



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 08:29 AM UTC

PDB ID : 8G0A / pdb_00008g0a
EMDB ID : EMD-29651
Title : Cryo-EM structure of SQ31f-bound Mycobacterium smegmatis ATP synthase rotational state 3
Authors : Courbon, G.M.; Rubinstein, J.L.
Deposited on : 2023-01-31
Resolution : 2.90 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:

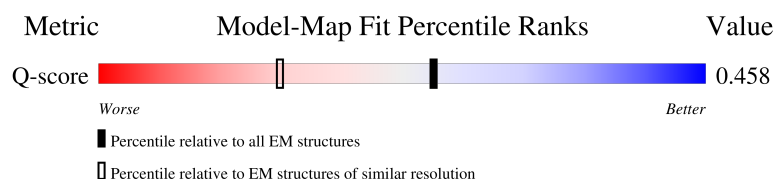
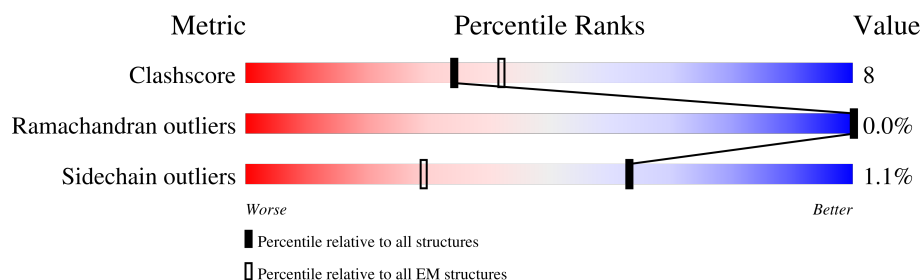
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	548	 79% 14% 6%
1	B	548	 81% 11% 7%
1	C	548	 85% 9% 6%
2	D	475	 84% 14% .

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Mol	Chain	Length	Quality of chain
2	E	475	 80% 17% ..
2	F	475	 78% 18% ..
3	G	307	 76% 15% • 9%
4	H	121	 69% 27% ..
5	b	170	 64% 16% • 17%
6	d	445	 76% 19% ..
7	1	86	 24% 80% 13% • 6%
7	2	86	 15% 80% 14% 6%
7	3	86	 10% 78% 16% 6%
7	4	86	 22% 73% 19% .. 6%
7	5	86	 28% 72% 21% • 6%
7	6	86	 24% 73% 21% 6%
7	7	86	 23% 81% 12% • 6%
7	8	86	 19% 76% 19% 6%
7	9	86	 23% 80% 13% • 6%
8	a	252	 22% 77% 16% 7%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 35630 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 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	514	Total	C	N	O	S	0	0
			3827	2413	671	733	10		
1	B	507	Total	C	N	O	S	0	0
			3733	2354	660	709	10		
1	C	514	Total	C	N	O	S	0	0
			3797	2403	673	711	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	464	Total	C	N	O	S	0	0
			3505	2222	609	661	13		
2	E	464	Total	C	N	O	S	0	0
			3508	2223	609	663	13		
2	F	464	Total	C	N	O	S	0	0
			3527	2232	609	673	13		

- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	279	Total	C	N	O	S	0	0
			2094	1322	391	375	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	117	Total	C	N	O		0	0
			838	531	159	148			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	141	Total	C	N	O	S	0	0
			941	593	177	170	1		

- Molecule 6 is a protein called ATP synthase subunit b-delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	433	Total	C	N	O	S	0	0
			2875	1805	549	518	3		

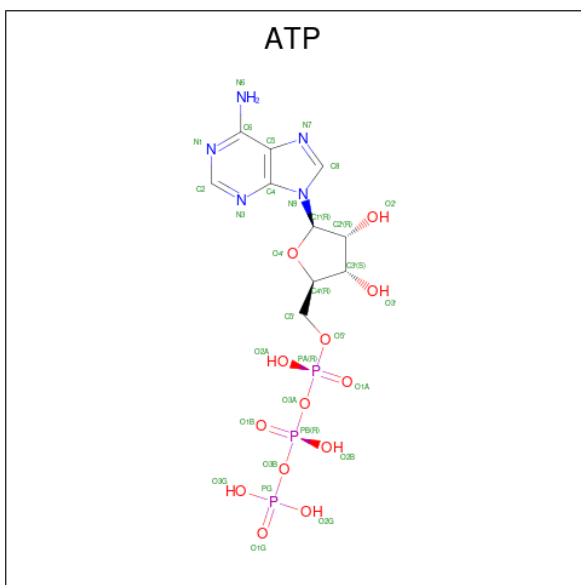
- Molecule 7 is a protein called ATP synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2	81	Total	C	N	O	S	0	0
			556	368	91	95	2		
7	3	81	Total	C	N	O	S	0	0
			554	367	89	96	2		
7	4	81	Total	C	N	O	S	0	0
			556	368	91	95	2		
7	5	81	Total	C	N	O	S	0	0
			560	370	92	96	2		
7	6	81	Total	C	N	O	S	0	0
			560	370	92	96	2		
7	7	81	Total	C	N	O	S	0	0
			560	370	92	96	2		
7	8	81	Total	C	N	O	S	0	0
			560	370	92	96	2		
7	9	81	Total	C	N	O	S	0	0
			556	368	91	95	2		
7	1	81	Total	C	N	O	S	0	0
			556	368	91	95	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	235	Total	C	N	O	S	0	0
			1808	1223	287	292	6		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

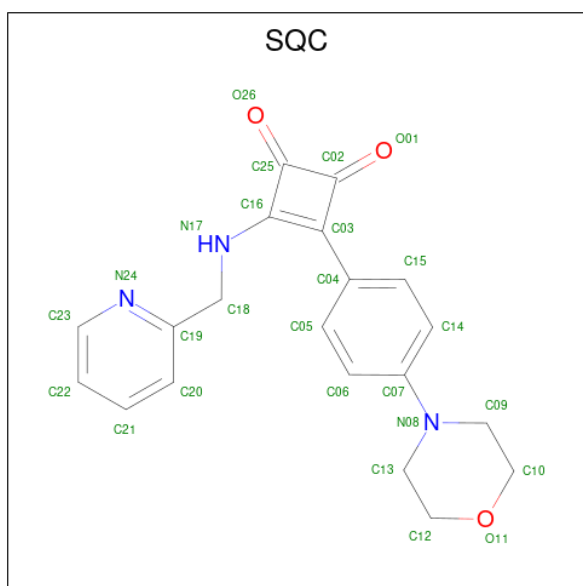
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	
10	B	1	Total	Mg	0
			1	1	
10	C	1	Total	Mg	0
			1	1	
10	E	1	Total	Mg	0
			1	1	

- Molecule 11 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
11	F	1	Total	O	P	0
			5	4	1	

- Molecule 12 is 3-[4-(morpholin-4-yl)phenyl]-4-[[pyridin-2-yl)methyl]amino}cyclobut-3-ene-1,2-dione (CCD ID: SQC) (formula: $C_{20}H_{19}N_3O_3$) (labeled as "Ligand of Interest" by depositor).

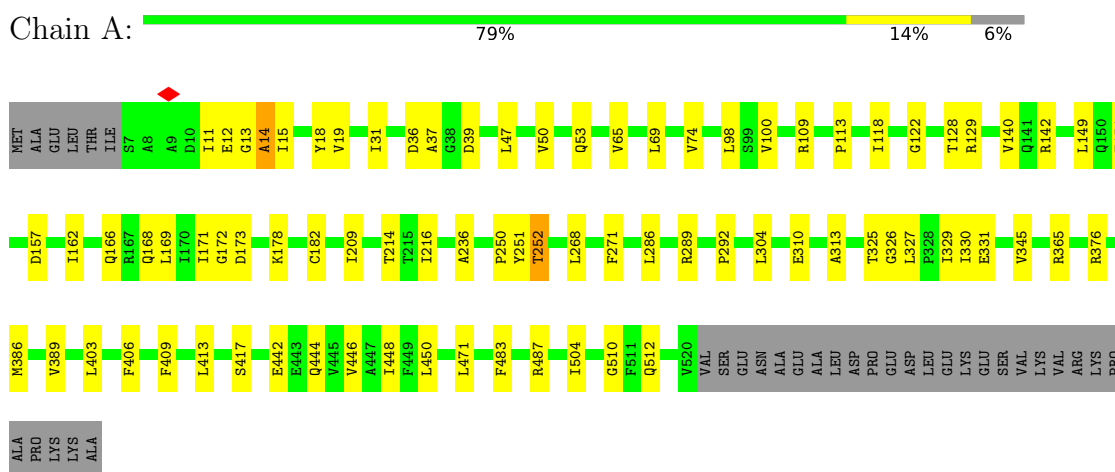


Mol	Chain	Residues	Atoms				AltConf
12	1	1	Total	C	N	O	0
			26	20	3	3	

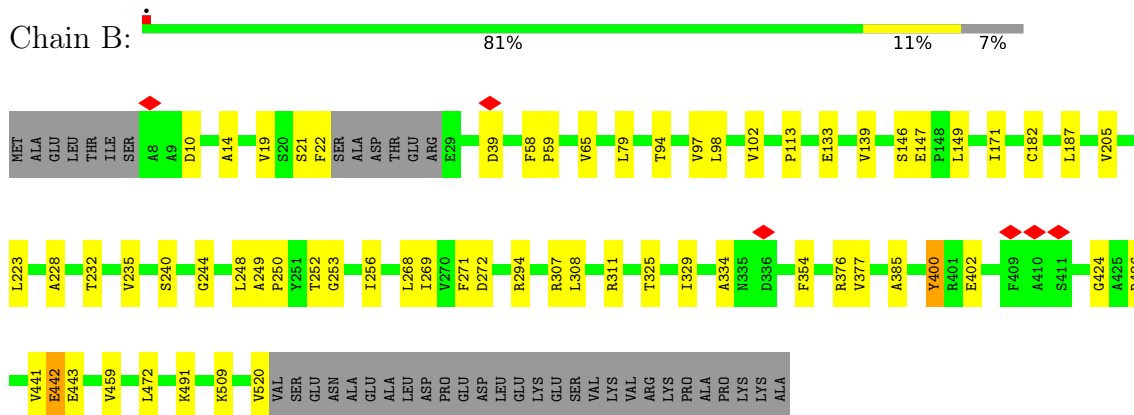
3 Residue-property plots

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.

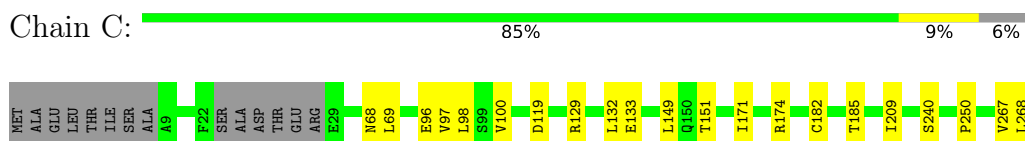
• Molecule 1: ATP synthase subunit alpha

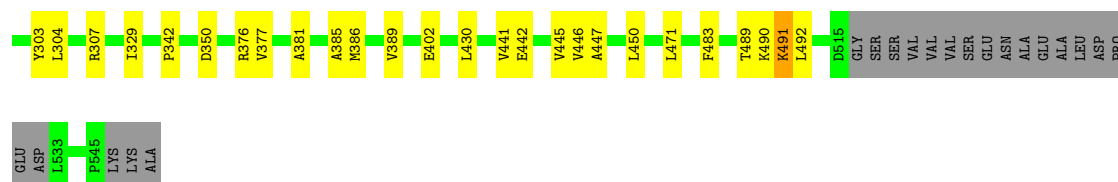


• Molecule 1: ATP synthase subunit alpha



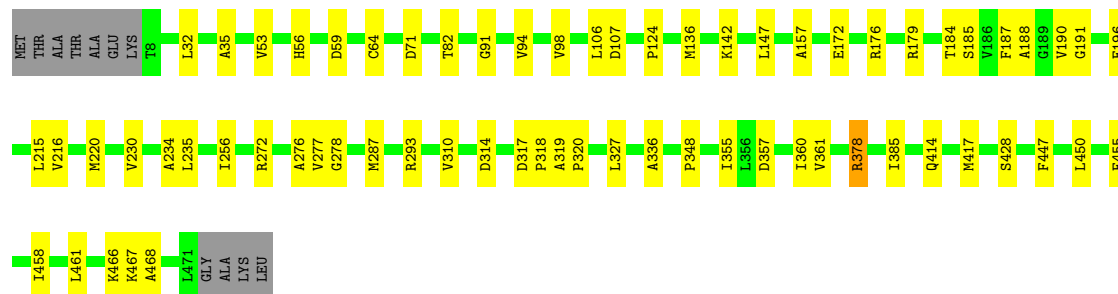
• Molecule 1: ATP synthase subunit alpha





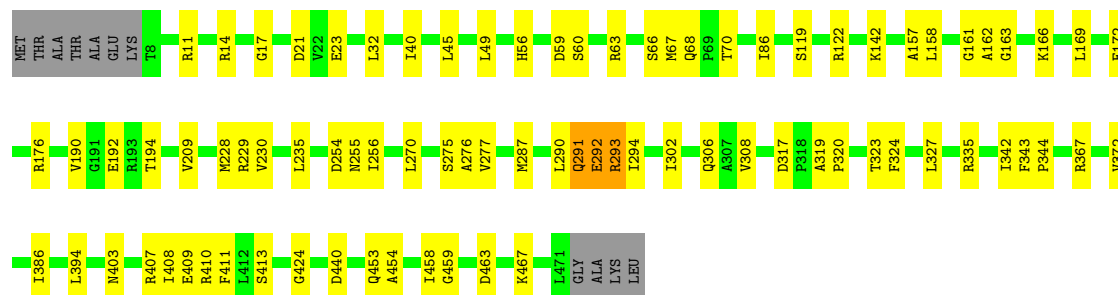
• Molecule 2: ATP synthase subunit beta

Chain D: 84% 14%



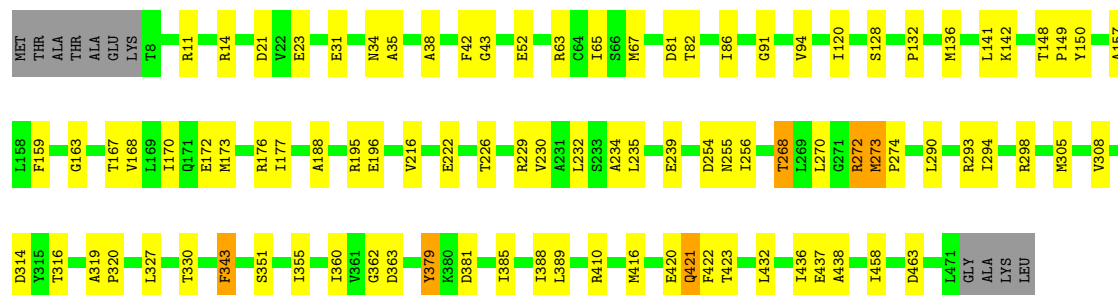
• Molecule 2: ATP synthase subunit beta

Chain E: 80% 17%



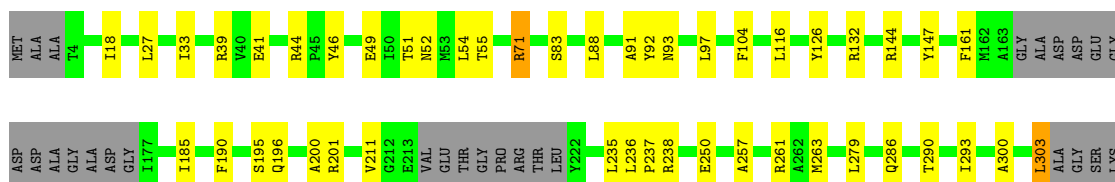
• Molecule 2: ATP synthase subunit beta

Chain F: 78% 18%

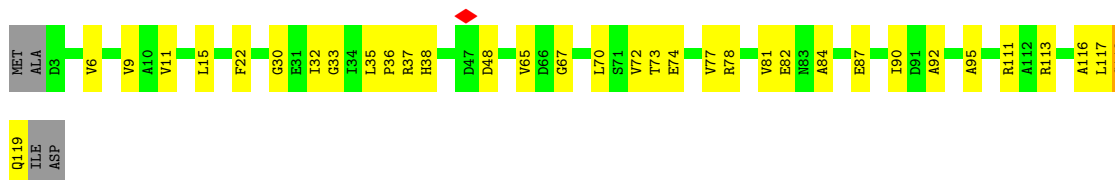


• Molecule 3: ATP synthase gamma chain

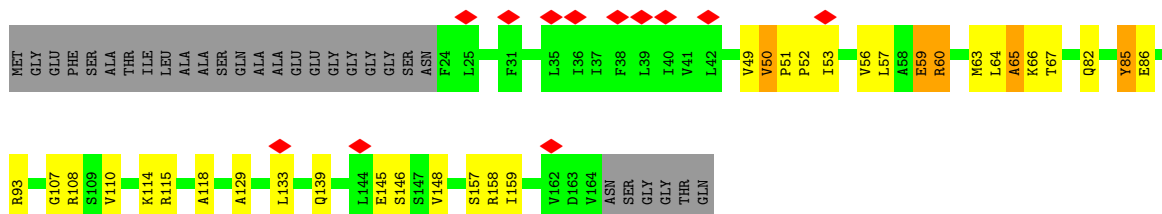
Chain G: 76% 15% 9%



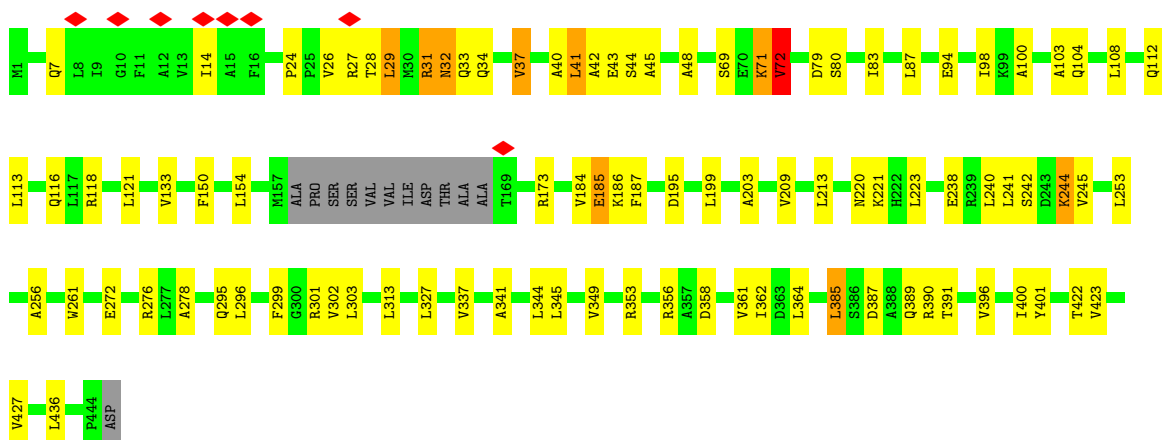
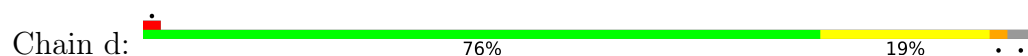
- Molecule 4: ATP synthase epsilon chain



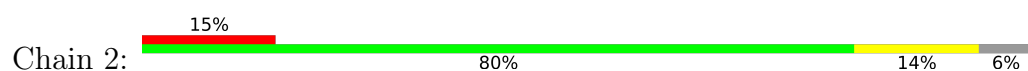
- Molecule 5: ATP synthase subunit b



- Molecule 6: ATP synthase subunit b-delta

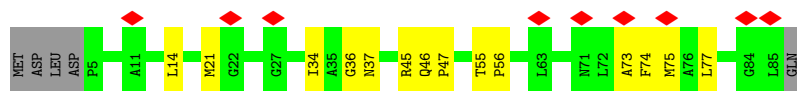
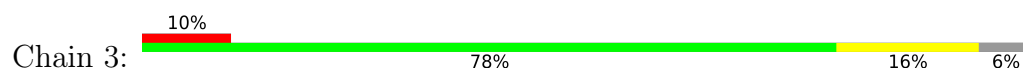


- Molecule 7: ATP synthase subunit c

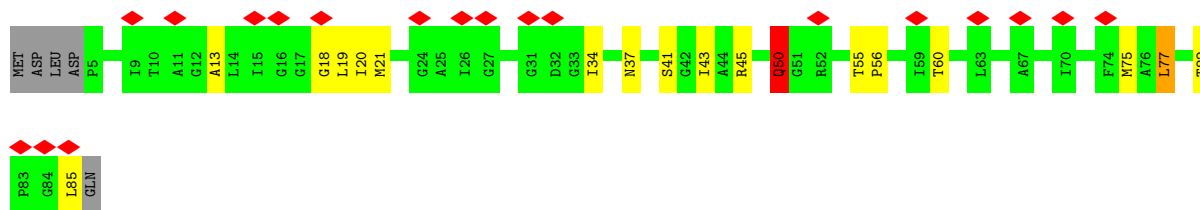
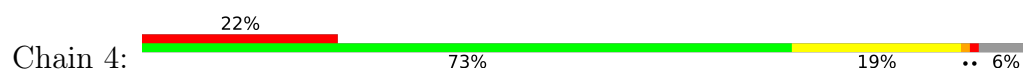




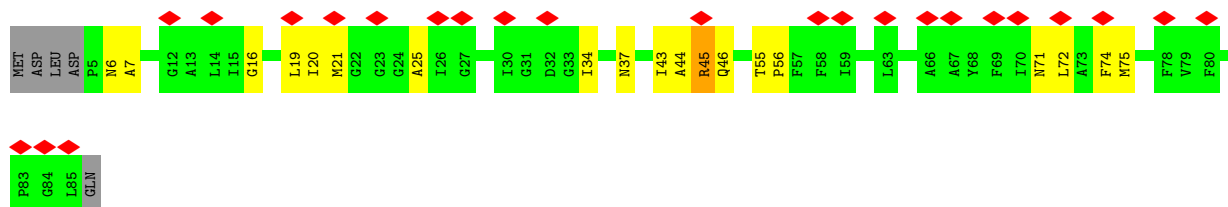
- Molecule 7: ATP synthase subunit c



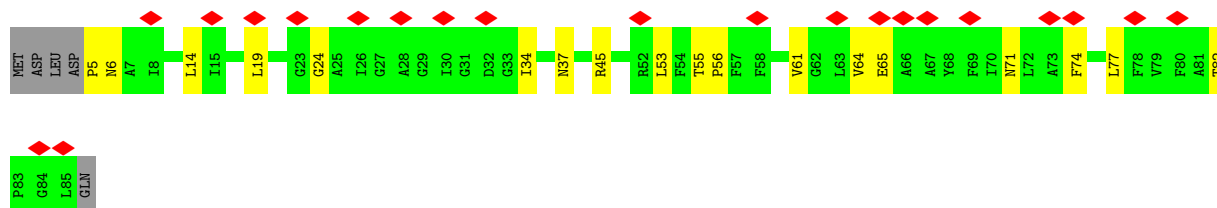
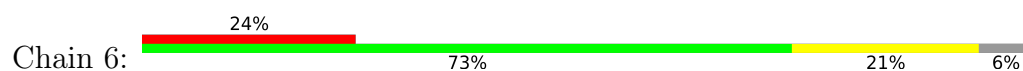
- Molecule 7: ATP synthase subunit c



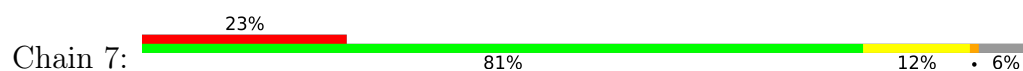
- Molecule 7: ATP synthase subunit c

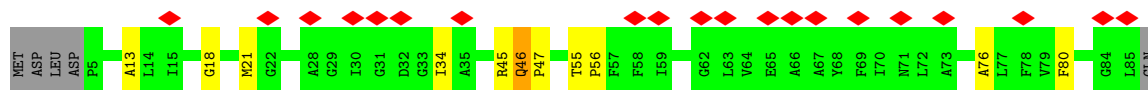


- Molecule 7: ATP synthase subunit c

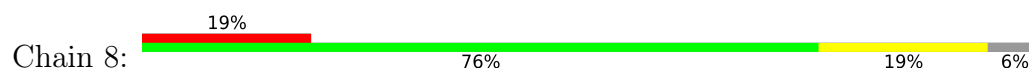


- Molecule 7: ATP synthase subunit c

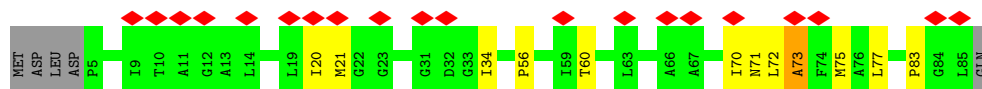
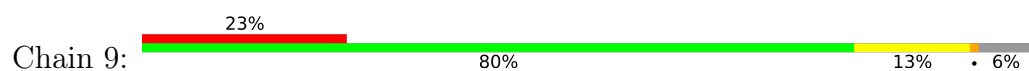




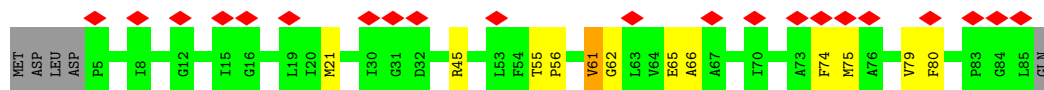
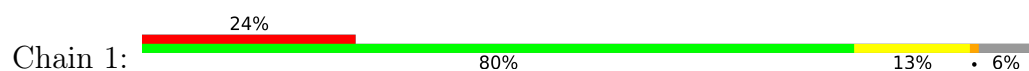
- Molecule 7: ATP synthase subunit c



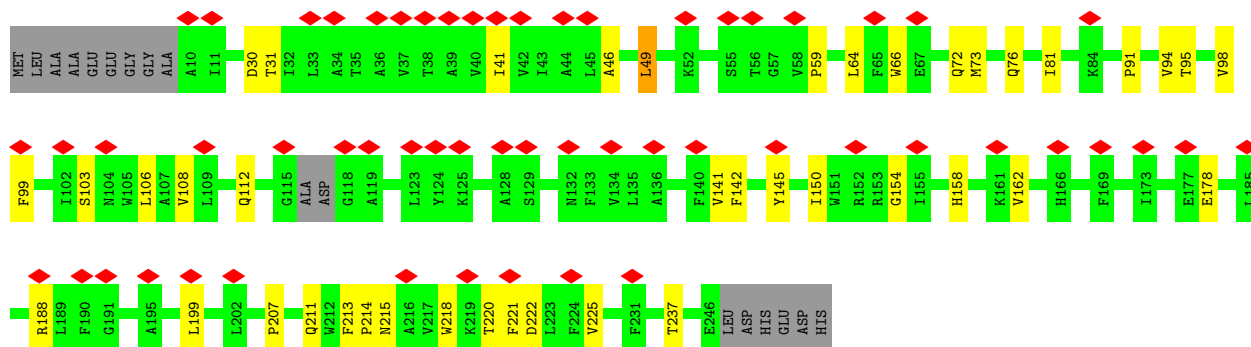
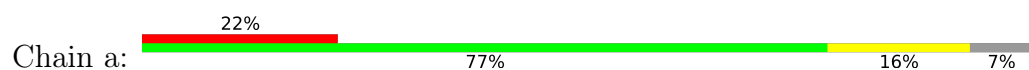
- Molecule 7: ATP synthase subunit c



- Molecule 7: ATP synthase subunit c



- Molecule 8: ATP synthase subunit a



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79965	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 ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.843	Depositor
Minimum map value	-1.052	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.096	Depositor
Recommended contour level	0.46	Depositor
Map size (Å)	329.59998, 329.59998, 329.59998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SQC, MG, ATP, 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	A	0.38	2/3887 (0.1%)	0.50	2/5266 (0.0%)
1	B	0.35	1/3790 (0.0%)	0.54	3/5137 (0.1%)
1	C	0.33	0/3856	0.51	0/5223
2	D	0.44	2/3570 (0.1%)	0.53	2/4845 (0.0%)
2	E	0.44	5/3573 (0.1%)	0.53	3/4849 (0.1%)
2	F	0.65	8/3592 (0.2%)	0.59	4/4873 (0.1%)
3	G	0.45	1/2122 (0.0%)	0.58	1/2872 (0.0%)
4	H	0.28	0/849	0.61	1/1158 (0.1%)
5	b	0.62	0/949	0.83	6/1291 (0.5%)
6	d	0.48	1/2900 (0.0%)	0.65	10/3963 (0.3%)
7	1	0.80	6/567 (1.1%)	0.59	1/769 (0.1%)
7	2	0.17	0/567	0.37	0/769
7	3	0.46	0/565	0.38	0/767
7	4	0.77	2/567 (0.4%)	0.63	0/769
7	5	0.88	4/571 (0.7%)	0.65	2/774 (0.3%)
7	6	0.58	2/571 (0.4%)	0.49	0/774
7	7	0.36	0/571	0.53	2/774 (0.3%)
7	8	0.24	0/571	0.42	0/774
7	9	0.54	1/567 (0.2%)	0.40	0/769
8	a	0.52	2/1860 (0.1%)	0.45	0/2543
All	All	0.47	37/36065 (0.1%)	0.55	37/48959 (0.1%)

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	272	ARG	CA-C	-8.08	1.43	1.52
2	E	454	ALA	CA-C	-8.04	1.41	1.52
8	a	221	PHE	C-O	-7.90	1.14	1.24
7	6	6	ASN	C-O	-7.74	1.15	1.24
2	F	379	TYR	CA-C	-7.37	1.42	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	118	GLY	N-CA-C	-9.14	103.32	115.21
1	B	10	ASP	N-CA-C	-9.01	101.37	111.82
2	D	467	LYS	N-CA-C	-7.71	103.89	113.38
2	E	293	ARG	N-CA-C	-7.71	104.11	113.97
6	d	98	ILE	N-CA-C	7.30	118.09	110.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3827	0	3831	60	0
1	B	3733	0	3707	53	0
1	C	3797	0	3796	34	0
2	D	3505	0	3491	44	0
2	E	3508	0	3492	70	0
2	F	3527	0	3511	70	0
3	G	2094	0	2121	44	0
4	H	838	0	813	36	0
5	b	941	0	907	35	0
6	d	2875	0	2735	83	0
7	1	556	0	571	10	0
7	2	556	0	571	13	0
7	3	554	0	566	21	0
7	4	556	0	571	16	0
7	5	560	0	577	16	0
7	6	560	0	577	14	0
7	7	560	0	577	11	0
7	8	560	0	577	16	0
7	9	556	0	571	14	0
8	a	1808	0	1858	34	0
9	A	31	0	12	0	0
9	B	31	0	12	0	0
9	C	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	31	0	12	3	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	E	1	0	0	0	0
11	F	5	0	0	0	0
12	1	26	0	0	1	0
All	All	35630	0	35468	575	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 8.

The worst 5 of 575 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:B:249:ALA:O	1:B:252:THR:HG22	1.52	1.09
1:B:235:VAL:HG11	1:B:252:THR:CG2	1.86	1.04
1:B:235:VAL:HG11	1:B:252:THR:HG21	1.57	0.84
7:7:45:ARG:HG2	7:7:46:GLN:HG3	1.62	0.82
2:F:148:THR:HG21	2:F:351:SER:OG	1.80	0.80

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/548 (93%)	500 (98%)	11 (2%)	1 (0%)	43	72
1	B	503/548 (92%)	489 (97%)	14 (3%)	0	100	100
1	C	508/548 (93%)	493 (97%)	15 (3%)	0	100	100
2	D	462/475 (97%)	453 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	462/475 (97%)	449 (97%)	13 (3%)	0	100	100
2	F	462/475 (97%)	453 (98%)	9 (2%)	0	100	100
3	G	273/307 (89%)	270 (99%)	3 (1%)	0	100	100
4	H	115/121 (95%)	113 (98%)	2 (2%)	0	100	100
5	b	139/170 (82%)	136 (98%)	2 (1%)	1 (1%)	18	48
6	d	429/445 (96%)	419 (98%)	10 (2%)	0	100	100
7	1	79/86 (92%)	77 (98%)	2 (2%)	0	100	100
7	2	79/86 (92%)	74 (94%)	5 (6%)	0	100	100
7	3	79/86 (92%)	78 (99%)	1 (1%)	0	100	100
7	4	79/86 (92%)	76 (96%)	3 (4%)	0	100	100
7	5	79/86 (92%)	79 (100%)	0	0	100	100
7	6	79/86 (92%)	78 (99%)	1 (1%)	0	100	100
7	7	79/86 (92%)	77 (98%)	2 (2%)	0	100	100
7	8	79/86 (92%)	77 (98%)	2 (2%)	0	100	100
7	9	79/86 (92%)	77 (98%)	2 (2%)	0	100	100
8	a	231/252 (92%)	226 (98%)	5 (2%)	0	100	100
All	All	4807/5138 (94%)	4694 (98%)	111 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	b	65	ALA
1	A	11	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/441 (90%)	393 (99%)	3 (1%)	73	90
1	B	377/441 (86%)	376 (100%)	1 (0%)	86	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	383/441 (87%)	380 (99%)	3 (1%)	73	90
2	D	367/388 (95%)	365 (100%)	2 (0%)	81	93
2	E	368/388 (95%)	368 (100%)	0	100	100
2	F	373/388 (96%)	368 (99%)	5 (1%)	61	86
3	G	202/238 (85%)	200 (99%)	2 (1%)	68	89
4	H	73/96 (76%)	72 (99%)	1 (1%)	59	85
5	b	75/124 (60%)	67 (89%)	8 (11%)	6	22
6	d	228/347 (66%)	221 (97%)	7 (3%)	35	69
7	1	49/56 (88%)	49 (100%)	0	100	100
7	2	49/56 (88%)	49 (100%)	0	100	100
7	3	49/56 (88%)	49 (100%)	0	100	100
7	4	49/56 (88%)	46 (94%)	3 (6%)	17	46
7	5	50/56 (89%)	48 (96%)	2 (4%)	28	62
7	6	50/56 (89%)	49 (98%)	1 (2%)	48	78
7	7	50/56 (89%)	50 (100%)	0	100	100
7	8	50/56 (89%)	50 (100%)	0	100	100
7	9	49/56 (88%)	49 (100%)	0	100	100
8	a	184/200 (92%)	183 (100%)	1 (0%)	81	93
All	All	3471/3996 (87%)	3432 (99%)	39 (1%)	63	88

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	d	71	LYS
7	5	45	ARG
6	d	72	VAL
7	4	21	MET
7	6	45	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	400	GLN
7	9	71	ASN
2	E	425	GLN

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Mol	Chain	Res	Type
7	3	46	GLN
2	E	326	HIS

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$
9	ATP	A	600	10	32,33,33	0.41	0	48,52,52	0.68	0
9	ATP	E	600	10	32,33,33	0.51	0	48,52,52	0.69	0
9	ATP	C	600	10	32,33,33	0.47	0	48,52,52	0.67	0
12	SQC	1	601	-	28,29,29	1.81	6 (21%)	39,40,40	1.18	2 (5%)
11	PO4	F	600	-	4,4,4	1.04	0	6,6,6	0.44	0
9	ATP	B	600	10	32,33,33	0.39	0	48,52,52	0.67	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
9	ATP	A	600	10	-	3/22/38/38	0/3/3/3
9	ATP	E	600	10	-	8/22/38/38	0/3/3/3
9	ATP	C	600	10	-	10/22/38/38	0/3/3/3
12	SQC	1	601	-	-	4/13/37/37	0/4/4/4
9	ATP	B	600	10	-	6/22/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	1	601	SQC	C16-N17	6.01	1.46	1.33
12	1	601	SQC	C03-C02	3.23	1.53	1.45
12	1	601	SQC	C07-N08	3.09	1.47	1.38
12	1	601	SQC	C16-C25	3.04	1.52	1.47
12	1	601	SQC	C04-C03	2.96	1.55	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	1	601	SQC	C23-N24-C19	2.89	121.46	117.41
12	1	601	SQC	C22-C21-C20	-2.45	117.21	120.24

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	600	ATP	PB-O3B-PG-O2G
9	A	600	ATP	C5'-O5'-PA-O1A
9	B	600	ATP	PB-O3B-PG-O3G
9	C	600	ATP	C5'-O5'-PA-O2A
9	E	600	ATP	C5'-O5'-PA-O2A

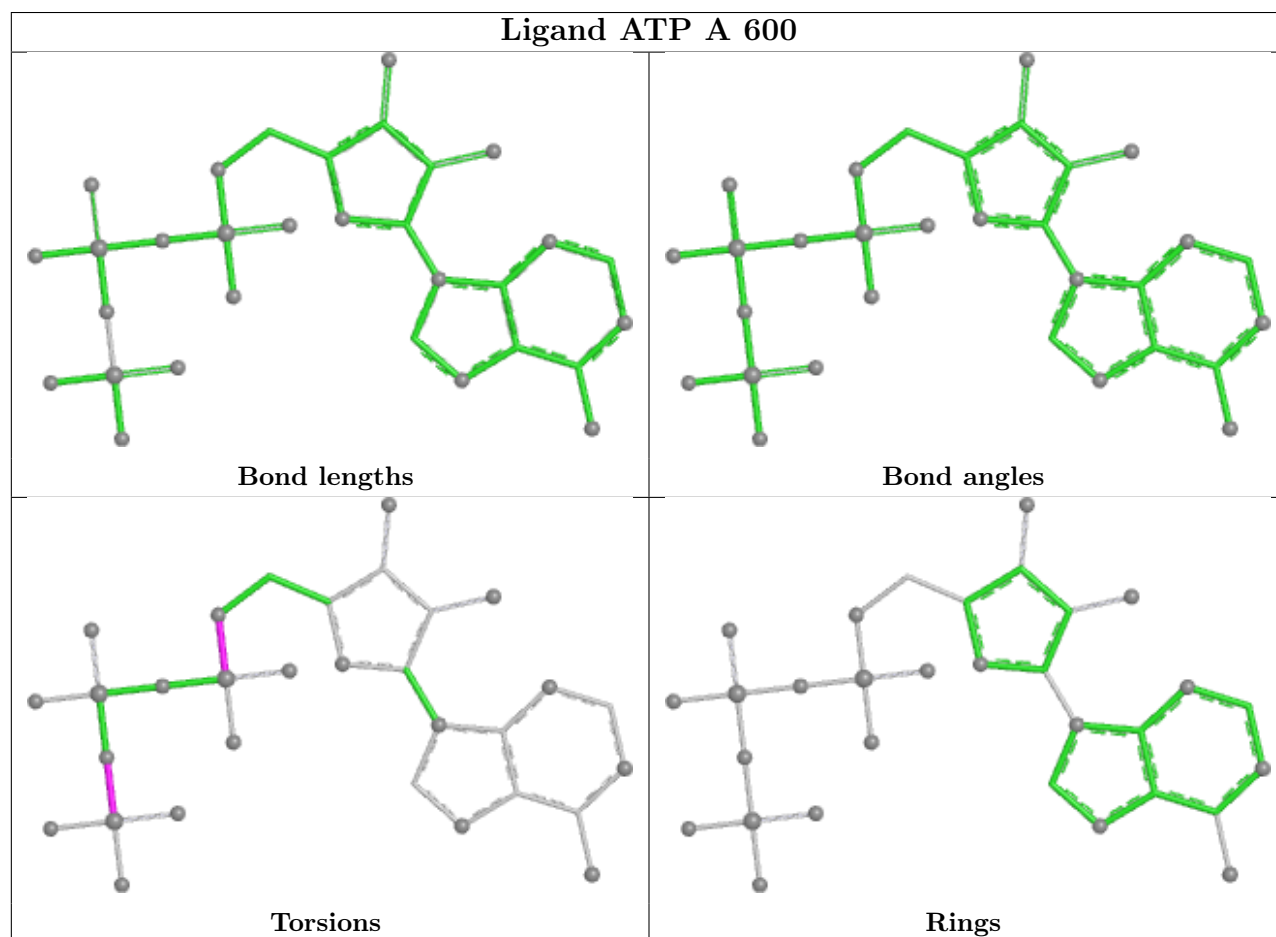
There are no ring outliers.

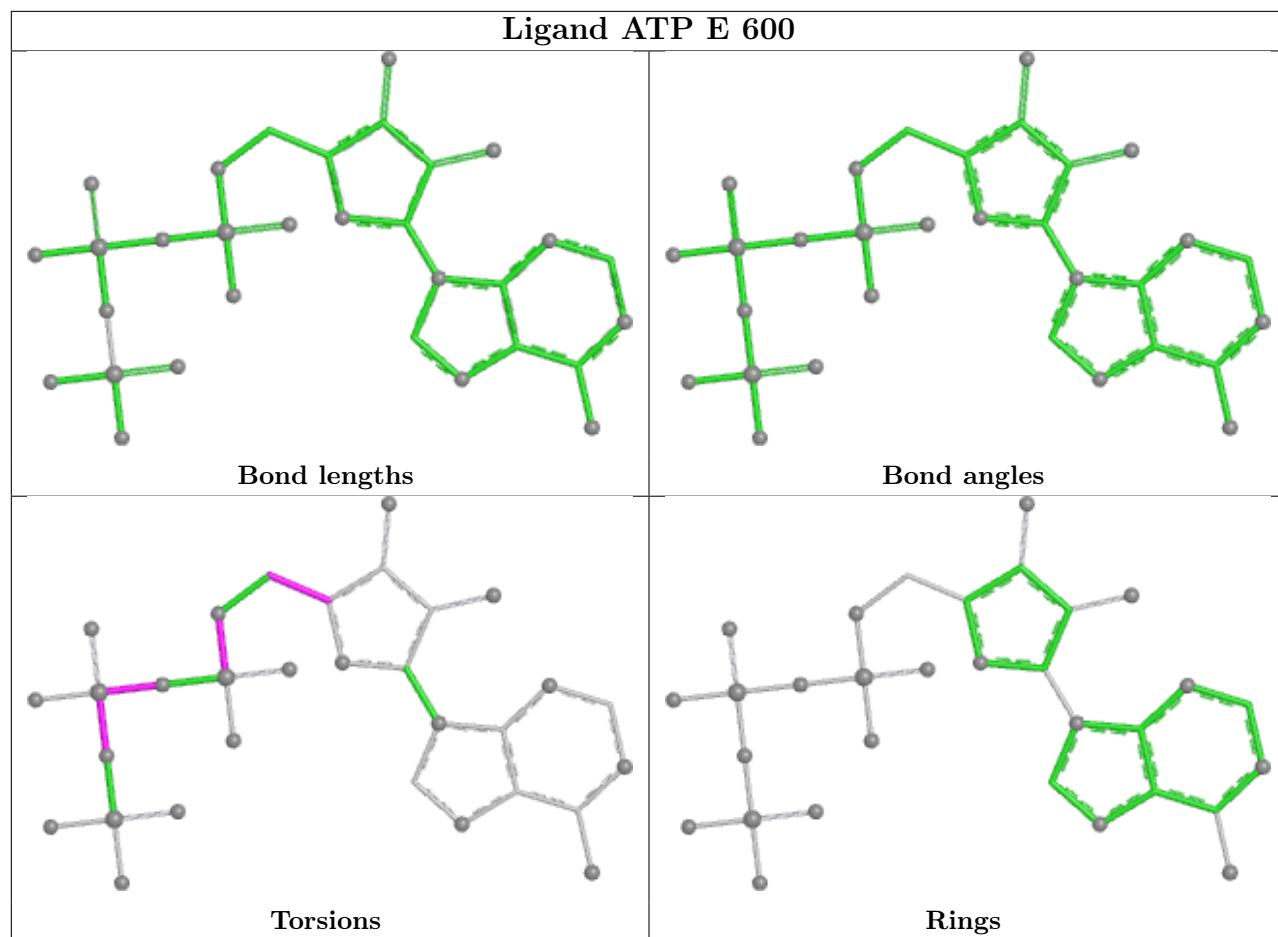
2 monomers are involved in 4 short contacts:

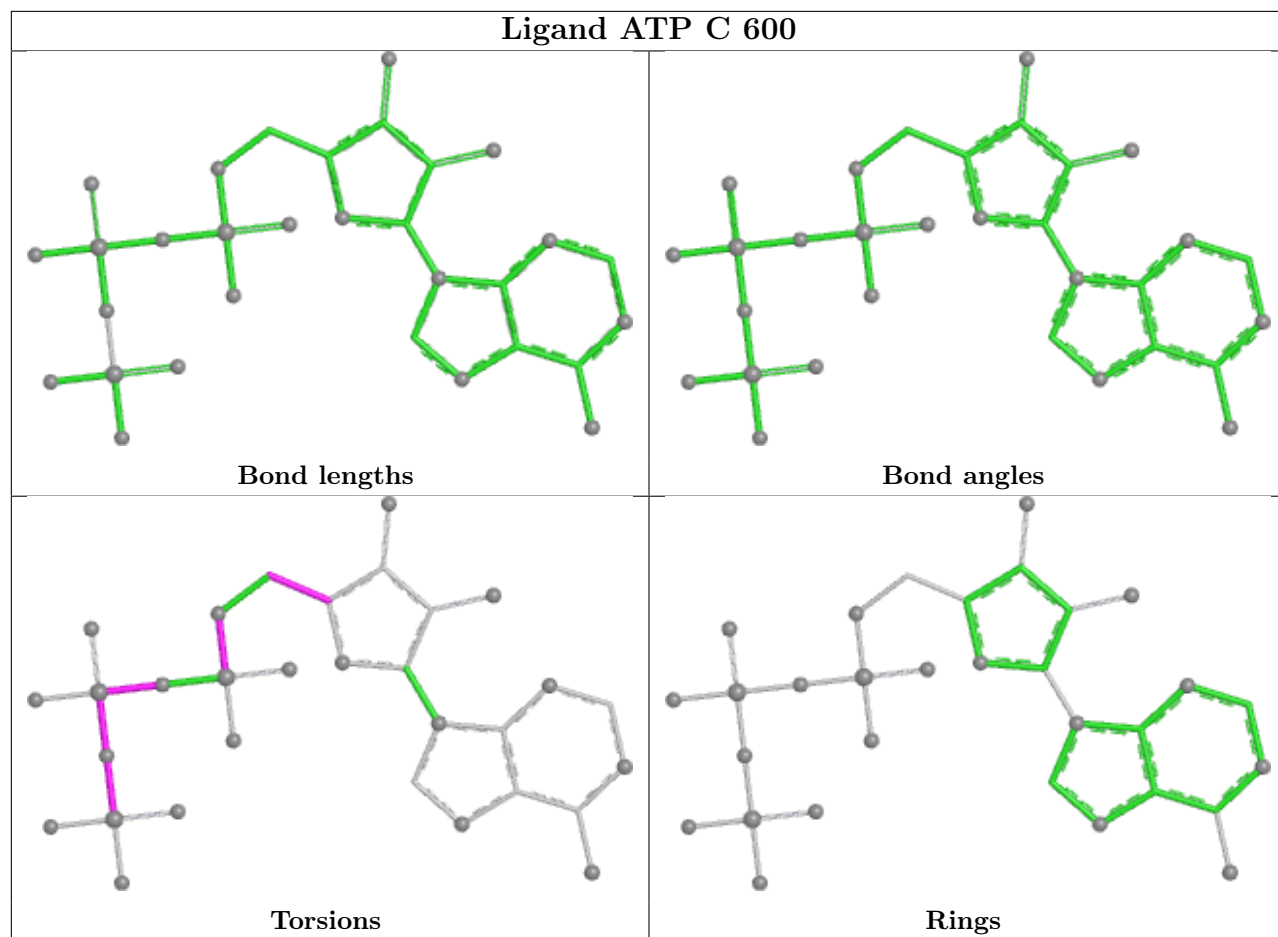
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	600	ATP	3	0
12	1	601	SQC	1	0

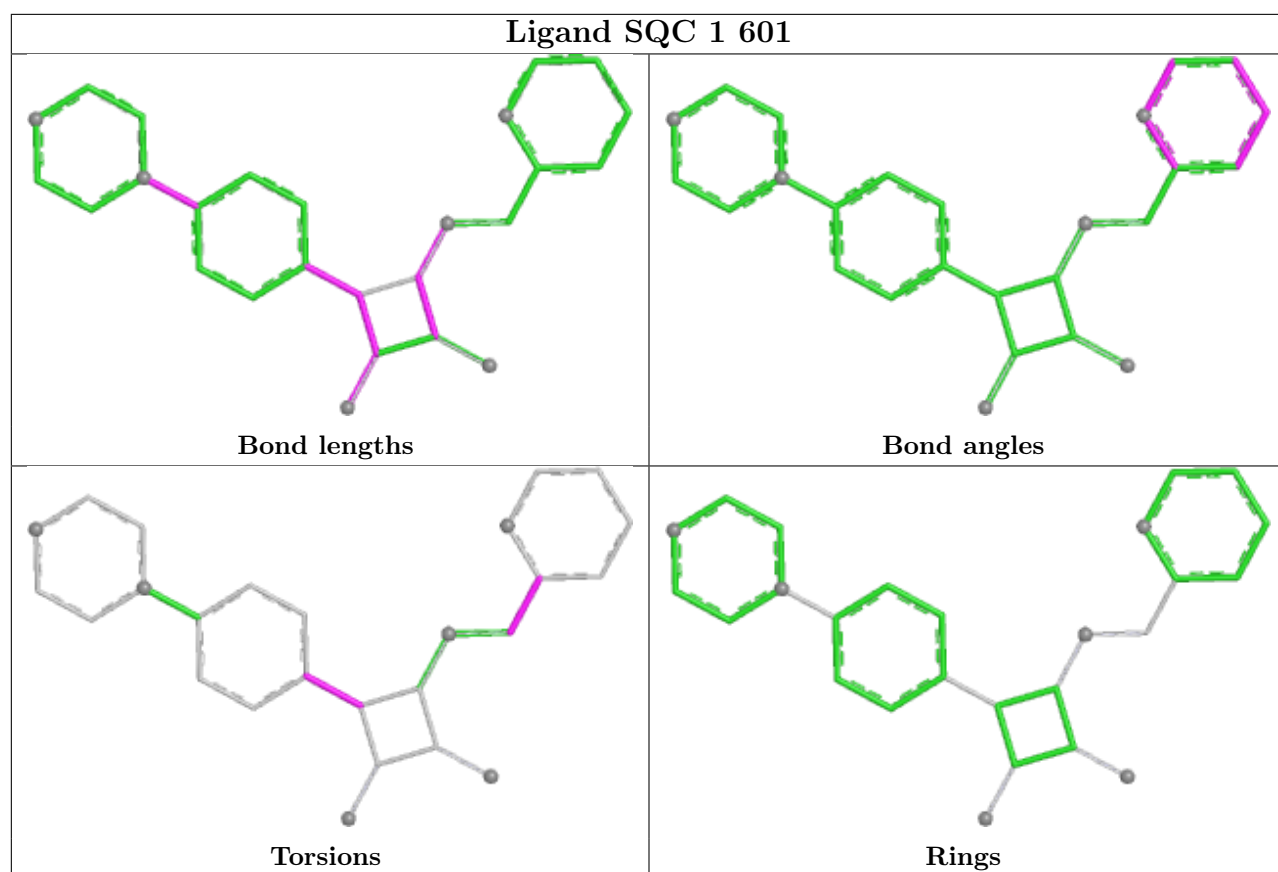
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

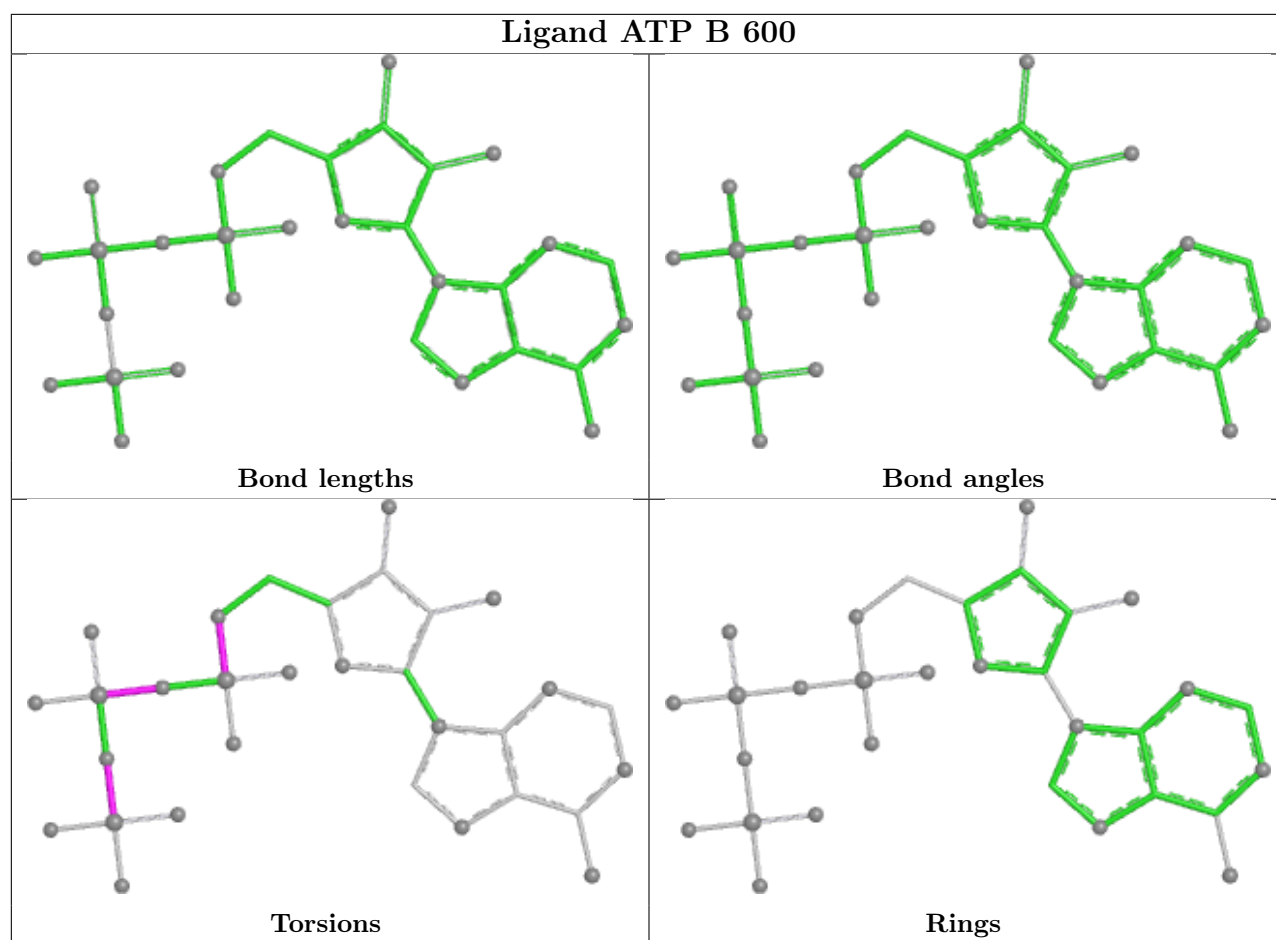
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

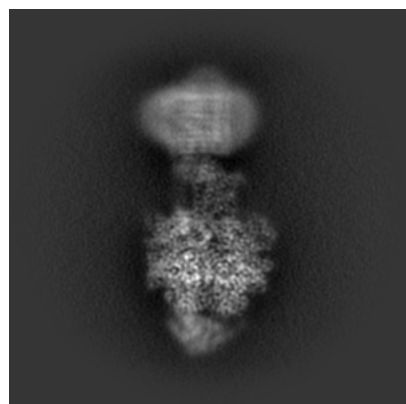
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29651. These allow visual inspection of the internal detail of the map and identification of artifacts.

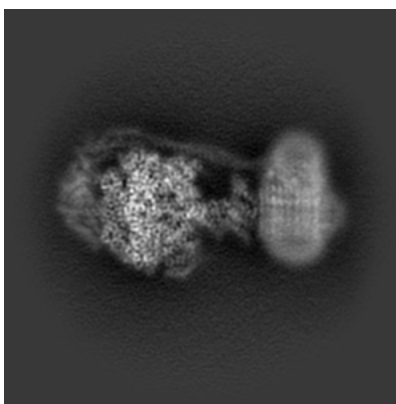
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

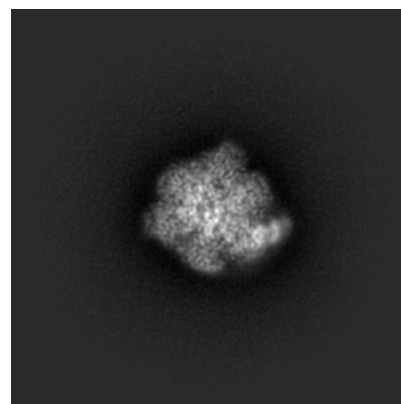
6.1.1 Primary map



X

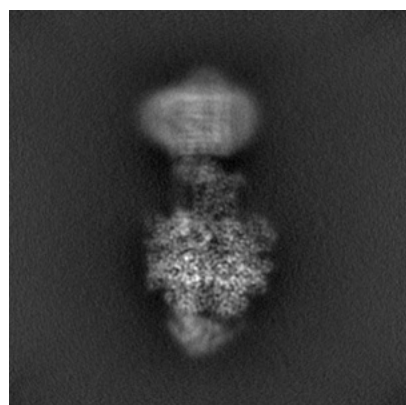


Y

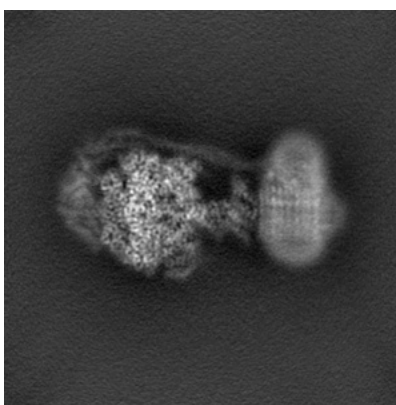


Z

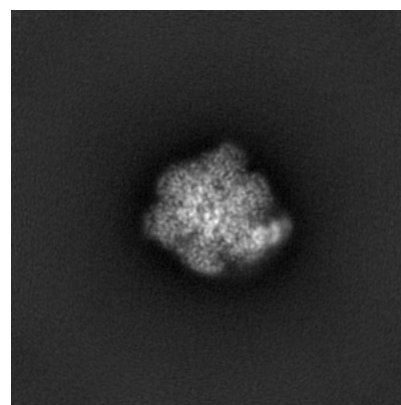
6.1.2 Raw map



X



Y

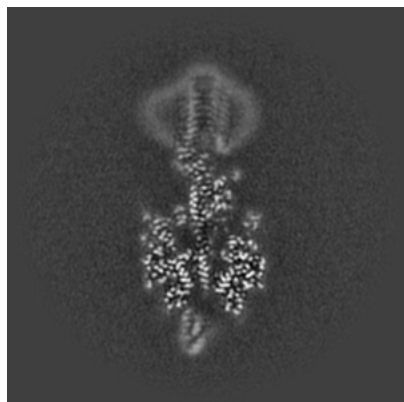


Z

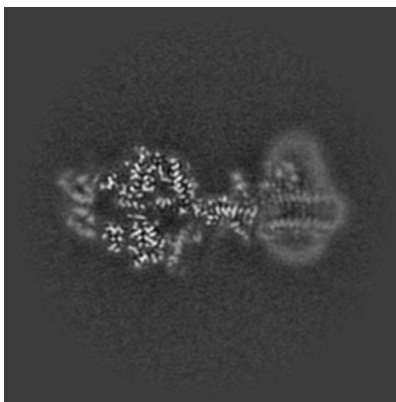
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

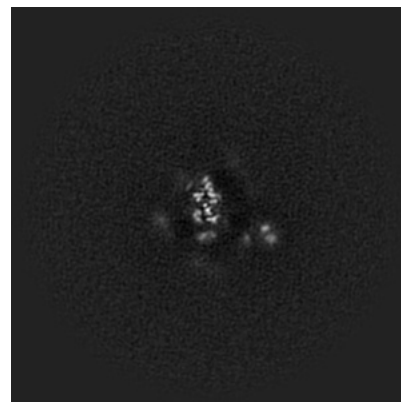
6.2.1 Primary map



X Index: 160

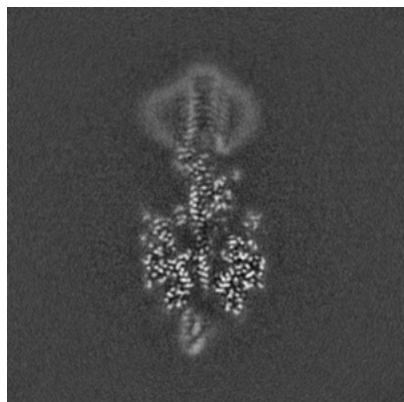


Y Index: 160

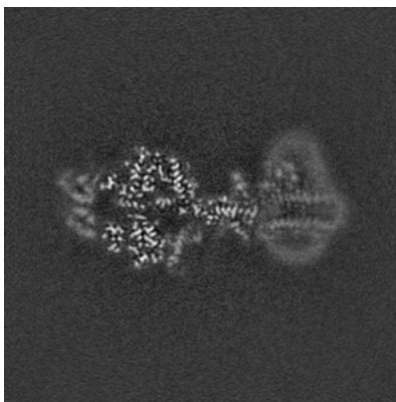


Z Index: 160

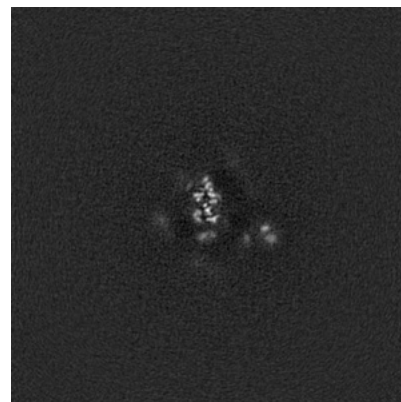
6.2.2 Raw map



X Index: 160



Y Index: 160

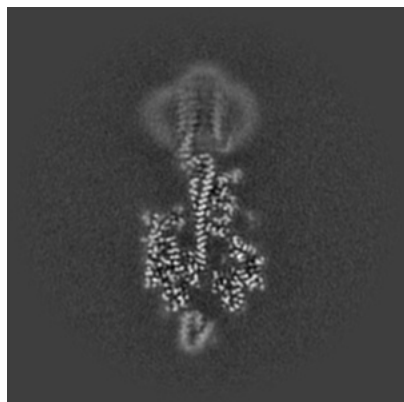


Z Index: 160

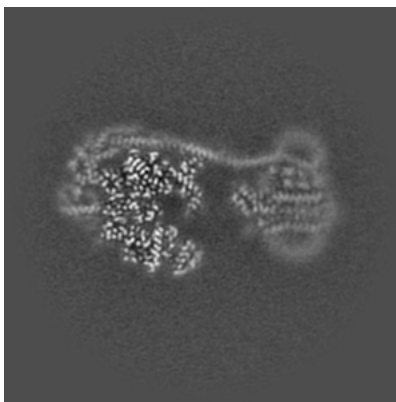
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

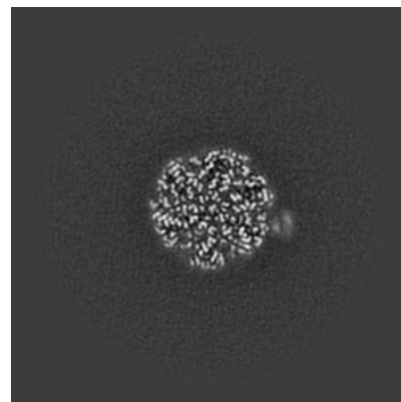
6.3.1 Primary map



X Index: 157

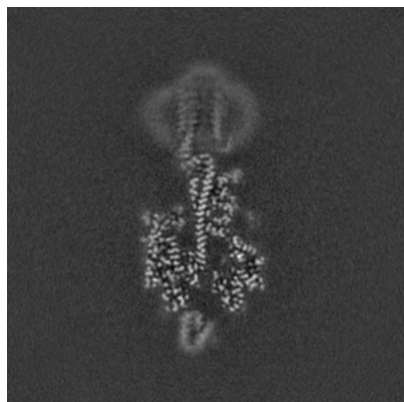


Y Index: 142

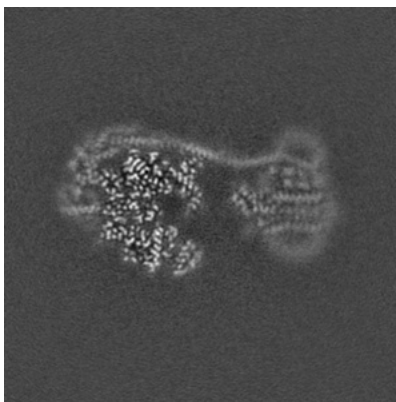


Z Index: 105

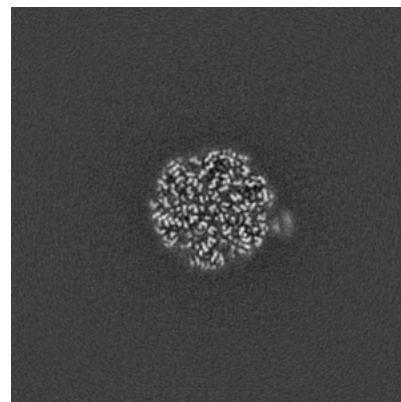
6.3.2 Raw map



X Index: 157



Y Index: 142

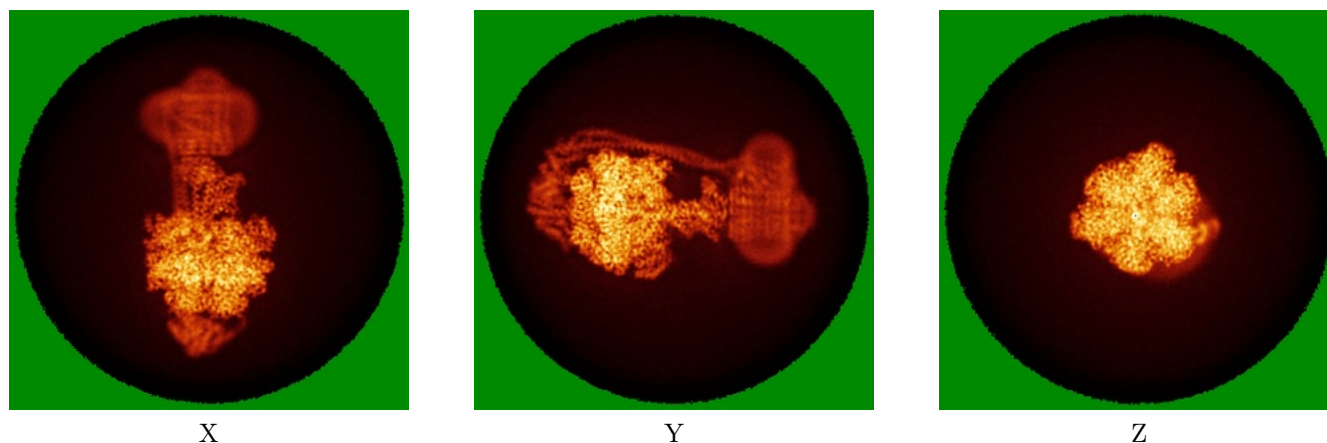


Z Index: 105

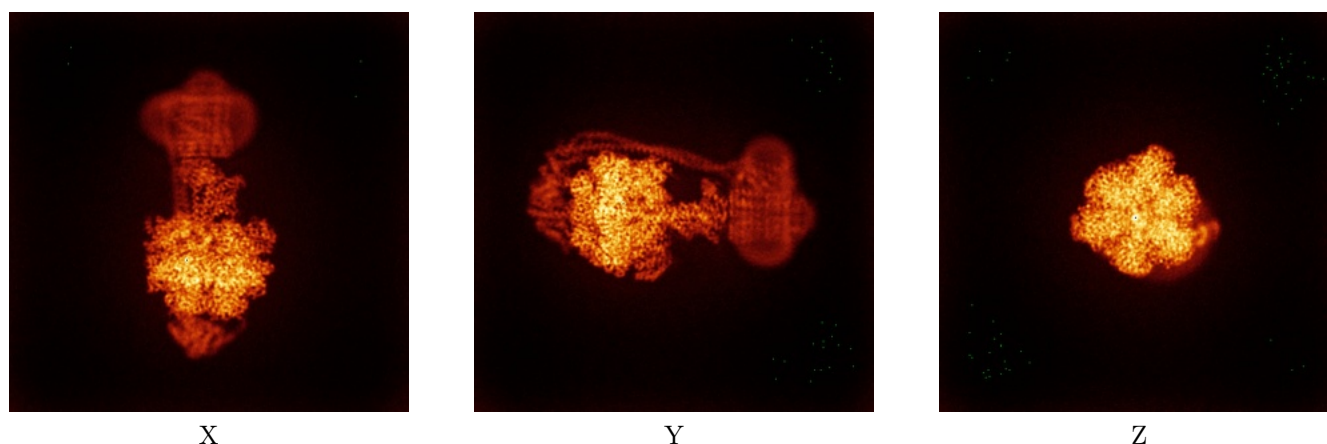
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

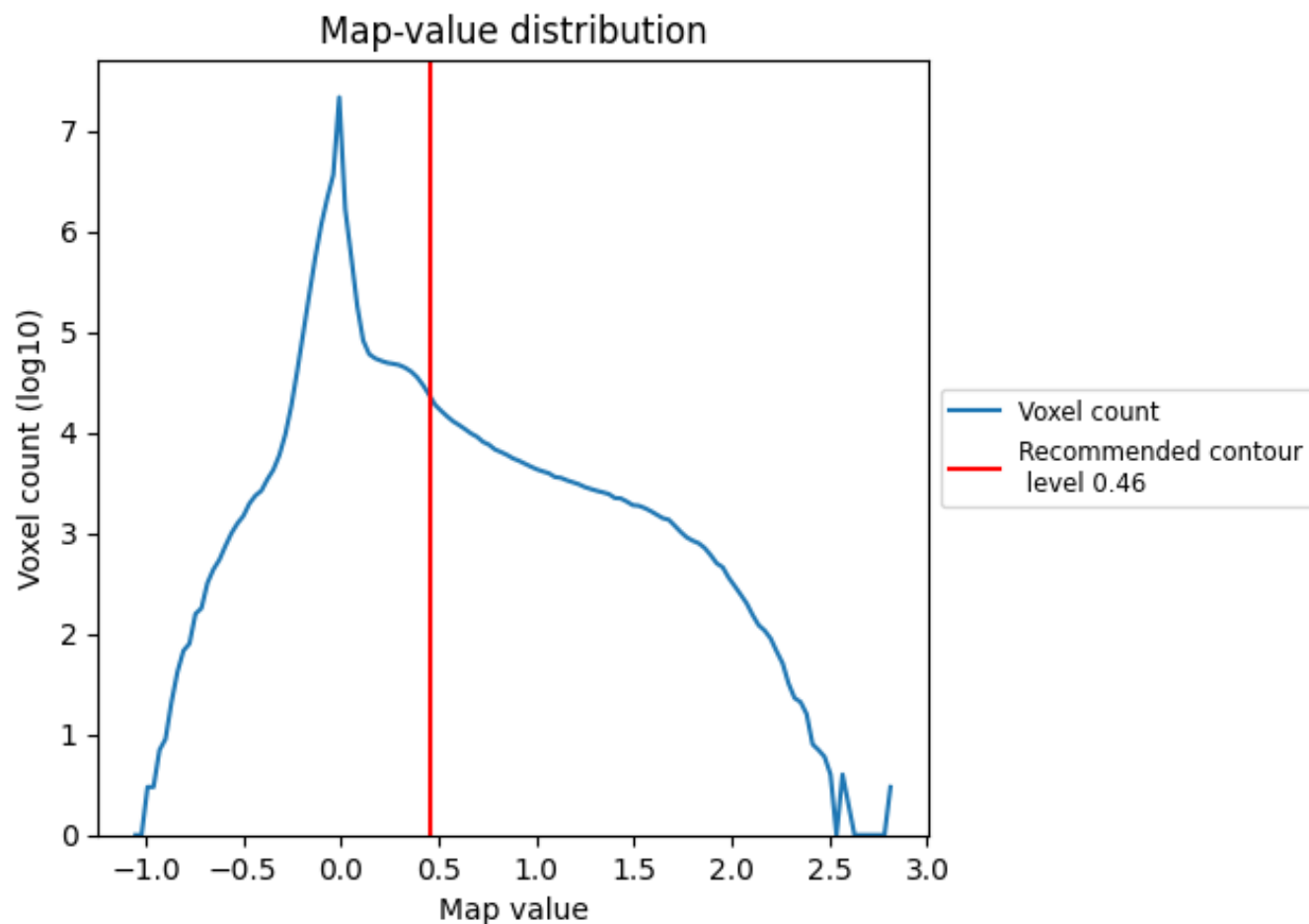
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

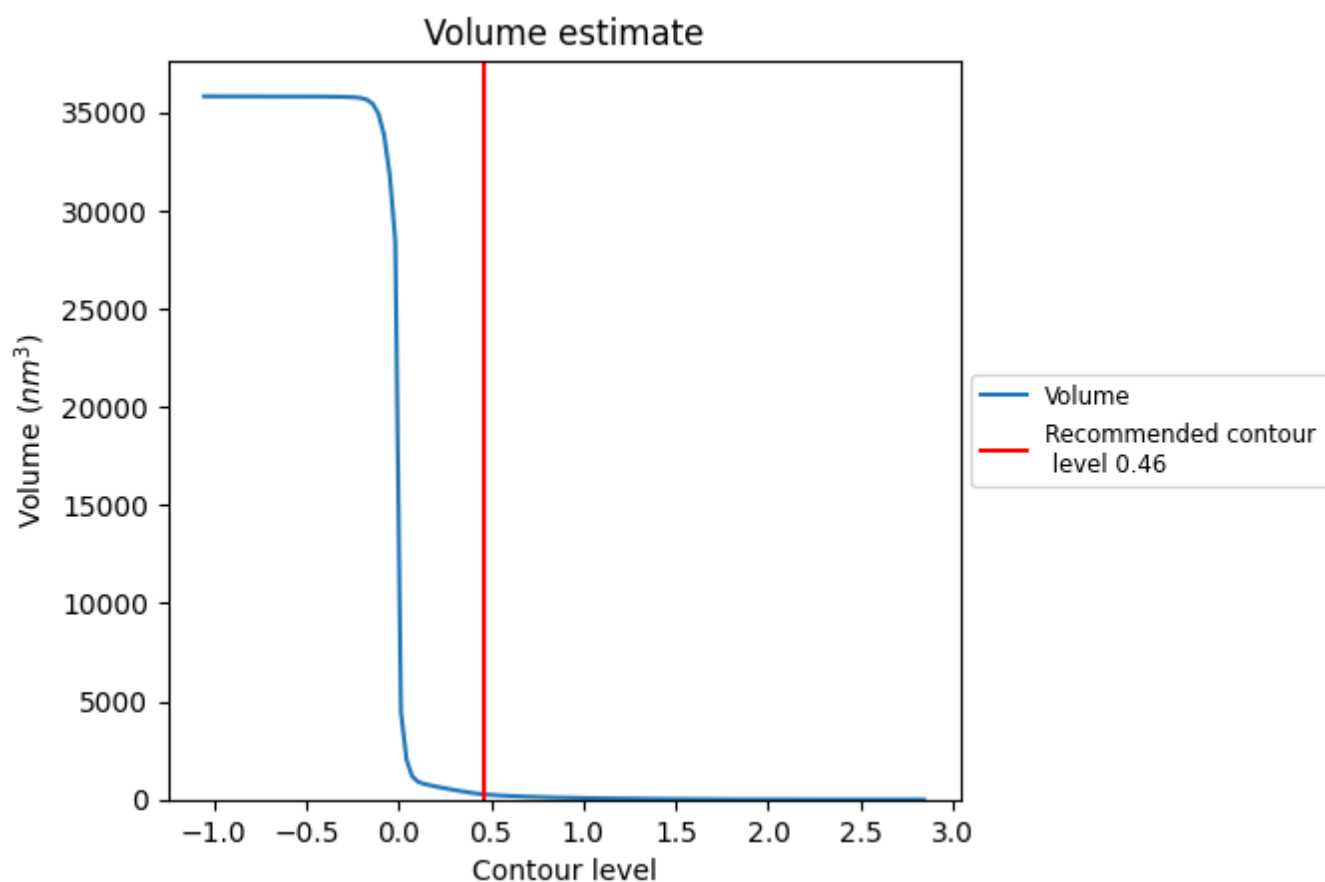
This section contains the results of statistical analysis of the map.

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.

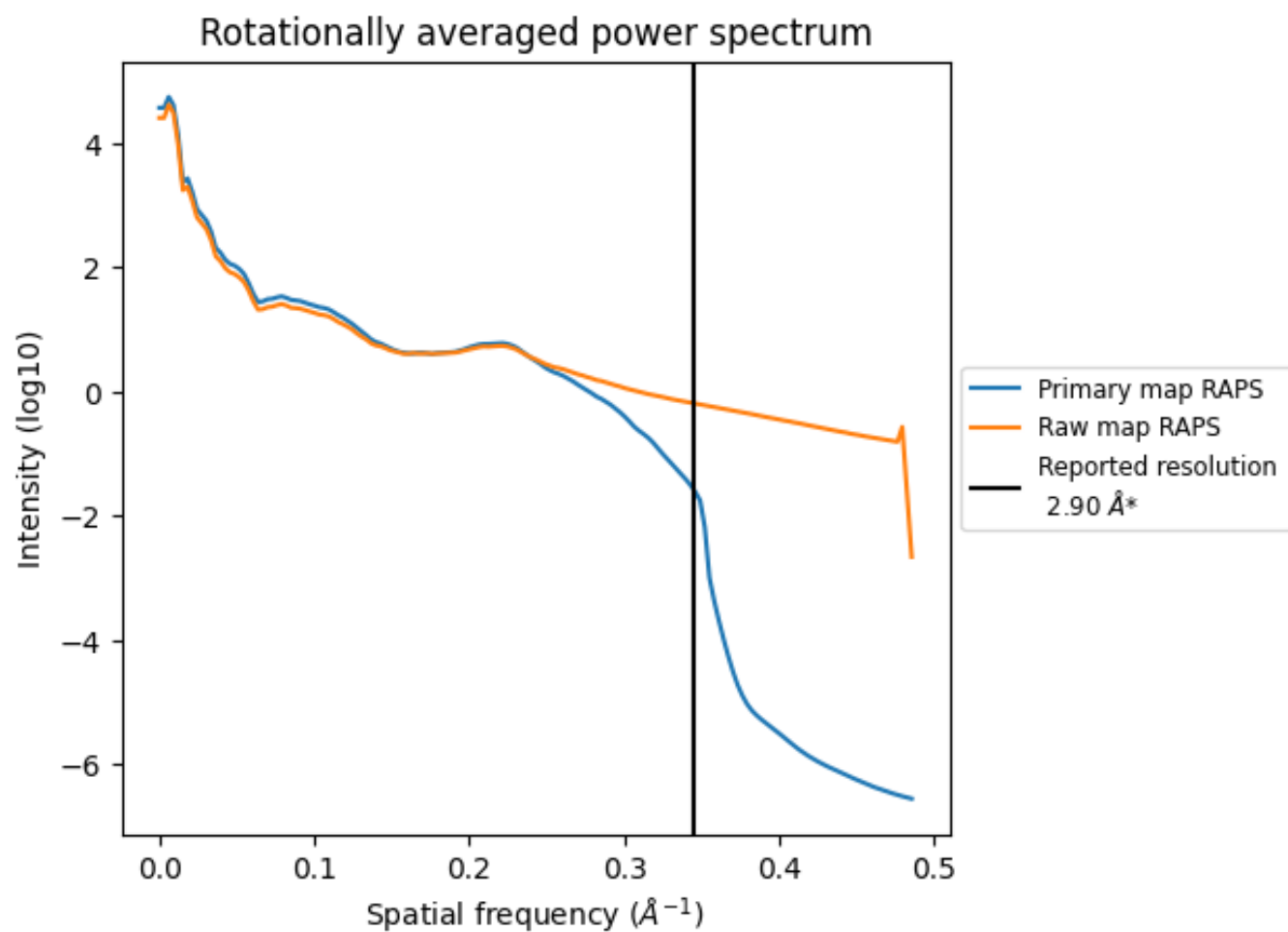
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 269 nm³; this corresponds to an approximate mass of 243 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 ⓘ

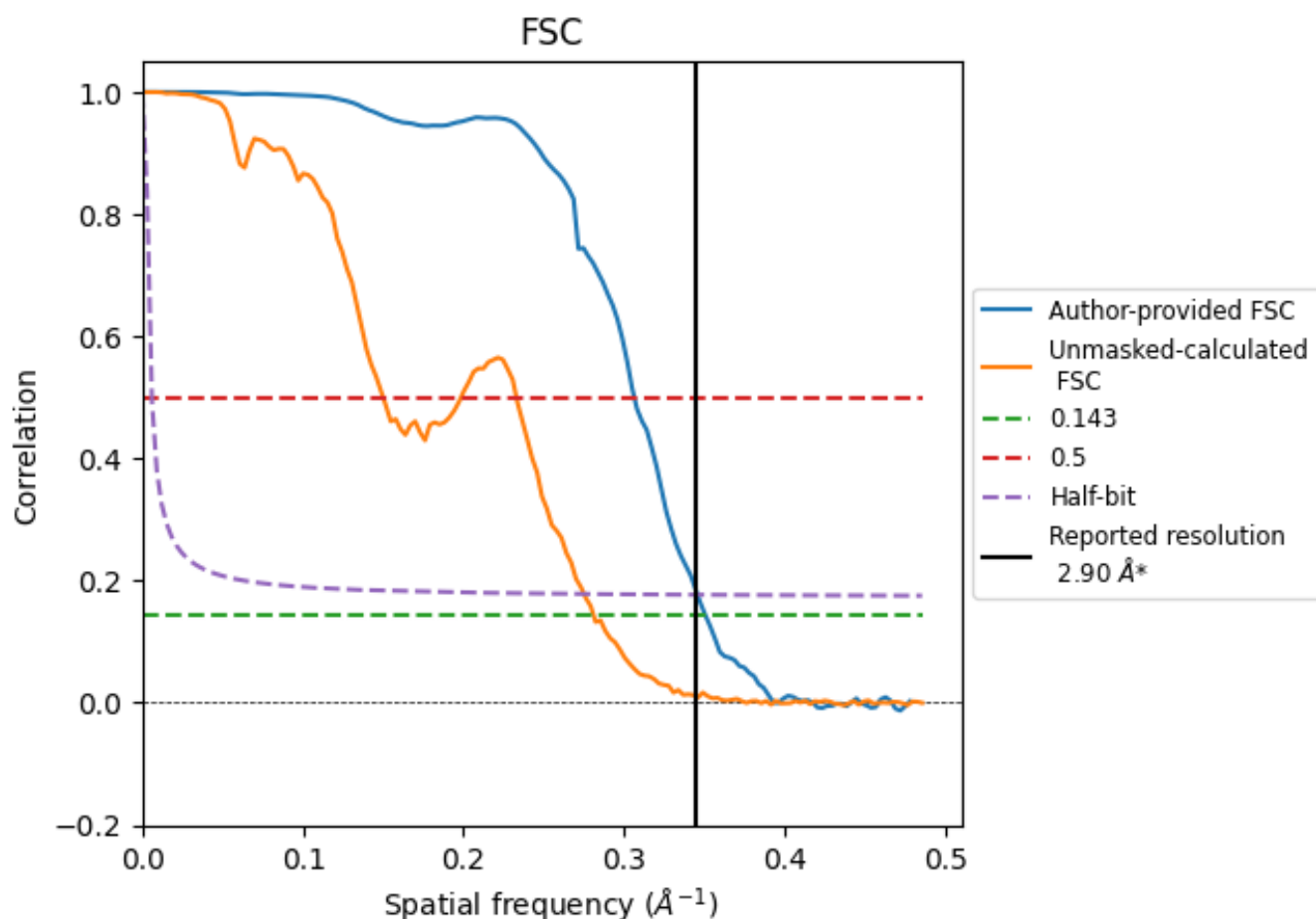


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

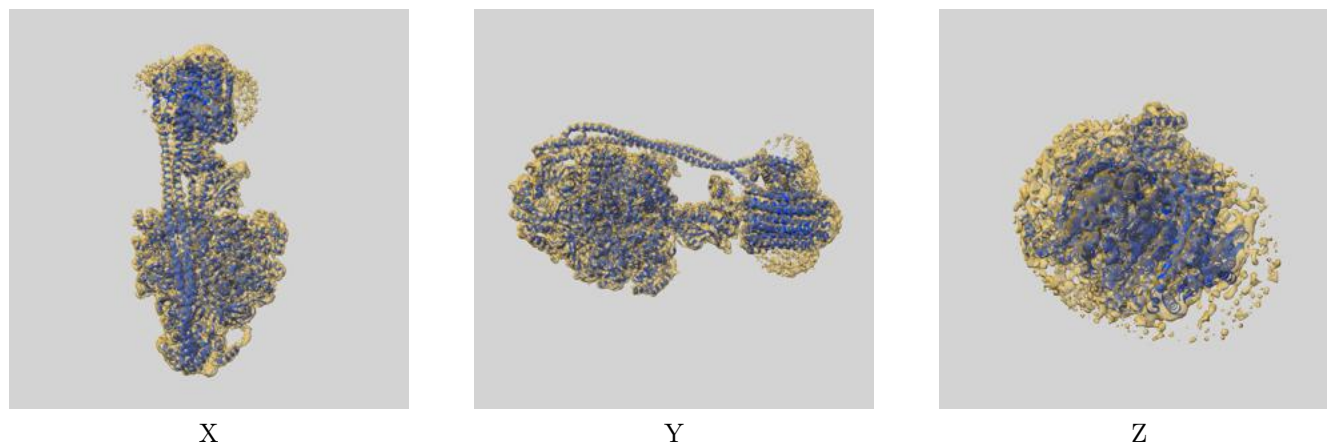
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.85	3.26	2.89
Unmasked-calculated*	3.56	6.67	3.64

*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 3.56 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

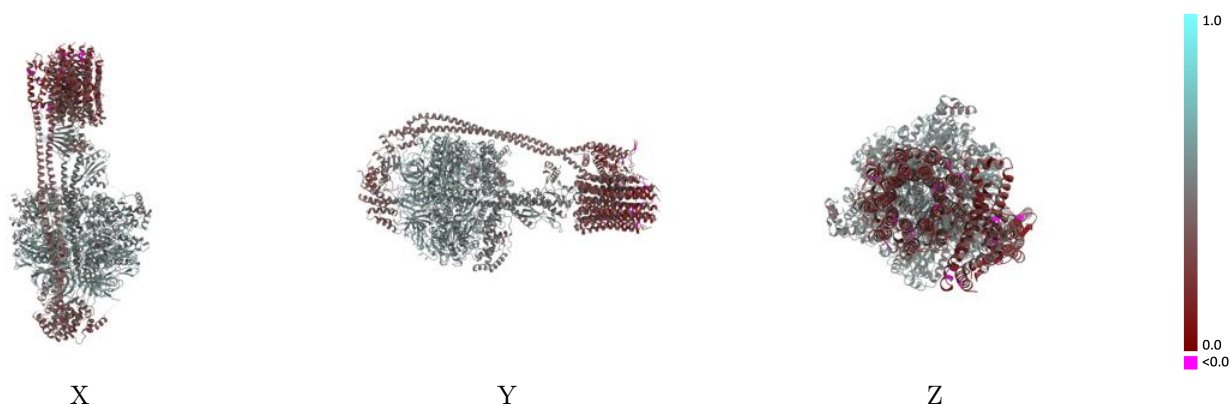
This section contains information regarding the fit between EMDB map EMD-29651 and PDB model 8G0A. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



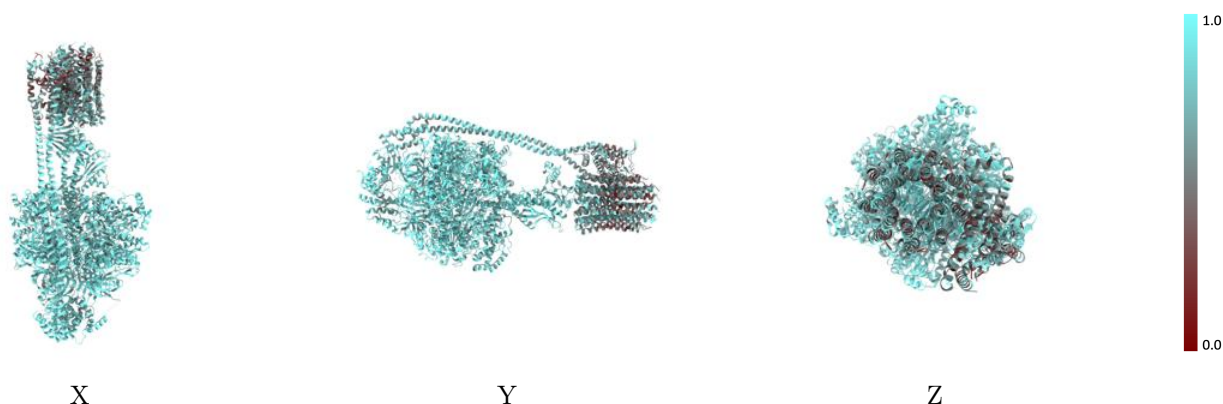
The images above show the 3D surface view of the map at the recommended contour level 0.46 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



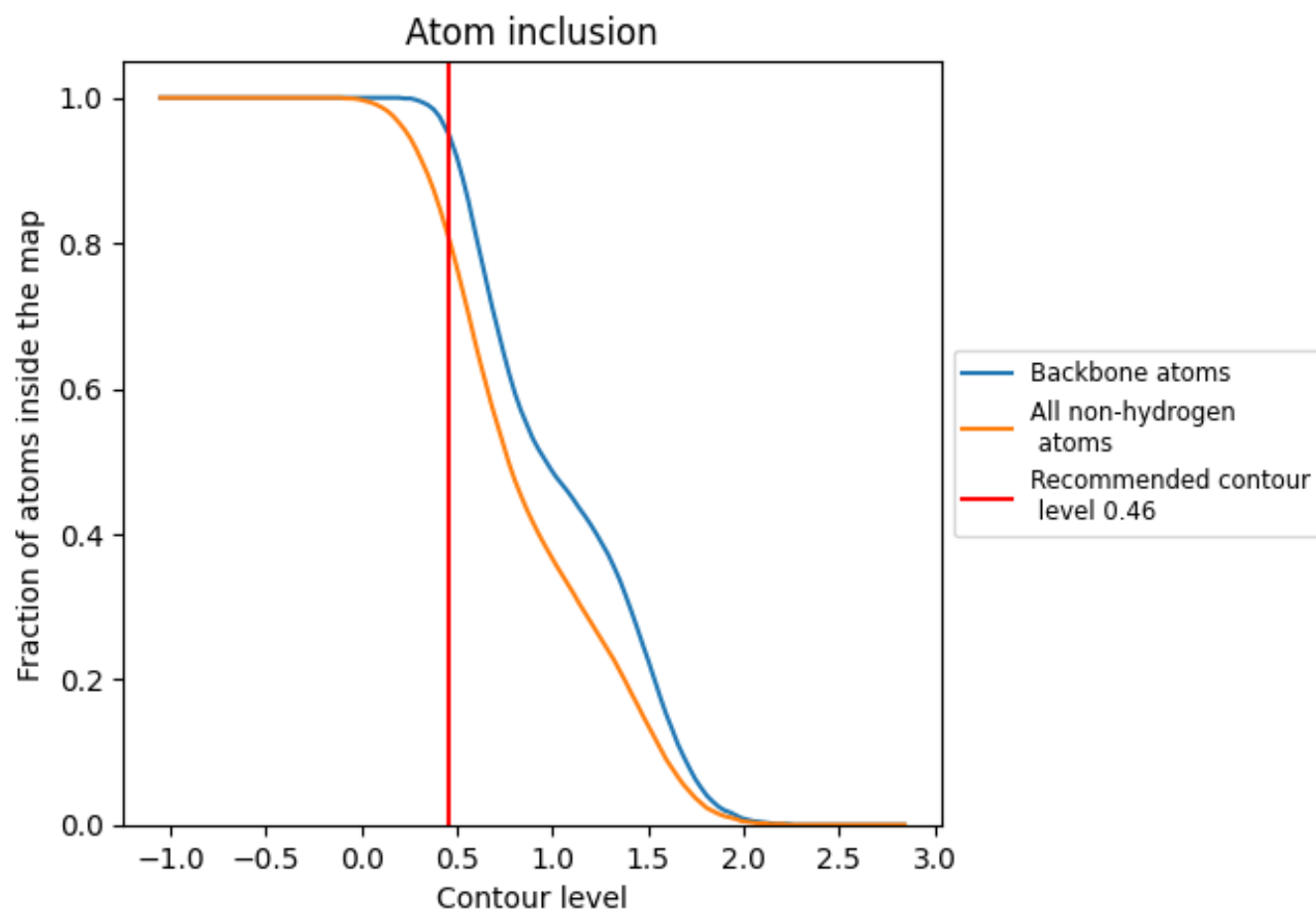
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.46).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 80% 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 (0.46) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8050	 0.4580
1	 0.5530	 0.2900
2	 0.5990	 0.3190
3	 0.6280	 0.3230
4	 0.5530	 0.2870
5	 0.5510	 0.2700
6	 0.5780	 0.2530
7	 0.5660	 0.2360
8	 0.5600	 0.2410
9	 0.5320	 0.2700
A	 0.8760	 0.5300
B	 0.8630	 0.5190
C	 0.8900	 0.5290
D	 0.8880	 0.5340
E	 0.8840	 0.5340
F	 0.8740	 0.5360
G	 0.8660	 0.5000
H	 0.8050	 0.4620
a	 0.5480	 0.2370
b	 0.7430	 0.3510
d	 0.7890	 0.3710

