



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 06:17 PM UTC

PDB ID : 6N30 / pdb_00006n30
EMDB ID : EMD-9335
Title : Bacillus PS3 ATP synthase class 3
Authors : Guo, H.; Rubinstein, J.L.
Deposited on : 2018-11-14
Resolution : 3.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

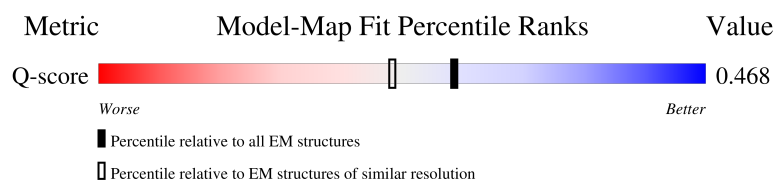
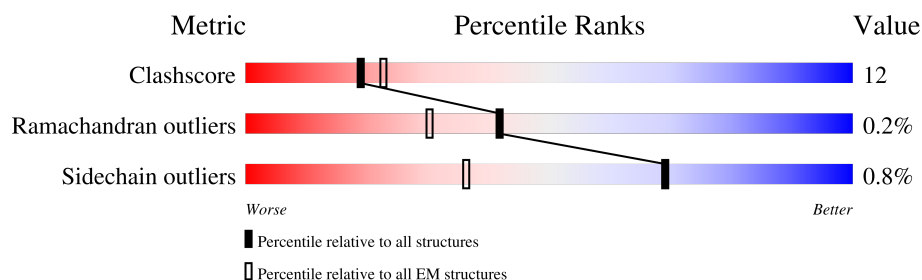
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



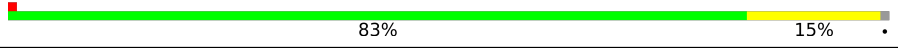
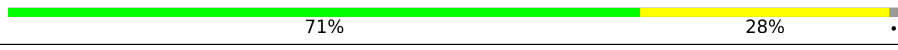
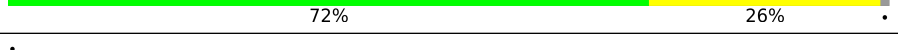
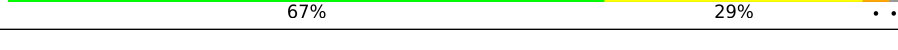
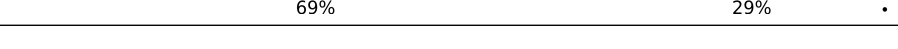
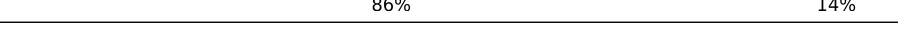
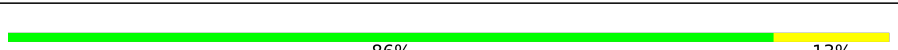
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	217187	24013	-
Ramachandran outliers	211220	23611	-
Sidechain outliers	210688	23127	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	b2	168	
2	b1	168	
3	a	237	
4	c0	72	

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Mol	Chain	Length	Quality of chain
4	c1	72	
4	c2	72	
4	c3	72	
4	c4	72	
4	c5	72	
4	c6	72	
4	c7	72	
4	c8	72	
4	c9	72	
5	A	502	
5	B	502	
5	C	502	
6	D	473	
6	E	473	
6	F	473	
7	G	285	
8	H	133	
9	I	178	

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 34851 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 Bacillus PS3 ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	b2	151	Total	C	N	O	S	0	0
			854	534	164	154	2		

- Molecule 2 is a protein called Bacillus PS3 ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b1	157	Total	C	N	O	S	0	0
			889	557	167	164	1		

- Molecule 3 is a protein called Bacillus PS3 ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	203	Total	C	N	O	S	0	0
			1486	990	238	250	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c3	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
4	c4	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
4	c5	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
4	c6	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
4	c7	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
4	c8	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
4	c9	71	Total	C	N	O	S	0	0
			507	333	86	87	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	c0	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
4	c1	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
4	c2	71	Total	C	N	O	S	0	0
			507	333	86	87	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	494	Total	C	N	O	S	0	0
			3736	2367	655	705	9		
5	A	500	Total	C	N	O	S	0	0
			3794	2402	663	720	9		
5	B	499	Total	C	N	O	S	0	0
			3780	2399	659	713	9		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	PRO	ARG	conflict	UNP A0A0M3VGF9
C	193	SER	CYS	conflict	UNP A0A0M3VGF9
C	463	PHE	TRP	conflict	UNP A0A0M3VGF9
A	132	PRO	ARG	conflict	UNP A0A0M3VGF9
A	193	SER	CYS	conflict	UNP A0A0M3VGF9
A	463	PHE	TRP	conflict	UNP A0A0M3VGF9
B	132	PRO	ARG	conflict	UNP A0A0M3VGF9
B	193	SER	CYS	conflict	UNP A0A0M3VGF9
B	463	PHE	TRP	conflict	UNP A0A0M3VGF9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	470	Total	C	N	O	S	0	0
			3610	2279	626	692	13		
6	D	469	Total	C	N	O	S	0	0
			3581	2262	624	683	12		
6	E	471	Total	C	N	O	S	0	0
			3614	2284	627	690	13		

- Molecule 7 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	284	Total	C	N	O	S	0	0
			2196	1387	385	416	8		

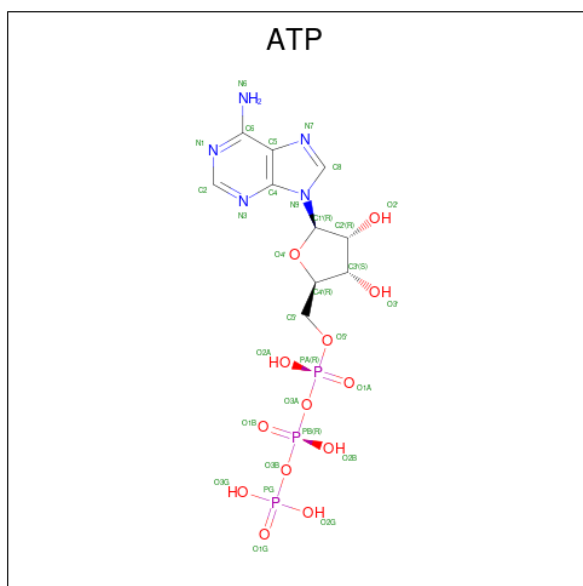
- Molecule 8 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	128	Total	C	N	O	S	0	0
			924	584	168	170	2		

- Molecule 9 is a protein called Bacillus PS3 ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	175	Total	C	N	O		0	0
			1188	765	213	210			

- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

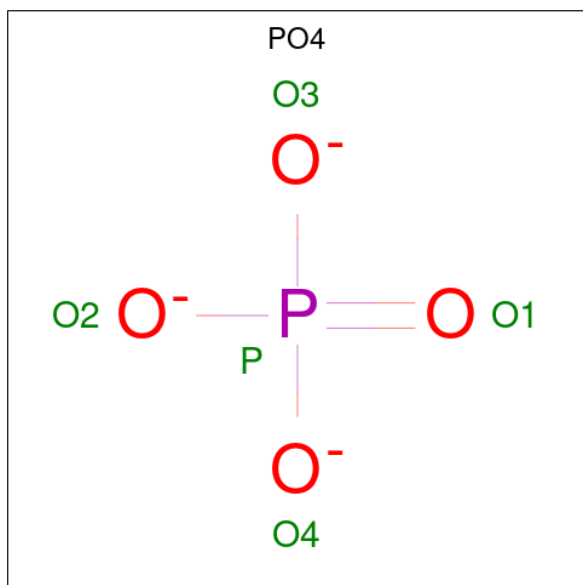


Mol	Chain	Residues	Atoms					AltConf
10	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

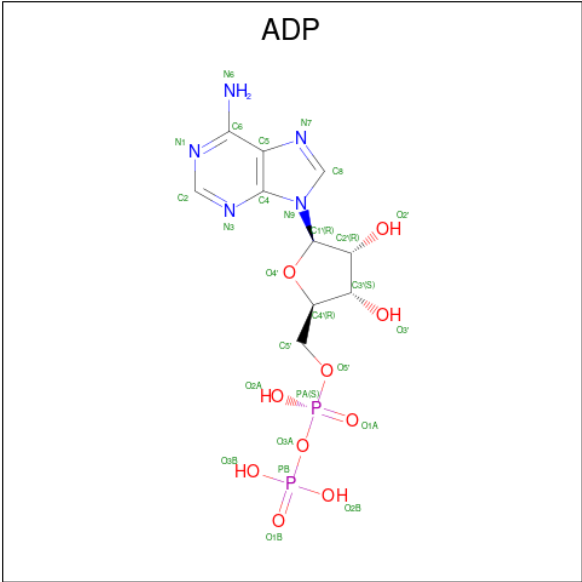
Mol	Chain	Residues	Atoms		AltConf
11	C	1	Total	Mg	0
			1	1	
11	A	1	Total	Mg	0
			1	1	
11	B	1	Total	Mg	0
			1	1	
11	E	1	Total	Mg	0
			1	1	

- Molecule 12 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			AltConf
12	D	1	Total	O	P	0
			5	4	1	

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

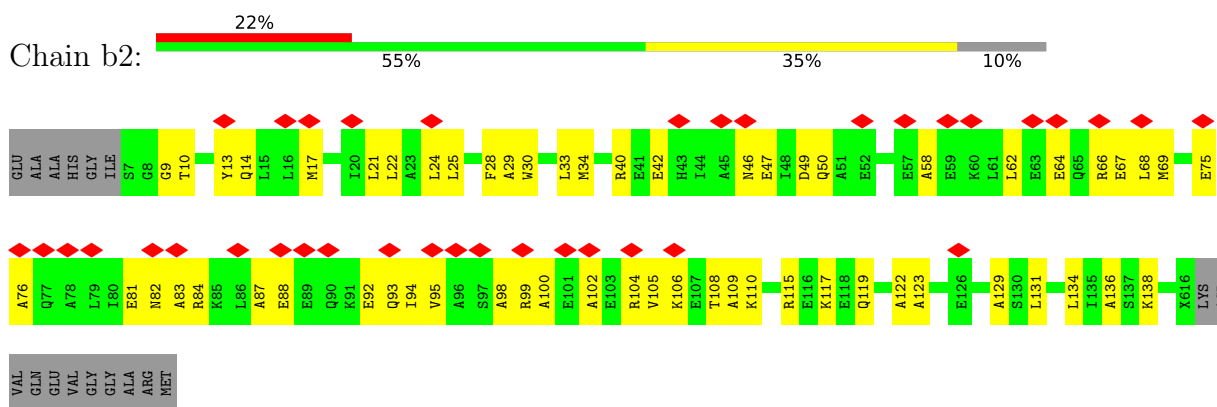


Mol	Chain	Residues	Atoms					AltConf
13	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

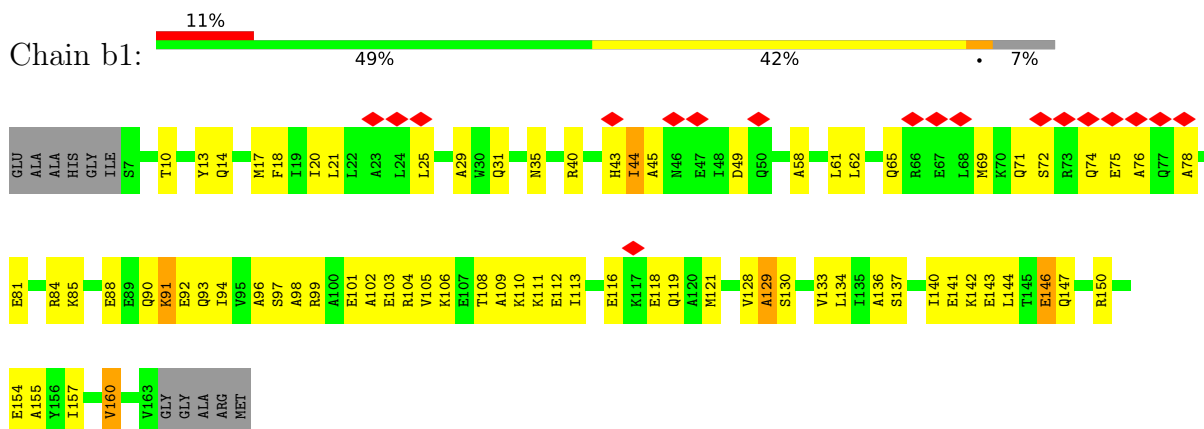
3 Residue-property plots

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.

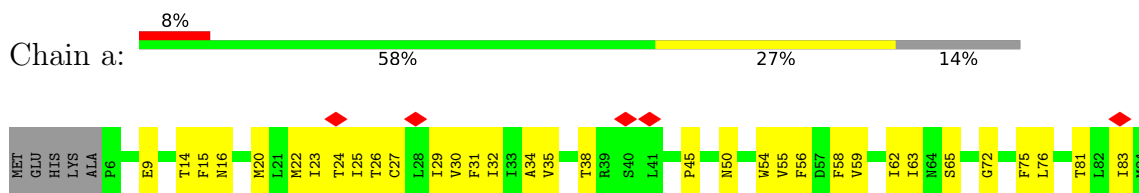
- Molecule 1: Bacillus PS3 ATP synthase subunit b

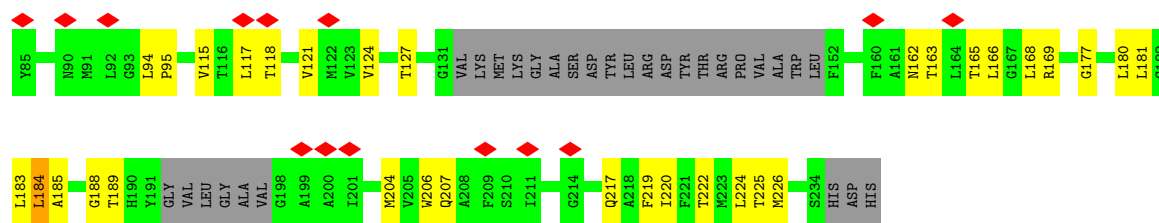


- Molecule 2: Bacillus PS3 ATP synthase subunit b

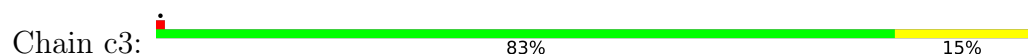


- Molecule 3: Bacillus PS3 ATP synthase subunit a





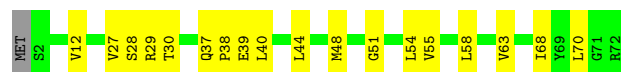
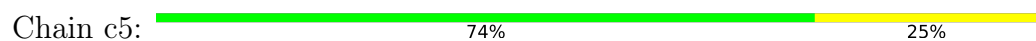
- Molecule 4: ATP synthase subunit c



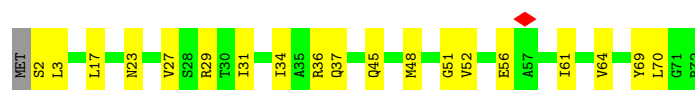
- Molecule 4: ATP synthase subunit c



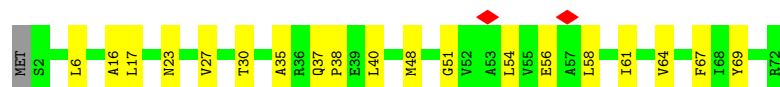
- Molecule 4: ATP synthase subunit c



- Molecule 4: ATP synthase subunit c

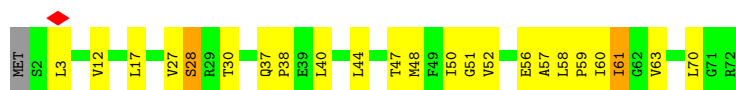


- Molecule 4: ATP synthase subunit c



- Molecule 4: ATP synthase subunit c

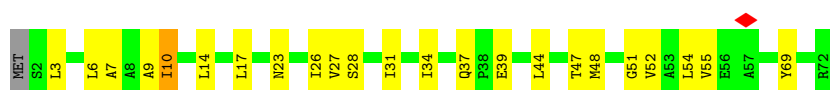




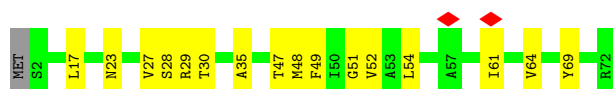
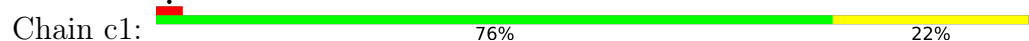
- Molecule 4: ATP synthase subunit c



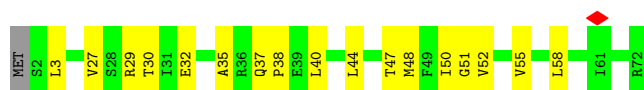
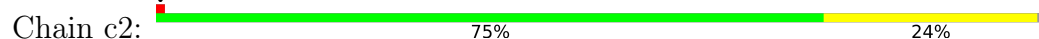
- Molecule 4: ATP synthase subunit c



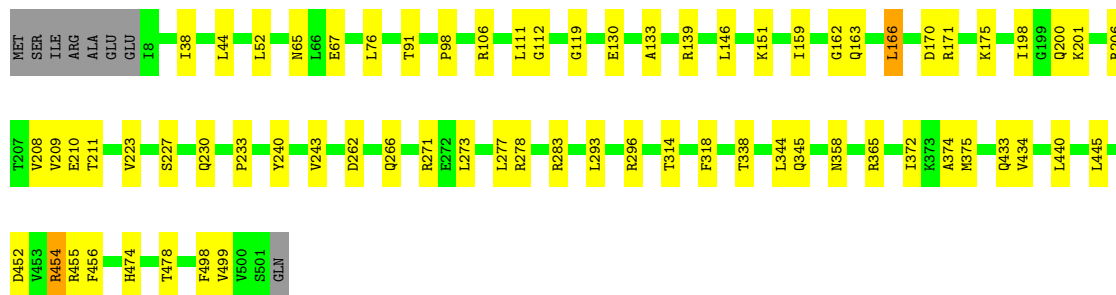
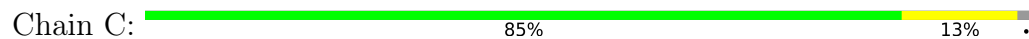
- Molecule 4: ATP synthase subunit c



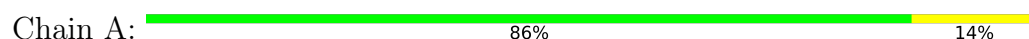
- Molecule 4: ATP synthase subunit c



- Molecule 5: ATP synthase subunit alpha



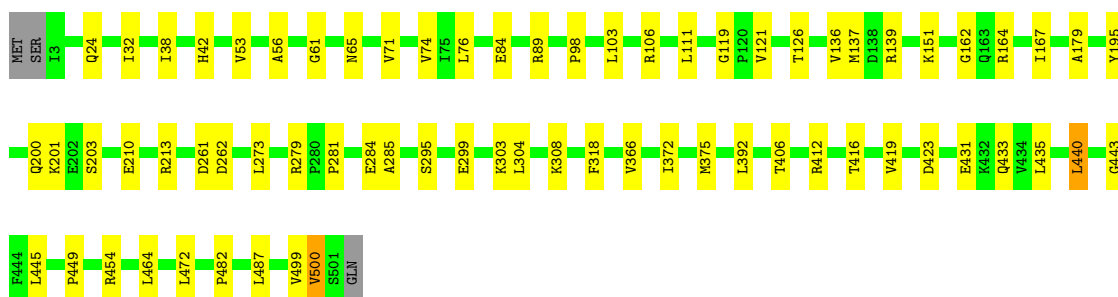
- Molecule 5: ATP synthase subunit alpha





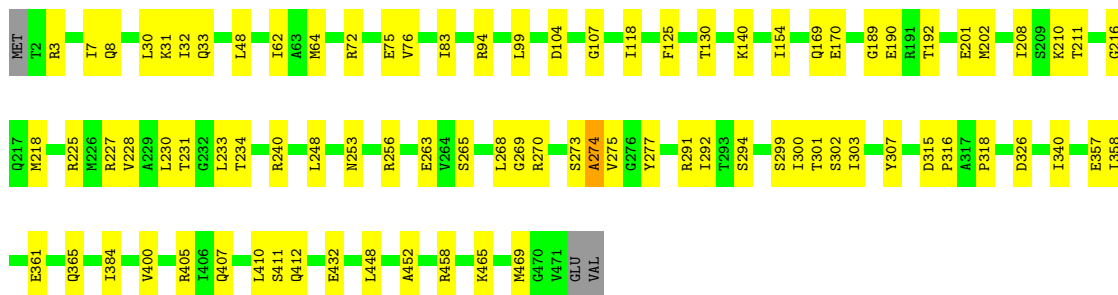
• Molecule 5: ATP synthase subunit alpha

Chain B: 85% 14%



• Molecule 6: ATP synthase subunit beta

Chain F: 81% 18%

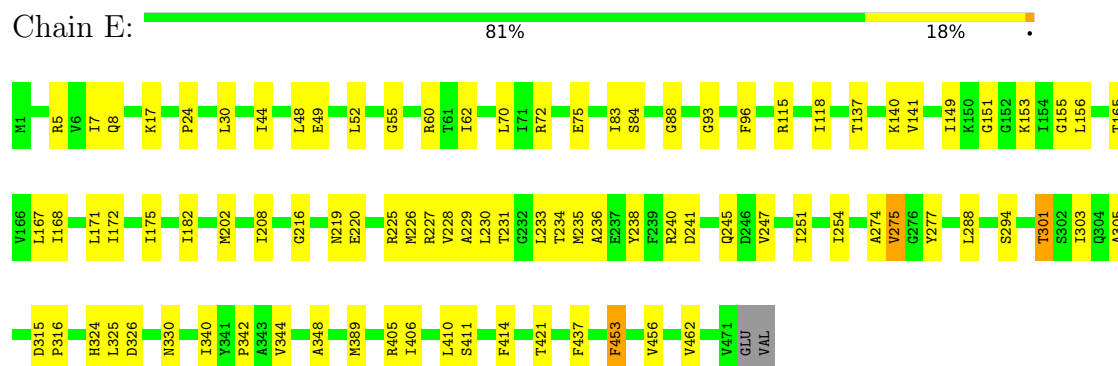


• Molecule 6: ATP synthase subunit beta

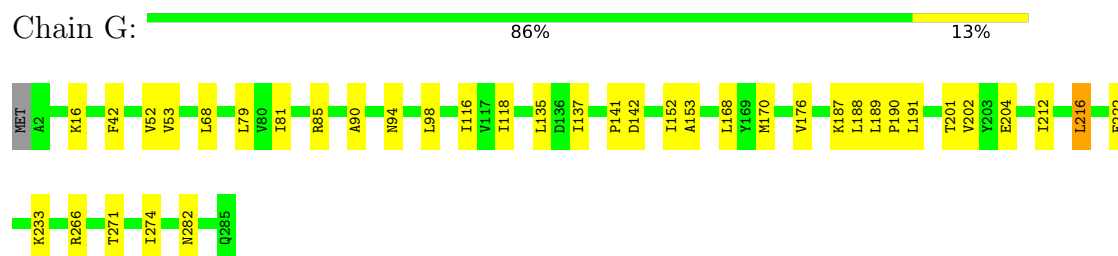
Chain D: 80% 18%



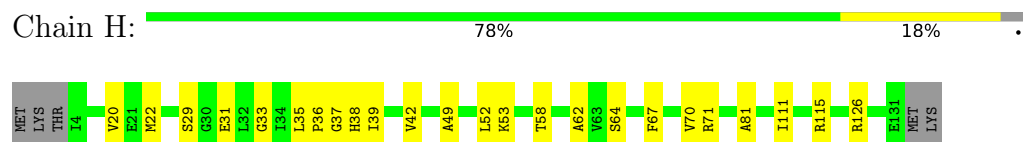
- Molecule 6: ATP synthase subunit beta



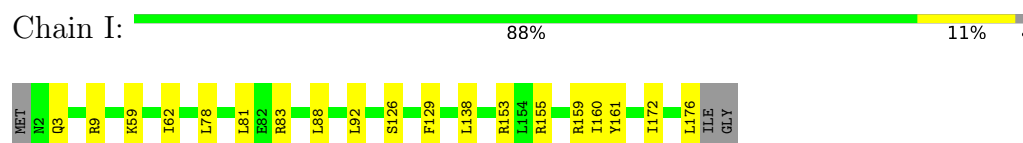
- Molecule 7: ATP synthase gamma chain



- Molecule 8: ATP synthase epsilon chain



- Molecule 9: Bacillus PS3 ATP synthase subunit delta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	175694	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.71	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	132075	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	7.682	Depositor
Minimum map value	-4.475	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.171	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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, ADP, PO4

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	b2	1.95	18/776 (2.3%)	2.17	45/1073 (4.2%)
2	b1	2.16	37/895 (4.1%)	2.31	62/1241 (5.0%)
3	a	0.27	0/1520	0.64	0/2079
4	c0	0.36	0/513	0.76	0/697
4	c1	0.34	0/513	0.70	0/697
4	c2	0.36	0/513	0.71	0/697
4	c3	0.34	0/513	0.68	0/697
4	c4	0.36	0/513	0.67	0/697
4	c5	0.33	0/513	0.70	0/697
4	c6	0.34	0/513	0.67	0/697
4	c7	0.30	0/513	0.65	0/697
4	c8	0.32	0/513	0.77	2/697 (0.3%)
4	c9	0.33	0/513	0.72	0/697
5	A	0.37	0/3854	0.60	1/5226 (0.0%)
5	B	0.38	0/3841	0.64	2/5210 (0.0%)
5	C	0.36	0/3796	0.59	0/5147
6	D	0.36	0/3644	0.63	3/4942 (0.1%)
6	E	0.40	0/3677	0.61	0/4980
6	F	0.37	0/3673	0.62	1/4978 (0.0%)
7	G	0.32	0/2229	0.65	2/3021 (0.1%)
8	H	0.27	0/935	0.65	0/1269
9	I	0.19	0/1203	0.47	0/1643
All	All	0.57	55/35173 (0.2%)	0.79	118/47779 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	B	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
All	All	0	3

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b1	130	SER	N-CA	-10.03	1.34	1.46
2	b1	137	SER	CA-C	-8.22	1.42	1.52
2	b1	109	ALA	N-CA	-8.09	1.36	1.46
2	b1	137	SER	CA-CB	7.45	1.65	1.53
2	b1	62	LEU	N-CA	-7.35	1.37	1.46

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b1	58	ALA	CA-C-N	11.20	135.28	120.28
2	b1	58	ALA	C-N-CA	11.20	135.28	120.28
6	F	274	ALA	N-CA-C	10.69	122.51	111.07
2	b1	65	GLN	O-C-N	-9.49	112.06	122.12
2	b1	103	GLU	O-C-N	-9.48	111.34	122.15

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	366	VAL	Peptide
5	B	482	PRO	Peptide
7	G	189	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	b2	854	0	551	153	0
2	b1	889	0	595	87	0
3	a	1486	0	1455	269	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	c0	507	0	552	23	0
4	c1	507	0	552	13	0
4	c2	507	0	552	13	0
4	c3	507	0	552	14	0
4	c4	507	0	552	35	0
4	c5	507	0	552	48	0
4	c6	507	0	552	20	0
4	c7	507	0	552	31	0
4	c8	507	0	552	46	0
4	c9	507	0	552	20	0
5	A	3794	0	3834	43	0
5	B	3780	0	3823	47	0
5	C	3736	0	3769	49	0
6	D	3581	0	3570	70	0
6	E	3614	0	3622	54	0
6	F	3610	0	3614	67	0
7	G	2196	0	2225	27	0
8	H	924	0	931	72	0
9	I	1188	0	1109	18	0
10	A	31	0	12	0	0
10	B	31	0	12	0	0
10	C	31	0	12	0	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	E	1	0	0	0	0
12	D	5	0	0	0	0
13	E	27	0	12	0	0
All	All	34851	0	34666	830	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 12.

The worst 5 of 830 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:b2:40:ARG:HH12	3:a:45:PRO:CD	1.14	1.59
1:b2:17:MET:CE	3:a:24:THR:HG22	1.35	1.52
2:b1:13:TYR:CE2	3:a:188:GLY:HA3	1.42	1.50
1:b2:17:MET:HE1	3:a:24:THR:CG2	1.39	1.48
1:b2:40:ARG:NH1	2:b1:44:ILE:CD1	1.76	1.47

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	b2	132/168 (79%)	131 (99%)	1 (1%)	0	100	100
2	b1	155/168 (92%)	152 (98%)	1 (1%)	2 (1%)	9	40
3	a	197/237 (83%)	186 (94%)	11 (6%)	0	100	100
4	c0	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
4	c1	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
4	c2	69/72 (96%)	67 (97%)	2 (3%)	0	100	100
4	c3	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
4	c4	69/72 (96%)	67 (97%)	2 (3%)	0	100	100
4	c5	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
4	c6	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
4	c7	69/72 (96%)	67 (97%)	2 (3%)	0	100	100
4	c8	69/72 (96%)	69 (100%)	0	0	100	100
4	c9	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
5	A	498/502 (99%)	484 (97%)	14 (3%)	0	100	100
5	B	497/502 (99%)	477 (96%)	20 (4%)	0	100	100
5	C	492/502 (98%)	472 (96%)	20 (4%)	0	100	100
6	D	467/473 (99%)	443 (95%)	21 (4%)	3 (1%)	21	56
6	E	469/473 (99%)	447 (95%)	20 (4%)	2 (0%)	30	62
6	F	468/473 (99%)	446 (95%)	22 (5%)	0	100	100
7	G	282/285 (99%)	257 (91%)	25 (9%)	0	100	100
8	H	126/133 (95%)	111 (88%)	15 (12%)	0	100	100
9	I	173/178 (97%)	166 (96%)	7 (4%)	0	100	100
All	All	4646/4814 (96%)	4450 (96%)	189 (4%)	7 (0%)	42	73

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b1	146	GLU
2	b1	144	LEU
6	D	209	SER
6	D	310	ALA
6	E	24	PRO

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	b2	26/124 (21%)	26 (100%)	0	100	100
2	b1	29/140 (21%)	28 (97%)	1 (3%)	32	64
3	a	143/198 (72%)	142 (99%)	1 (1%)	76	83
4	c0	51/52 (98%)	50 (98%)	1 (2%)	48	72
4	c1	51/52 (98%)	51 (100%)	0	100	100
4	c2	51/52 (98%)	50 (98%)	1 (2%)	48	72
4	c3	51/52 (98%)	51 (100%)	0	100	100
4	c4	51/52 (98%)	51 (100%)	0	100	100
4	c5	51/52 (98%)	51 (100%)	0	100	100
4	c6	51/52 (98%)	51 (100%)	0	100	100
4	c7	51/52 (98%)	51 (100%)	0	100	100
4	c8	51/52 (98%)	50 (98%)	1 (2%)	48	72
4	c9	51/52 (98%)	50 (98%)	1 (2%)	48	72
5	A	398/412 (97%)	395 (99%)	3 (1%)	73	82
5	B	395/412 (96%)	391 (99%)	4 (1%)	68	80
5	C	390/412 (95%)	386 (99%)	4 (1%)	68	80
6	D	375/389 (96%)	374 (100%)	1 (0%)	86	88
6	E	384/389 (99%)	380 (99%)	4 (1%)	68	80
6	F	383/389 (98%)	382 (100%)	1 (0%)	86	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	232/240 (97%)	229 (99%)	3 (1%)	61	78
8	H	89/108 (82%)	88 (99%)	1 (1%)	65	79
9	I	95/146 (65%)	95 (100%)	0	100	100
All	All	3449/3879 (89%)	3422 (99%)	27 (1%)	69	82

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	440	LEU
6	F	170	GLU
7	G	176	VAL
5	B	500	VAL
6	D	175	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	425	HIS
6	D	259	GLN
6	F	179	HIS
6	F	365	GLN
6	D	324	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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
10	ATP	B	600	11	32,33,33	1.34	5 (15%)	48,52,52	1.72	7 (14%)
10	ATP	A	600	11	32,33,33	1.31	5 (15%)	48,52,52	1.74	8 (16%)
10	ATP	C	600	11	32,33,33	1.36	5 (15%)	48,52,52	1.76	7 (14%)
12	PO4	D	600	-	4,4,4	1.04	0	6,6,6	0.40	0
13	ADP	E	600	11	28,29,29	1.42	5 (17%)	43,45,45	1.80	9 (20%)

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	ADP	E	600	11	-	5/16/32/32	0/3/3/3
10	ATP	B	600	11	-	4/22/38/38	0/3/3/3
10	ATP	A	600	11	-	1/22/38/38	0/3/3/3
10	ATP	C	600	11	-	6/22/38/38	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	600	ATP	C5-C4	4.53	1.47	1.39
10	B	600	ATP	C5-C4	4.51	1.47	1.39
13	E	600	ADP	C5-C4	4.48	1.47	1.39
10	A	600	ATP	C5-C4	4.33	1.46	1.39
13	E	600	ADP	C5-N7	-2.79	1.34	1.39

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	600	ATP	C5-C4-N3	-5.73	118.82	126.72
10	A	600	ATP	C5-C4-N3	-5.72	118.83	126.72
13	E	600	ADP	C5-C4-N3	-5.68	118.90	126.72
10	B	600	ATP	C5-C4-N3	-5.58	119.04	126.72
10	C	600	ATP	N3-C4-N9	4.71	135.18	127.17

There are no chirality outliers.

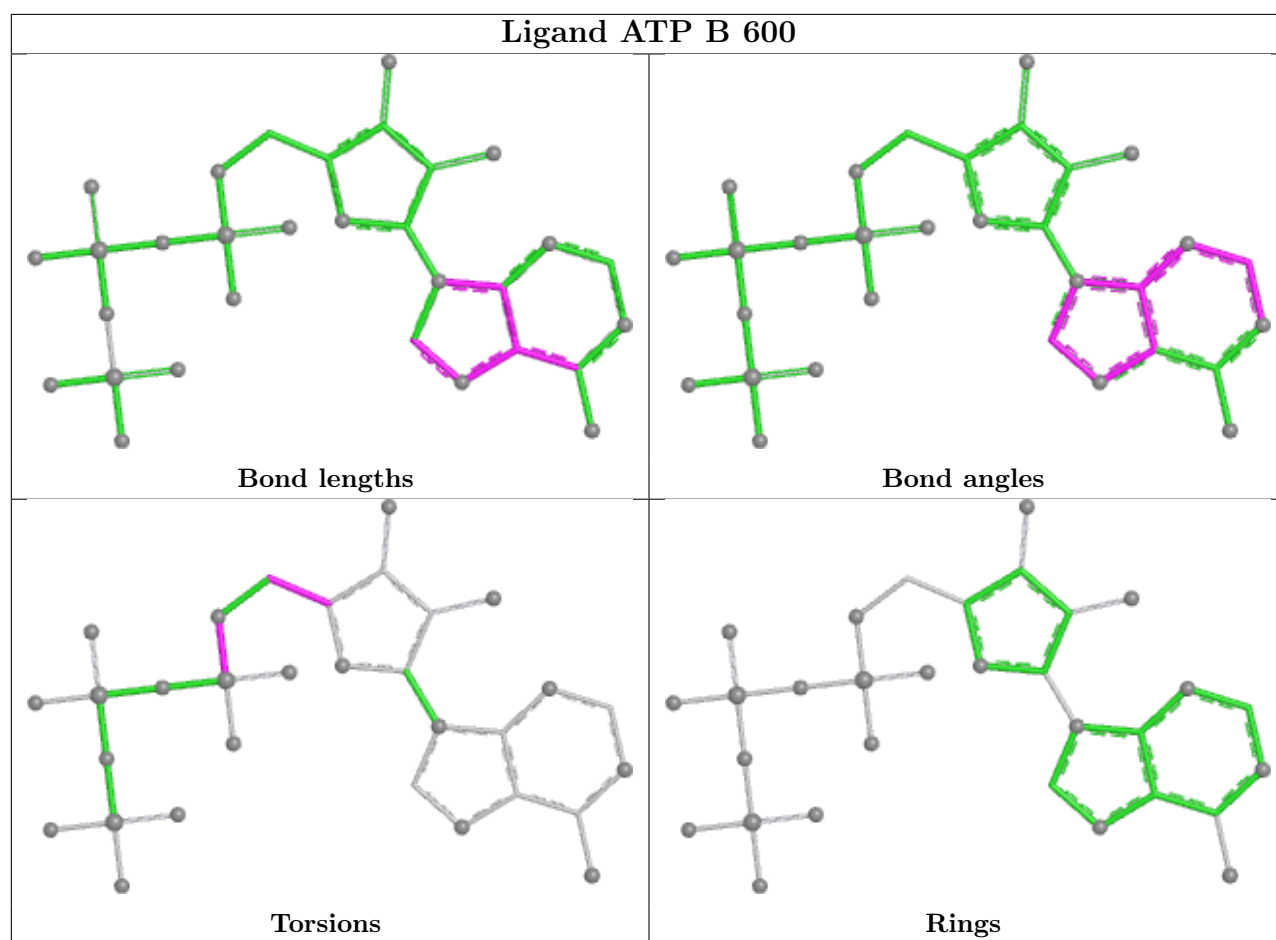
5 of 16 torsion outliers are listed below:

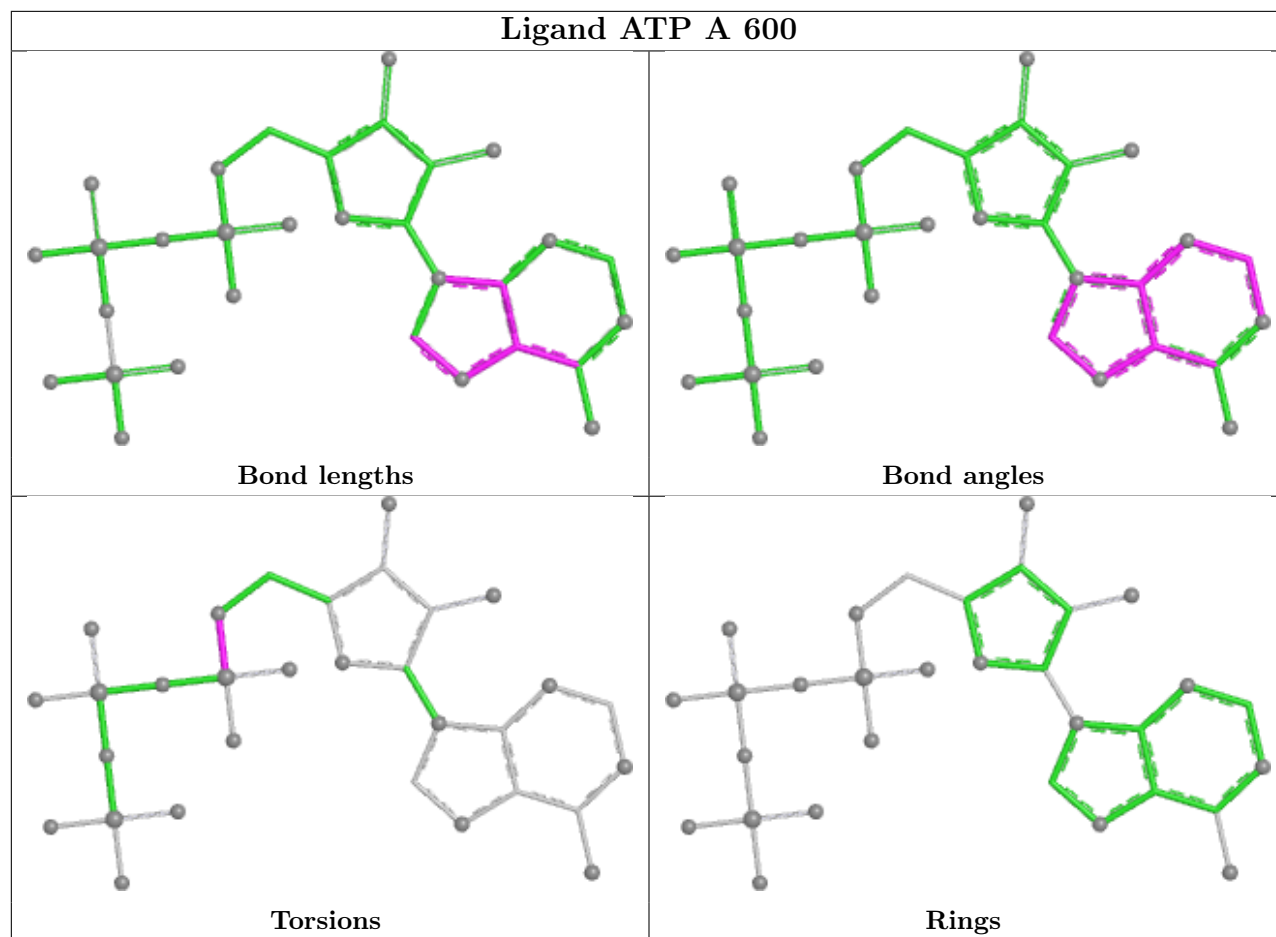
Mol	Chain	Res	Type	Atoms
10	C	600	ATP	C5'-O5'-PA-O1A
10	A	600	ATP	C5'-O5'-PA-O2A
10	B	600	ATP	C5'-O5'-PA-O1A
10	B	600	ATP	C5'-O5'-PA-O3A
13	E	600	ADP	C5'-O5'-PA-O1A

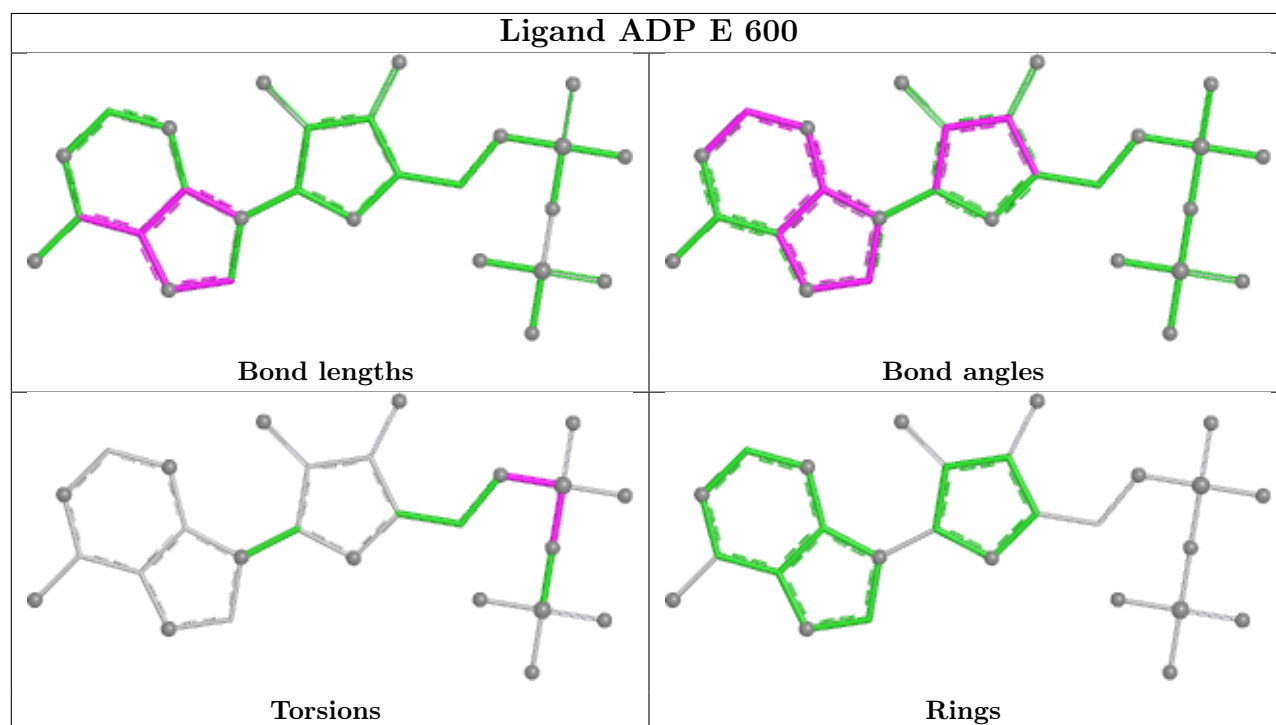
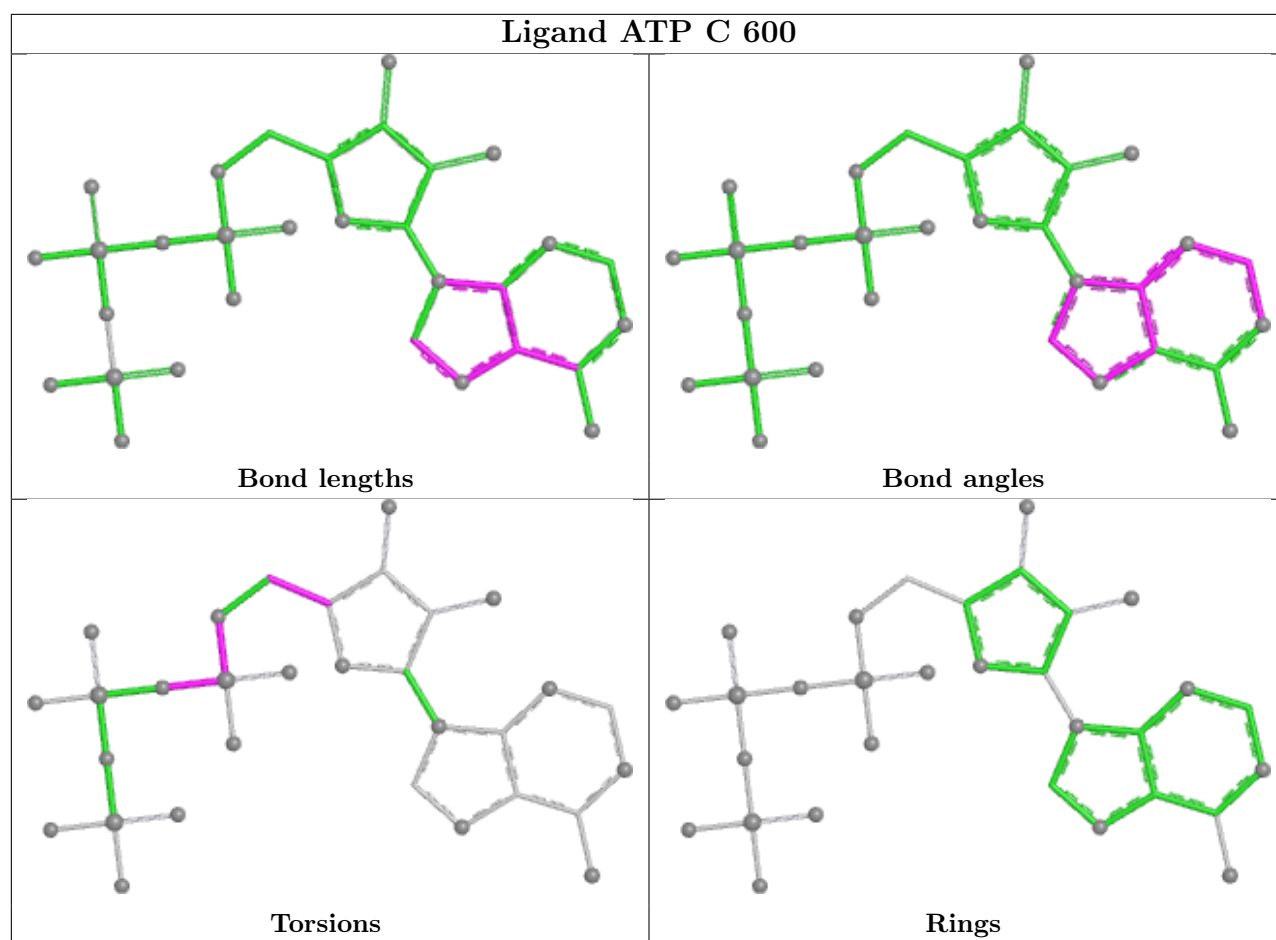
There are no ring outliers.

No monomer is involved in short contacts.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	b2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b2	140:ILE	C	600:UNK	N	14.20

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9335. These allow visual inspection of the internal detail of the map and identification of artifacts.

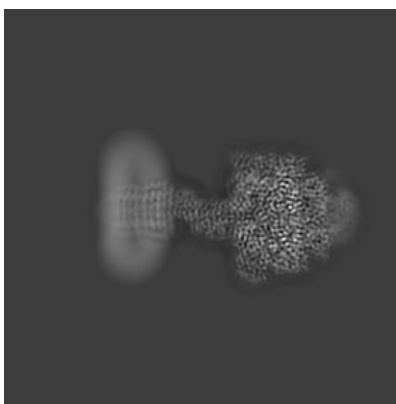
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

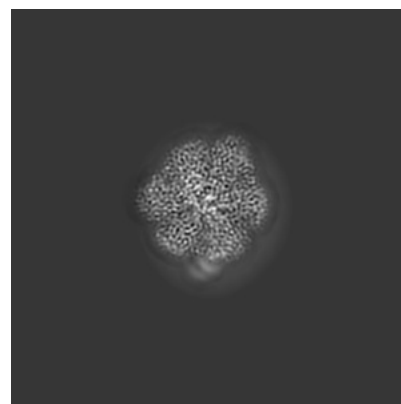
6.1.1 Primary map



X

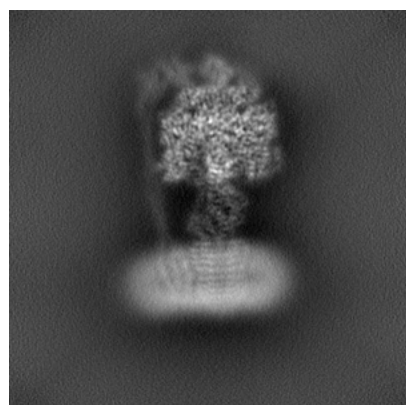


Y

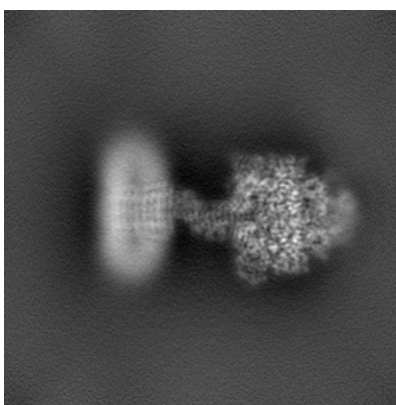


Z

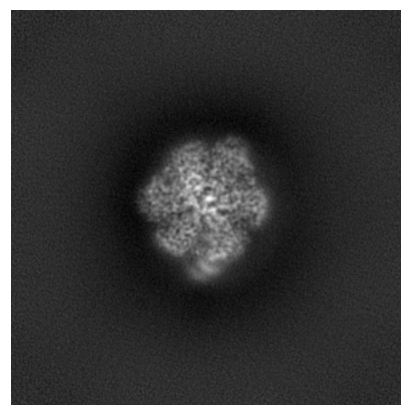
6.1.2 Raw map



X



Y



Z

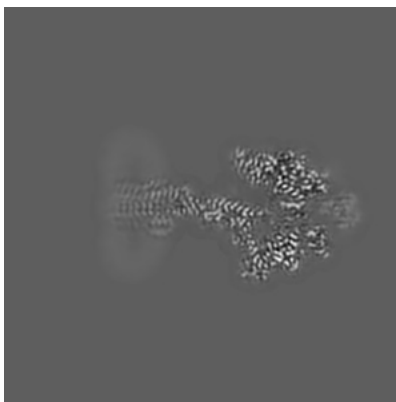
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

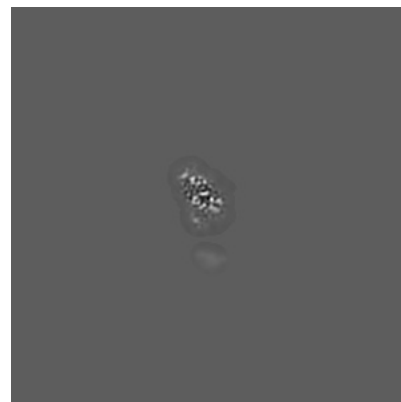
6.2.1 Primary map



X Index: 160



Y Index: 160

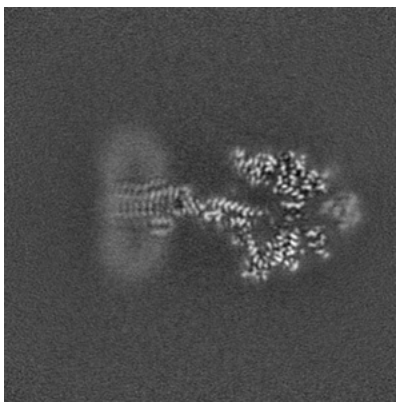


Z Index: 160

6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

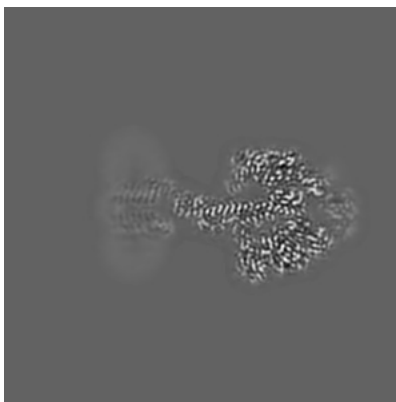
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

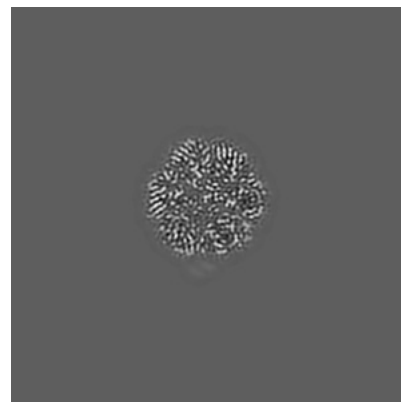
6.3.1 Primary map



X Index: 142

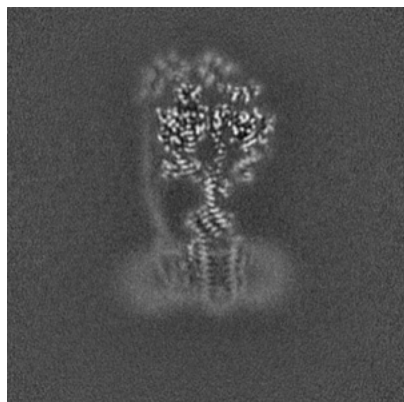


Y Index: 167

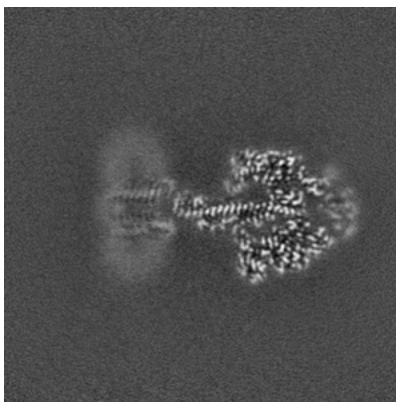


Z Index: 226

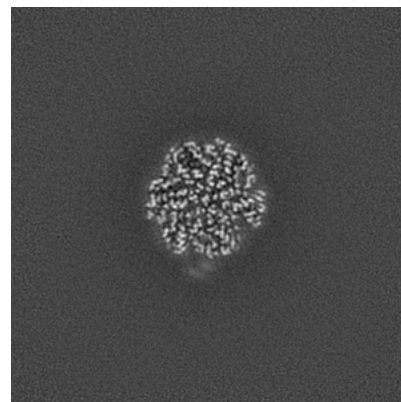
6.3.2 Raw map



X Index: 163



Y Index: 167

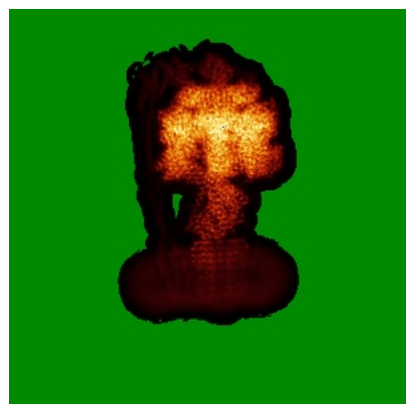


Z Index: 231

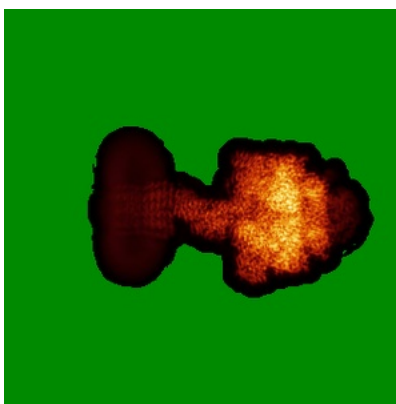
The images above show the largest variance slices of the map in three orthogonal directions.

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

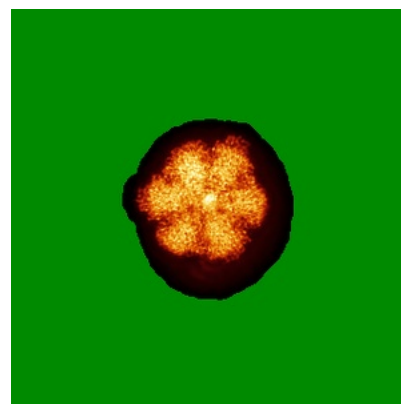
6.4.1 Primary map



X

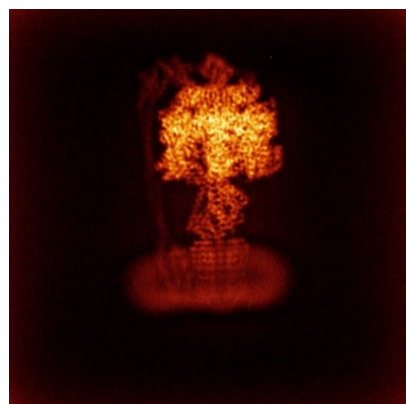


Y

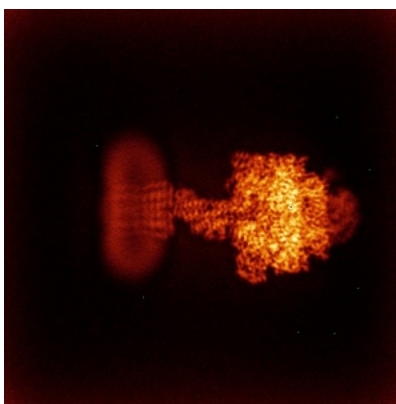


Z

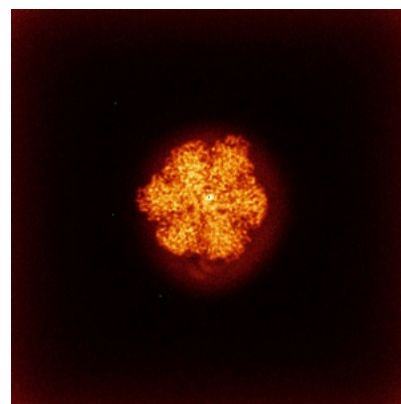
6.4.2 Raw map



X



Y

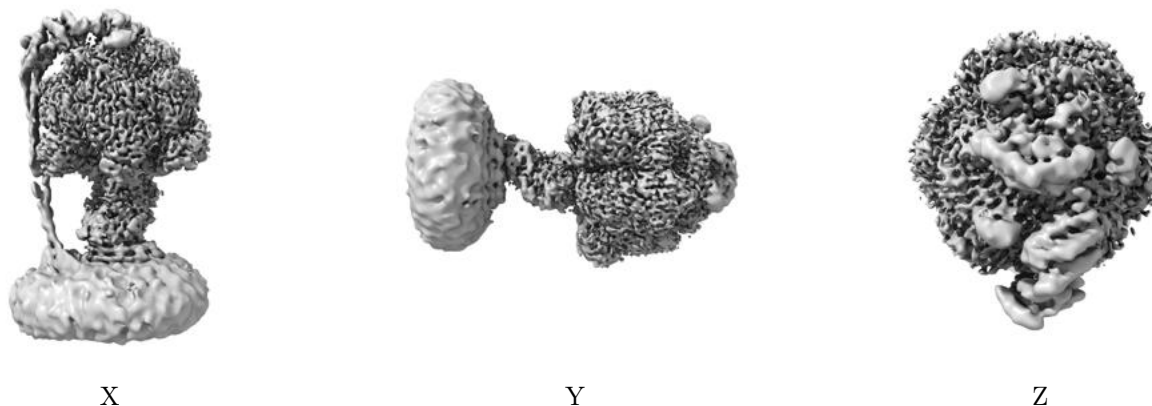


Z

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.

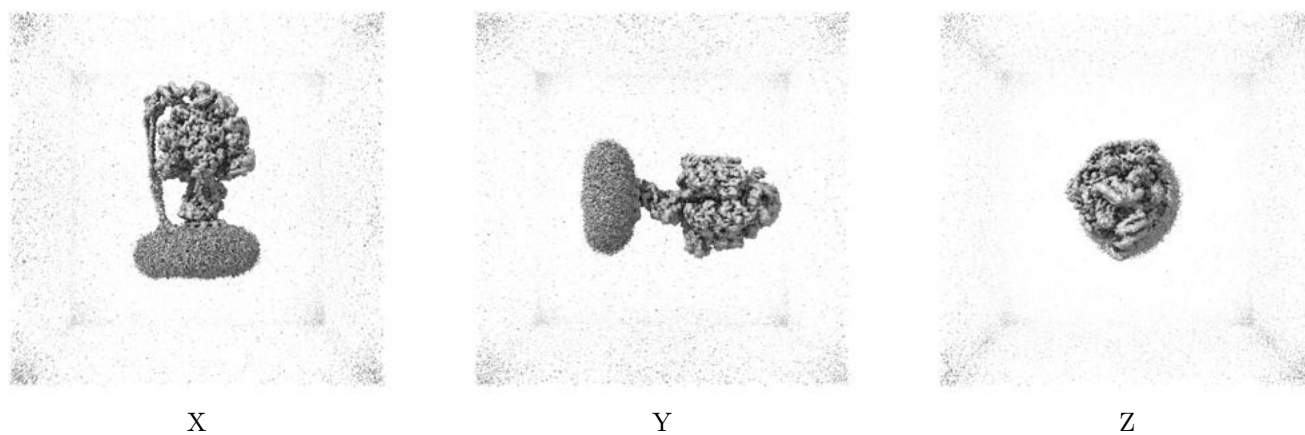
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

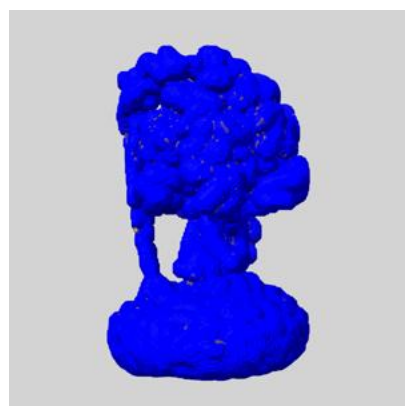
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

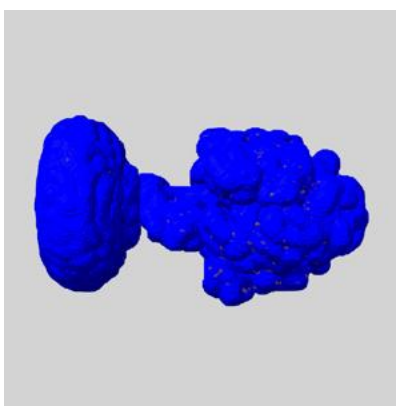
A mask typically either:

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

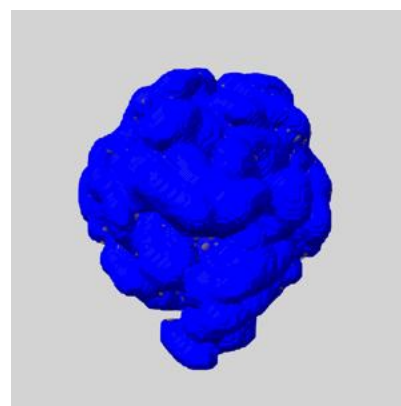
6.6.1 emd_9335_msk_1.map [i](#)



X



Y

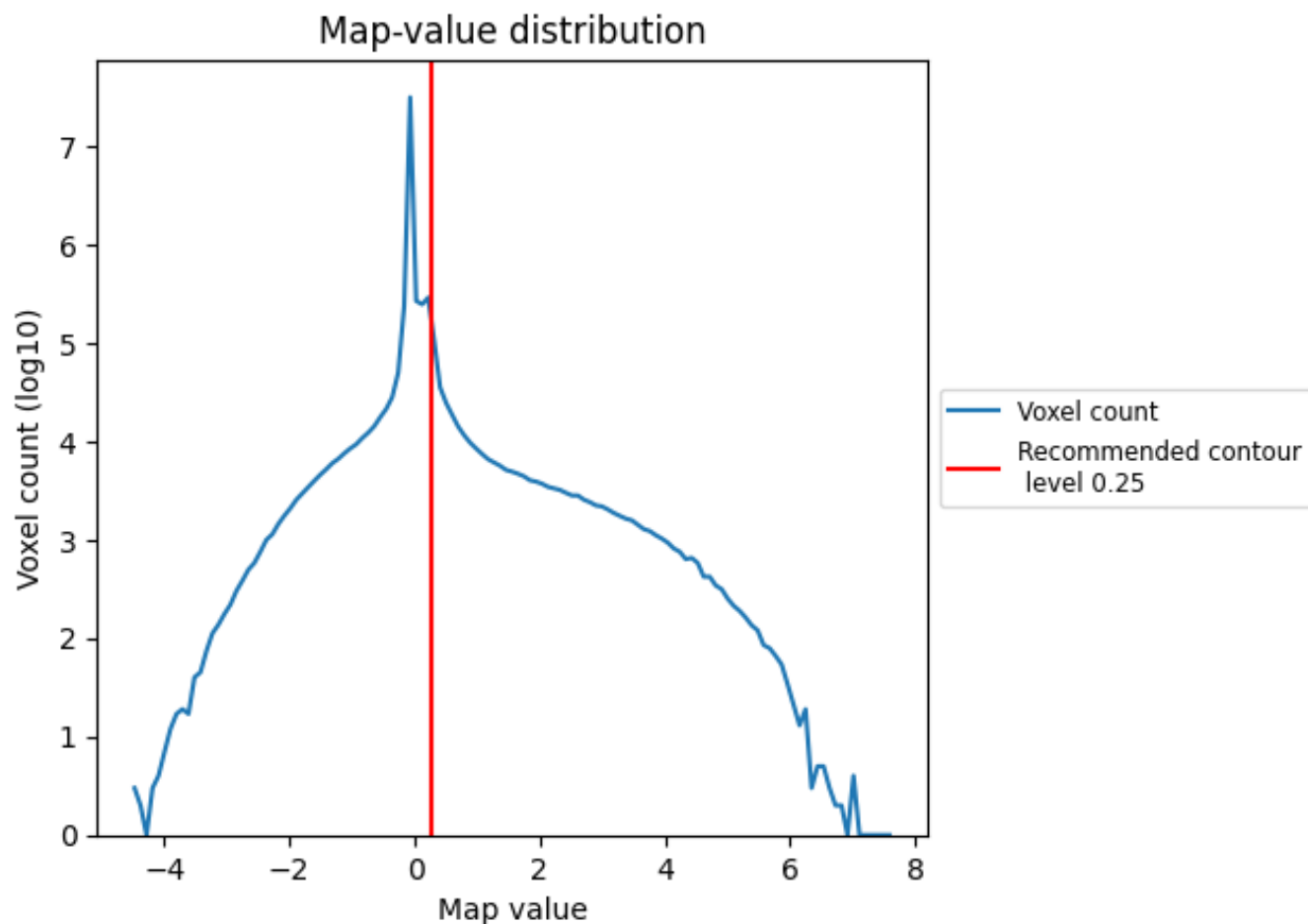


Z

7 Map analysis [i](#)

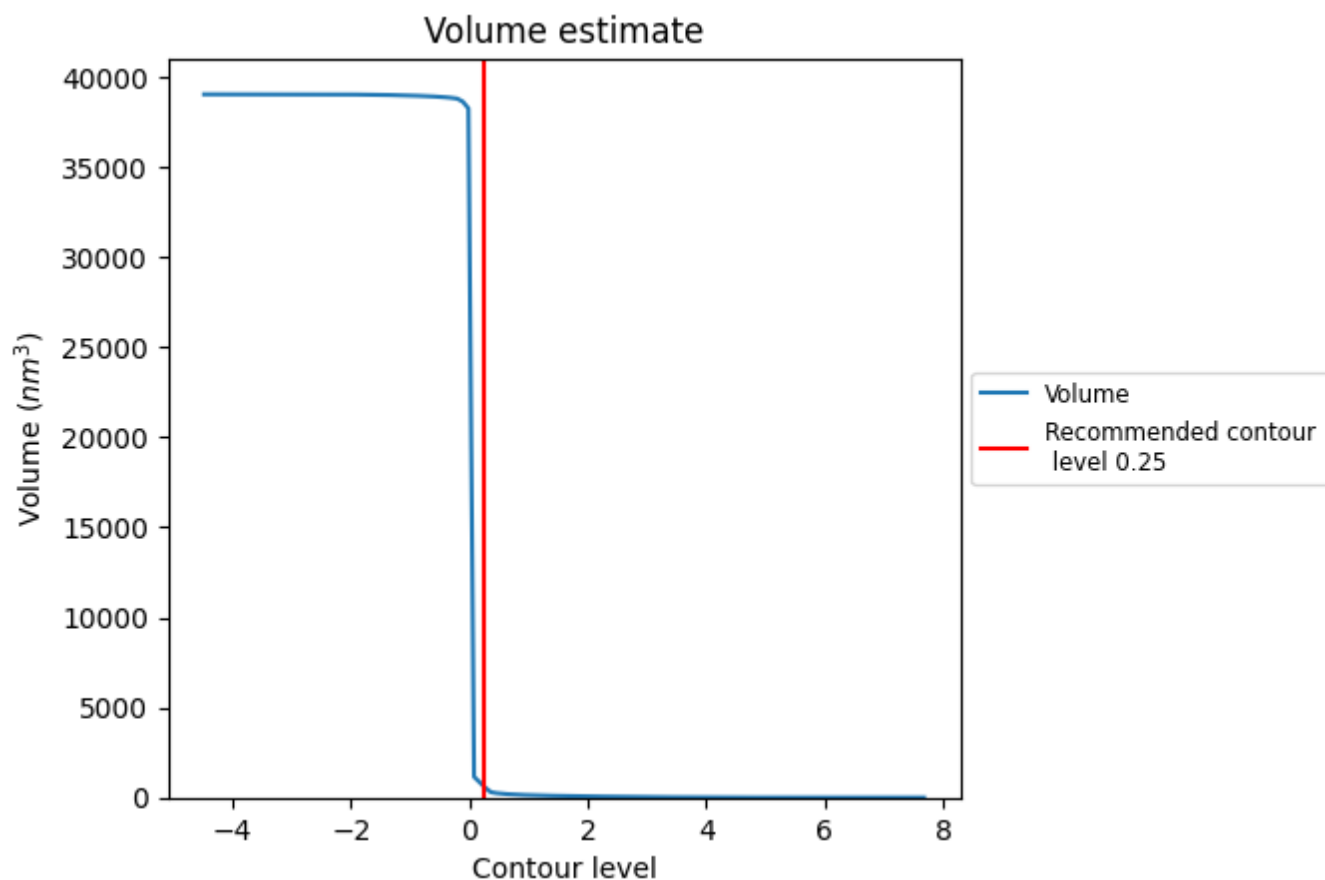
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

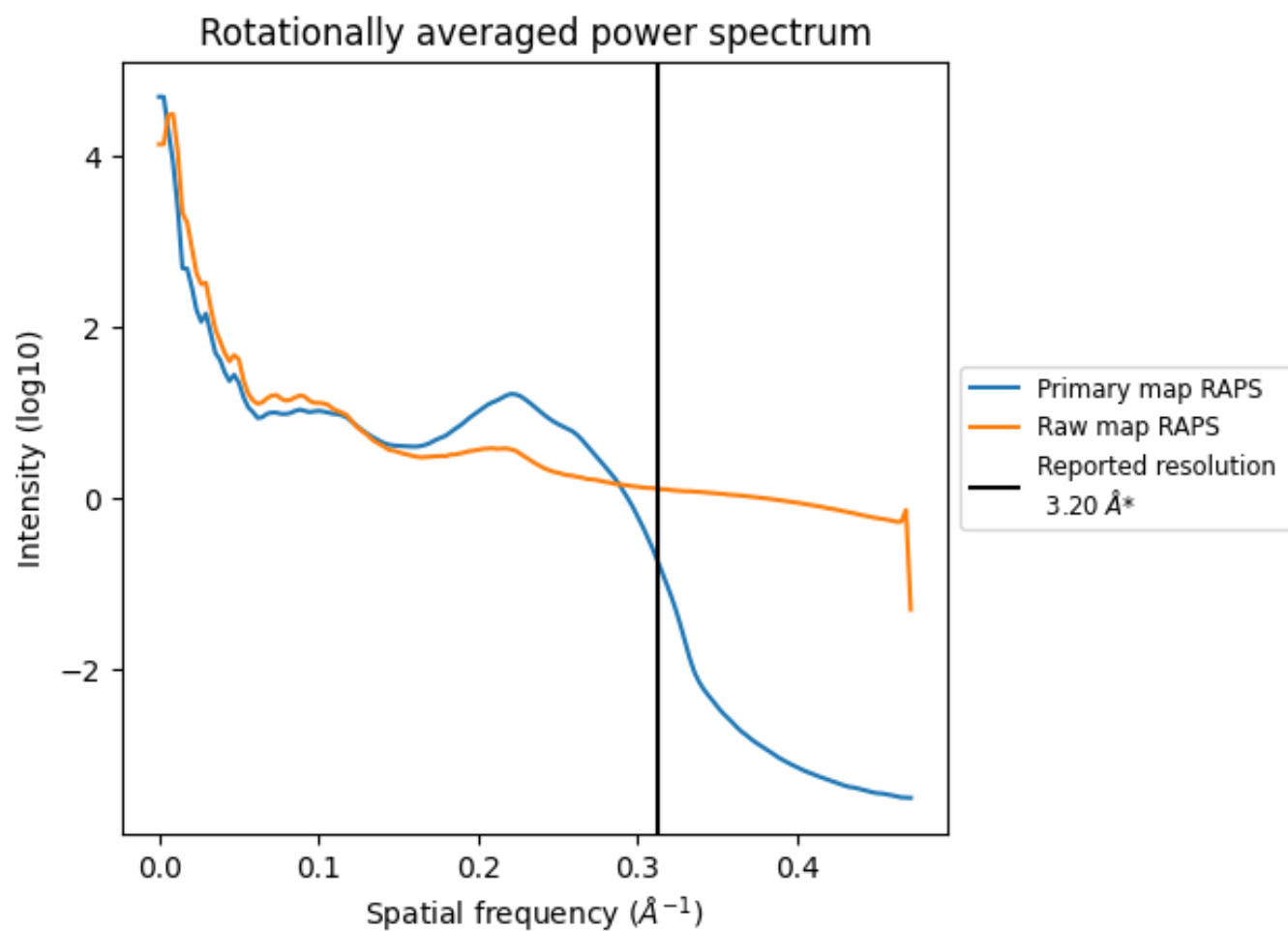
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 620 nm^3 ; this corresponds to an approximate mass of 560 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 ⓘ

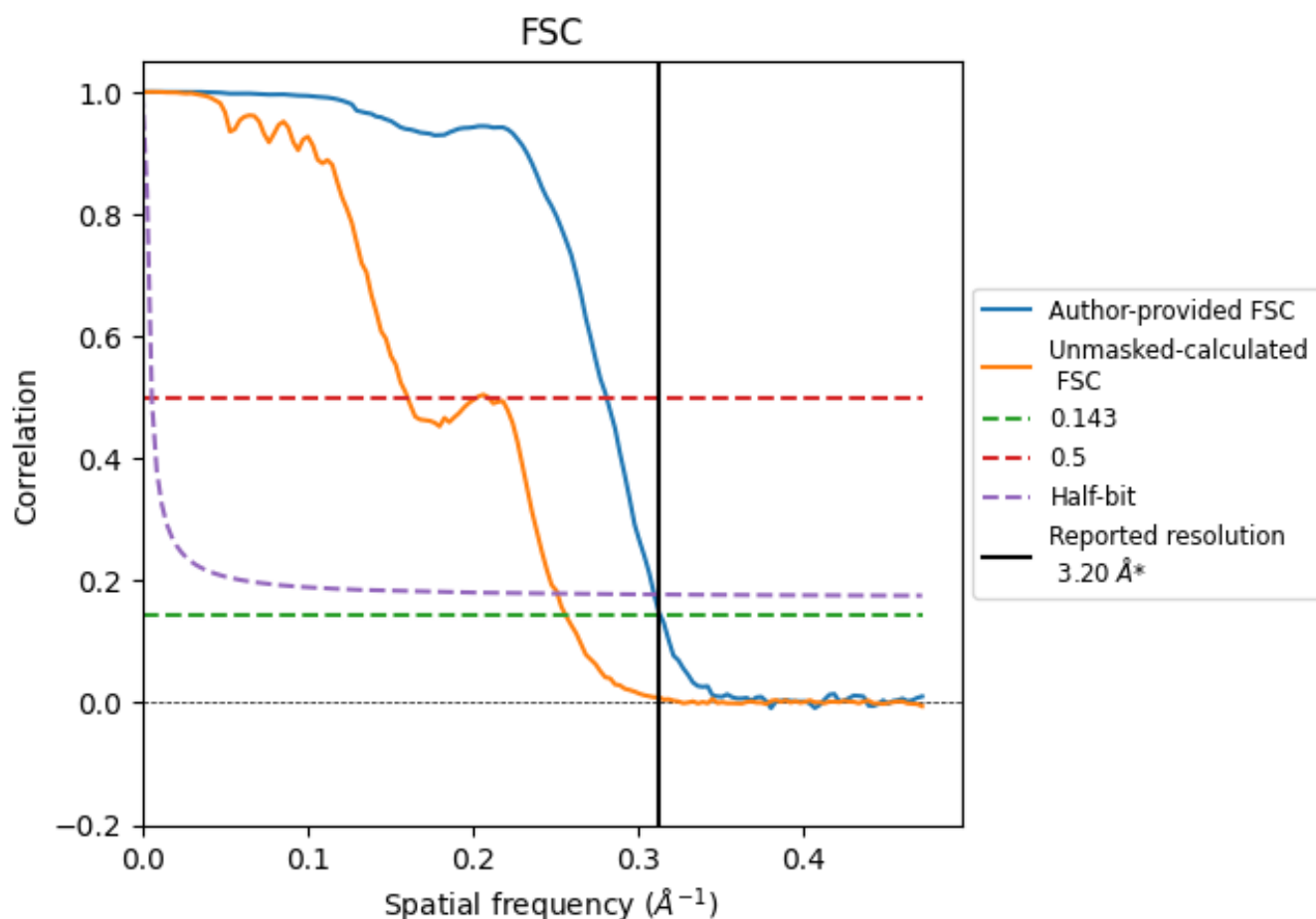


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

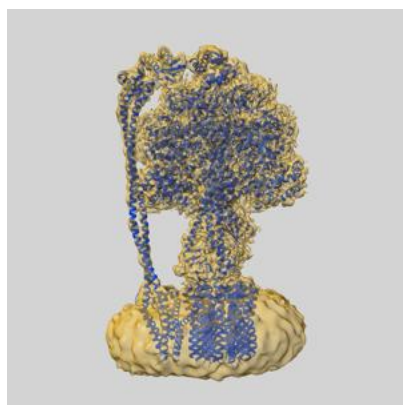
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.56	3.23
Unmasked-calculated*	3.90	6.23	3.98

*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 3.90 differs from the reported value 3.2 by more than 10 %

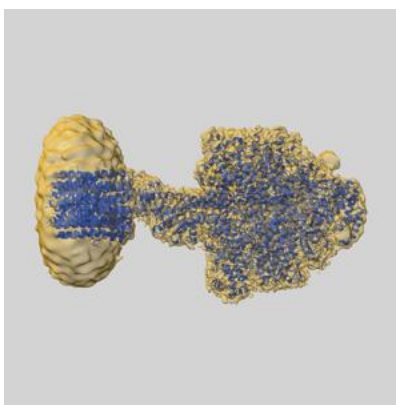
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9335 and PDB model 6N30. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

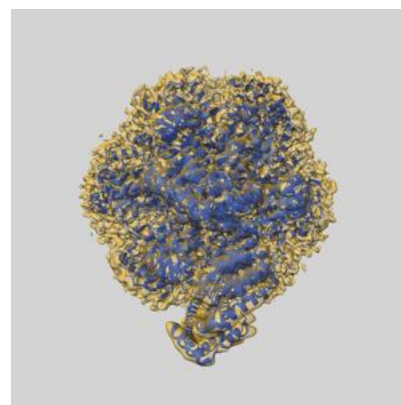
9.1 Map-model overlay [i](#)



X



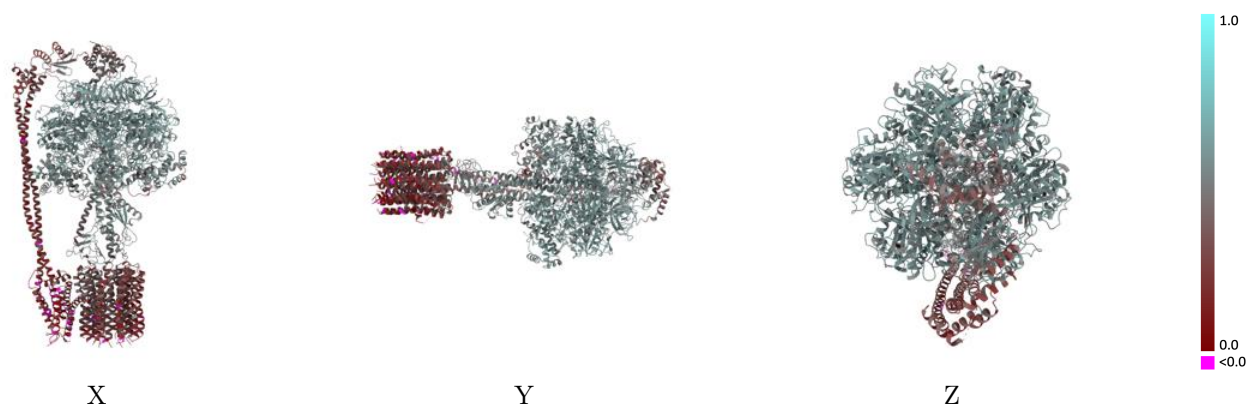
Y



Z

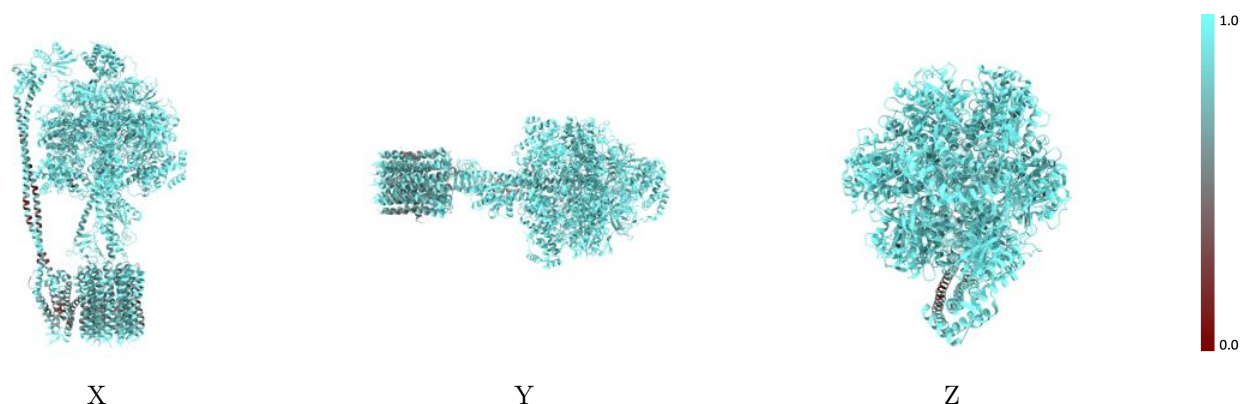
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



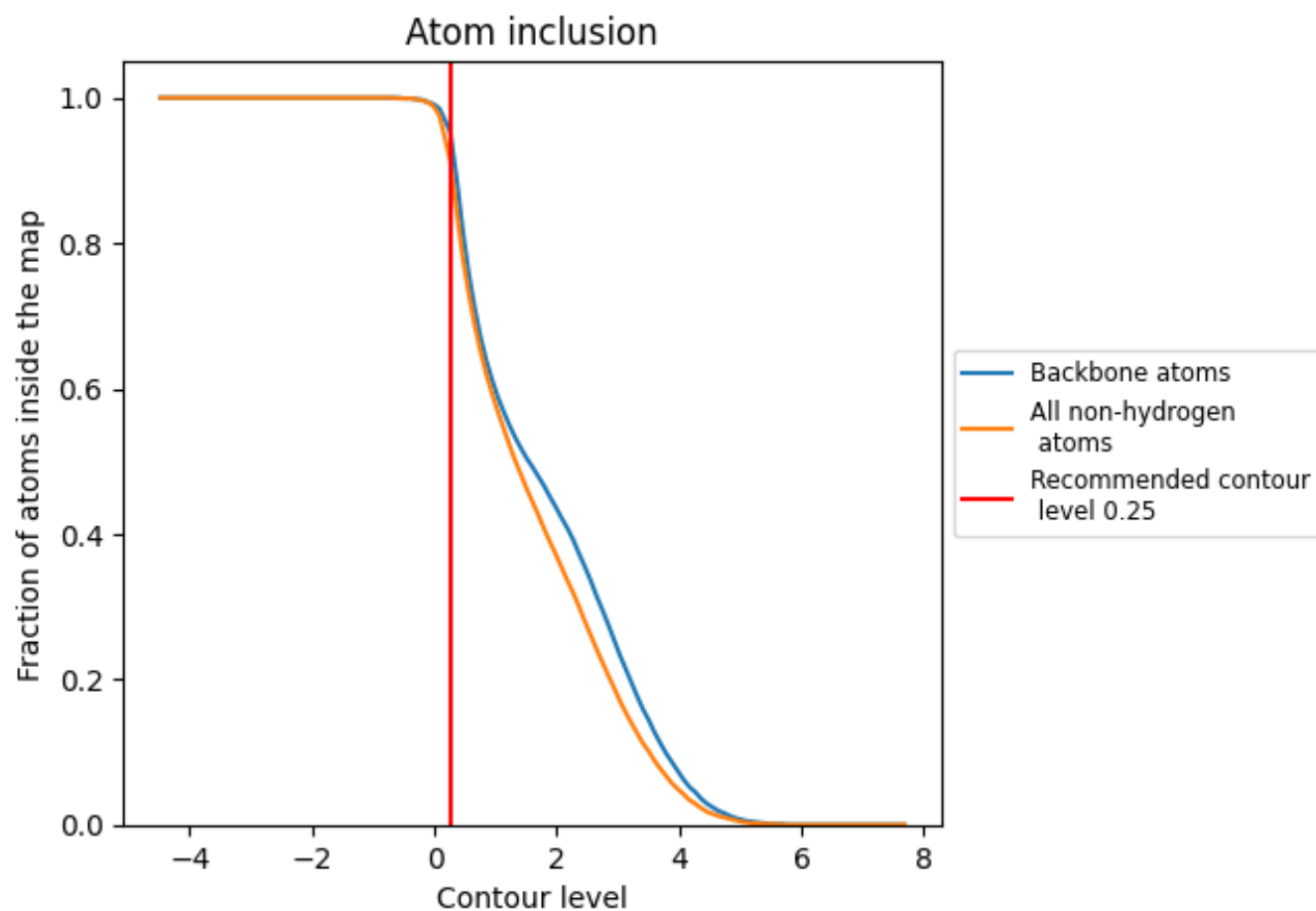
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9170	 0.4680
A	 0.9560	 0.5430
B	 0.9700	 0.5550
C	 0.9650	 0.5430
D	 0.9670	 0.5430
E	 0.9710	 0.5690
F	 0.9680	 0.5510
G	 0.9480	 0.5190
H	 0.9340	 0.4730
I	 0.9390	 0.4120
a	 0.7160	 0.1600
b1	 0.7830	 0.2050
b2	 0.6730	 0.2070
c0	 0.8090	 0.2420
c1	 0.7970	 0.2480
c2	 0.7950	 0.2640
c3	 0.8130	 0.3030
c4	 0.8270	 0.3230
c5	 0.8150	 0.3090
c6	 0.8290	 0.2960
c7	 0.7850	 0.2610
c8	 0.8050	 0.2570
c9	 0.7810	 0.2290

