CDL	CB2-C1-CA2-OA2
19	R	201	CDL	C36-C37-C38-C39
19	R	201	CDL	C11-C12-C13-C14
19	R	201	CDL	C1-CA2-OA2-PA1
19	R	201	CDL	OA6-CA4-CA6-OA8
19	R	201	CDL	CA3-CA4-CA6-OA8
19	S	201	CDL	C19-C20-C21-C22
17	D	601	ATP	O4'-C4'-C5'-O5'
17	D	601	ATP	C5'-O5'-PA-O1A
19	R	201	CDL	CA2-OA2-PA1-OA3
19	R	201	CDL	CA3-OA5-PA1-OA2
19	R	201	CDL	CA3-OA5-PA1-OA3
19	R	201	CDL	CA3-OA5-PA1-OA4
19	R	201	CDL	CB2-OB2-PB2-OB4
19	R	201	CDL	CB3-OB5-PB2-OB2
19	S	201	CDL	CA3-OA5-PA1-OA3
19	S	201	CDL	CB3-OB5-PB2-OB4
19	R	201	CDL	C17-C18-C19-C20
19	S	201	CDL	CA3-CA4-OA6-CA5
19	R	201	CDL	C76-C77-C78-C79
19	S	201	CDL	C72-C73-C74-C75
19	S	201	CDL	C32-C33-C34-C35
19	R	201	CDL	C77-C78-C79-C80
19	S	201	CDL	C53-C54-C55-C56
19	S	201	CDL	C1-CB2-OB2-PB2
19	S	201	CDL	C33-C34-C35-C36
17	D	601	ATP	PA-O3A-PB-O2B
19	S	201	CDL	C35-C36-C37-C38
19	S	201	CDL	CA6-CA4-OA6-CA5
17	B	601	ATP	PA-O3A-PB-O2B
19	R	201	CDL	C12-C11-CA5-OA6
19	R	201	CDL	C78-C79-C80-C81
19	R	201	CDL	C37-C38-C39-C40
19	S	201	CDL	CA3-CA4-CA6-OA8
17	B	601	ATP	PB-O3B-PG-O1G
19	R	201	CDL	C64-C65-C66-C67

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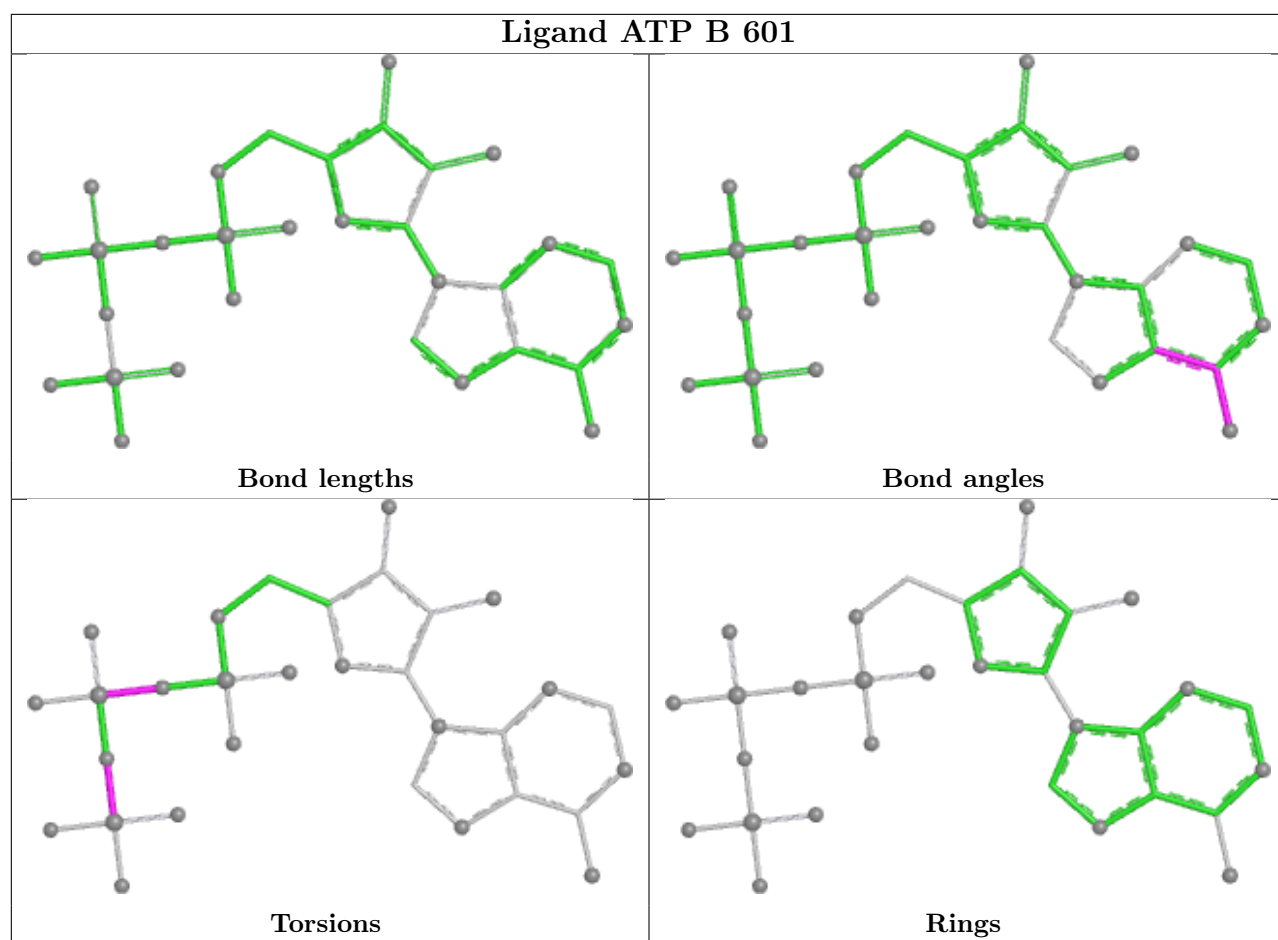
Mol	Chain	Res	Type	Atoms
19	R	201	CDL	C12-C11-CA5-OA7
19	S	201	CDL	C56-C57-C58-C59

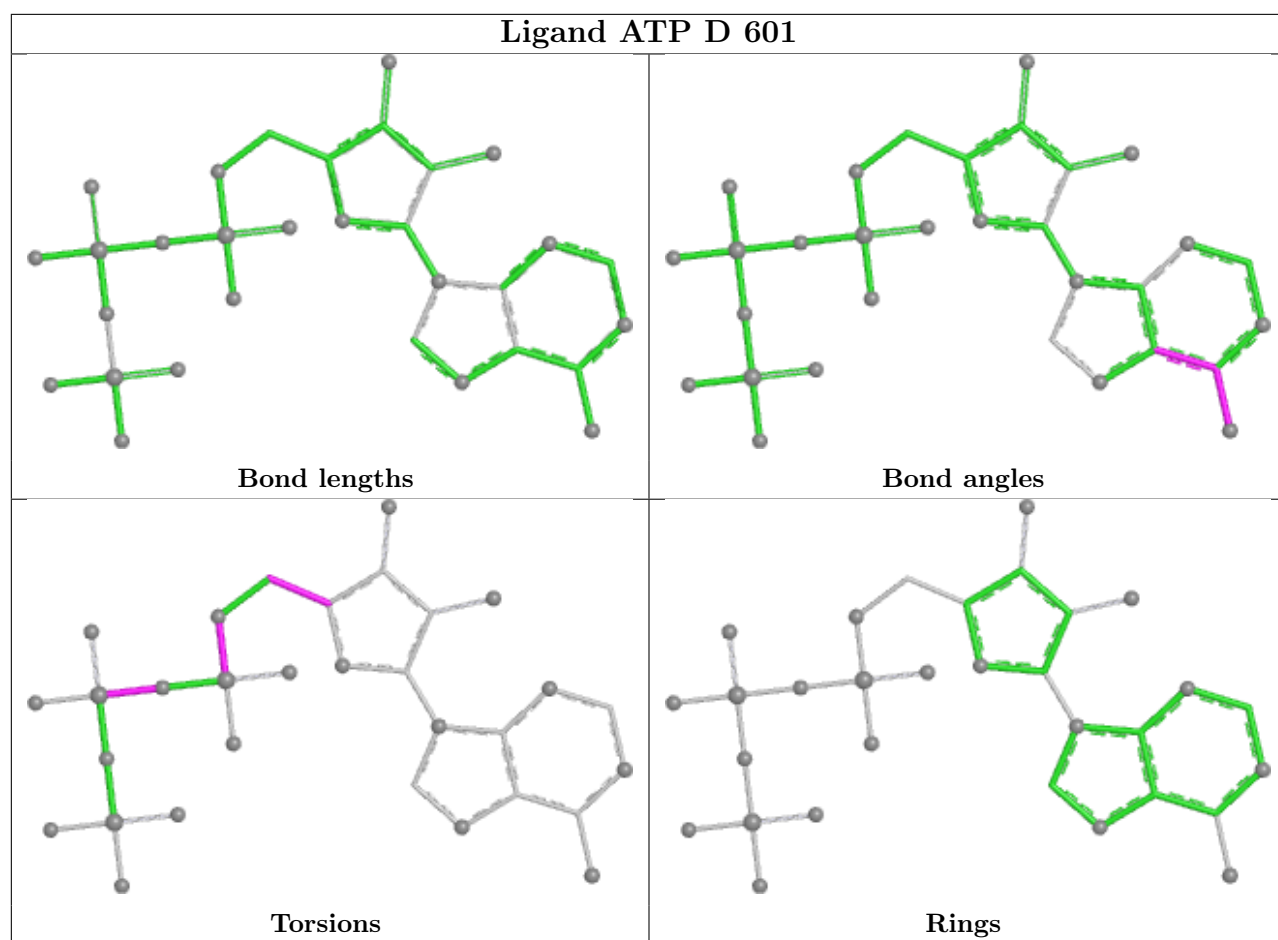
There are no ring outliers.

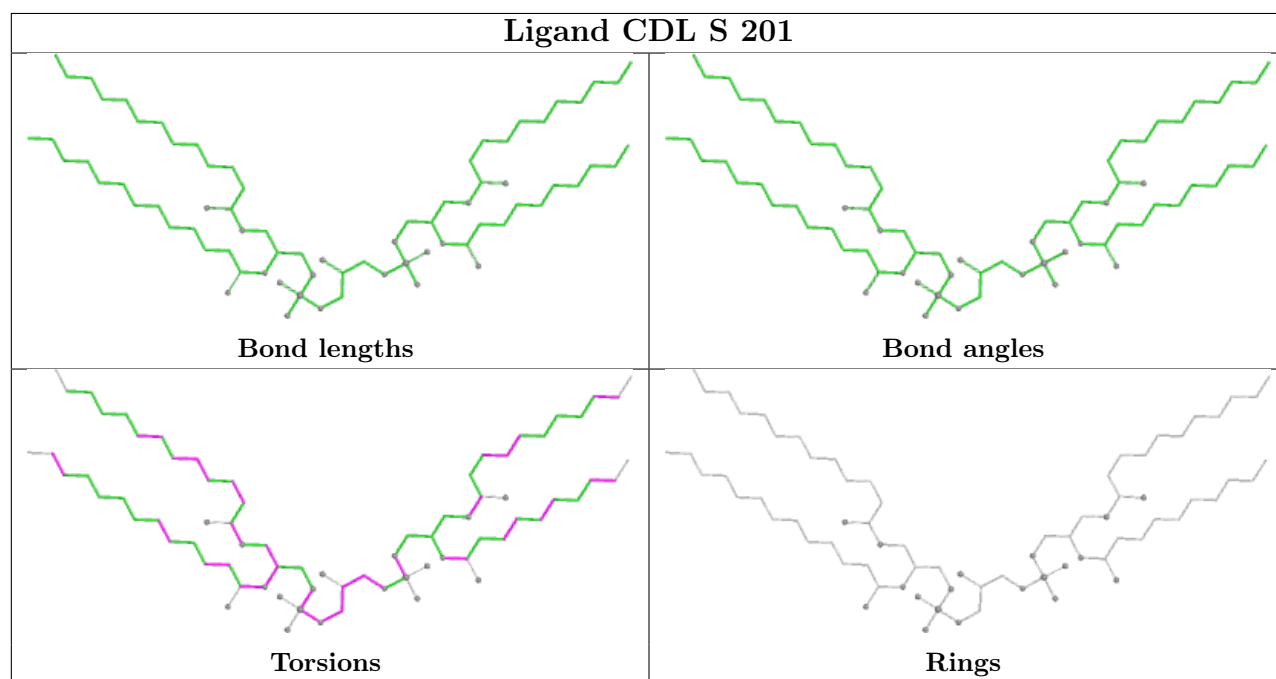
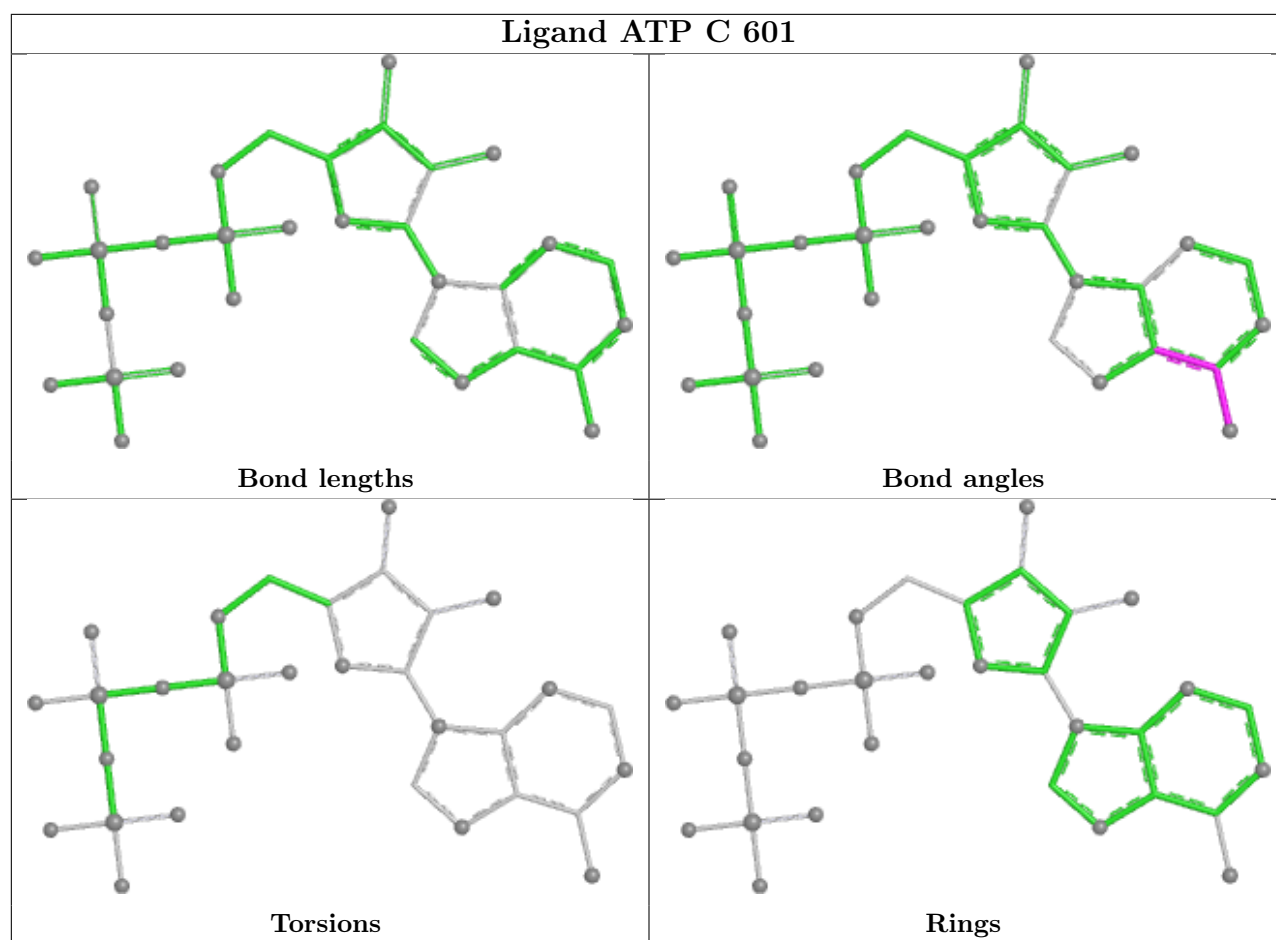
2 monomers are involved in 4 short contacts:

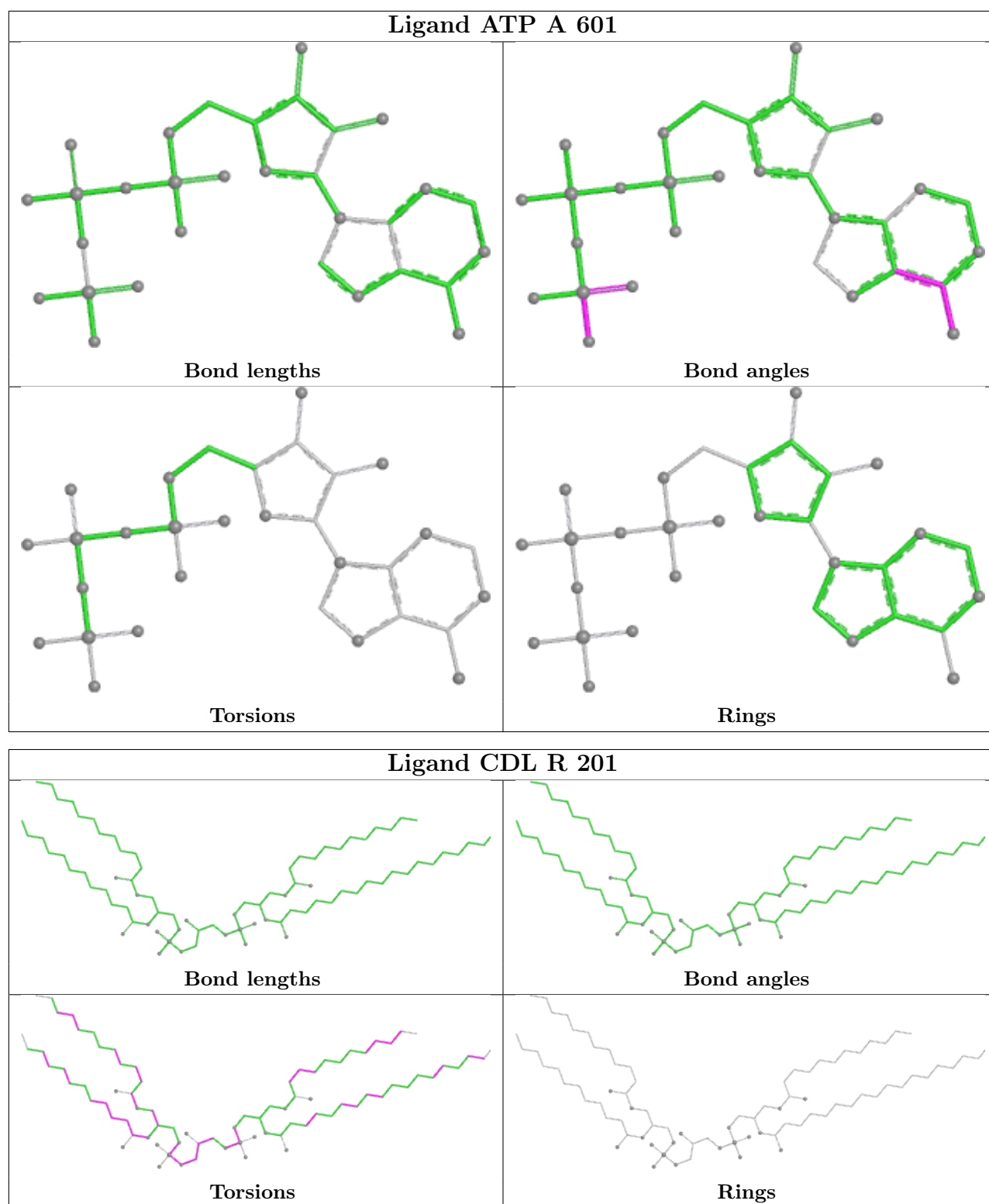
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	C	601	ATP	1	0
19	R	201	CDL	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

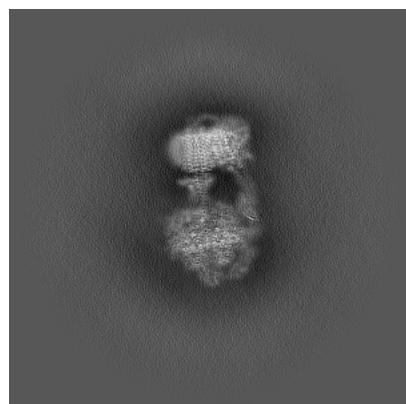
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44142. These allow visual inspection of the internal detail of the map and identification of artifacts.

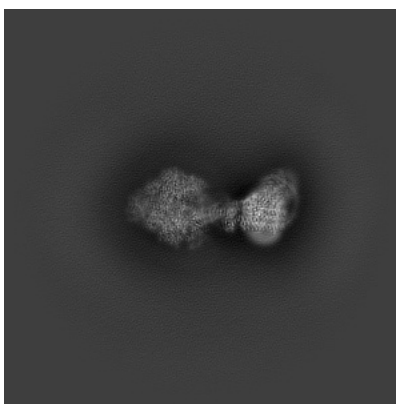
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

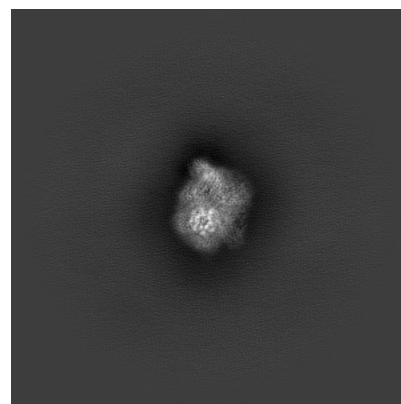
6.1.1 Primary map



X

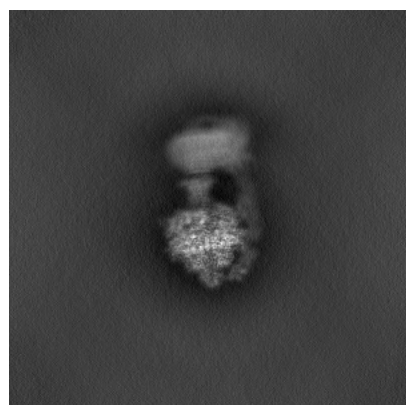


Y

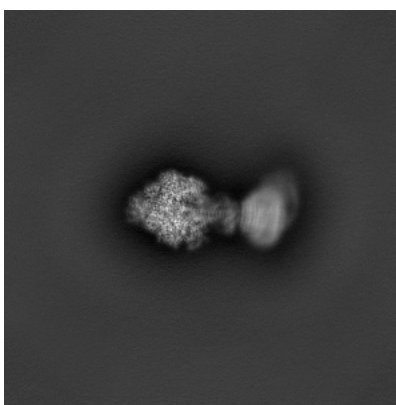


Z

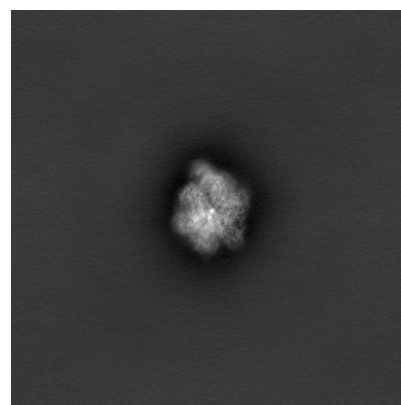
6.1.2 Raw map



X



Y

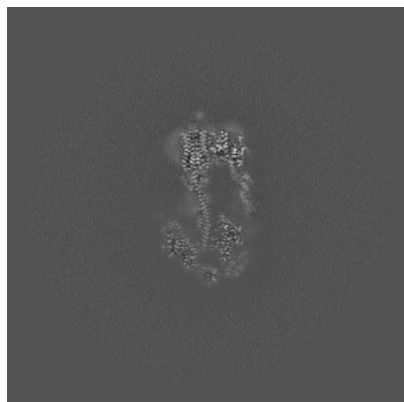


Z

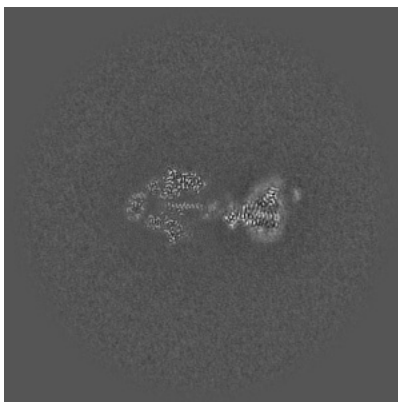
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

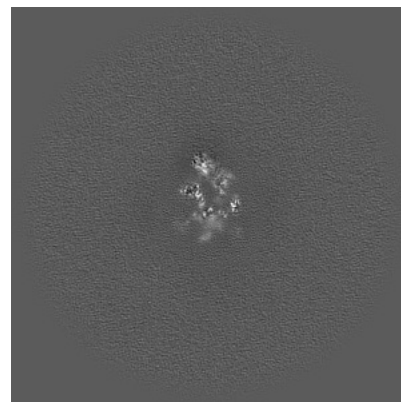
6.2.1 Primary map



X Index: 256



Y Index: 256

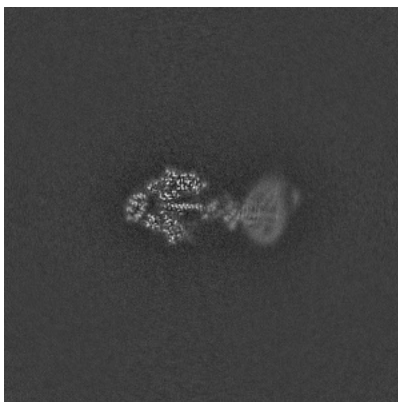


Z Index: 256

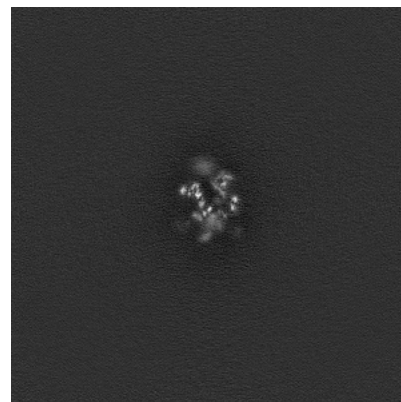
6.2.2 Raw map



X Index: 256



Y Index: 256

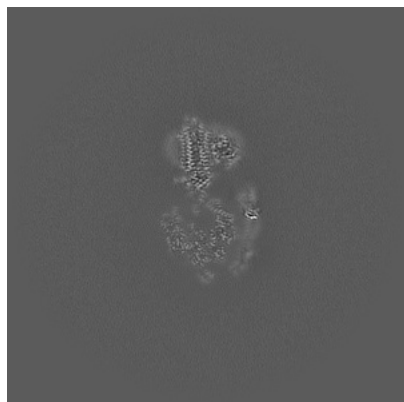


Z Index: 256

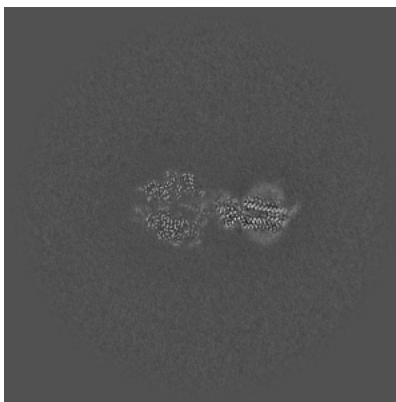
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

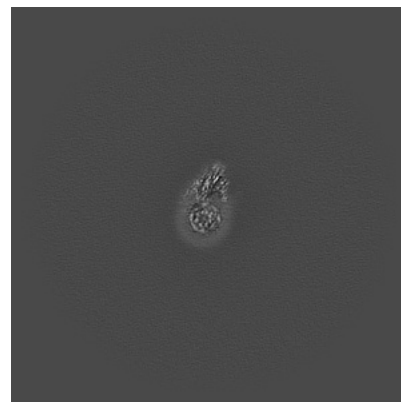
6.3.1 Primary map



X Index: 243

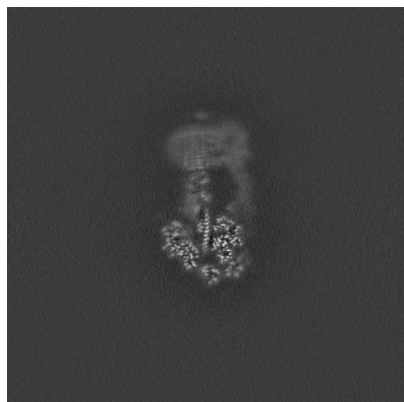


Y Index: 244

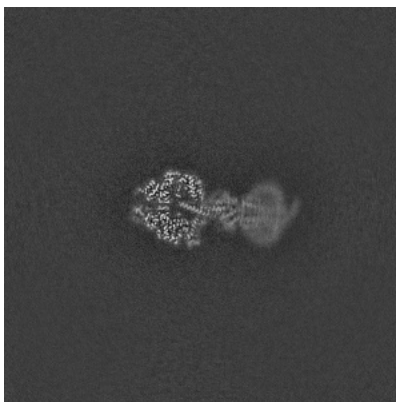


Z Index: 322

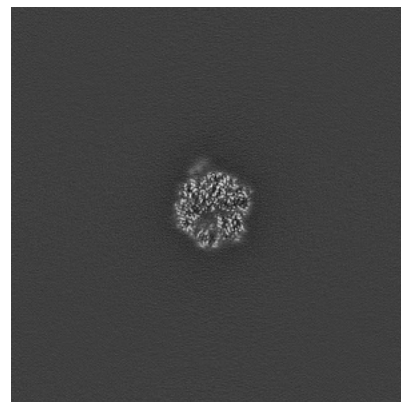
6.3.2 Raw map



X Index: 258



Y Index: 246

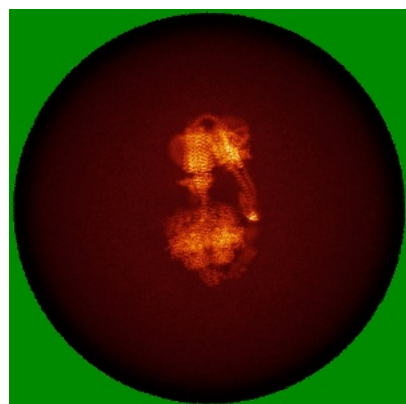


Z Index: 214

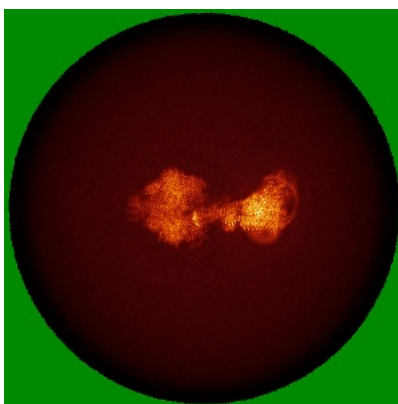
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

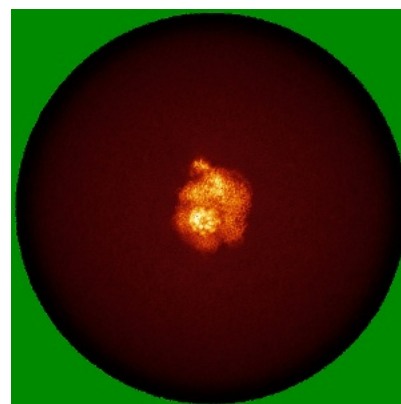
6.4.1 Primary map



X

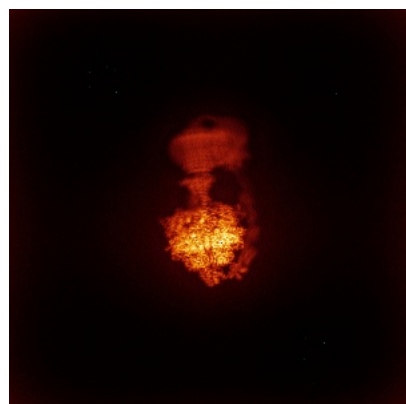


Y

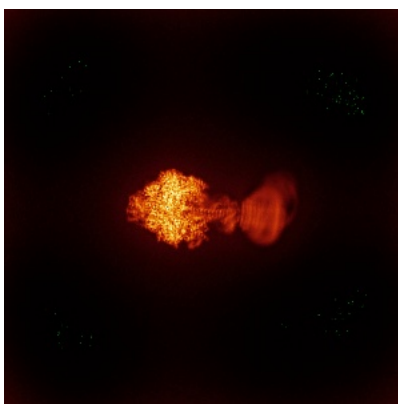


Z

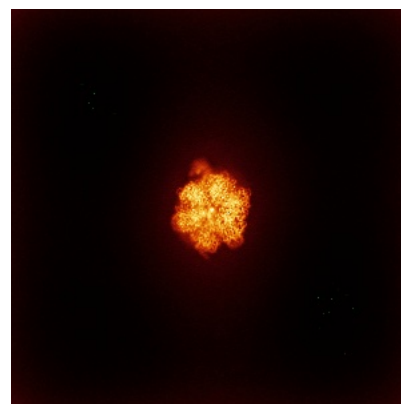
6.4.2 Raw map



X



Y

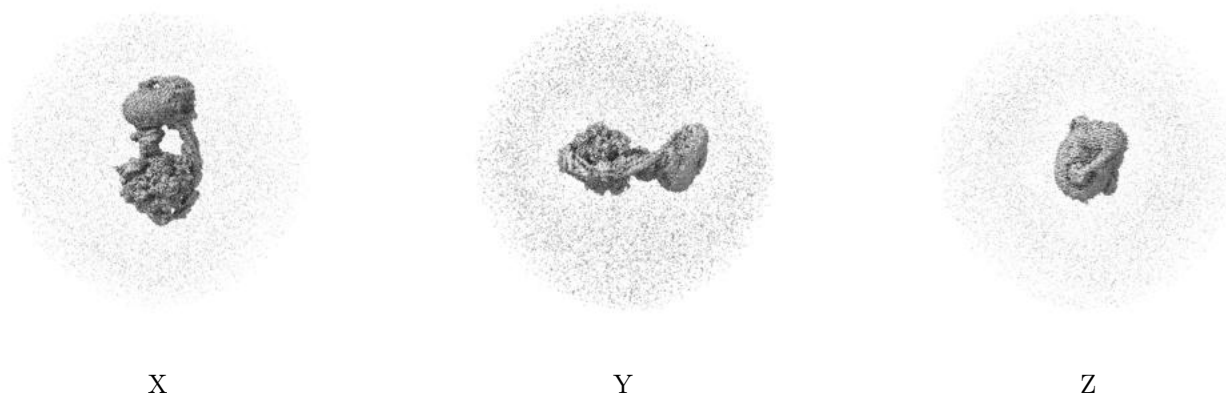


Z

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.

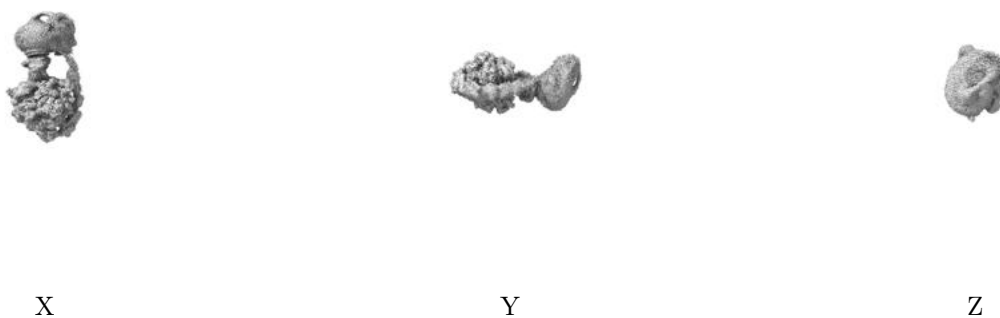
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.55. 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.

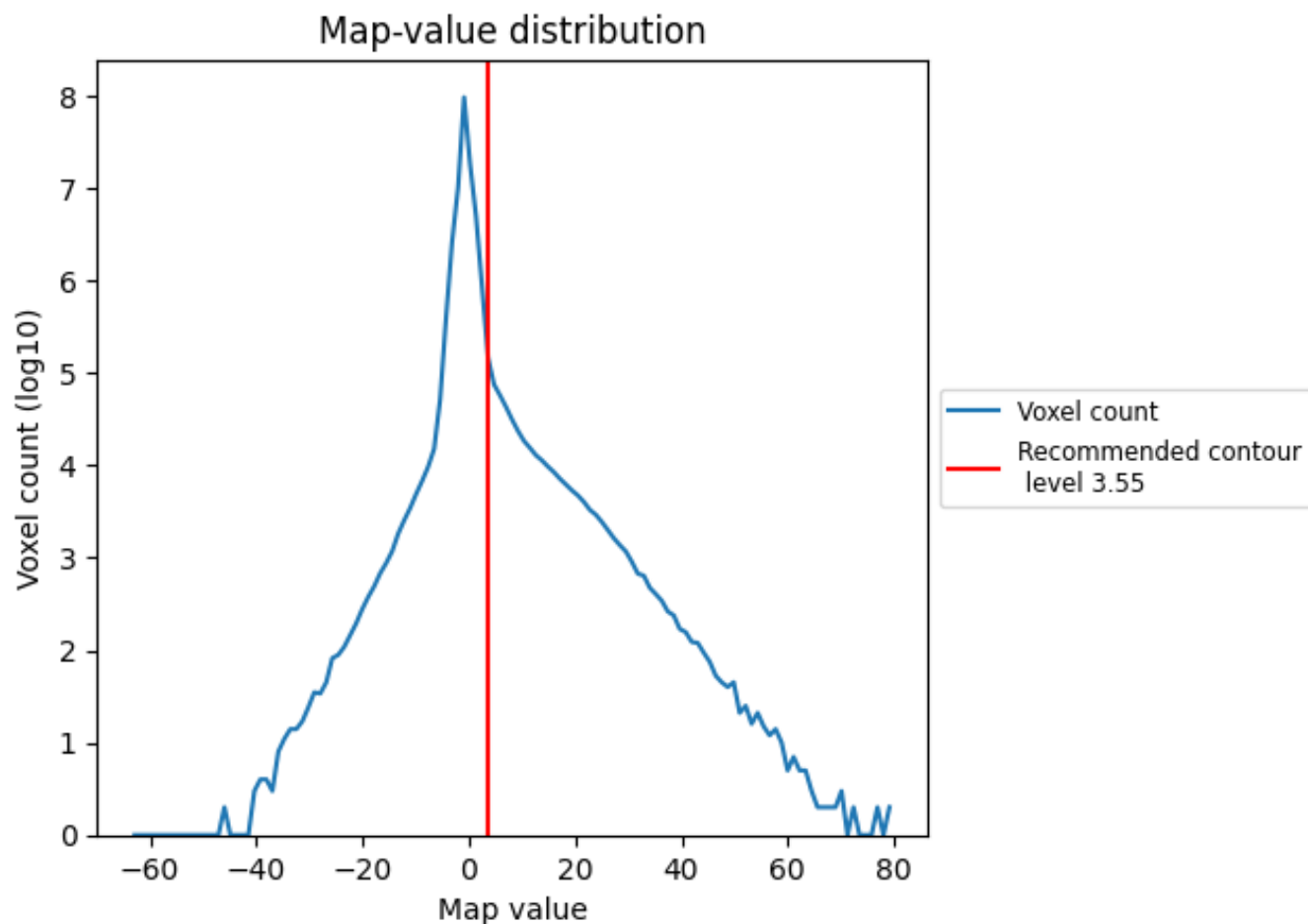
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

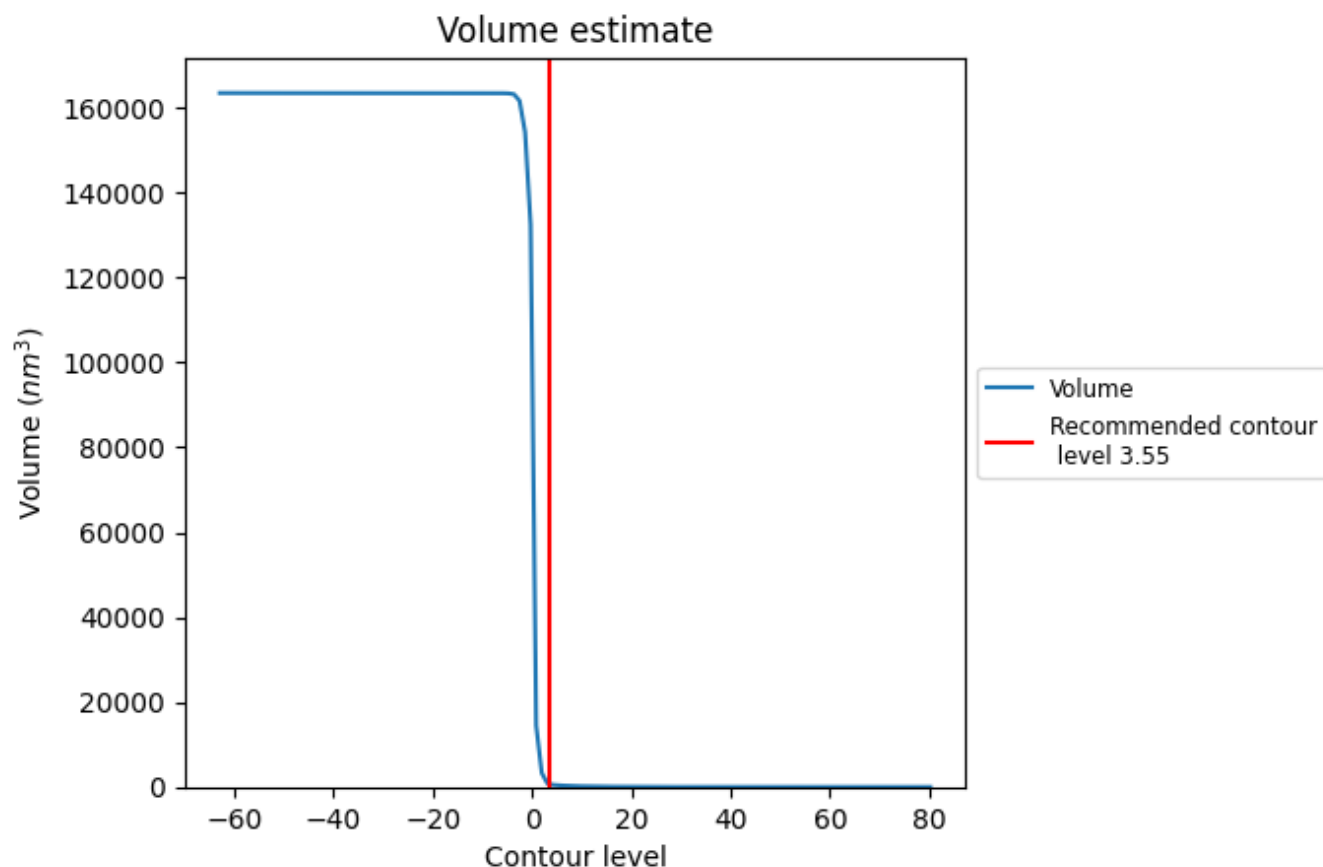
This section contains the results of statistical analysis of the map.

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.

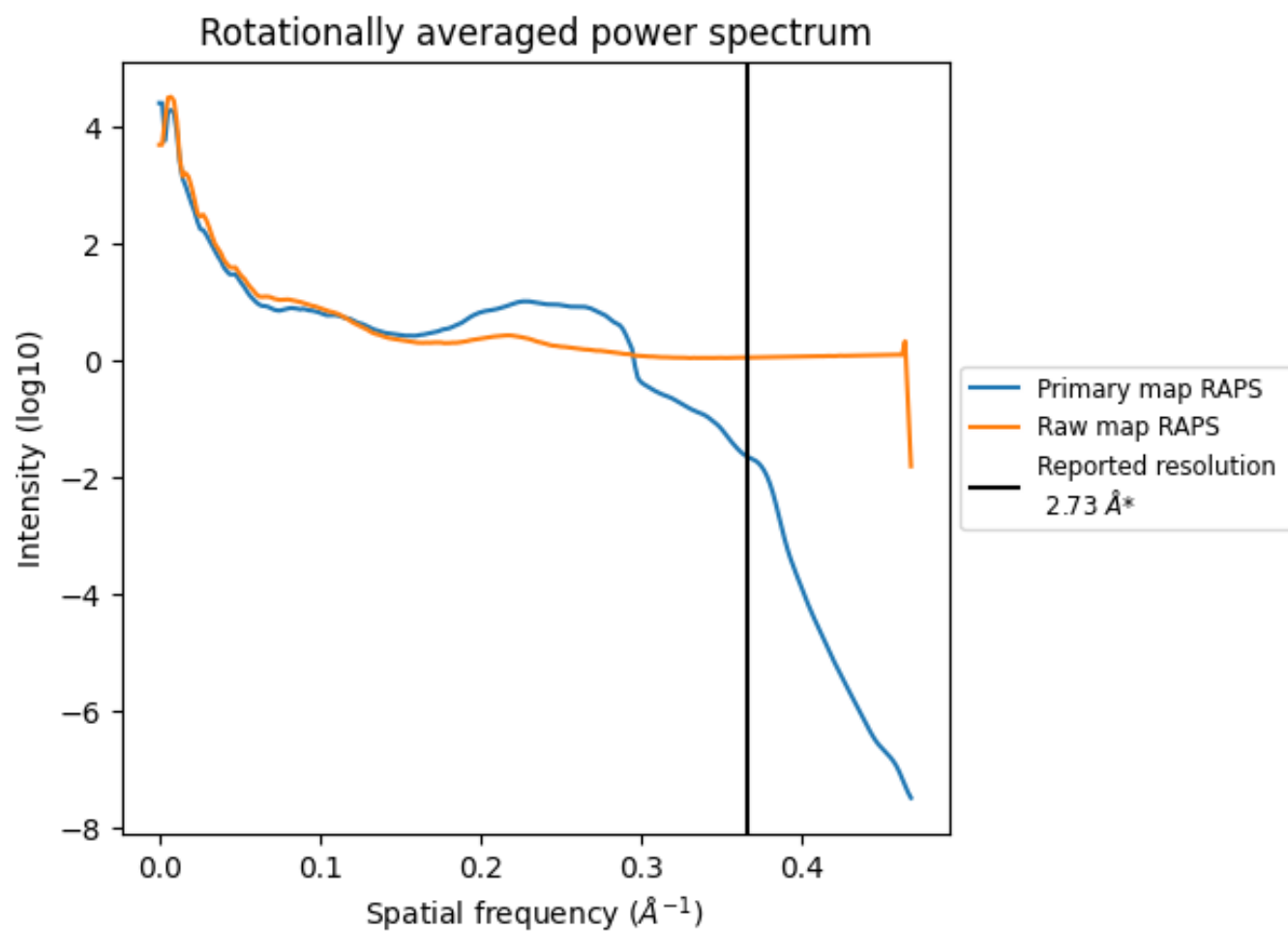
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 701 nm^3 ; this corresponds to an approximate mass of 633 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 ⓘ

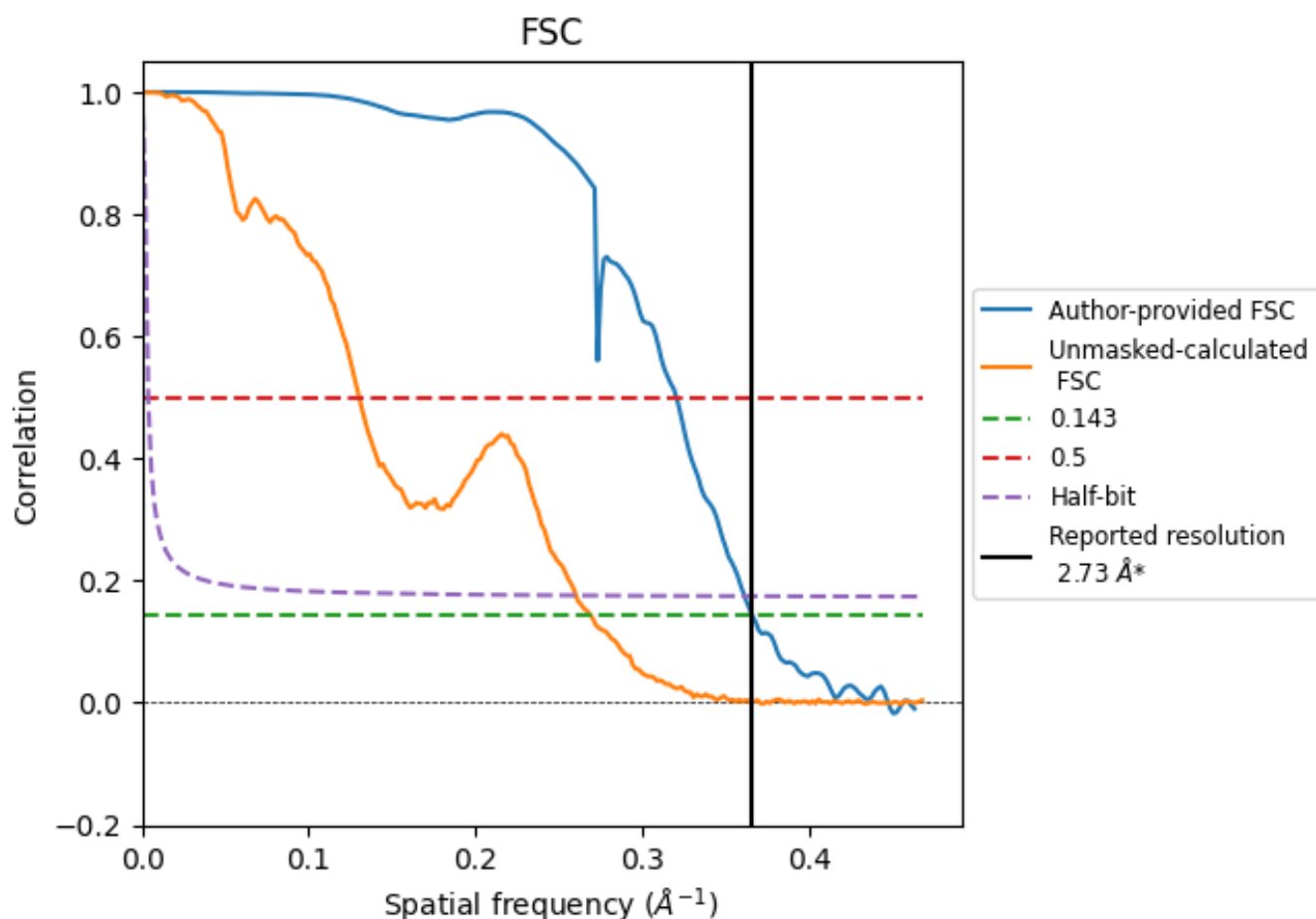


*Reported resolution corresponds to spatial frequency of 0.366 Å⁻¹

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 0.366 \AA^{-1}

8.2 Resolution estimates [i](#)

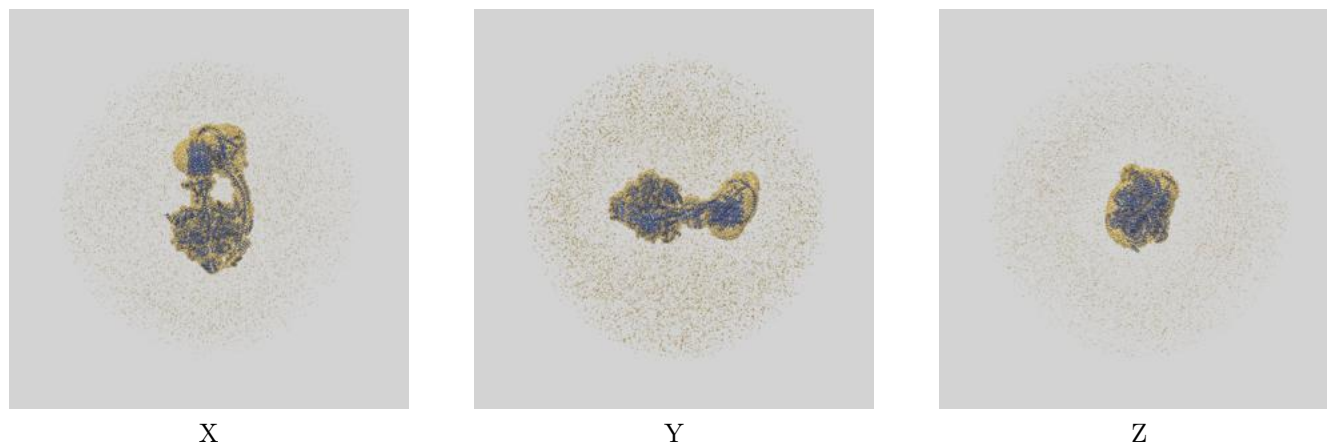
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.73	3.12	2.77
Unmasked-calculated*	3.71	7.68	3.84

*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 3.71 differs from the reported value 2.73 by more than 10 %

9 Map-model fit [i](#)

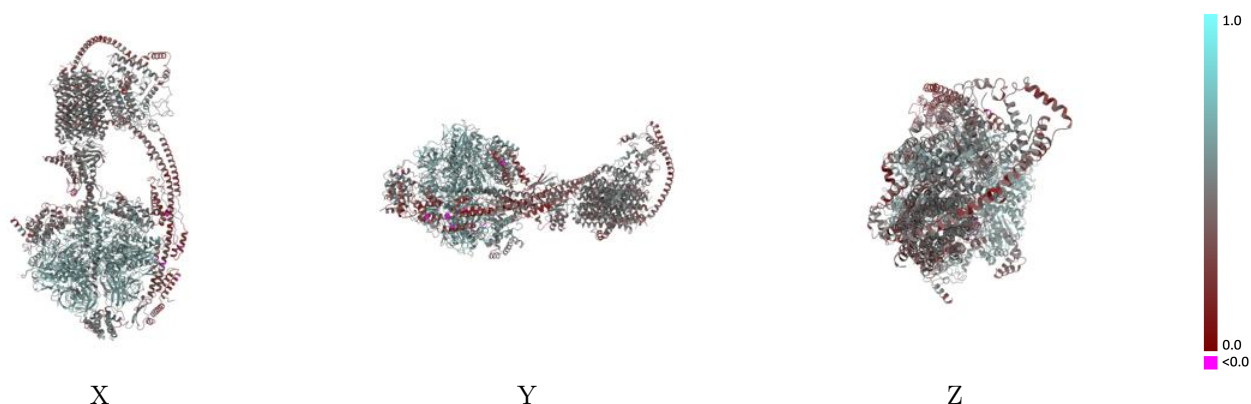
This section contains information regarding the fit between EMDB map EMD-44142 and PDB model 9B3J. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



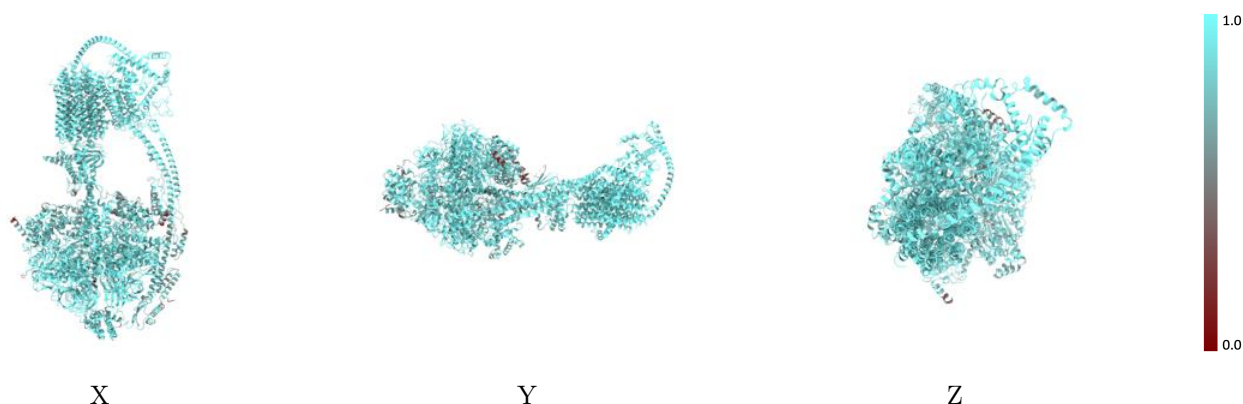
The images above show the 3D surface view of the map at the recommended contour level 3.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



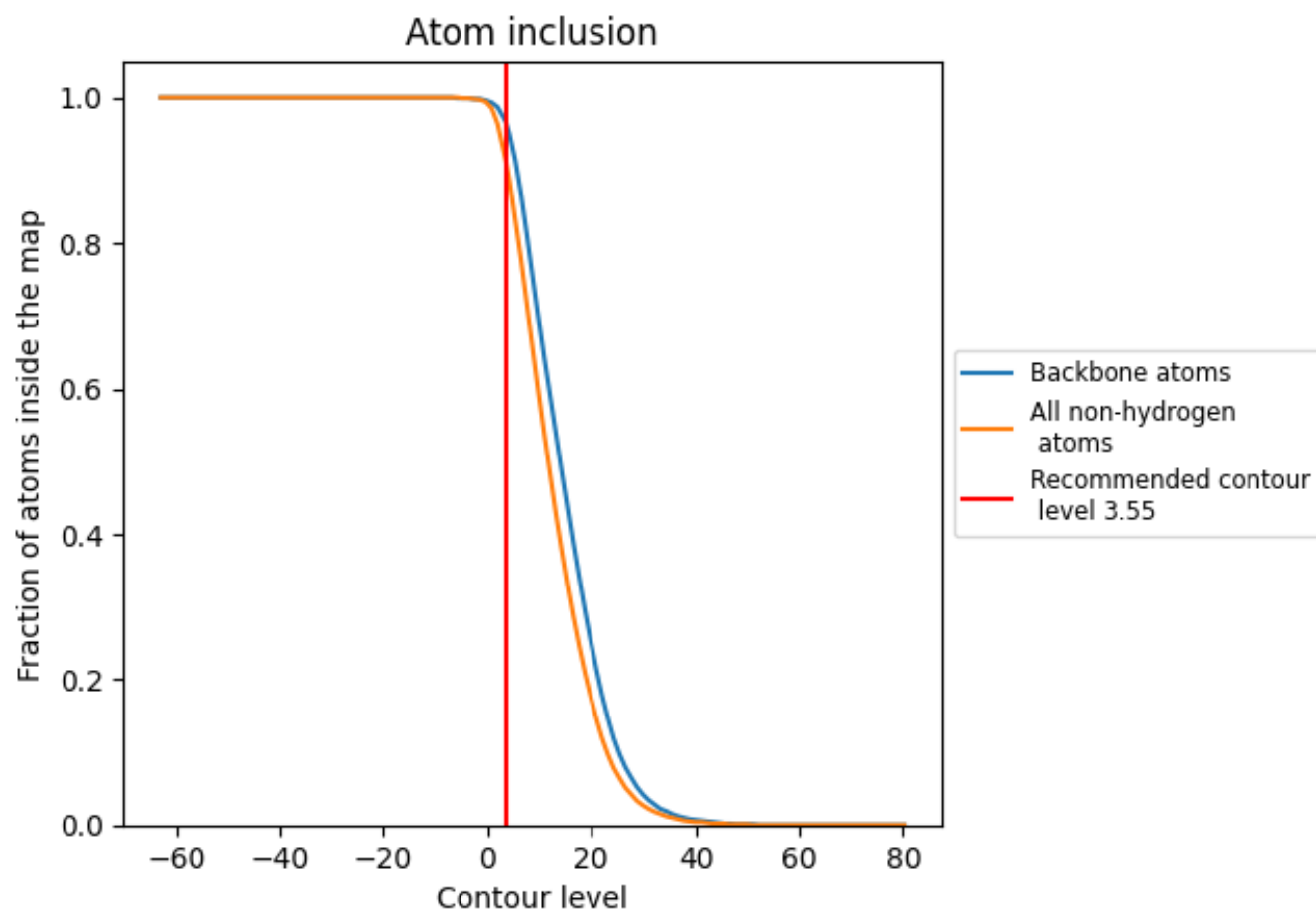
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.55).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 91% 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 (3.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9140	 0.4860
1	 0.9570	 0.4590
2	 0.9570	 0.4490
3	 0.9380	 0.4400
4	 0.9440	 0.4350
5	 0.9400	 0.4270
6	 0.9360	 0.4320
7	 0.9510	 0.4460
8	 0.9630	 0.4530
A	 0.8760	 0.5210
B	 0.9130	 0.5420
C	 0.9040	 0.5400
D	 0.9590	 0.5840
E	 0.9000	 0.5210
F	 0.9470	 0.5770
G	 0.8840	 0.4310
H	 0.9160	 0.4150
I	 0.7970	 0.3380
K	 0.9040	 0.3670
L	 0.8050	 0.2340
M	 0.8740	 0.2960
N	 0.9560	 0.4480
O	 0.8310	 0.4240
P	 0.9730	 0.4330
Q	 0.9320	 0.4070
R	 0.9440	 0.4700
S	 0.9320	 0.4060
T	 0.9330	 0.3540

