



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 02:11 AM UTC

PDB ID : 9BYK / pdb_00009byk
EMDB ID : EMD-45036
Title : Cryo-EM structure of ATP synthase E state
Authors : Zhang, Z.; Maharjan, R.; Tringides, M.
Deposited on : 2024-05-23
Resolution : 3.03 Å(reported)

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

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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

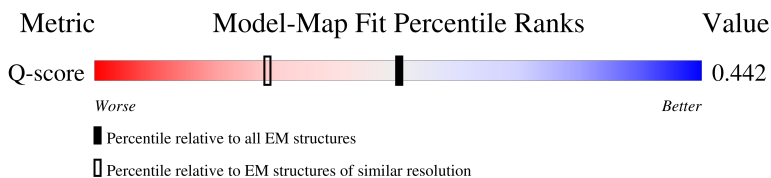
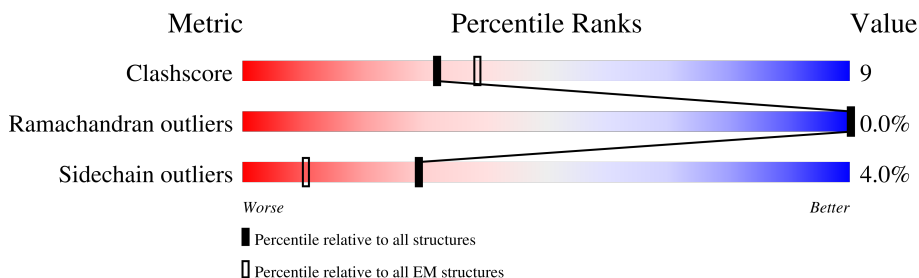
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.03 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.







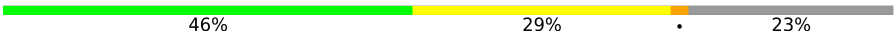


















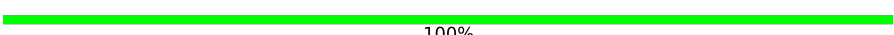

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13929 (2.53 - 3.53)

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	8	67	
2	A	550	
2	B	550	
2	C	550	

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Mol	Chain	Length	Quality of chain
3	D	570	
3	E	570	
3	F	570	
4	G	273	
5	H	168	
6	I	136	
7	J	108	
8	K	141	
8	L	141	
8	M	141	
8	N	141	
8	O	141	
8	P	141	
8	Q	141	
8	R	141	
9	S	213	
10	T	103	
11	a	226	
12	b	238	
13	c	76	
14	d	166	
15	e	71	
16	i	58	
17	k	26	
18	f	88	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 37263 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 protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	29	Total	C	N	O	S	0	0
			237	159	33	43	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	503	Total	C	N	O	S	0	0
			3828	2412	675	729	12		
2	C	482	Total	C	N	O	S	0	0
			3678	2320	650	696	12		
2	B	499	Total	C	N	O	S	0	0
			3796	2389	670	725	12		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	THR	GLY	conflict	UNP A0A8D1XYK3
C	4	THR	GLY	conflict	UNP A0A8D1XYK3
B	4	THR	GLY	conflict	UNP A0A8D1XYK3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	468	Total	C	N	O	S	0	0
			3541	2245	600	684	12		
3	E	465	Total	C	N	O	S	0	0
			3522	2234	597	679	12		
3	F	466	Total	C	N	O	S	0	0
			3527	2237	598	680	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	272	Total	C	N	O	S	0	0
			2106	1329	363	407	7		

- Molecule 5 is a protein called ATP synthase F1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	129	Total	C	N	O	S	0	0
			945	593	161	190	1		

- Molecule 6 is a protein called ATP synthase F1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	46	Total	C	N	O	S	0	0
			353	225	64	63	1		

- Molecule 7 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	45	Total	C	N	O	S	0	0
			335	201	70	64			

- Molecule 8 is a protein called ATP synthase lipid-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	72	Total	C	N	O	S	0	0
			513	341	80	89	3		
8	L	72	Total	C	N	O	S	0	0
			513	341	80	89	3		
8	M	72	Total	C	N	O	S	0	0
			513	341	80	89	3		
8	N	72	Total	C	N	O	S	0	0
			510	339	80	89	2		
8	O	72	Total	C	N	O	S	0	0
			513	341	80	89	3		
8	P	72	Total	C	N	O	S	0	0
			513	341	80	89	3		
8	Q	72	Total	C	N	O	S	0	0
			513	341	80	89	3		
8	R	72	Total	C	N	O	S	0	0
			513	341	80	89	3		

- Molecule 9 is a protein called ATP synthase subunit O, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	187	Total	C	N	O	S	0	0
			1430	911	244	266	9		

- Molecule 10 is a protein called ATP synthase subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	T	43	Total	C	N	O	0	0
			317	203	52	62		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	215	Total	C	N	O	S	0	0
			1638	1090	259	278	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	b	199	Total	C	N	O	S	0	0
			1430	888	267	270	5		

- Molecule 13 is a protein called ATP synthase-coupling factor 6, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	c	69	Total	C	N	O	0	0
			417	255	82	80		

- Molecule 14 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	d	147	Total	C	N	O	0	0
			741	446	148	147		

- Molecule 15 is a protein called ATP synthase subunit e, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	e	41	Total	C	N	O	0	0
			259	164	48	47		

- Molecule 16 is a protein called ATP synthase membrane subunit K, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	i	38	Total	C	N	O	S	0	0
			277	183	45	47	2		

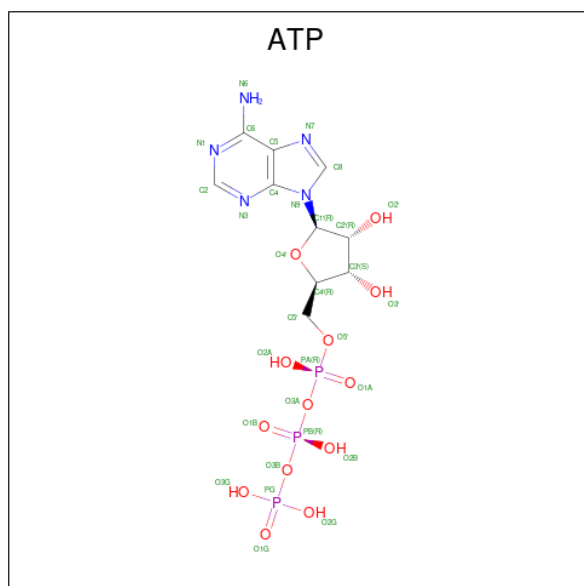
- Molecule 17 is a protein called unknown protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	k	26	Total	C	N	O		0	0
			130	78	26	26			

- Molecule 18 is a protein called ATP synthase subunit f, mitochondrial.

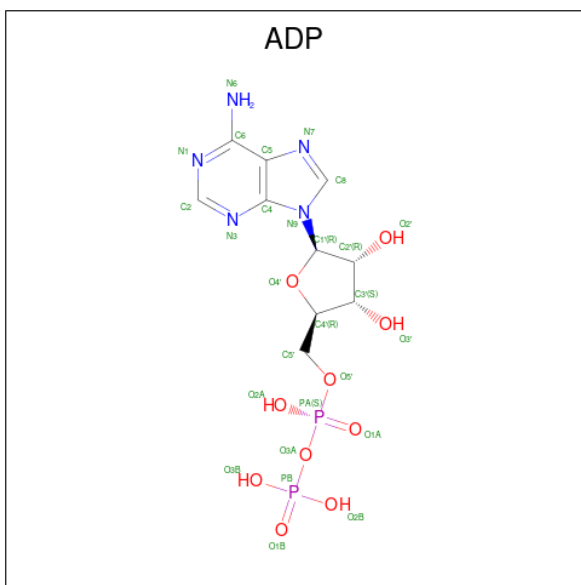
Mol	Chain	Residues	Atoms					AltConf	Trace
18	f	83	Total	C	N	O	S	0	0
			504	312	96	94	2		

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

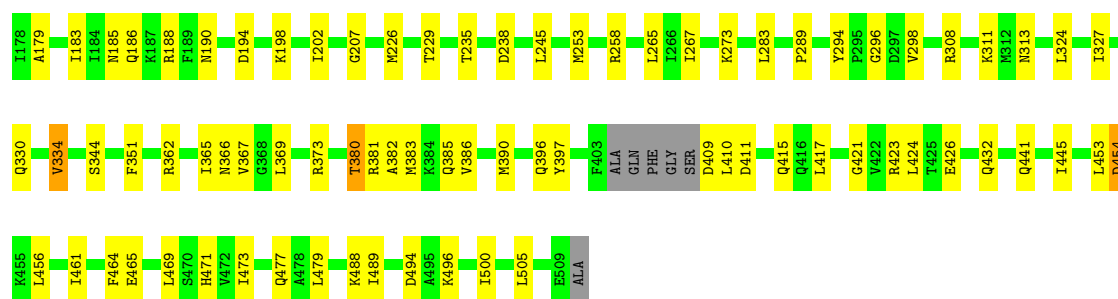


Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total Mg 1 1	0
20	D	1	Total Mg 1 1	0
20	F	1	Total Mg 1 1	0
20	C	1	Total Mg 1 1	0

- Molecule 21 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

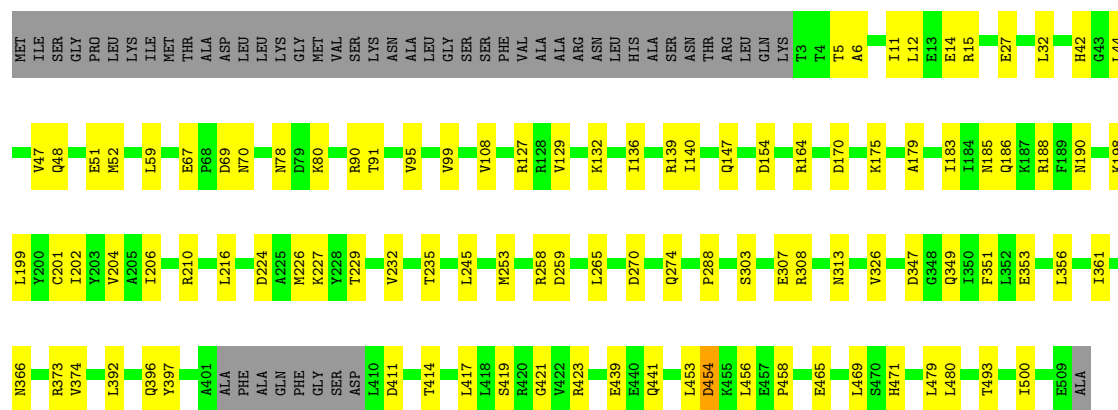


Mol	Chain	Residues	Atoms					AltConf
21	D	1	Total 27	C 10	N 5	O 10	P 2	0
21	F	1	Total 27	C 10	N 5	O 10	P 2	0



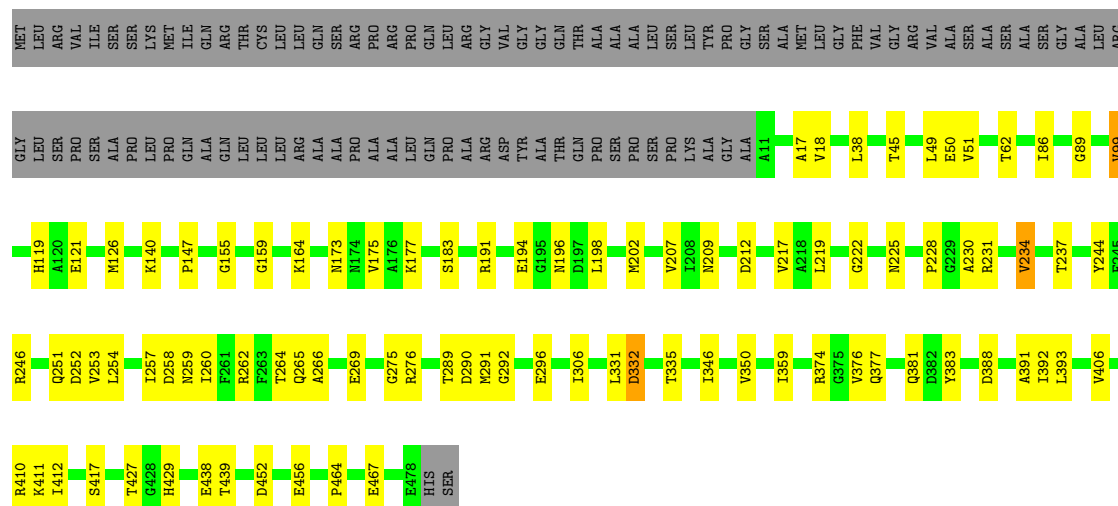
• Molecule 2: ATP synthase subunit alpha

Chain B: 73% 18% 9%



• Molecule 3: ATP synthase subunit beta

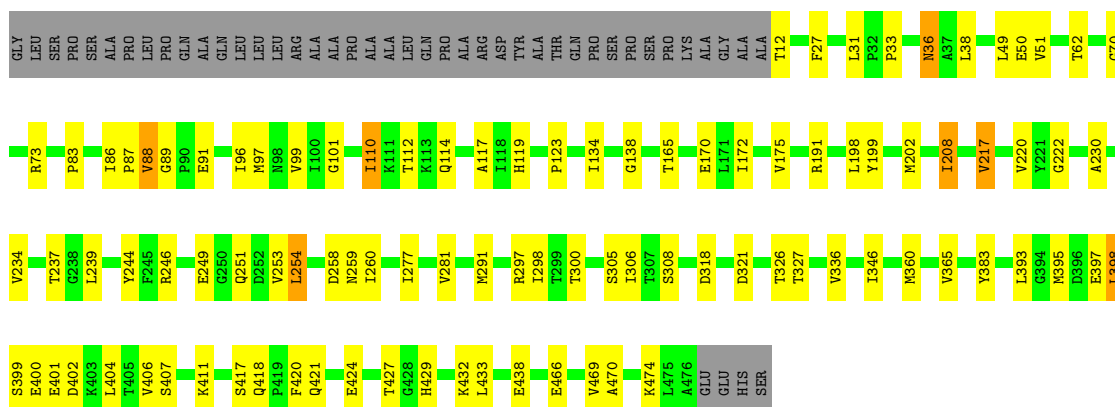
Chain D: 66% 15% 18%



• Molecule 3: ATP synthase subunit beta

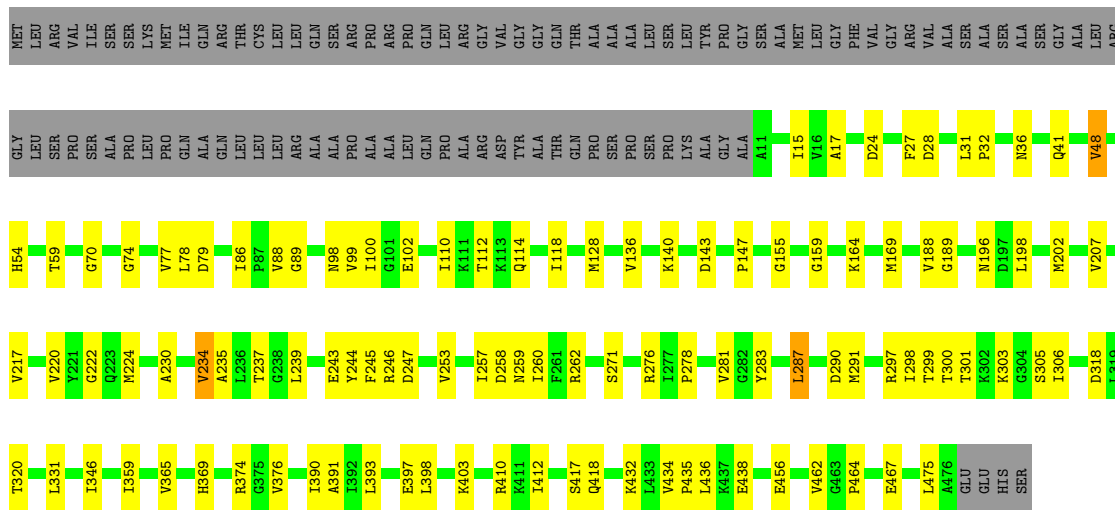
Chain E: 64% 16% 18%





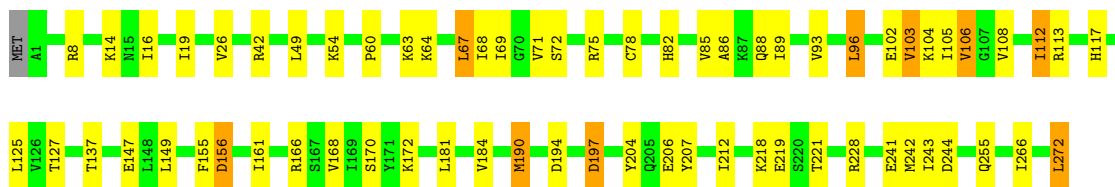
• Molecule 3: ATP synthase subunit beta

Chain F: 63% 18% 18%



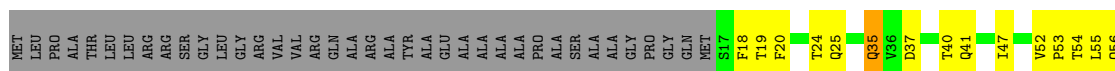
• Molecule 4: ATP synthase subunit gamma

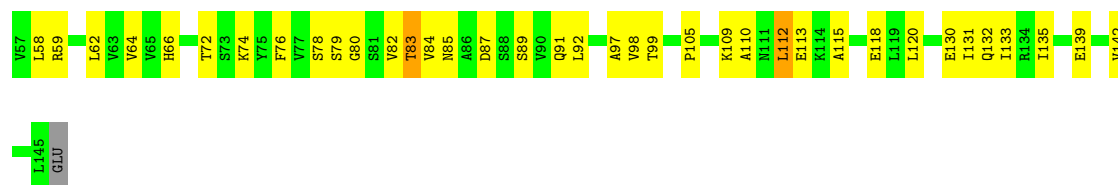
Chain G: 75% 21% 4%



• Molecule 5: ATP synthase F1 subunit delta

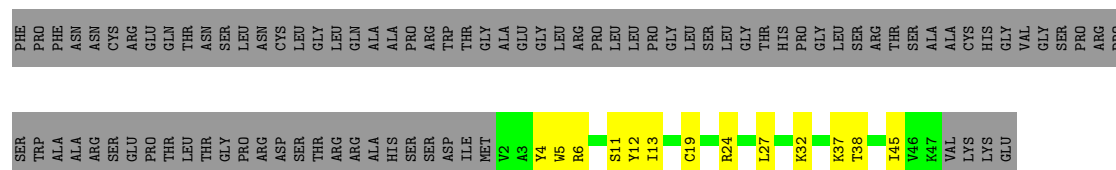
Chain H: 46% 29% 23%





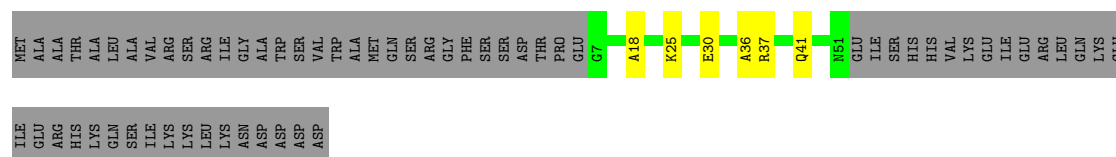
• Molecule 6: ATP synthase F1 subunit epsilon

Chain I: 24% 10% 66%



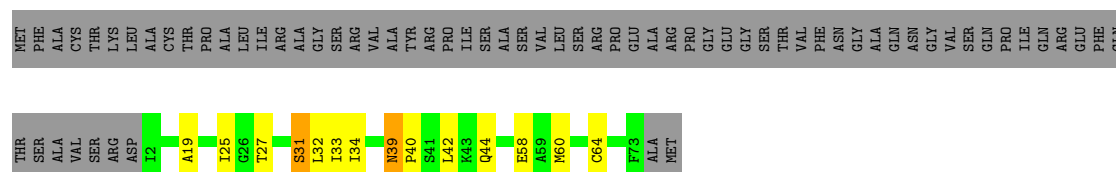
• Molecule 7: ATPase inhibitor, mitochondrial

Chain J: 36% 6% 58%



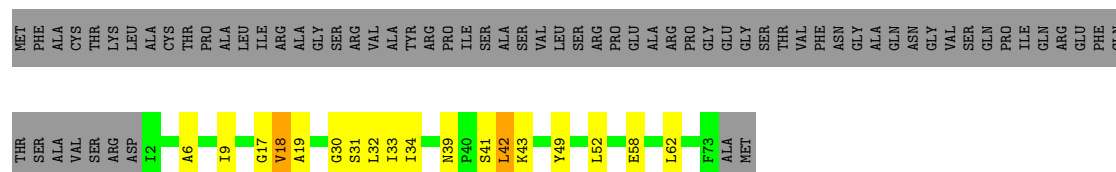
• Molecule 8: ATP synthase lipid-binding protein

Chain K: 41% 9% 49%



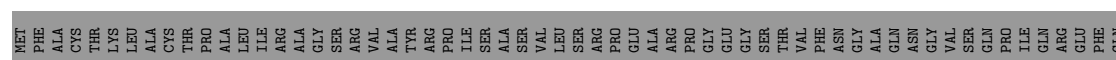
• Molecule 8: ATP synthase lipid-binding protein

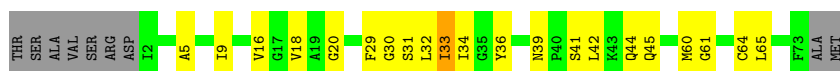
Chain L: 38% 11% 49%



• Molecule 8: ATP synthase lipid-binding protein

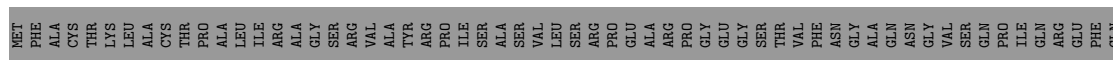
Chain M: 36% 14% 49%





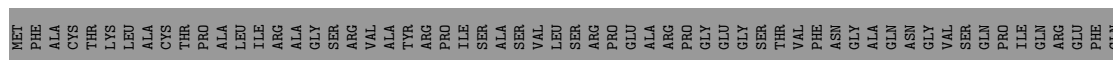
- Molecule 8: ATP synthase lipid-binding protein

Chain N: 34% 16% 49%



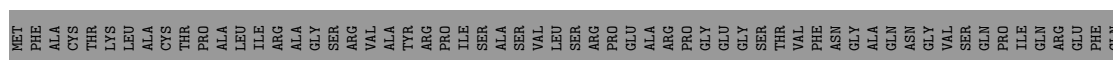
- Molecule 8: ATP synthase lipid-binding protein

Chain O: 41% 9% 49%



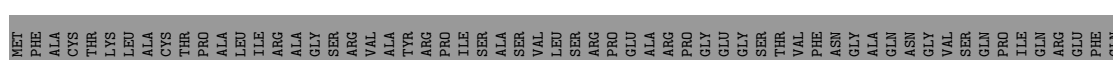
- Molecule 8: ATP synthase lipid-binding protein

Chain P: 38% 10% 49%



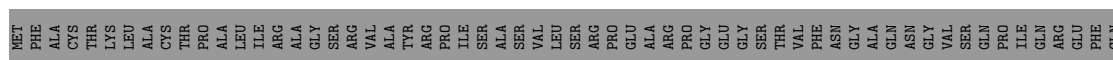
- Molecule 8: ATP synthase lipid-binding protein

Chain Q: 40% 11% 49%



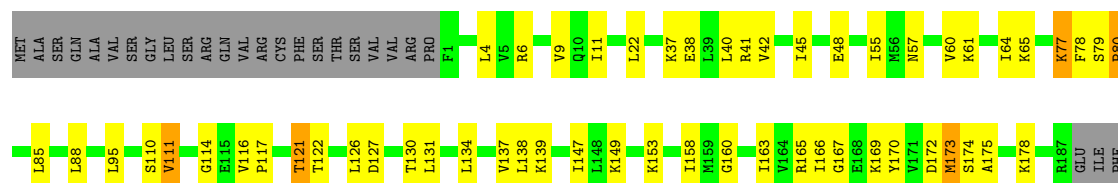
- Molecule 8: ATP synthase lipid-binding protein

Chain R: 32% 18% 49%



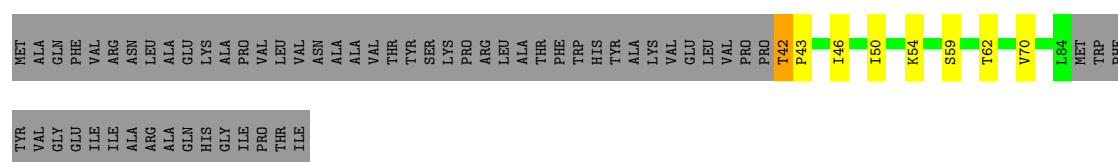
- Molecule 9: ATP synthase subunit O, mitochondrial

Chain S: 



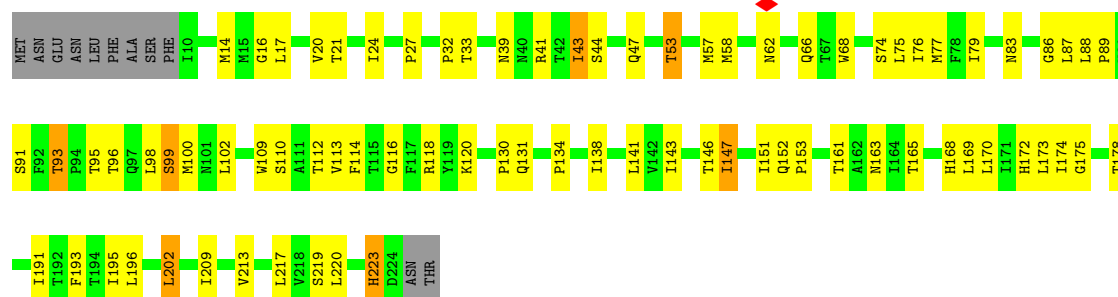
- Molecule 10: ATP synthase subunit

Chain T: 



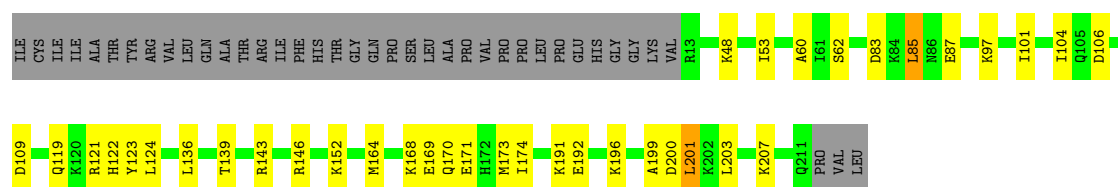
- Molecule 11: ATP synthase subunit a

Chain a: 




- Molecule 12: ATP synthase subunit b

Chain b: 




- Molecule 13: ATP synthase-coupling factor 6, mitochondrial

Chain c: 



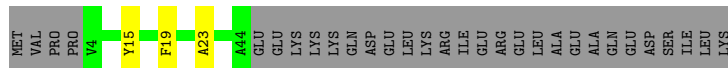
- Molecule 14: ATP synthase subunit d, mitochondrial

Chain d:  86% 11%



- Molecule 15: ATP synthase subunit e, mitochondrial

Chain e:  54% 42%



- Molecule 16: ATP synthase membrane subunit K, mitochondrial

Chain i:  47% 19% 34%




- Molecule 17: unknown protein

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: ATP synthase subunit f, mitochondrial

Chain f:  85% 9% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37533	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.253	Depositor
Minimum map value	-0.219	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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

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	8	0.11	0/242	0.35	0/328
2	A	0.12	0/3879	0.25	0/5235
2	B	0.16	0/3844	0.29	0/5187
2	C	0.13	0/3727	0.27	0/5028
3	D	0.12	0/3598	0.26	0/4880
3	E	0.12	0/3579	0.25	0/4854
3	F	0.12	0/3584	0.26	0/4861
4	G	0.11	0/2132	0.23	0/2867
5	H	0.09	0/958	0.27	0/1306
6	I	0.08	0/358	0.21	0/481
7	J	0.10	0/338	0.21	0/449
8	K	0.11	0/522	0.27	0/704
8	L	0.11	0/522	0.25	0/704
8	M	0.13	0/522	0.28	0/704
8	N	0.13	0/519	0.30	0/701
8	O	0.10	0/522	0.22	0/704
8	P	0.11	0/522	0.25	0/704
8	Q	0.25	0/522	0.39	0/704
8	R	0.35	0/522	0.51	0/704
9	S	0.24	0/1448	0.43	0/1948
10	T	0.10	0/319	0.26	0/433
11	a	0.13	0/1674	0.32	0/2293
12	b	0.12	0/1441	0.29	0/1944
13	c	0.08	0/420	0.20	0/573
14	d	0.10	0/742	0.26	0/1036
15	e	0.07	0/261	0.22	0/356
16	i	0.28	0/281	0.37	0/380
18	f	0.11	0/508	0.30	0/692
All	All	0.14	0/37506	0.28	0/50760

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	8	237	0	239	12	0
2	A	3828	0	3930	61	0
2	B	3796	0	3906	61	0
2	C	3678	0	3785	67	0
3	D	3541	0	3592	56	0
3	E	3522	0	3580	54	0
3	F	3527	0	3584	63	0
4	G	2106	0	2178	52	0
5	H	945	0	938	39	0
6	I	353	0	358	14	0
7	J	335	0	311	5	0
8	K	513	0	532	13	0
8	L	513	0	532	15	0
8	M	513	0	532	21	0
8	N	510	0	525	21	0
8	O	513	0	532	14	0
8	P	513	0	532	15	0
8	Q	513	0	532	14	0
8	R	513	0	532	18	0
9	S	1430	0	1537	41	0
10	T	317	0	344	6	0
11	a	1638	0	1734	48	0
12	b	1430	0	1320	24	0
13	c	417	0	285	8	0
14	d	741	0	348	3	0
15	e	259	0	226	3	0
16	i	277	0	270	7	0
17	k	130	0	28	0	0
18	f	504	0	366	5	0
19	A	31	0	12	0	0
19	B	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	C	31	0	12	0	0
20	A	1	0	0	0	0
20	C	1	0	0	0	0
20	D	1	0	0	0	0
20	F	1	0	0	0	0
21	D	27	0	12	1	0
21	F	27	0	12	2	0
All	All	37263	0	37168	640	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 9.

The worst 5 of 640 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)
5:H:78:SER:HG	6:I:19:CYS:HG	1.22	0.88
3:F:239:LEU:HD13	3:F:298:ILE:HG12	1.67	0.77
7:J:36:ALA:HB2	2:C:410:LEU:HD11	1.67	0.75
8:M:18:VAL:HG11	8:N:64:CYS:HB2	1.69	0.74
8:Q:19:ALA:HB2	8:R:17:GLY:HA2	1.68	0.74

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	8	27/67 (40%)	24 (89%)	3 (11%)	0	100	100
2	A	501/550 (91%)	489 (98%)	12 (2%)	0	100	100
2	B	495/550 (90%)	484 (98%)	11 (2%)	0	100	100
2	C	478/550 (87%)	471 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	466/570 (82%)	453 (97%)	13 (3%)	0	100	100
3	E	463/570 (81%)	449 (97%)	14 (3%)	0	100	100
3	F	464/570 (81%)	451 (97%)	13 (3%)	0	100	100
4	G	270/273 (99%)	267 (99%)	3 (1%)	0	100	100
5	H	127/168 (76%)	122 (96%)	5 (4%)	0	100	100
6	I	44/136 (32%)	44 (100%)	0	0	100	100
7	J	43/108 (40%)	43 (100%)	0	0	100	100
8	K	70/141 (50%)	69 (99%)	1 (1%)	0	100	100
8	L	70/141 (50%)	69 (99%)	1 (1%)	0	100	100
8	M	70/141 (50%)	68 (97%)	2 (3%)	0	100	100
8	N	70/141 (50%)	69 (99%)	1 (1%)	0	100	100
8	O	70/141 (50%)	68 (97%)	2 (3%)	0	100	100
8	P	70/141 (50%)	67 (96%)	3 (4%)	0	100	100
8	Q	70/141 (50%)	66 (94%)	4 (6%)	0	100	100
8	R	70/141 (50%)	66 (94%)	4 (6%)	0	100	100
9	S	185/213 (87%)	170 (92%)	14 (8%)	1 (0%)	24	57
10	T	41/103 (40%)	41 (100%)	0	0	100	100
11	a	213/226 (94%)	202 (95%)	11 (5%)	0	100	100
12	b	197/238 (83%)	190 (96%)	7 (4%)	0	100	100
13	c	67/76 (88%)	66 (98%)	1 (2%)	0	100	100
14	d	145/166 (87%)	140 (97%)	4 (3%)	1 (1%)	18	49
15	e	39/71 (55%)	39 (100%)	0	0	100	100
16	i	36/58 (62%)	33 (92%)	3 (8%)	0	100	100
18	f	79/88 (90%)	73 (92%)	6 (8%)	0	100	100
All	All	4940/6479 (76%)	4793 (97%)	145 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	S	80	PRO
14	d	126	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	8	28/66 (42%)	26 (93%)	2 (7%)	13	40
2	A	405/444 (91%)	399 (98%)	6 (2%)	57	77
2	B	403/444 (91%)	394 (98%)	9 (2%)	45	71
2	C	389/444 (88%)	381 (98%)	8 (2%)	47	72
3	D	376/452 (83%)	366 (97%)	10 (3%)	39	68
3	E	375/452 (83%)	359 (96%)	16 (4%)	26	57
3	F	375/452 (83%)	363 (97%)	12 (3%)	34	64
4	G	229/231 (99%)	218 (95%)	11 (5%)	23	54
5	H	101/127 (80%)	93 (92%)	8 (8%)	11	36
6	I	34/109 (31%)	34 (100%)	0	100	100
7	J	27/85 (32%)	26 (96%)	1 (4%)	30	61
8	K	49/103 (48%)	46 (94%)	3 (6%)	17	46
8	L	49/103 (48%)	47 (96%)	2 (4%)	27	58
8	M	49/103 (48%)	46 (94%)	3 (6%)	17	46
8	N	48/103 (47%)	43 (90%)	5 (10%)	7	25
8	O	49/103 (48%)	47 (96%)	2 (4%)	27	58
8	P	49/103 (48%)	44 (90%)	5 (10%)	7	26
8	Q	49/103 (48%)	46 (94%)	3 (6%)	17	46
8	R	49/103 (48%)	47 (96%)	2 (4%)	27	58
9	S	162/186 (87%)	154 (95%)	8 (5%)	22	53
10	T	36/85 (42%)	34 (94%)	2 (6%)	19	49
11	a	181/199 (91%)	159 (88%)	22 (12%)	5	19
12	b	124/207 (60%)	119 (96%)	5 (4%)	28	59
13	c	20/69 (29%)	19 (95%)	1 (5%)	22	53
14	d	1/144 (1%)	1 (100%)	0	100	100
15	e	17/60 (28%)	17 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	i	26/47 (55%)	25 (96%)	1 (4%)	29	60
18	f	26/76 (34%)	25 (96%)	1 (4%)	29	60
All	All	3726/5203 (72%)	3578 (96%)	148 (4%)	29	59

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	a	147	ILE
2	B	216	LEU
11	a	178	THR
2	C	95	VAL
4	G	103	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	330	GLN
2	B	341	ASN
2	C	366	ASN
18	f	70	ASN
5	H	35	GLN

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 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	$\# Z > 2$
19	ATP	A	601	20	32,33,33	0.35	0	48,52,52	0.29	0
19	ATP	B	601	-	32,33,33	0.33	0	48,52,52	0.30	0
19	ATP	C	601	20	32,33,33	0.35	0	48,52,52	0.28	0
21	ADP	D	501	20	28,29,29	1.39	4 (14%)	43,45,45	1.84	8 (18%)
21	ADP	F	501	20	28,29,29	1.39	4 (14%)	43,45,45	1.87	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
19	ATP	A	601	20	-	1/22/38/38	0/3/3/3
19	ATP	B	601	-	-	5/22/38/38	0/3/3/3
19	ATP	C	601	20	-	5/22/38/38	0/3/3/3
21	ADP	D	501	20	-	3/16/32/32	0/3/3/3
21	ADP	F	501	20	-	1/16/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	501	ADP	C5-C4	4.62	1.47	1.39
21	F	501	ADP	C5-C4	4.59	1.47	1.39
21	D	501	ADP	C5-C6	2.69	1.48	1.41
21	F	501	ADP	C5-C6	2.66	1.48	1.41
21	F	501	ADP	C5-N7	-2.37	1.34	1.39

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	F	501	ADP	C5-C4-N3	-5.91	118.58	126.72
21	D	501	ADP	C5-C4-N3	-5.86	118.65	126.72
21	D	501	ADP	N3-C4-N9	4.71	135.18	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	F	501	ADP	N3-C4-N9	4.71	135.17	127.17
21	D	501	ADP	C2-N3-C4	3.70	120.88	111.83

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

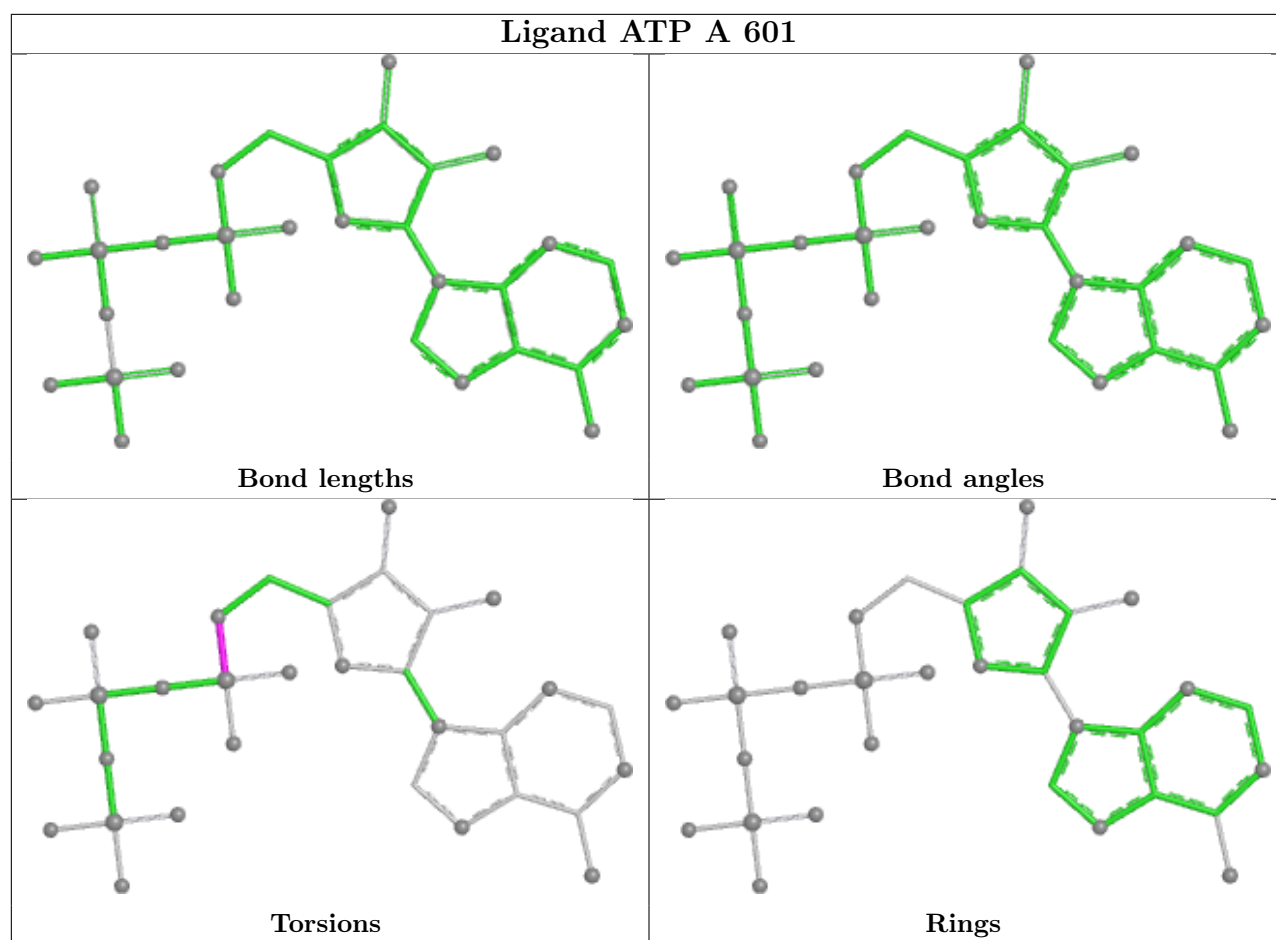
Mol	Chain	Res	Type	Atoms
19	C	601	ATP	C5'-O5'-PA-O1A
19	C	601	ATP	C5'-O5'-PA-O2A
19	C	601	ATP	C5'-O5'-PA-O3A
19	B	601	ATP	C5'-O5'-PA-O1A
19	B	601	ATP	C5'-O5'-PA-O3A

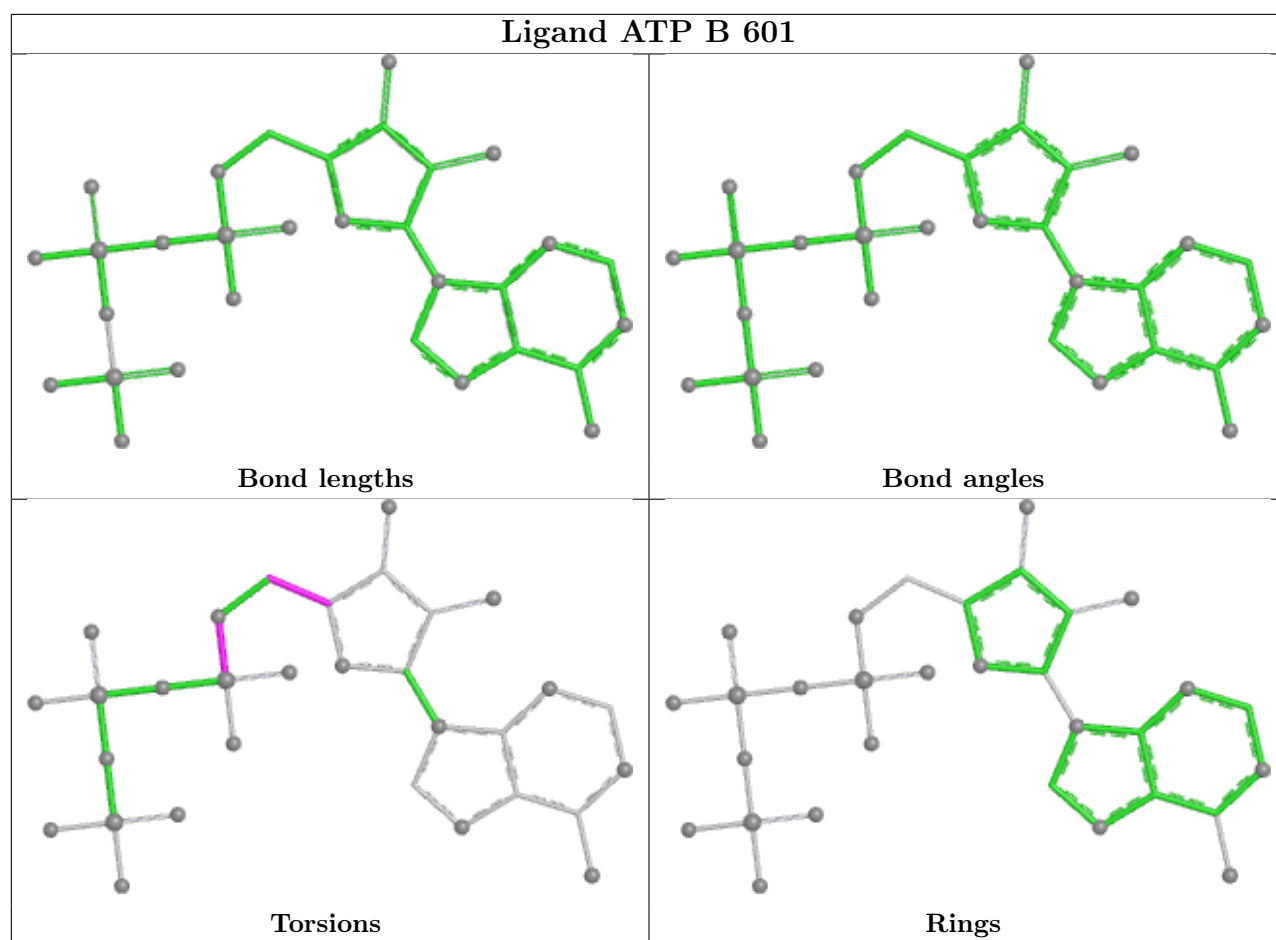
There are no ring outliers.

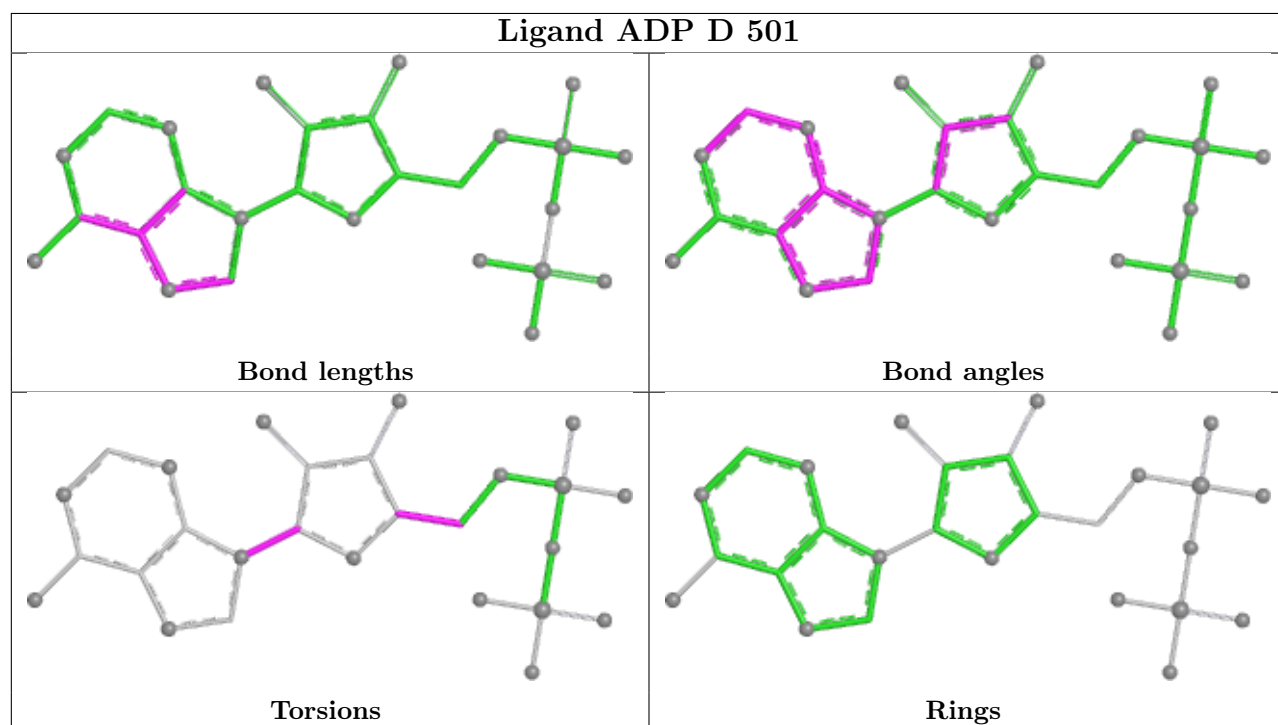
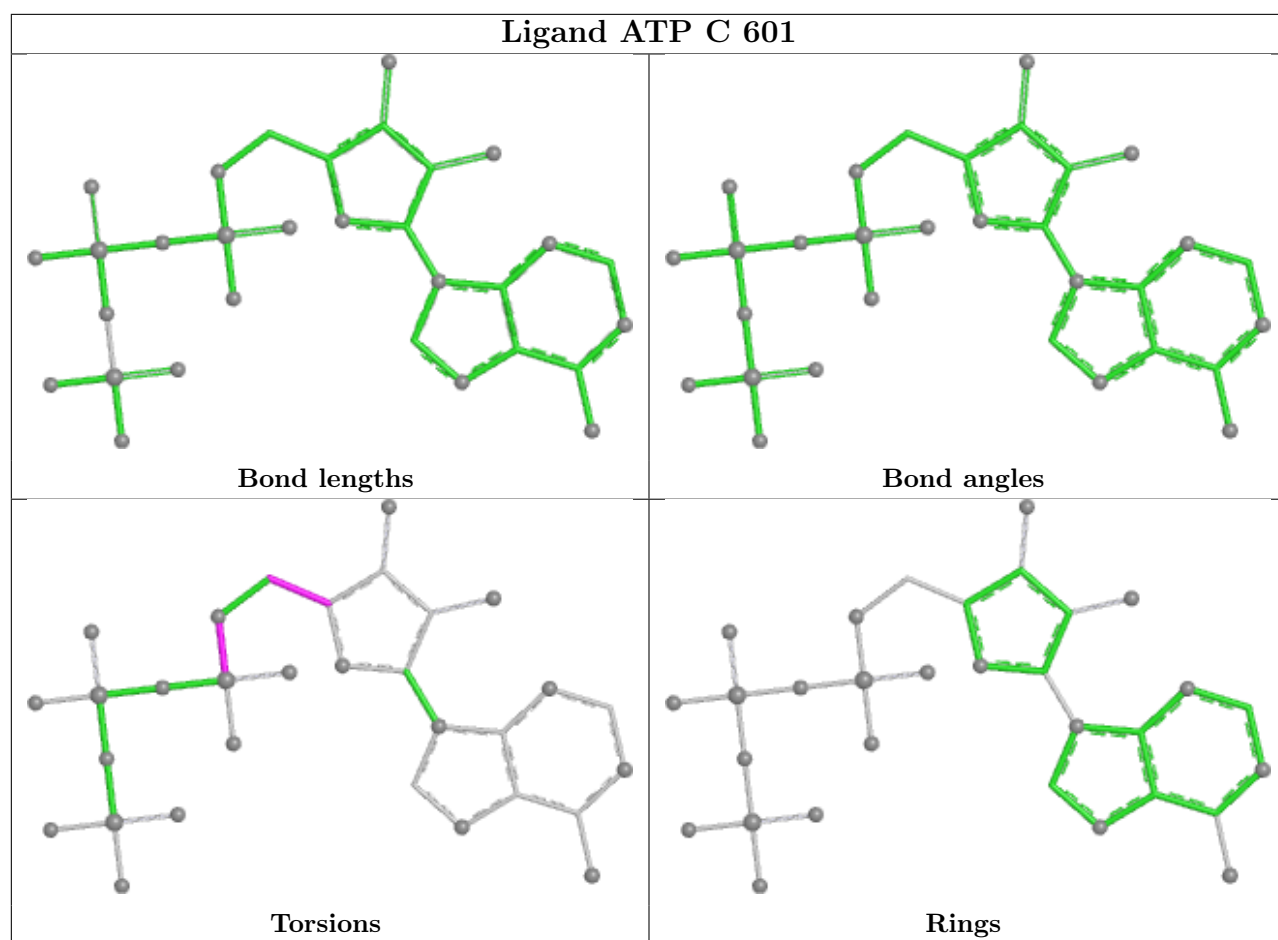
3 monomers are involved in 4 short contacts:

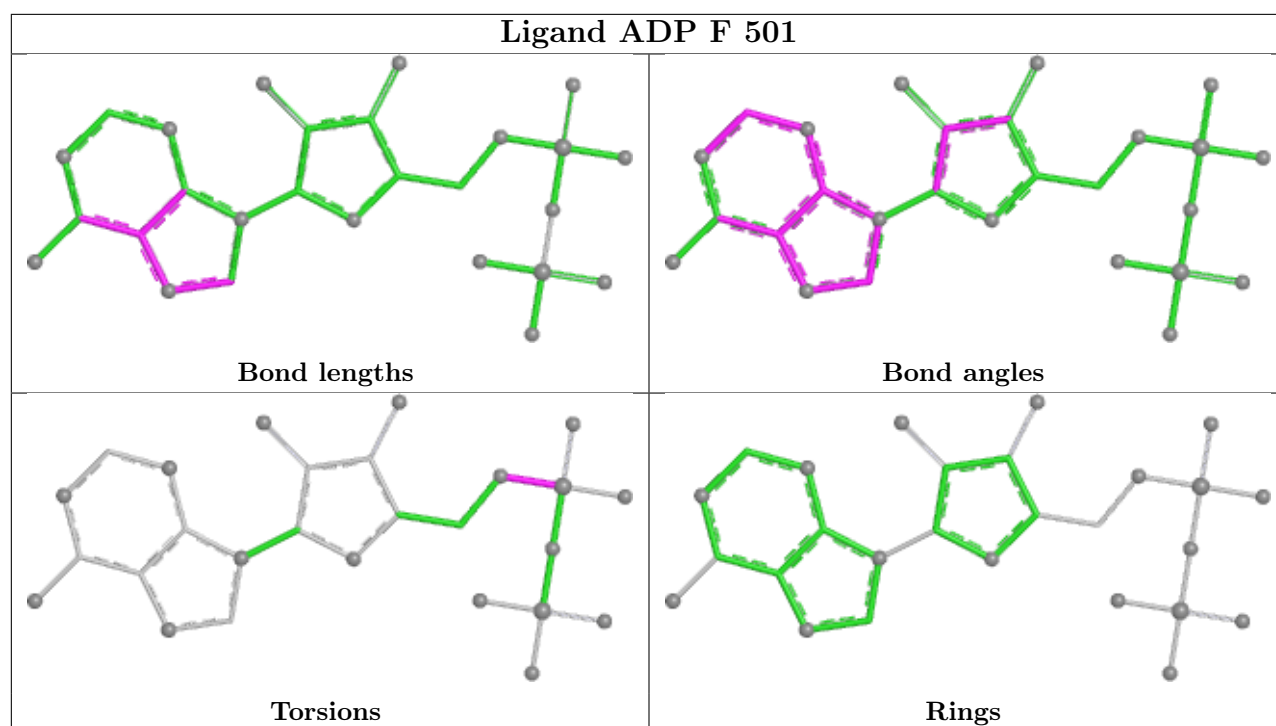
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	601	ATP	1	0
21	D	501	ADP	1	0
21	F	501	ADP	2	0

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.

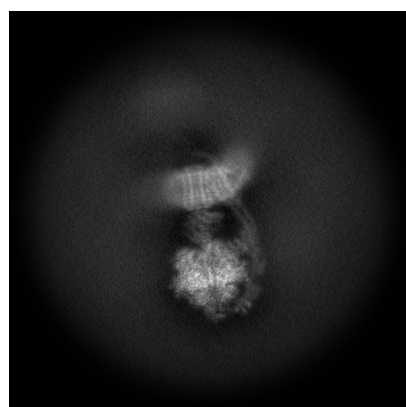
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45036. These allow visual inspection of the internal detail of the map and identification of artifacts.

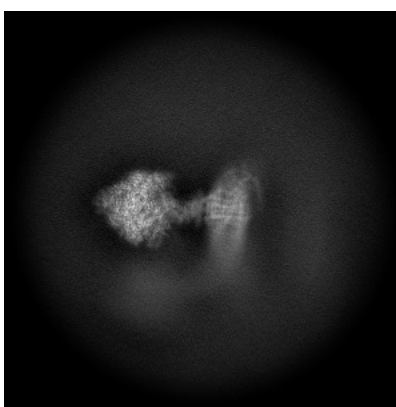
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

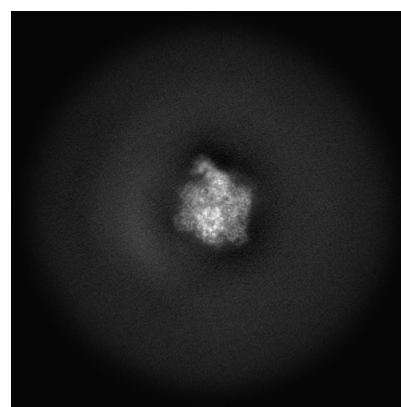
6.1.1 Primary map



X



Y

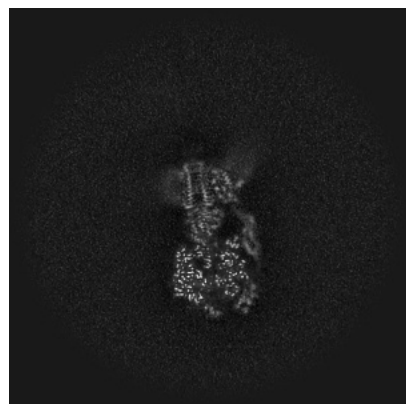


Z

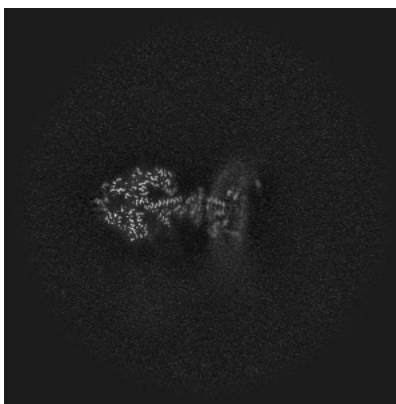
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

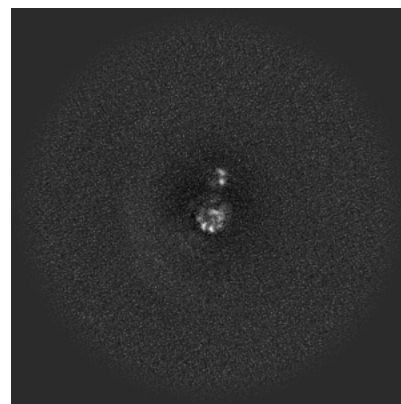
6.2.1 Primary map



X Index: 256



Y Index: 256

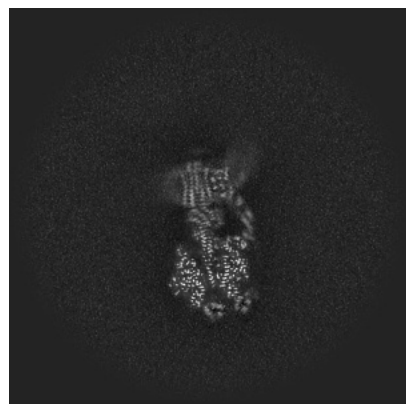


Z Index: 256

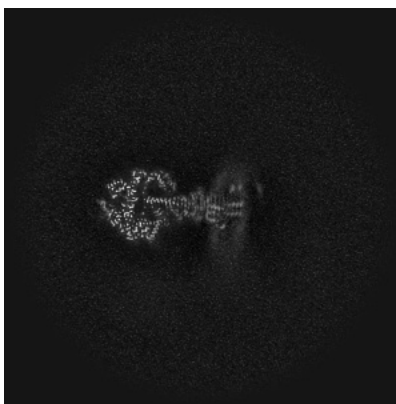
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

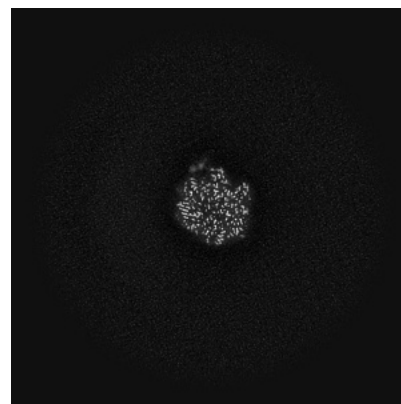
6.3.1 Primary map



X Index: 262



Y Index: 251

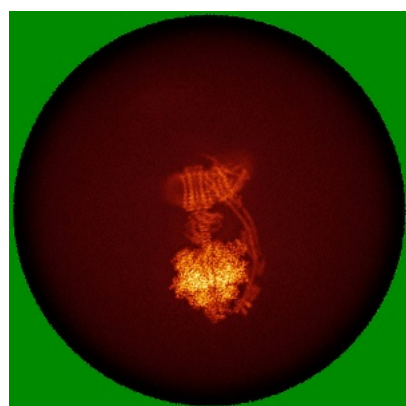


Z Index: 166

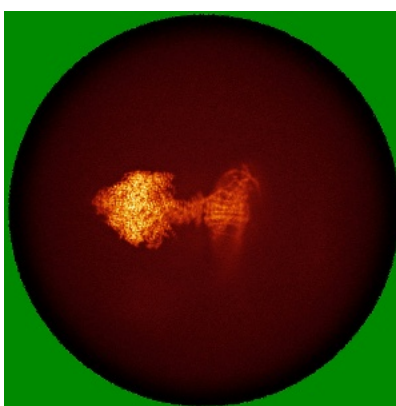
The images above show the largest variance slices of the map in three orthogonal directions.

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

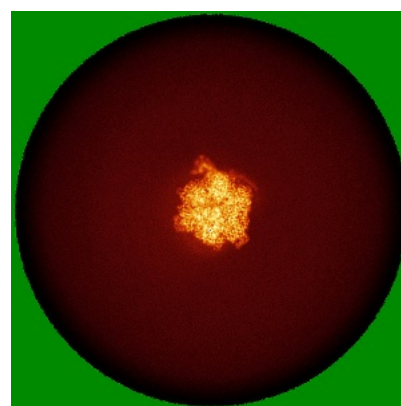
6.4.1 Primary map



X



Y

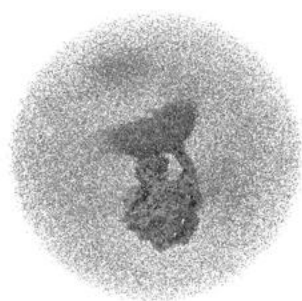


Z

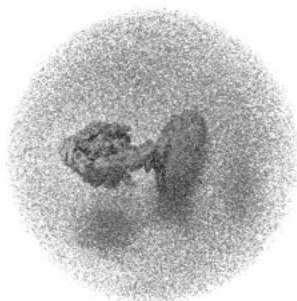
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

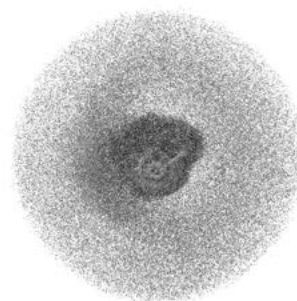
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

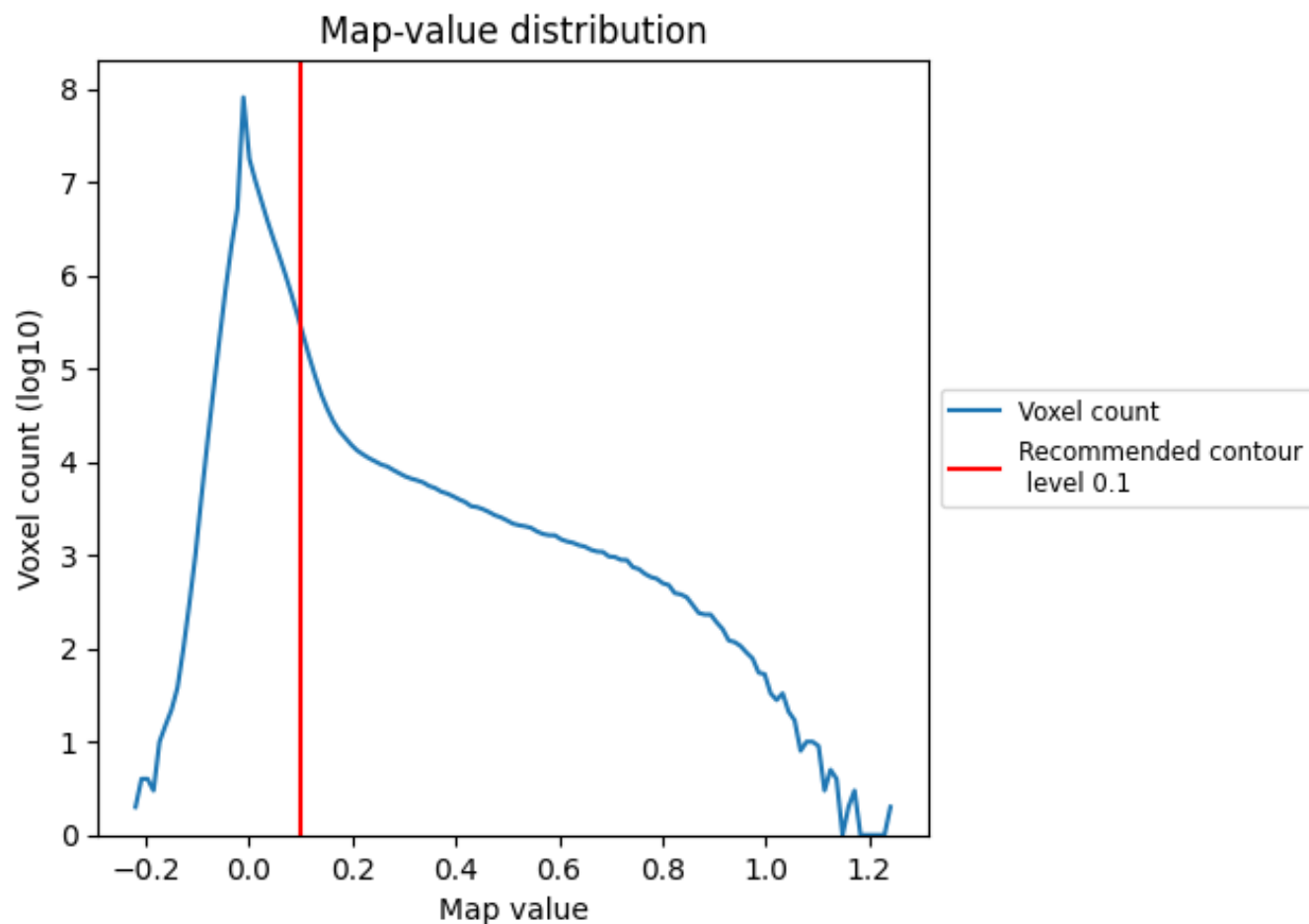
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

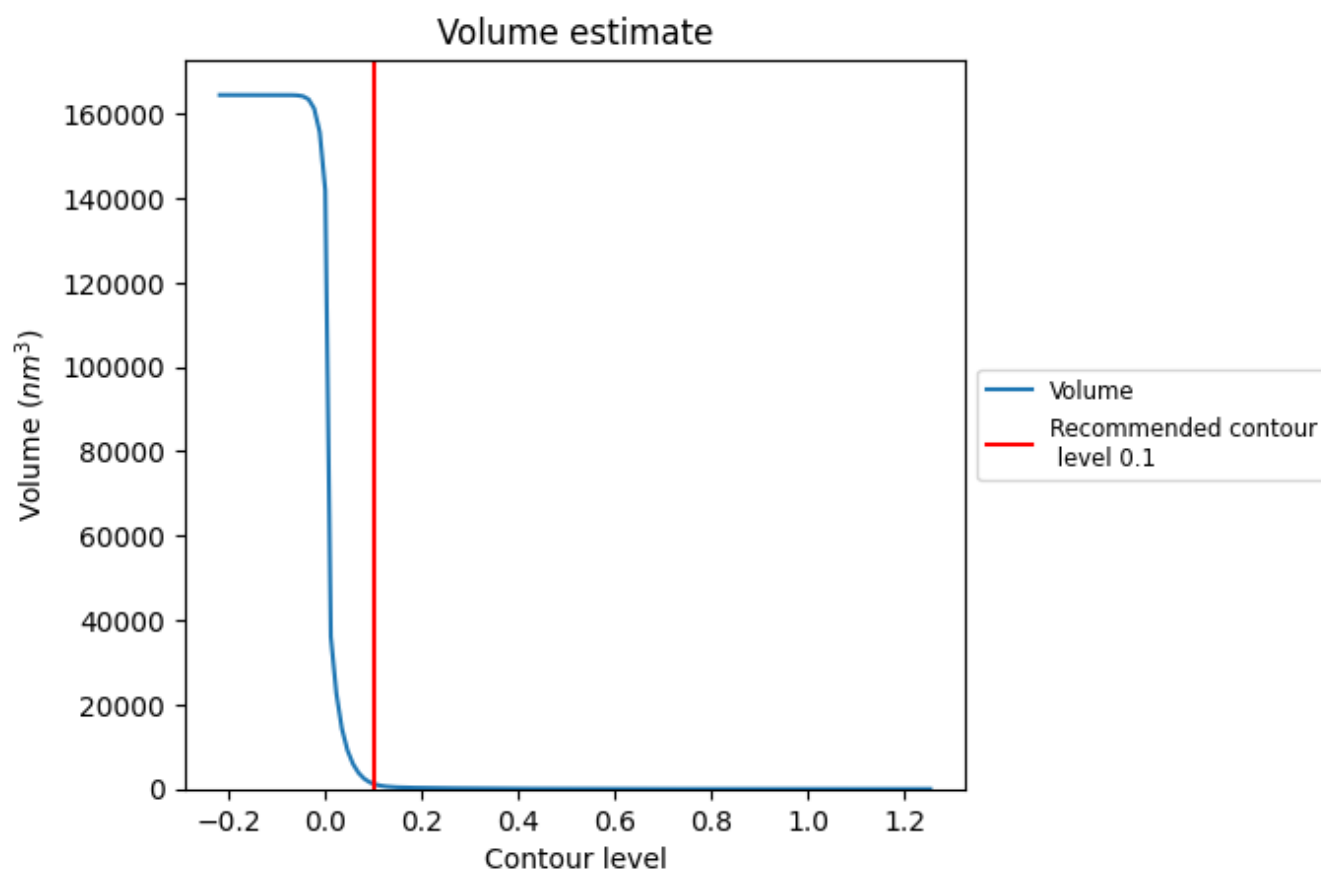
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

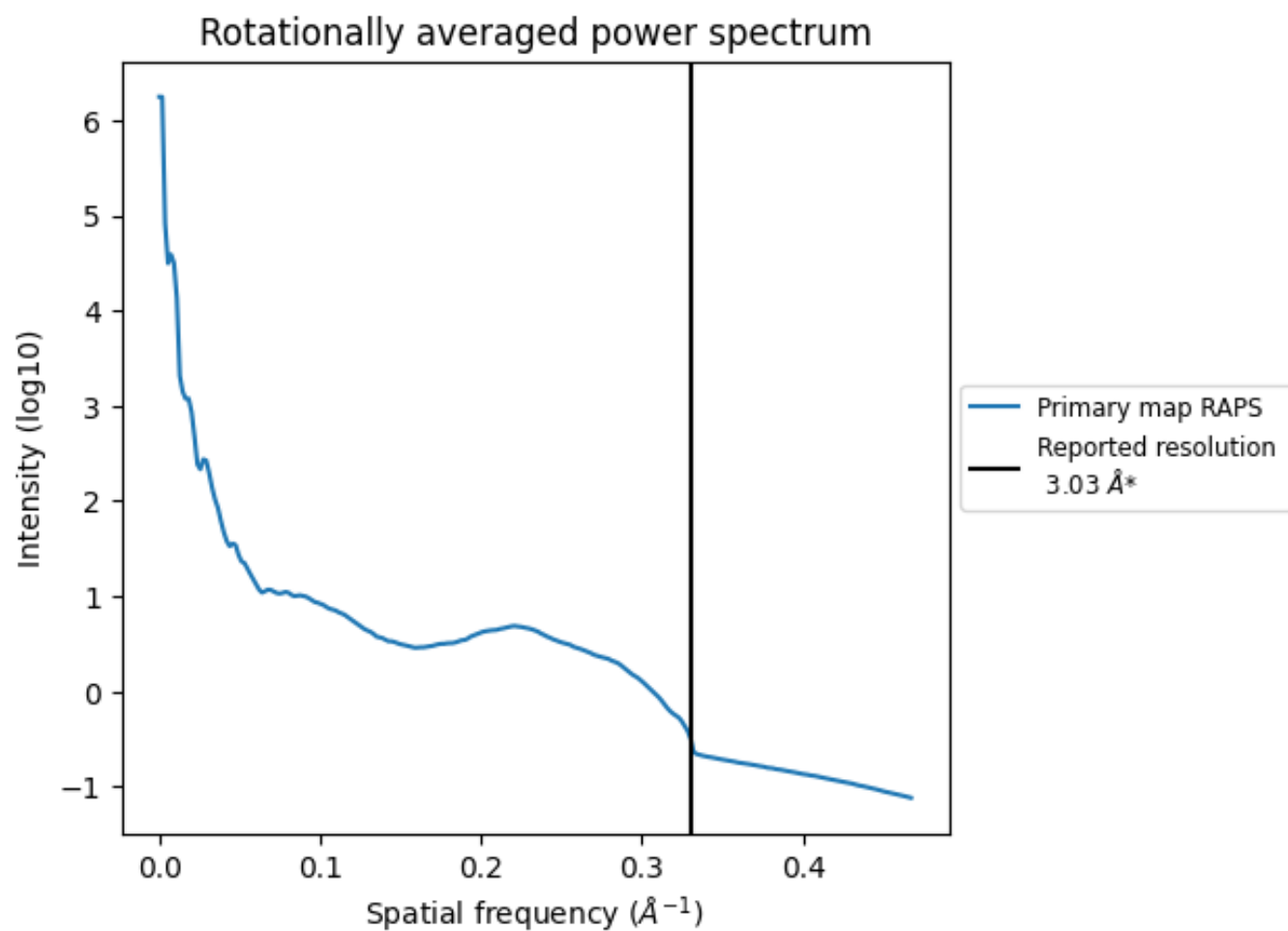
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1200 nm³; this corresponds to an approximate mass of 1084 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 0.330 Å⁻¹

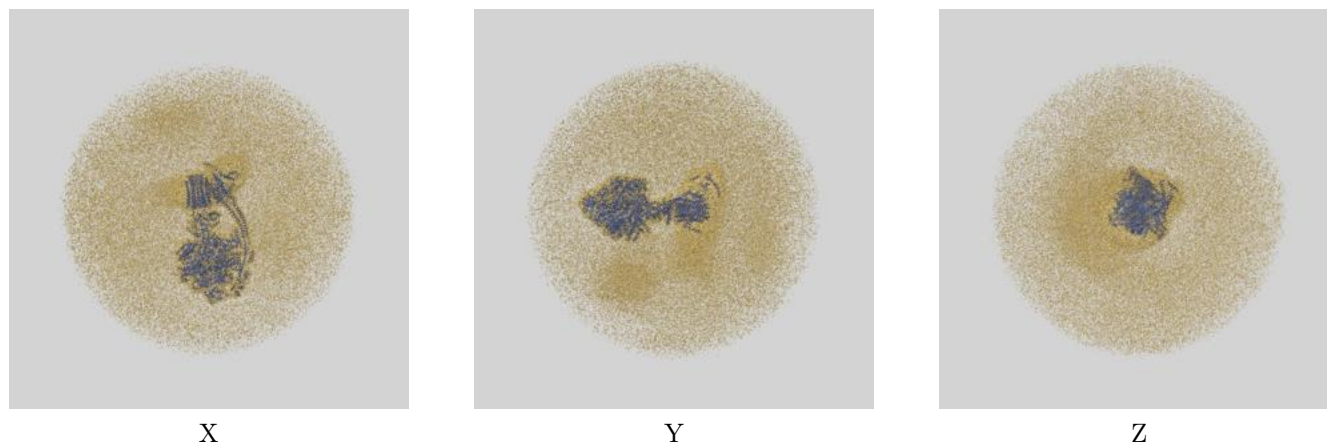
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

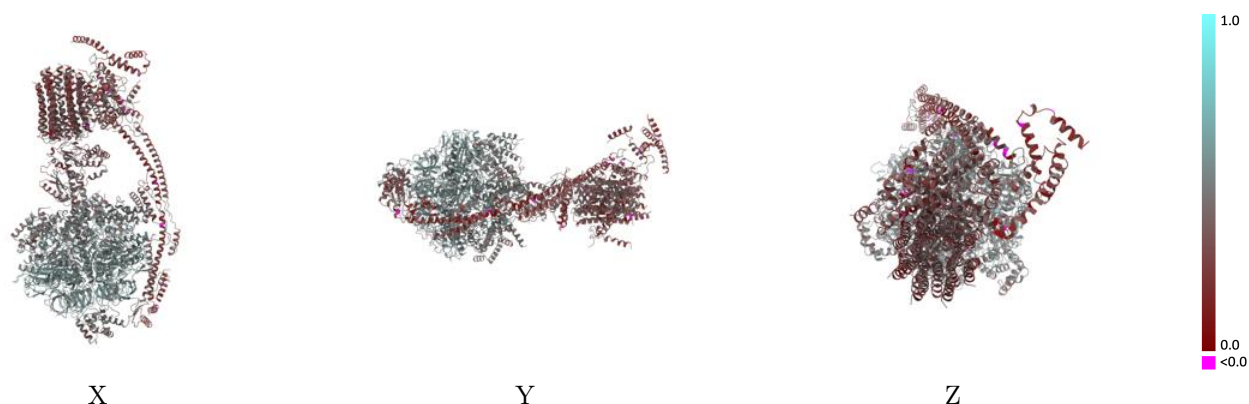
This section contains information regarding the fit between EMDB map EMD-45036 and PDB model 9BYK. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



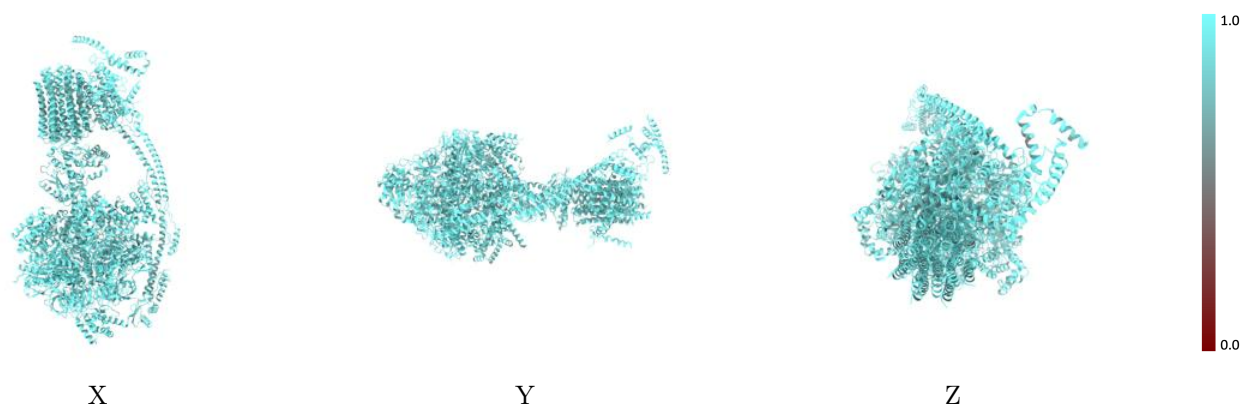
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



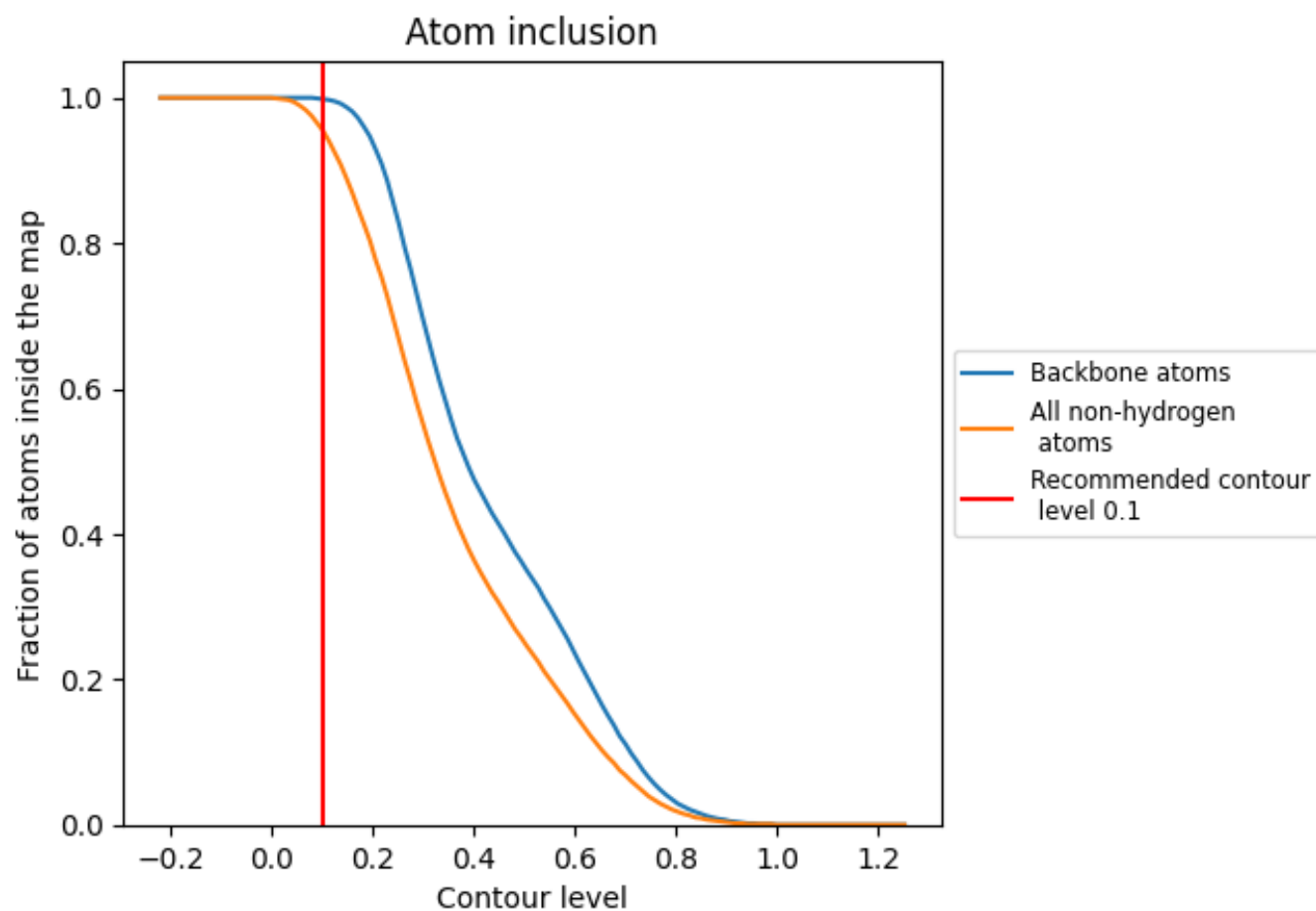
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).





























































9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 96% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9570	 0.4420
8	 0.9490	 0.3170
A	 0.9730	 0.5160
B	 0.9770	 0.5180
C	 0.9730	 0.5140
D	 0.9690	 0.5200
E	 0.9690	 0.5220
F	 0.9780	 0.5340
G	 0.9420	 0.4120
H	 0.9240	 0.3210
I	 0.9710	 0.3490
J	 0.9250	 0.4860
K	 0.9150	 0.2800
L	 0.9170	 0.3060
M	 0.9190	 0.3210
N	 0.9450	 0.3320
O	 0.9350	 0.3160
P	 0.9370	 0.2960
Q	 0.9430	 0.3120
R	 0.9230	 0.3120
S	 0.9280	 0.3920
T	 0.8740	 0.2190
a	 0.9270	 0.3210
b	 0.8980	 0.2330
c	 0.9490	 0.2860
d	 0.9890	 0.3290
e	 0.9220	 0.2580
f	 0.9680	 0.3400
i	 0.9490	 0.2800
k	 0.9770	 0.3350

