



wwPDB EM Validation Summary Report ⓘ

Apr 20, 2024 – 02:25 PM EDT

PDB ID : 8FL8
EMDB ID : EMD-29270
Title : Yeast ATP Synthase structure in presence of MgATP
Authors : Sharma, S.; Patel, H.; Luo, M.; Mueller, D.M.; Liao, M.
Deposited on : 2022-12-21
Resolution : 4.20 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.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

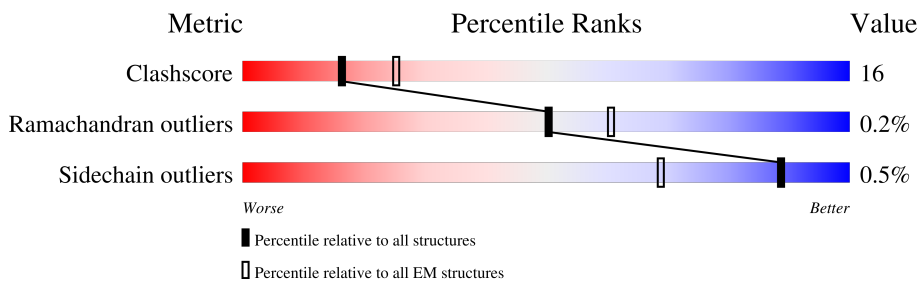
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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.






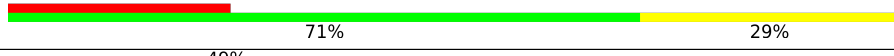
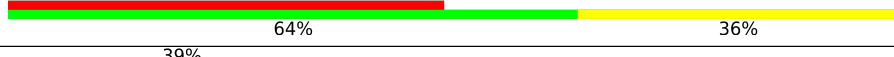




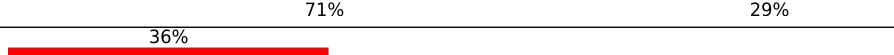



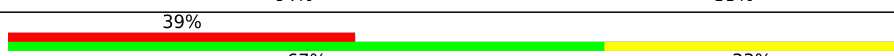
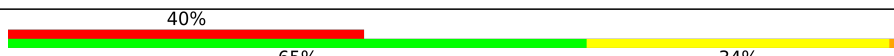
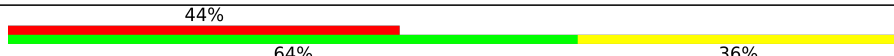



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	41	
2	J	37	
3	Y	166	
4	A	507	
4	B	507	
4	C	507	
5	D	473	
5	E	473	

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Mol	Chain	Length	Quality of chain
5	F	473	
6	G	270	
7	H	132	
8	I	59	
9	K	75	
9	L	75	
9	M	75	
9	N	75	
9	O	75	
9	P	75	
9	Q	75	
9	R	75	
9	S	75	
9	T	75	
10	X	224	
11	Z	155	
12	7	171	
13	6	89	
14	U	85	

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 38784 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
			Total	C	N	O	S		
1	8	41	356	250	51	52	3	0	0

- Molecule 2 is a protein called ATP18 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	J	37	292	197	45	48	2	0	0

- Molecule 3 is a protein called ATP synthase subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Y	166	1254	799	217	237	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	507	3858	2435	679	741	3	0	0
4	B	506	3846	2426	678	739	3	0	0
4	C	505	3844	2426	676	739	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	473	3572	2262	608	696	6	0	0
5	E	473	3572	2262	608	696	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	472	3566	2259	607	694	6	0	0

- Molecule 6 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	261	2032	1276	353	393	10	0	0

- Molecule 7 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	132	990	624	165	199	2	0	0

- Molecule 8 is a protein called ATP synthase subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	I	59	392	243	71	78	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	S	74	533	357	82	90	4	0	0
9	T	74	533	357	82	90	4	0	0
9	K	75	537	359	83	91	4	0	0
9	L	74	533	357	82	90	4	0	0
9	M	74	533	357	82	90	4	0	0
9	N	74	533	357	82	90	4	0	0
9	O	74	533	357	82	90	4	0	0
9	P	75	537	359	83	91	4	0	0
9	Q	74	533	357	82	90	4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	74	Total	C	N	O	S	0	0
			533	357	82	90	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	224	Total	C	N	O	S	0	0
			1772	1210	265	287	10		

- Molecule 11 is a protein called ATP synthase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Z	155	Total	C	N	O	S	0	0
			1232	778	211	242	1		

- Molecule 12 is a protein called ATP synthase subunit d, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	7	171	Total	C	N	O	S	0	0
			1363	856	236	268	3		

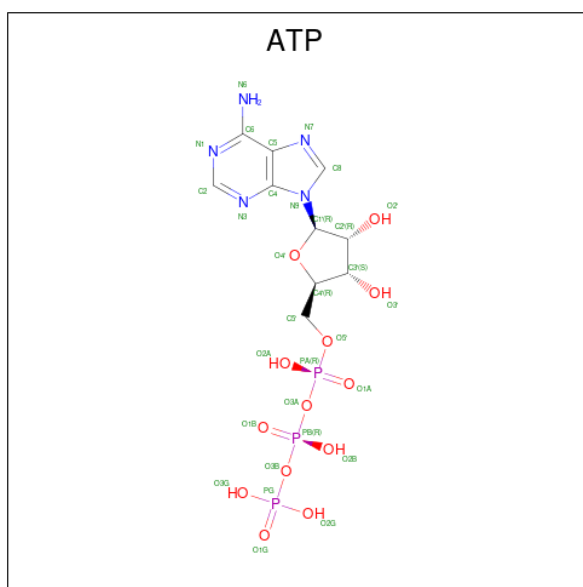
- Molecule 13 is a protein called ATP synthase subunit H, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	6	89	Total	C	N	O	0	0
			710	441	114	155		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	85	Total	C	N	O	S	0	0
			639	420	109	109	1		

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

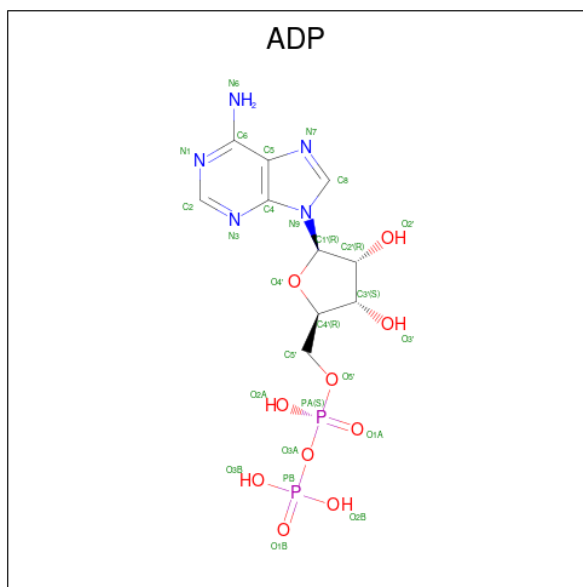


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
15	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
15	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
15	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
15	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

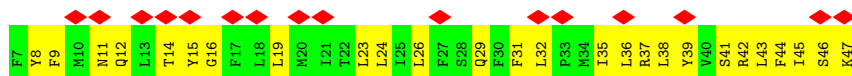


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
17	F	1	27	10	5	10	2	0

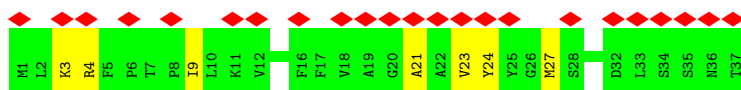
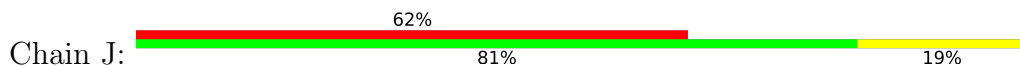
3 Residue-property plots [i](#)

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

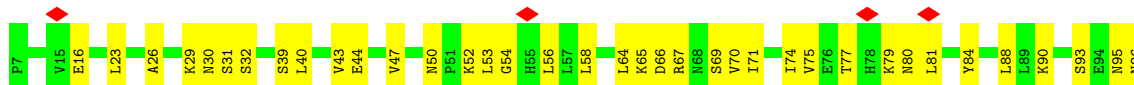
- Molecule 1: ATP synthase protein 8



- Molecule 2: ATP18 isoform 1



- Molecule 3: ATP synthase subunit 5, mitochondrial

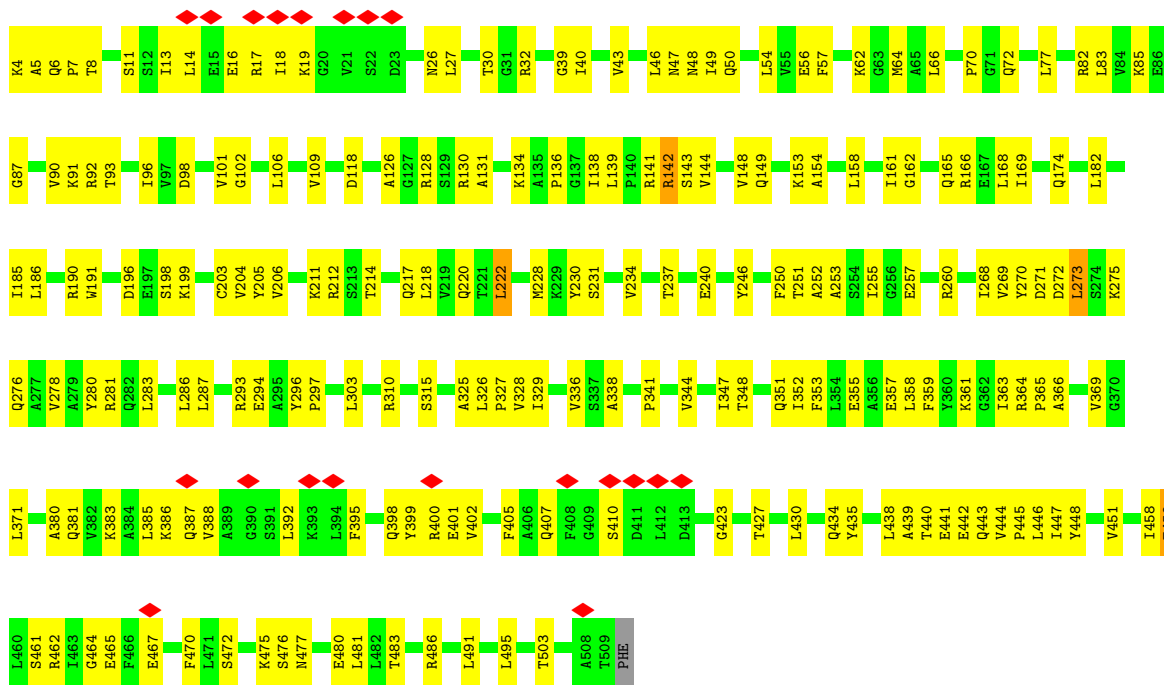


- Molecule 4: ATP synthase subunit alpha

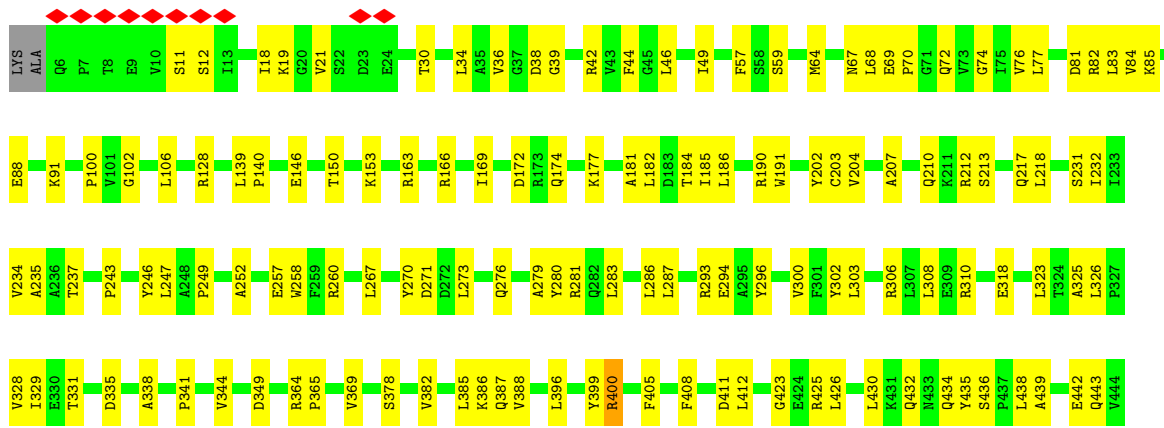


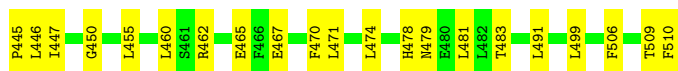


• Molecule 4: ATP synthase subunit alpha

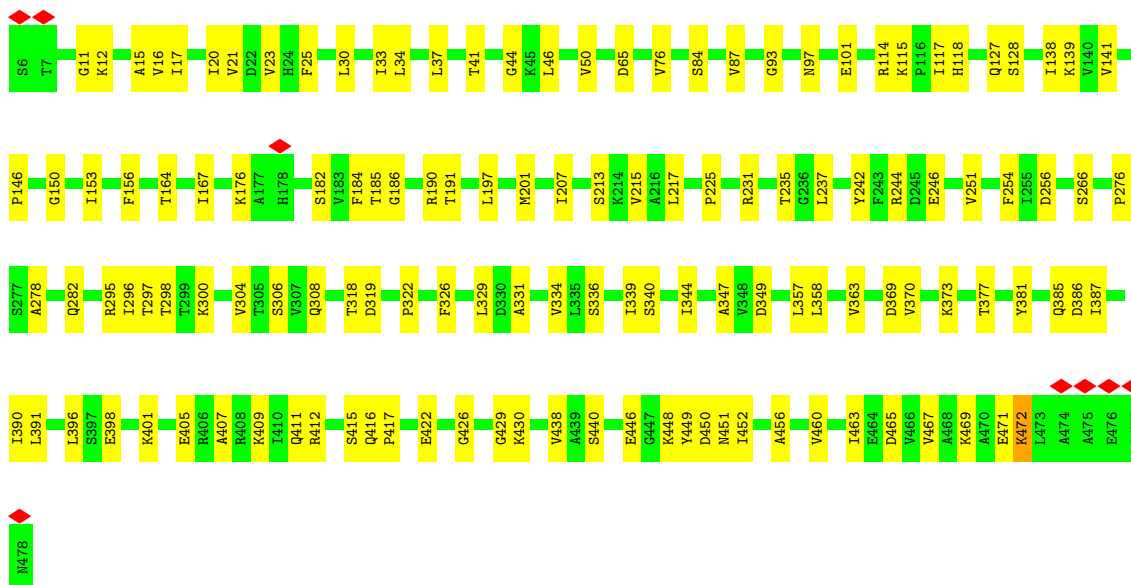


• Molecule 4: ATP synthase subunit alpha

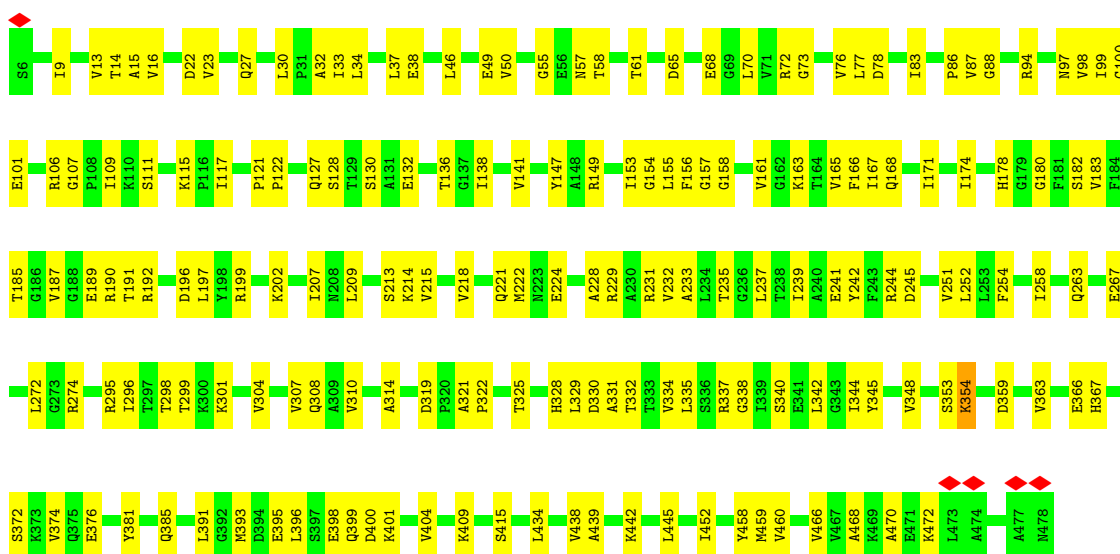




- Molecule 5: ATP synthase subunit beta

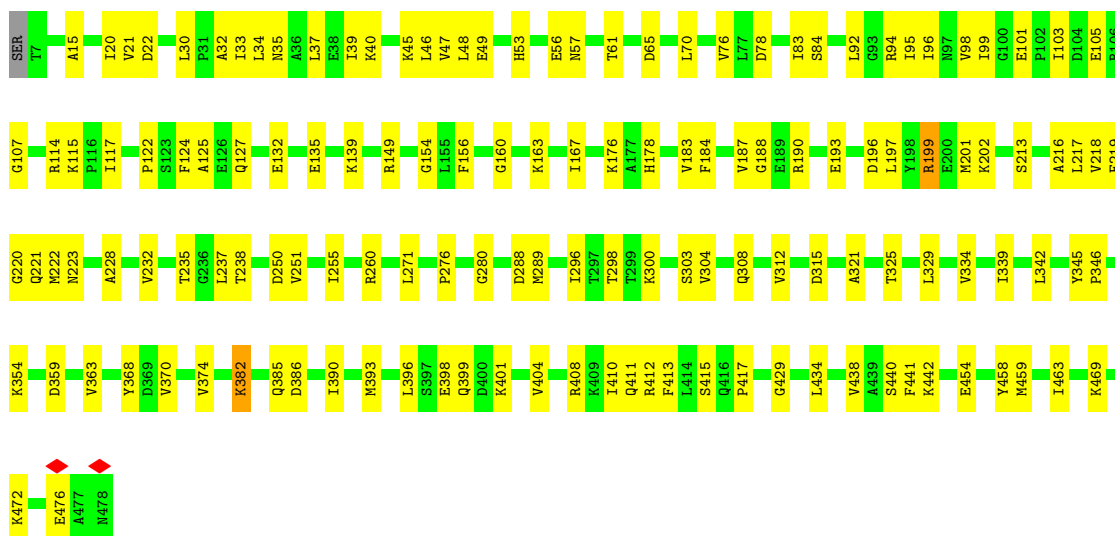


- Molecule 5: ATP synthase subunit beta

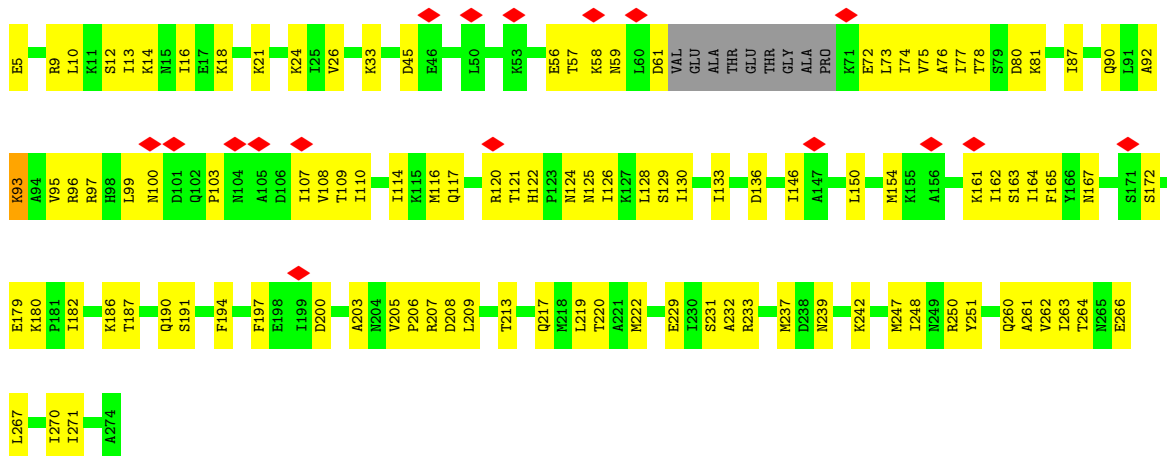


- Molecule 5: ATP synthase subunit beta

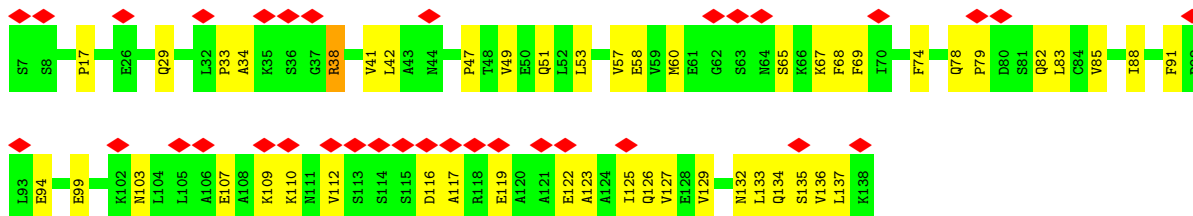




- Molecule 6: ATP synthase subunit gamma, mitochondrial

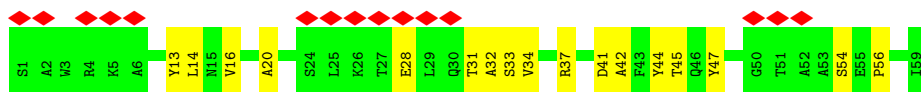


- Molecule 7: ATP synthase subunit delta, mitochondrial

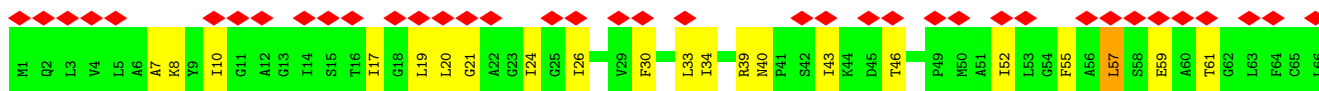


- Molecule 8: ATP synthase subunit epsilon, mitochondrial

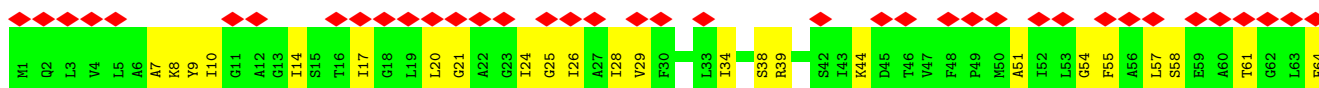




- Molecule 9: ATP synthase subunit 9, mitochondrial



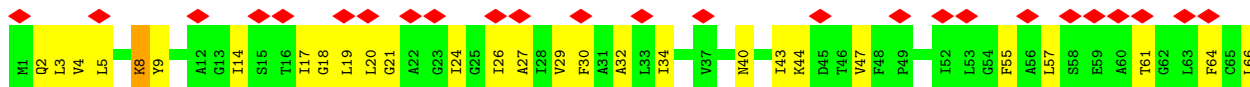
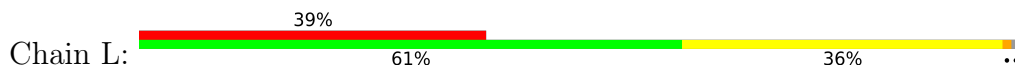
- Molecule 9: ATP synthase subunit 9, mitochondrial



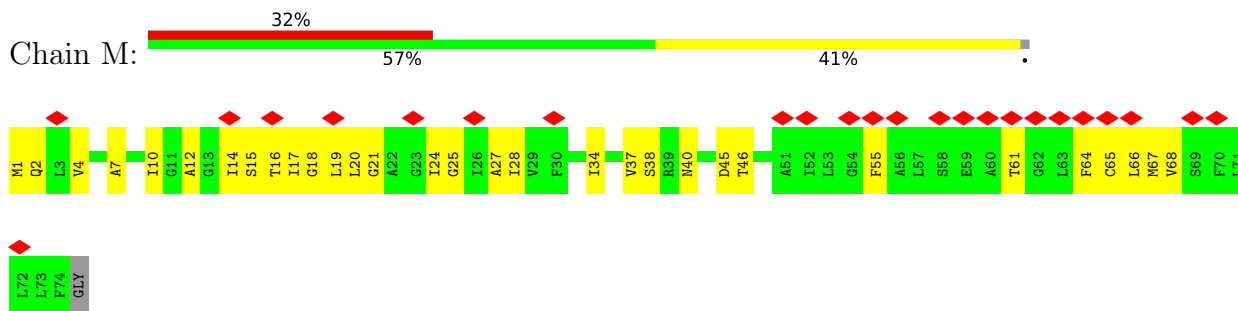
- Molecule 9: ATP synthase subunit 9, mitochondrial



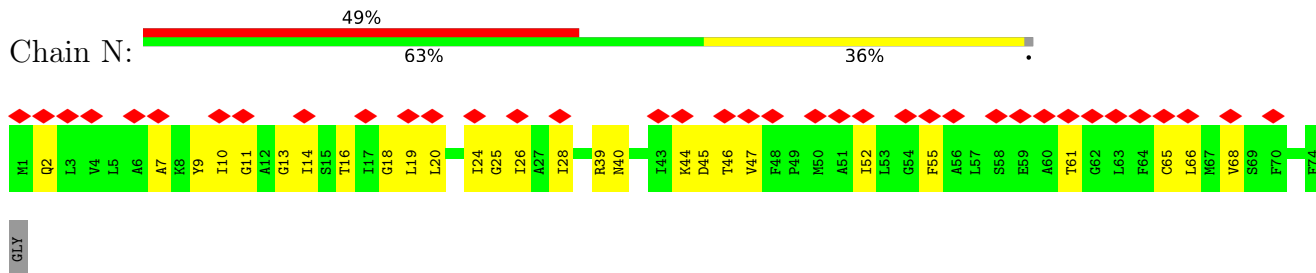
- Molecule 9: ATP synthase subunit 9, mitochondrial



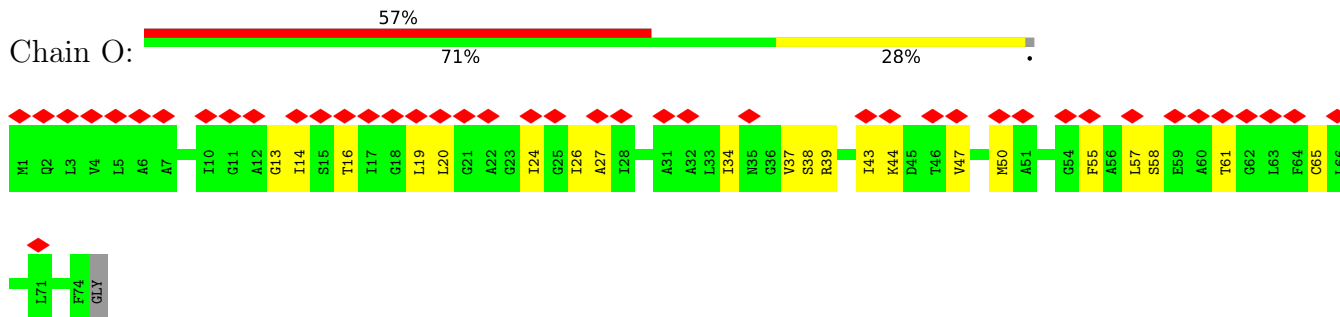
- Molecule 9: ATP synthase subunit 9, mitochondrial



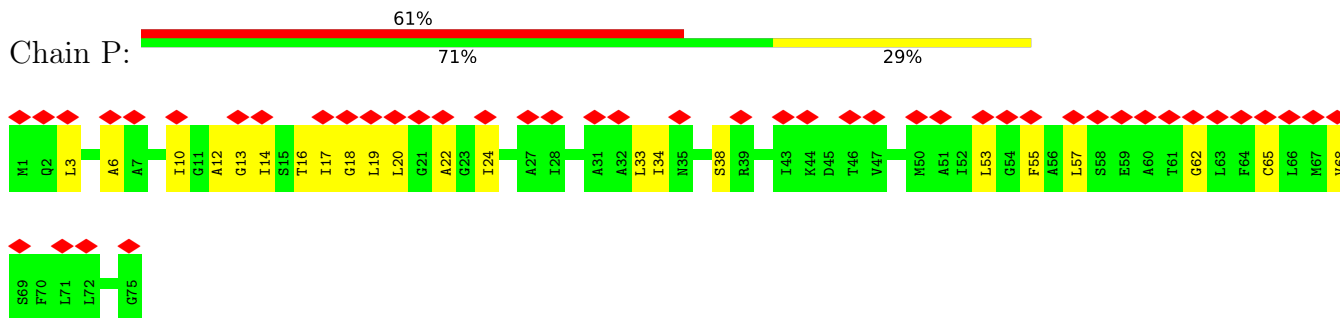
• Molecule 9: ATP synthase subunit 9, mitochondrial



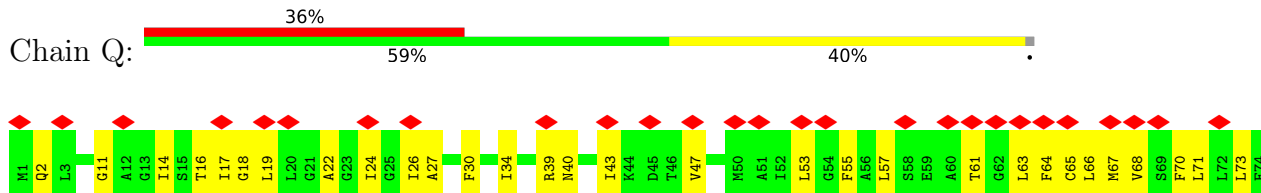
• Molecule 9: ATP synthase subunit 9, mitochondrial



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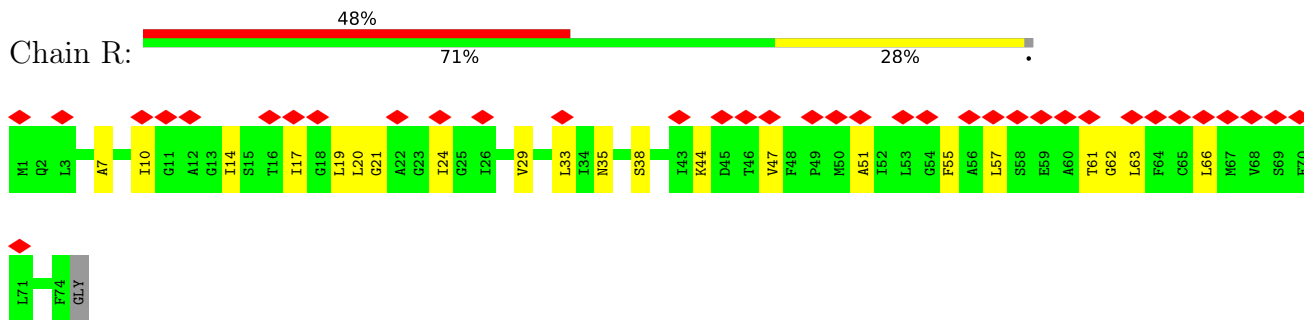


• Molecule 9: ATP synthase subunit 9, mitochondrial

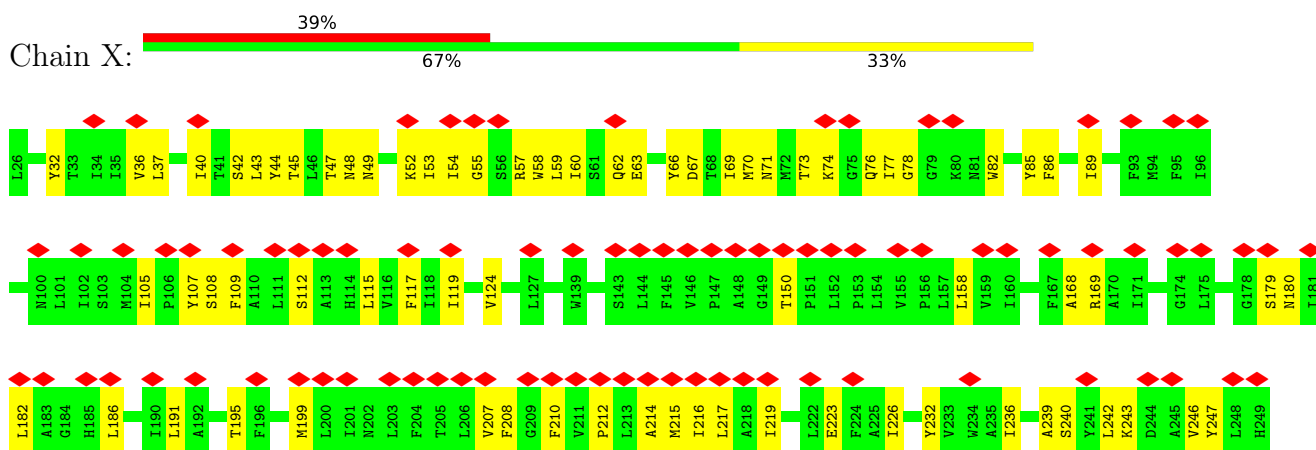


GLY

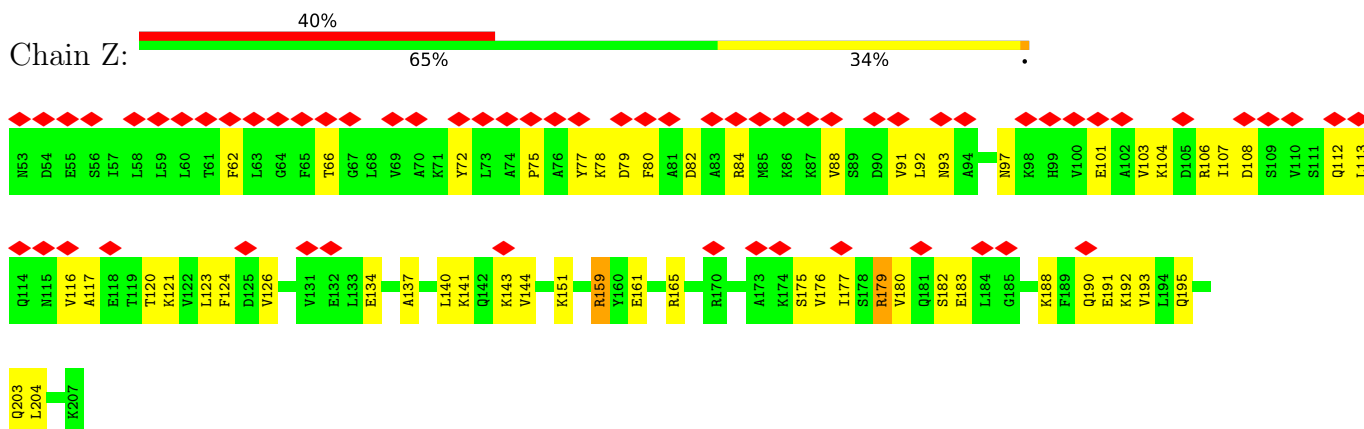
• Molecule 9: ATP synthase subunit 9, mitochondrial



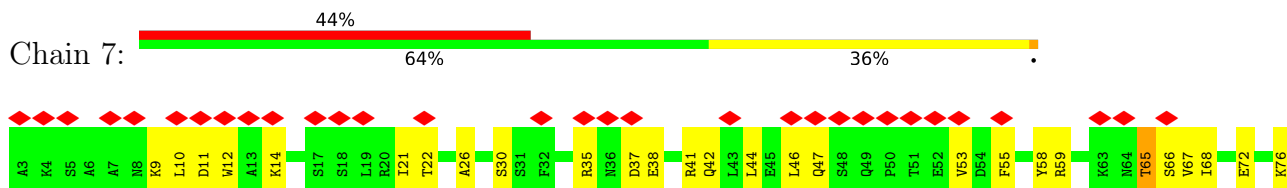
• Molecule 10: ATP synthase subunit a

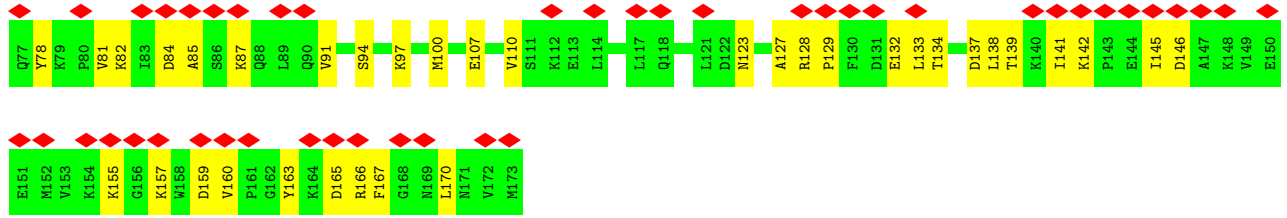


• Molecule 11: ATP synthase subunit 4, mitochondrial

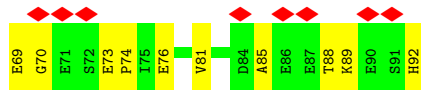
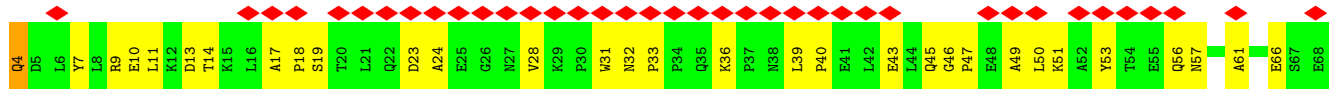


• Molecule 12: ATP synthase subunit d, mitochondrial

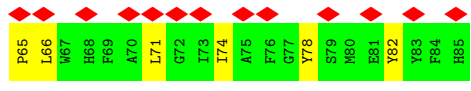
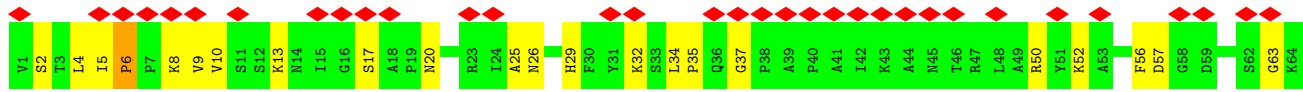




• Molecule 13: ATP synthase subunit H, mitochondrial



• Molecule 14: ATP synthase subunit f, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65559	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 ($e^-/\text{\AA}^2$)	51.07	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.045	Depositor
Minimum map value	-0.015	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.009	Depositor
Map size (\AA)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP, MG

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	0.28	0/366	0.52	0/492
2	J	0.27	0/302	0.55	0/410
3	Y	0.25	0/1272	0.51	0/1717
4	A	0.25	0/3916	0.52	0/5298
4	B	0.27	0/3903	0.56	2/5282 (0.0%)
4	C	0.26	0/3902	0.53	0/5280
5	D	0.25	0/3628	0.50	0/4919
5	E	0.26	0/3628	0.51	1/4919 (0.0%)
5	F	0.27	0/3622	0.52	0/4911
6	G	0.26	0/2057	0.52	0/2767
7	H	0.25	0/1004	0.45	0/1359
8	I	0.24	0/398	0.45	0/547
9	K	0.29	0/545	0.49	0/737
9	L	0.28	0/541	0.53	0/732
9	M	0.27	0/541	0.49	0/732
9	N	0.28	0/541	0.53	0/732
9	O	0.27	0/541	0.45	0/732
9	P	0.28	0/545	0.50	0/737
9	Q	0.32	0/541	0.50	0/732
9	R	0.27	0/541	0.50	0/732
9	S	0.27	0/541	0.53	1/732 (0.1%)
9	T	0.28	0/541	0.46	0/732
10	X	0.25	0/1820	0.47	0/2483
11	Z	0.24	0/1246	0.47	0/1678
12	7	0.24	0/1382	0.49	0/1858
13	6	0.24	0/725	0.50	0/988
14	U	0.26	0/659	0.49	0/895
All	All	0.26	0/39248	0.51	4/53133 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	S	57	LEU	CA-CB-CG	5.51	127.97	115.30
4	B	273	LEU	CA-CB-CG	5.38	127.68	115.30
4	B	222	LEU	CA-CB-CG	5.18	127.22	115.30
5	E	197	LEU	CA-CB-CG	5.18	127.22	115.30

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	8	356	0	379	26	0
2	J	292	0	298	8	0
3	Y	1254	0	1318	56	0
4	A	3858	0	3941	123	0
4	B	3846	0	3932	156	0
4	C	3844	0	3923	115	0
5	D	3572	0	3638	88	0
5	E	3572	0	3638	126	0
5	F	3566	0	3633	103	0
6	G	2032	0	2093	82	0
7	H	990	0	999	44	0
8	I	392	0	306	16	0
9	K	537	0	582	33	0
9	L	533	0	579	34	0
9	M	533	0	579	35	0
9	N	533	0	579	27	0
9	O	533	0	579	27	0
9	P	537	0	582	22	0
9	Q	533	0	579	33	0
9	R	533	0	579	27	0
9	S	533	0	579	21	0
9	T	533	0	579	27	0
10	X	1772	0	1873	59	0
11	Z	1232	0	1256	60	0
12	7	1363	0	1389	69	0
13	6	710	0	668	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	U	639	0	615	31	0
15	A	31	0	12	2	0
15	B	31	0	12	0	0
15	C	31	0	12	2	0
15	E	31	0	12	4	0
16	A	1	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	E	1	0	0	0	0
16	F	1	0	0	0	0
17	F	27	0	12	2	0
All	All	38784	0	39755	1240	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 16.

The worst 5 of 1240 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)
9:N:25:GLY:HA2	9:O:27:ALA:HB2	1.51	0.92
3:Y:136:ARG:HD3	3:Y:137:ILE:HG23	1.54	0.89
5:D:456:ALA:HA	5:D:469:LYS:HD2	1.56	0.86
11:Z:123:LEU:HD11	12:7:14:LYS:HB3	1.58	0.85
4:B:82:ARG:NH2	5:E:33:ILE:O	2.09	0.85

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	39/41 (95%)	34 (87%)	5 (13%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
3	Y	164/166 (99%)	141 (86%)	23 (14%)	0	100	100
4	A	505/507 (100%)	483 (96%)	22 (4%)	0	100	100
4	B	504/507 (99%)	474 (94%)	29 (6%)	1 (0%)	47	80
4	C	503/507 (99%)	477 (95%)	26 (5%)	0	100	100
5	D	471/473 (100%)	442 (94%)	28 (6%)	1 (0%)	47	80
5	E	471/473 (100%)	444 (94%)	25 (5%)	2 (0%)	34	72
5	F	470/473 (99%)	453 (96%)	17 (4%)	0	100	100
6	G	257/270 (95%)	239 (93%)	17 (7%)	1 (0%)	34	72
7	H	130/132 (98%)	118 (91%)	11 (8%)	1 (1%)	19	60
8	I	57/59 (97%)	52 (91%)	4 (7%)	1 (2%)	8	42
9	K	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
9	L	72/75 (96%)	71 (99%)	1 (1%)	0	100	100
9	M	72/75 (96%)	71 (99%)	1 (1%)	0	100	100
9	N	72/75 (96%)	71 (99%)	1 (1%)	0	100	100
9	O	72/75 (96%)	70 (97%)	2 (3%)	0	100	100
9	P	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
9	Q	72/75 (96%)	71 (99%)	1 (1%)	0	100	100
9	R	72/75 (96%)	70 (97%)	2 (3%)	0	100	100
9	S	72/75 (96%)	71 (99%)	1 (1%)	0	100	100
9	T	72/75 (96%)	71 (99%)	1 (1%)	0	100	100
10	X	222/224 (99%)	202 (91%)	20 (9%)	0	100	100
11	Z	153/155 (99%)	144 (94%)	9 (6%)	0	100	100
12	7	169/171 (99%)	155 (92%)	12 (7%)	2 (1%)	13	50
13	6	87/89 (98%)	72 (83%)	15 (17%)	0	100	100
14	U	83/85 (98%)	75 (90%)	7 (8%)	1 (1%)	13	50
All	All	5042/5119 (98%)	4747 (94%)	285 (6%)	10 (0%)	50	80

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	459	GLU
7	H	117	ALA

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Mol	Chain	Res	Type
8	I	56	PRO
5	E	354	LYS
6	G	57	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8	40/40 (100%)	40 (100%)	0	100	100
2	J	30/30 (100%)	30 (100%)	0	100	100
3	Y	139/139 (100%)	136 (98%)	3 (2%)	52	70
4	A	410/410 (100%)	409 (100%)	1 (0%)	93	96
4	B	409/410 (100%)	408 (100%)	1 (0%)	93	96
4	C	409/410 (100%)	408 (100%)	1 (0%)	93	96
5	D	382/382 (100%)	381 (100%)	1 (0%)	92	95
5	E	382/382 (100%)	381 (100%)	1 (0%)	92	95
5	F	381/382 (100%)	379 (100%)	2 (0%)	88	93
6	G	224/230 (97%)	223 (100%)	1 (0%)	91	94
7	H	111/111 (100%)	110 (99%)	1 (1%)	78	87
8	I	25/46 (54%)	25 (100%)	0	100	100
9	K	55/55 (100%)	55 (100%)	0	100	100
9	L	55/55 (100%)	54 (98%)	1 (2%)	59	76
9	M	55/55 (100%)	55 (100%)	0	100	100
9	N	55/55 (100%)	55 (100%)	0	100	100
9	O	55/55 (100%)	55 (100%)	0	100	100
9	P	55/55 (100%)	55 (100%)	0	100	100
9	Q	55/55 (100%)	55 (100%)	0	100	100
9	R	55/55 (100%)	55 (100%)	0	100	100
9	S	55/55 (100%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	T	55/55 (100%)	55 (100%)	0	100	100
10	X	193/193 (100%)	191 (99%)	2 (1%)	76	86
11	Z	137/138 (99%)	135 (98%)	2 (2%)	65	80
12	7	154/156 (99%)	153 (99%)	1 (1%)	86	92
13	6	79/79 (100%)	78 (99%)	1 (1%)	69	82
14	U	60/68 (88%)	59 (98%)	1 (2%)	60	78
All	All	4115/4156 (99%)	4095 (100%)	20 (0%)	89	93

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	X	180	ASN
12	7	123	ASN
14	U	50	ARG
13	6	4	GLN
5	D	472	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
9	S	2	GLN
12	7	47	GLN
4	C	387	GLN
5	F	53	HIS
5	F	223	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 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
17	ADP	F	501	16	24,29,29	0.96	1 (4%)	29,45,45	1.45	4 (13%)
15	ATP	A	601	16	26,33,33	0.59	0	31,52,52	0.74	2 (6%)
15	ATP	C	601	16	26,33,33	0.60	0	31,52,52	0.75	2 (6%)
15	ATP	E	501	16	26,33,33	0.59	0	31,52,52	0.76	2 (6%)
15	ATP	B	601	16	26,33,33	0.60	0	31,52,52	0.75	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	ADP	F	501	16	-	0/12/32/32	0/3/3/3
15	ATP	A	601	16	-	3/18/38/38	0/3/3/3
15	ATP	C	601	16	-	3/18/38/38	0/3/3/3
15	ATP	E	501	16	-	5/18/38/38	0/3/3/3
15	ATP	B	601	16	-	5/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	501	ADP	C5-C4	2.46	1.47	1.40

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	F	501	ADP	C3'-C2'-C1'	3.43	106.14	100.98
17	F	501	ADP	PA-O3A-PB	-3.38	121.21	132.83
17	F	501	ADP	N3-C2-N1	-3.13	123.79	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	F	501	ADP	C4-C5-N7	-2.62	106.67	109.40
15	C	601	ATP	C5-C6-N6	2.33	123.89	120.35

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

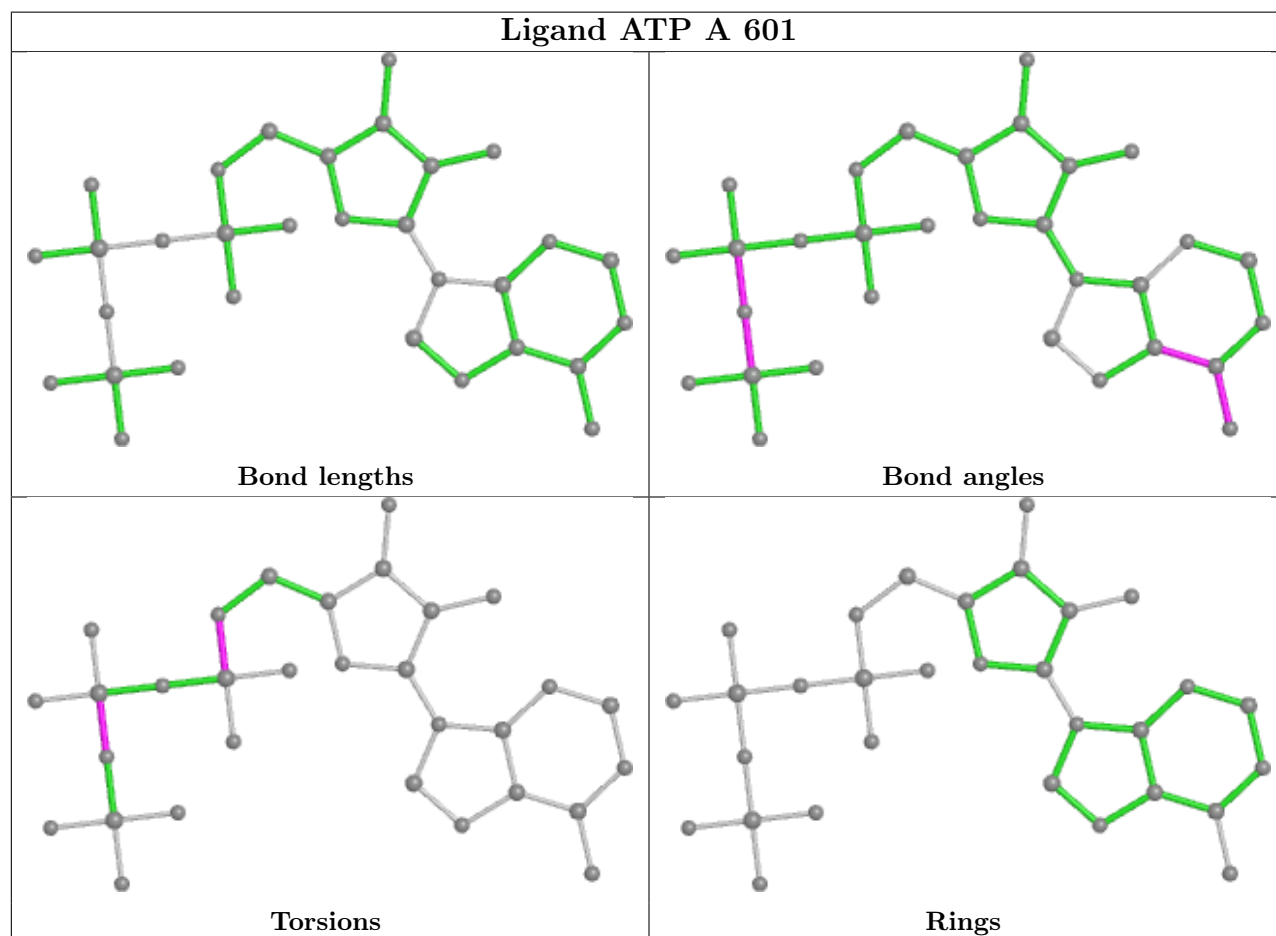
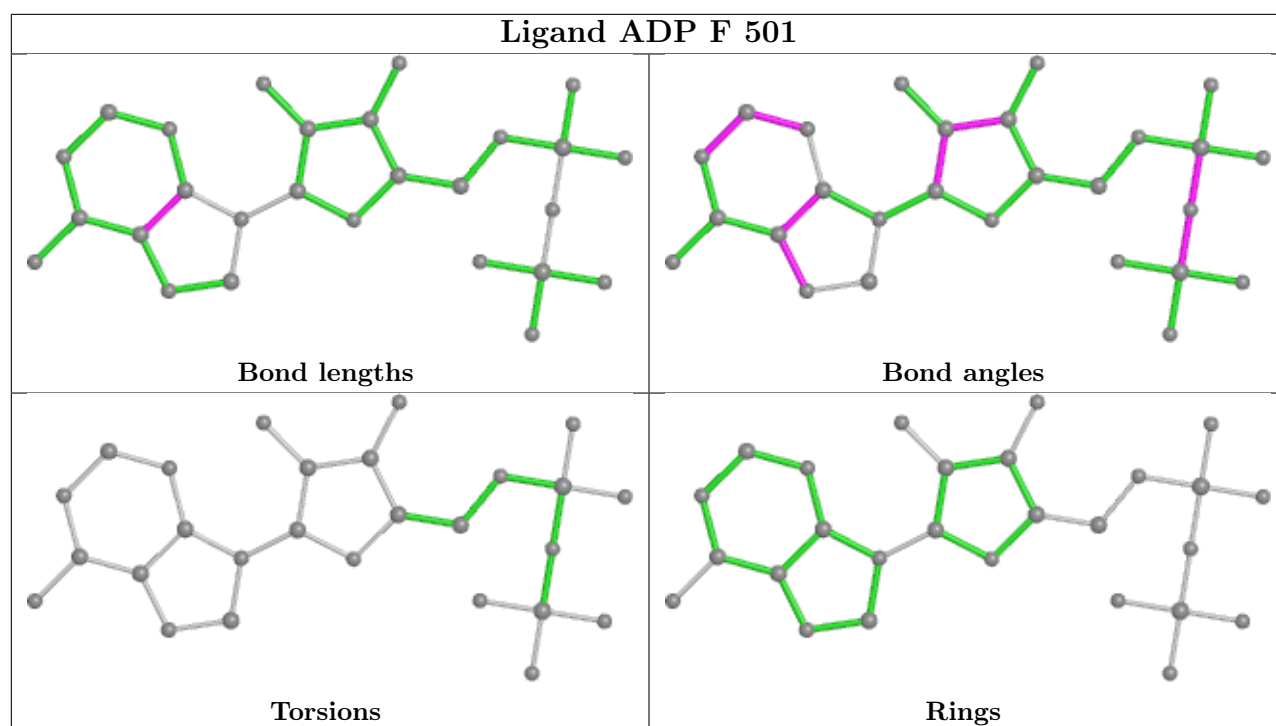
Mol	Chain	Res	Type	Atoms
15	B	601	ATP	C5'-O5'-PA-O1A
15	B	601	ATP	C5'-O5'-PA-O3A
15	C	601	ATP	C5'-O5'-PA-O1A
15	E	501	ATP	C5'-O5'-PA-O1A
15	E	501	ATP	C5'-O5'-PA-O3A

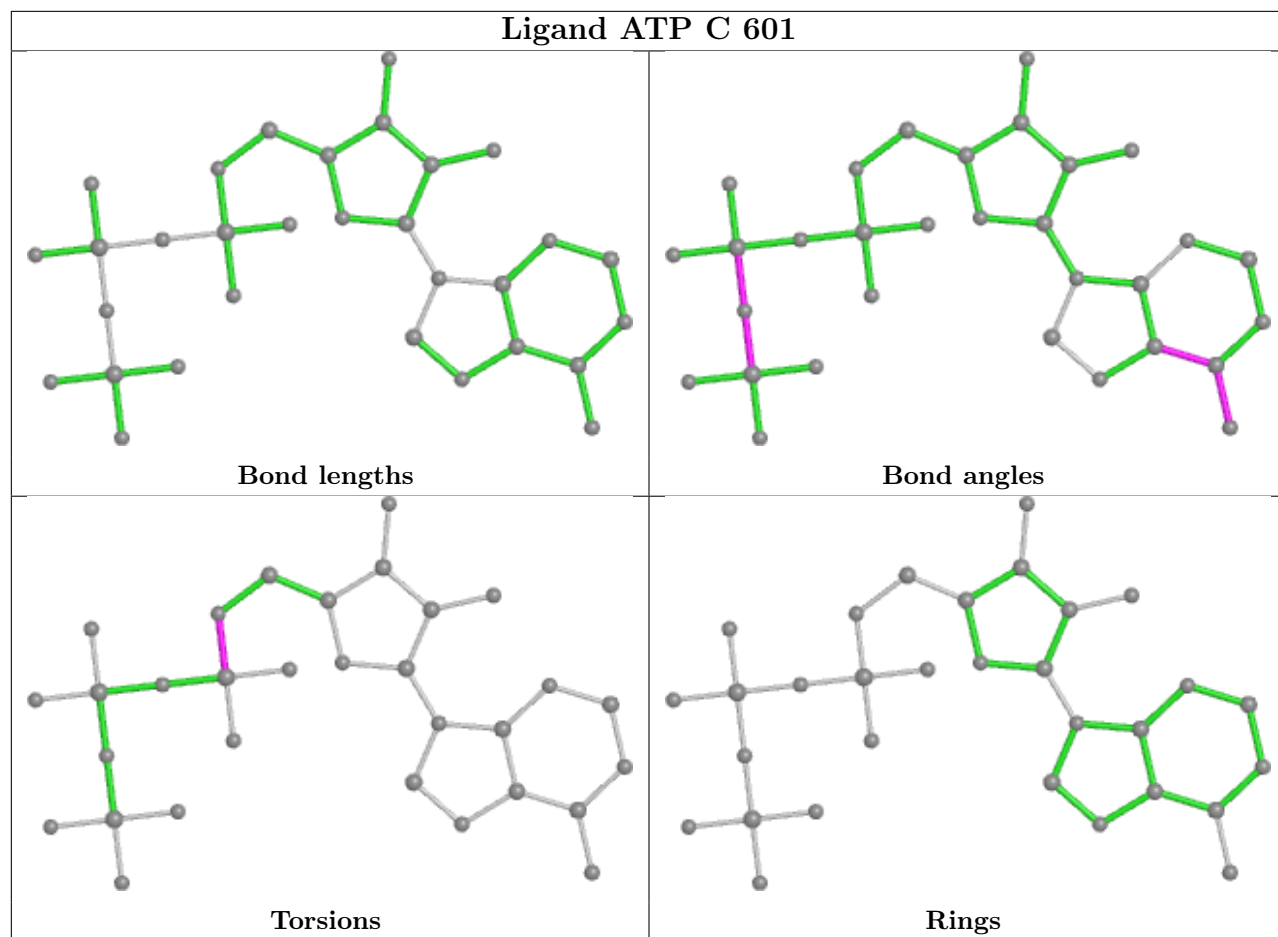
There are no ring outliers.

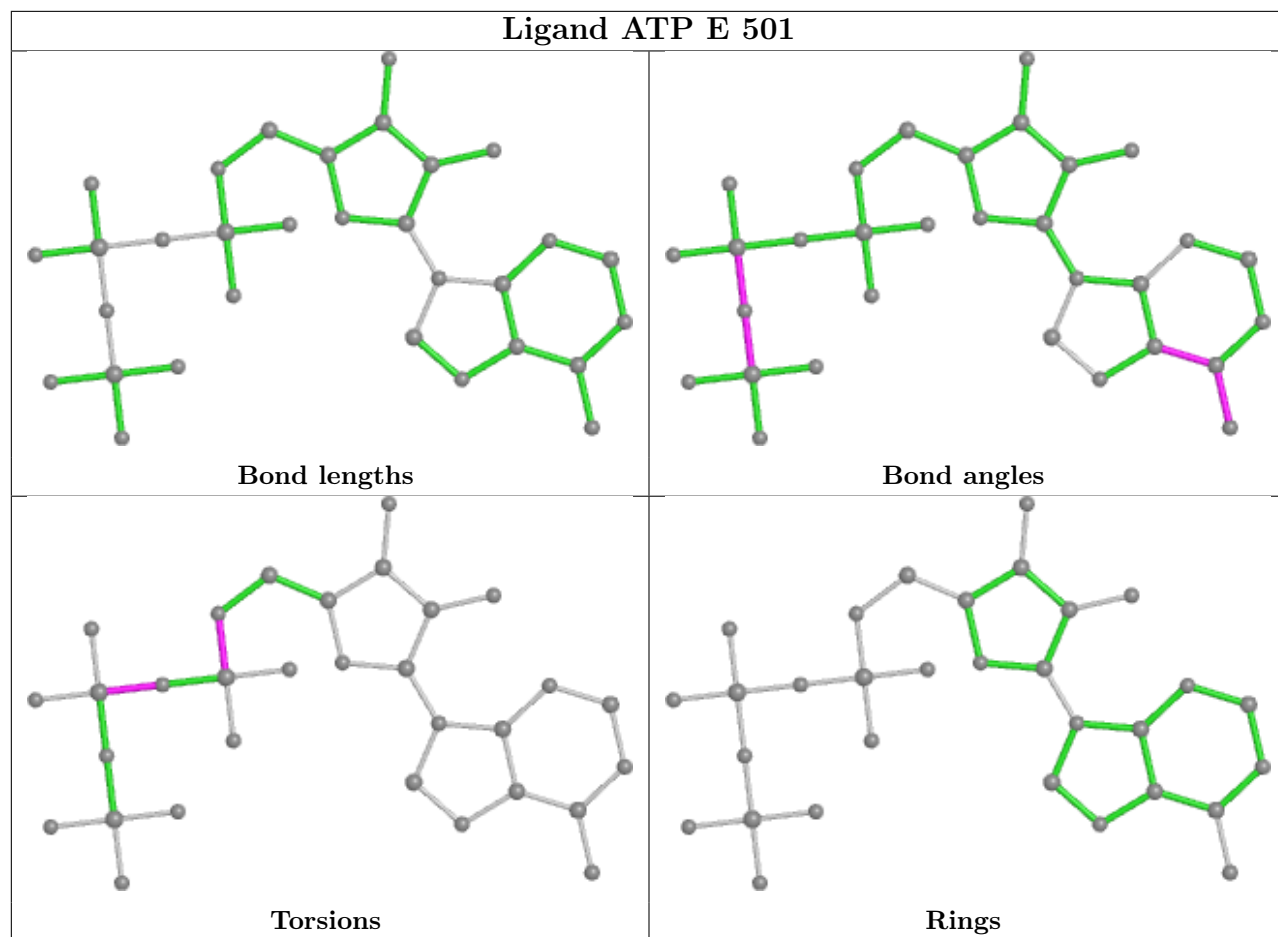
4 monomers are involved in 10 short contacts:

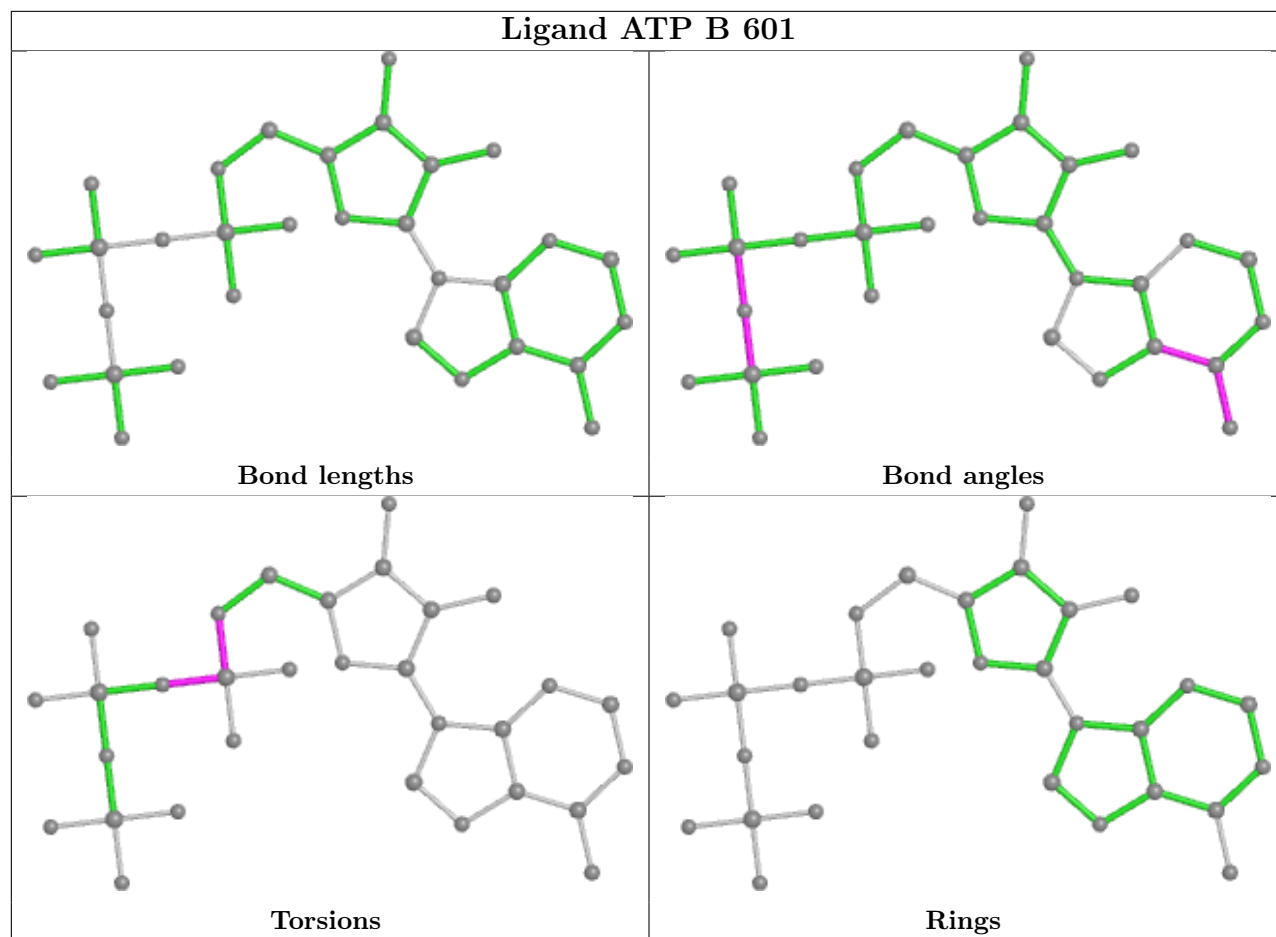
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	F	501	ADP	2	0
15	A	601	ATP	2	0
15	C	601	ATP	2	0
15	E	501	ATP	4	0

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.

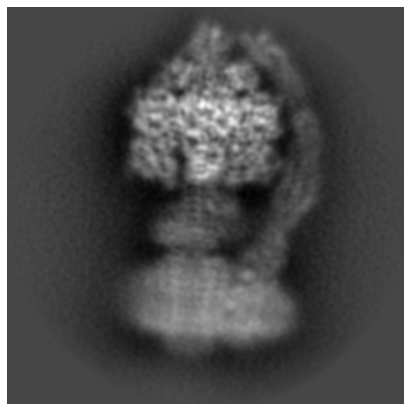
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29270. These allow visual inspection of the internal detail of the map and identification of artifacts.

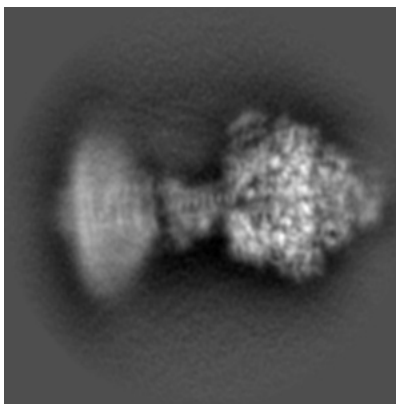
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

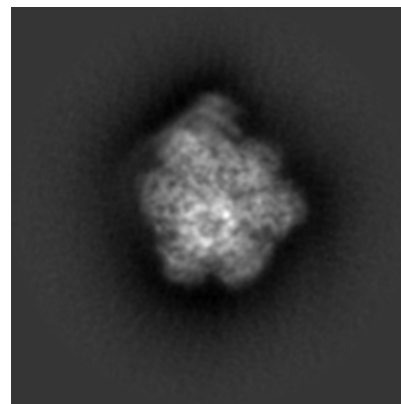
6.1.1 Primary map



X

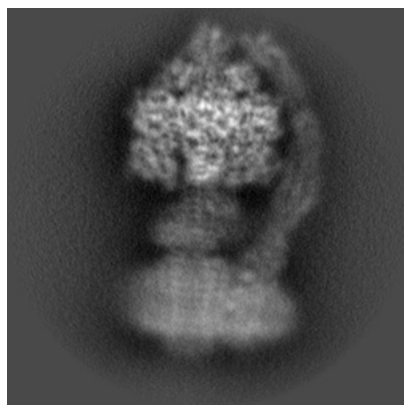


Y

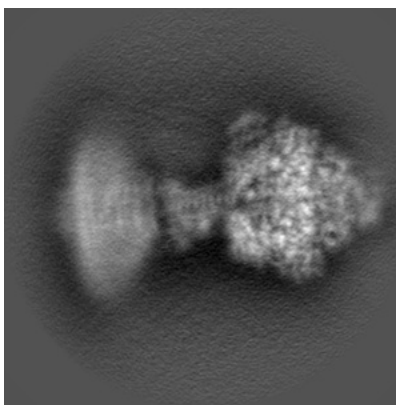


Z

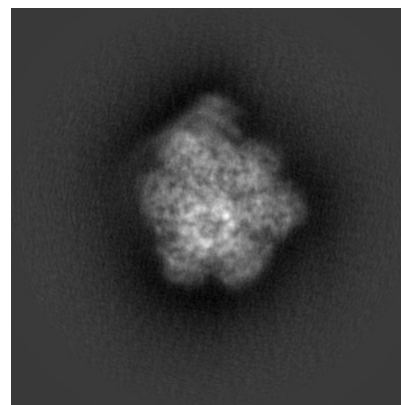
6.1.2 Raw map



X



Y

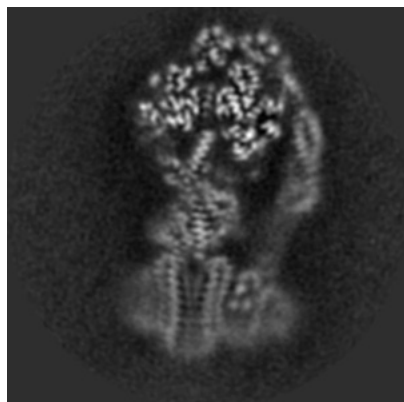


Z

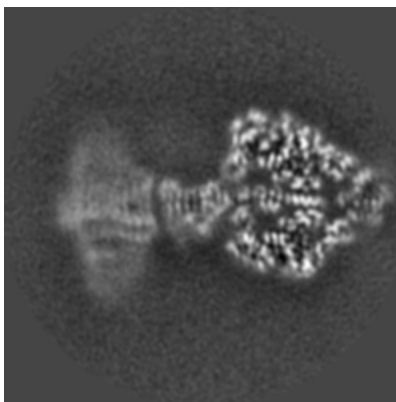
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

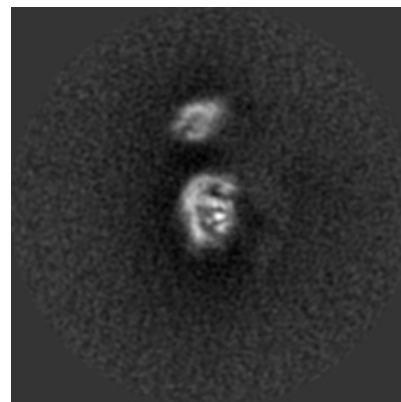
6.2.1 Primary map



X Index: 128

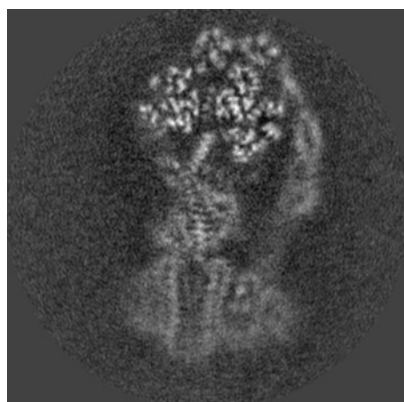


Y Index: 128

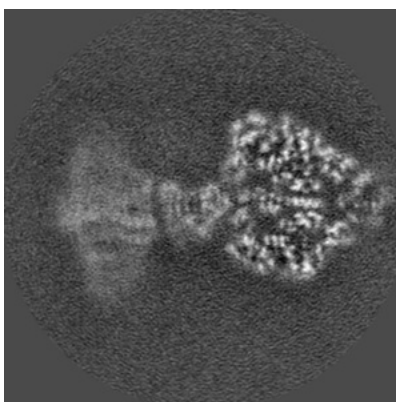


Z Index: 128

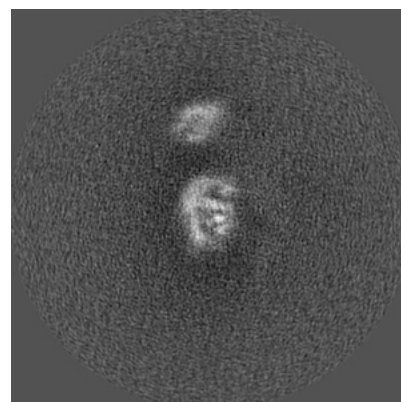
6.2.2 Raw map



X Index: 128



Y Index: 128

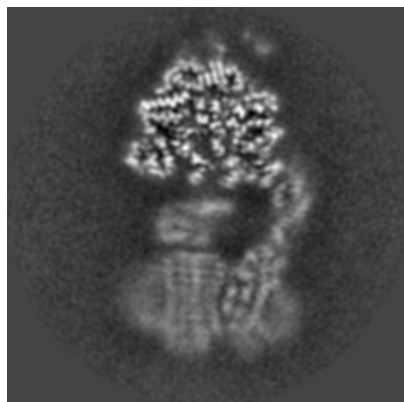


Z Index: 128

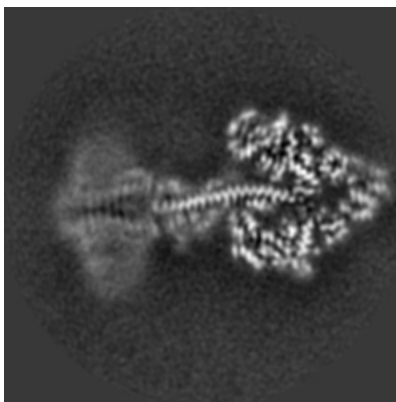
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

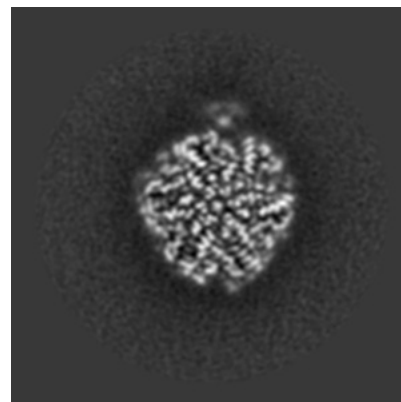
6.3.1 Primary map



X Index: 114

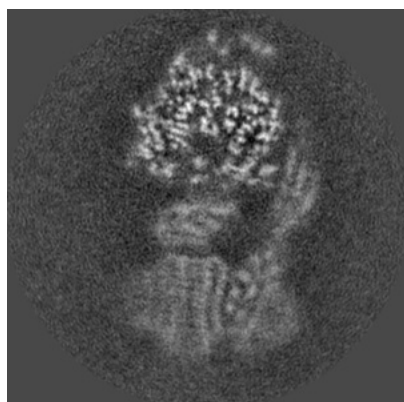


Y Index: 123

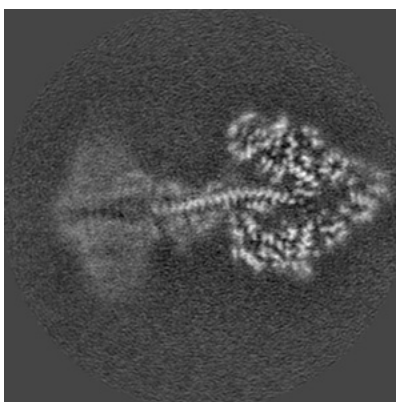


Z Index: 191

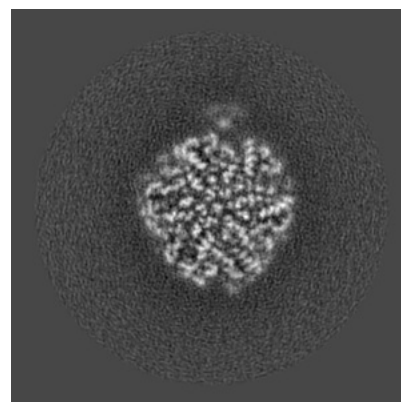
6.3.2 Raw map



X Index: 118



Y Index: 123

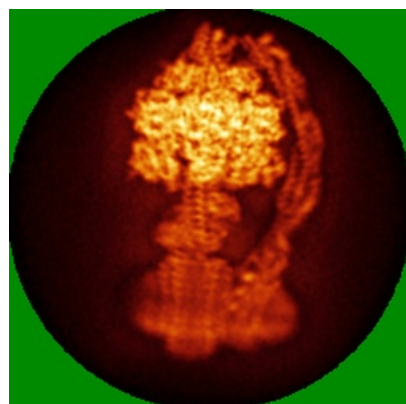


Z Index: 191

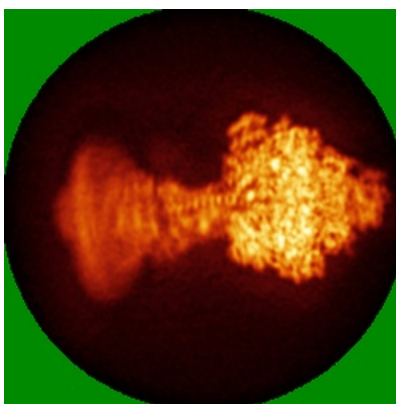
The images above show the largest variance slices of the map in three orthogonal directions.

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

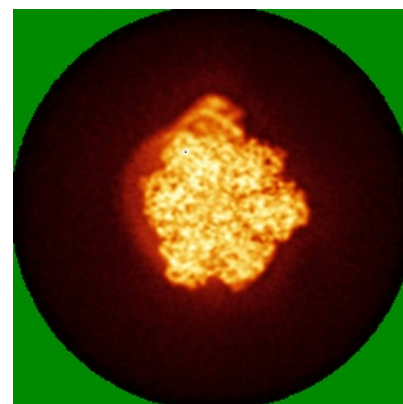
6.4.1 Primary map



X

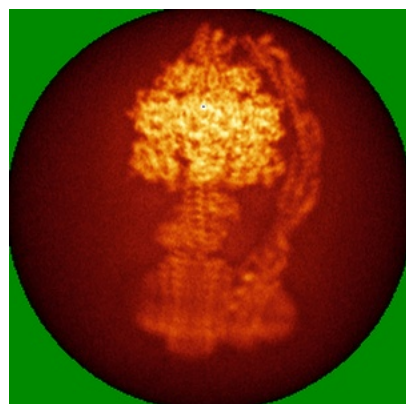


Y

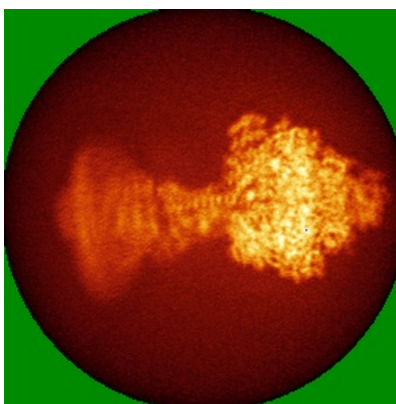


Z

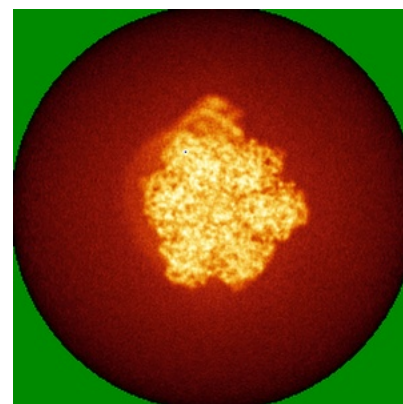
6.4.2 Raw map



X



Y

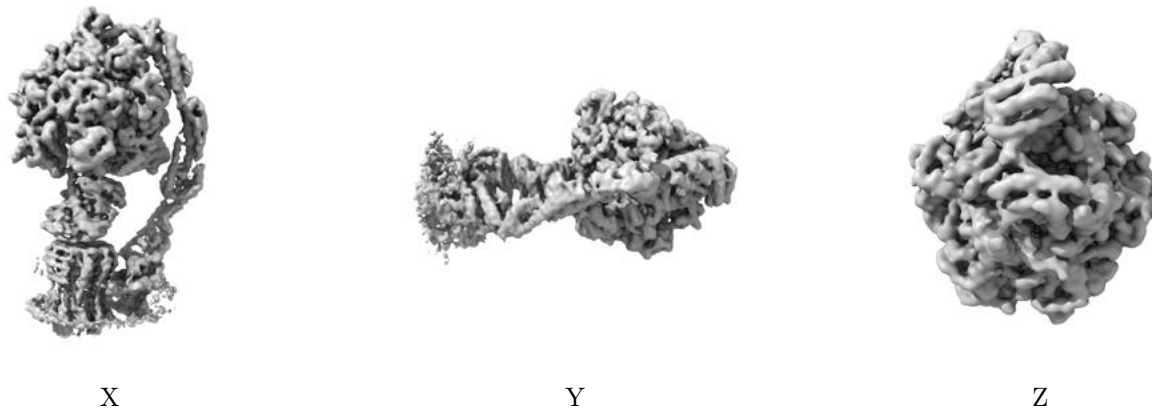


Z

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.

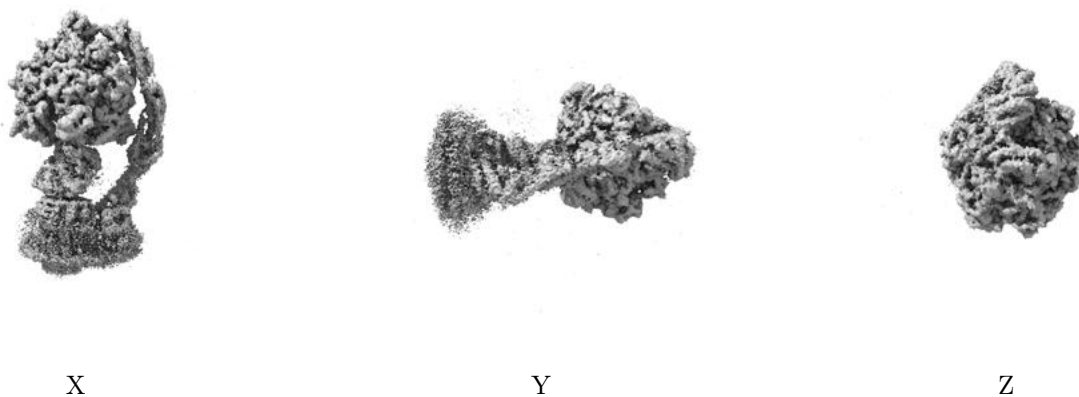
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

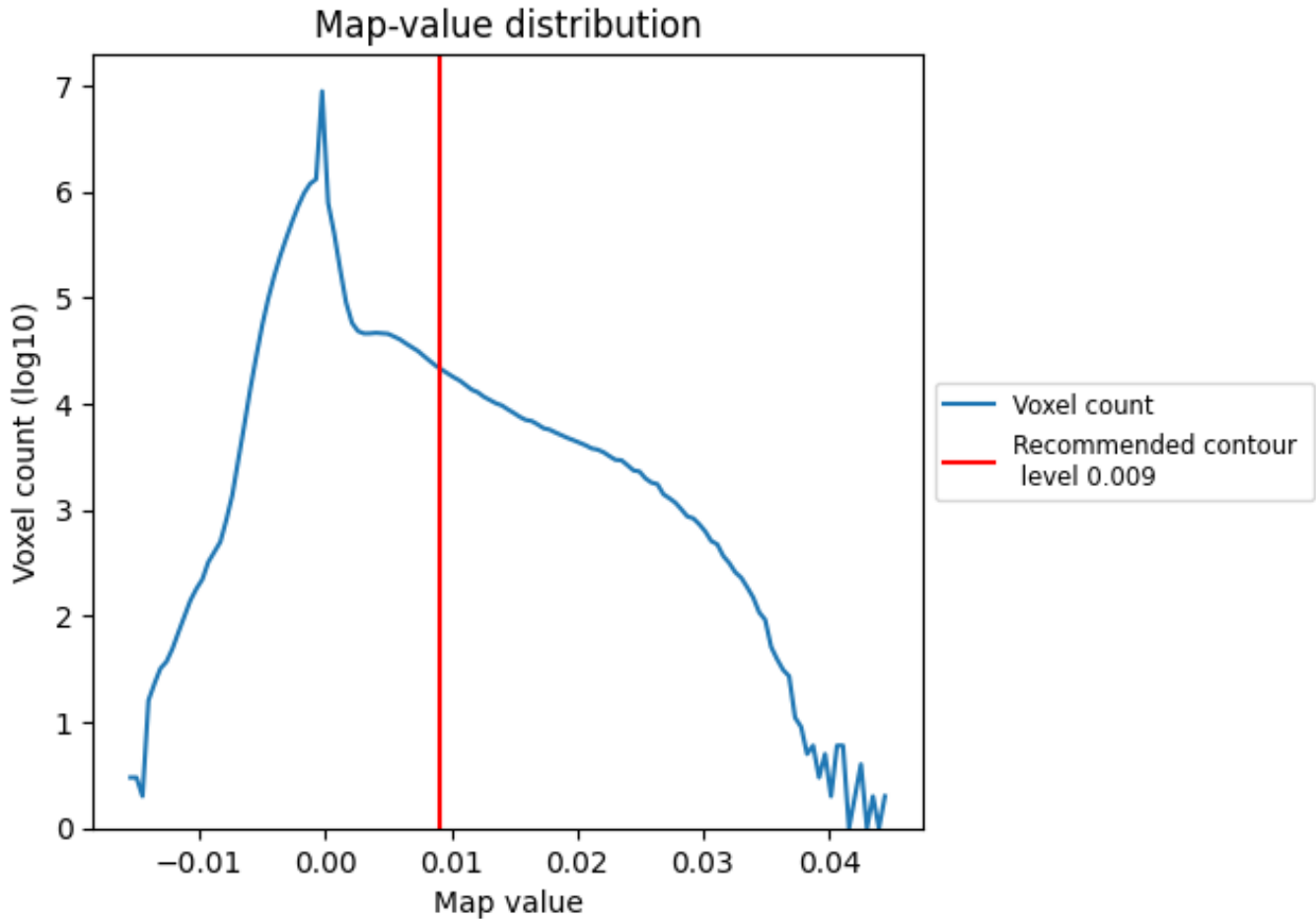
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

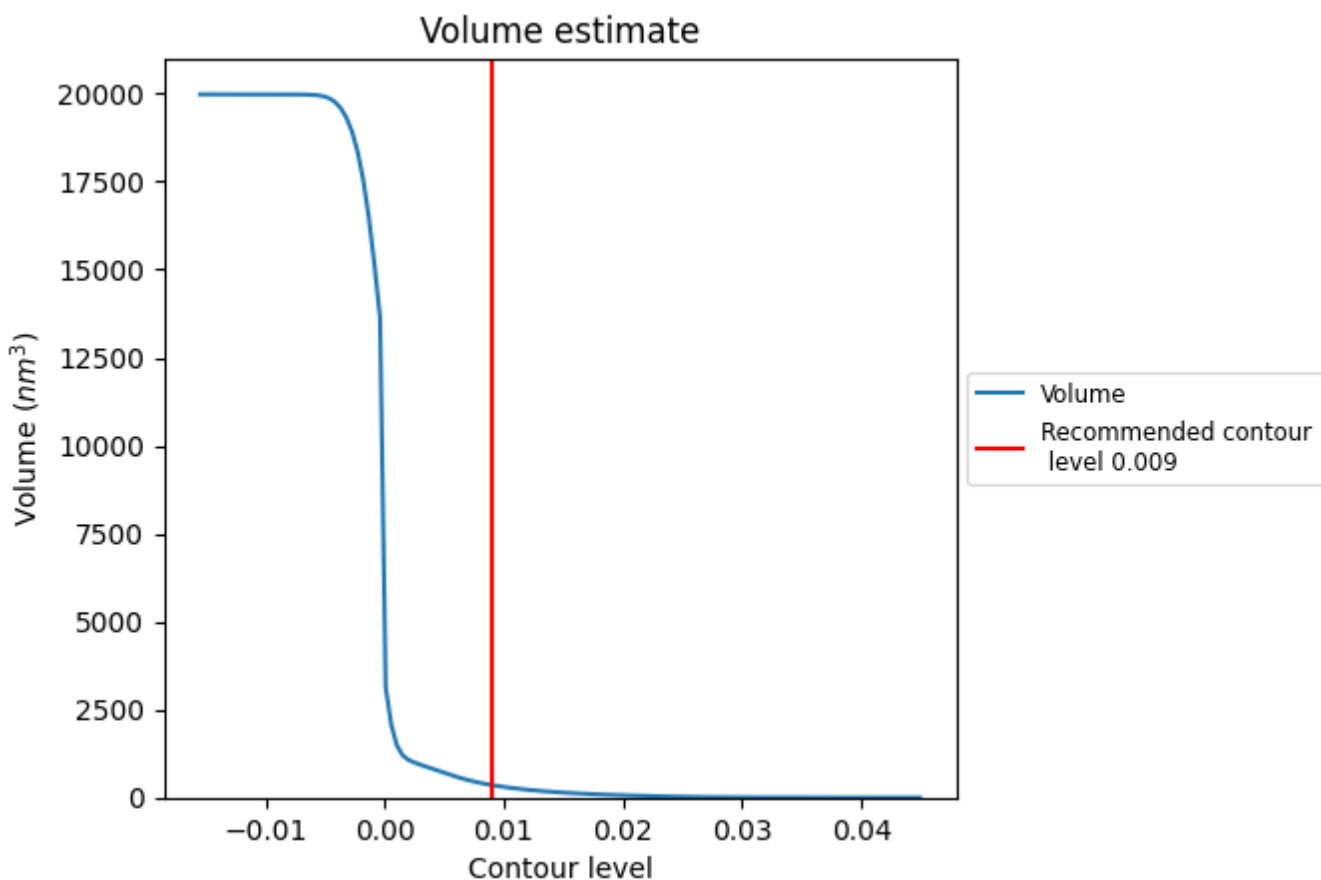
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

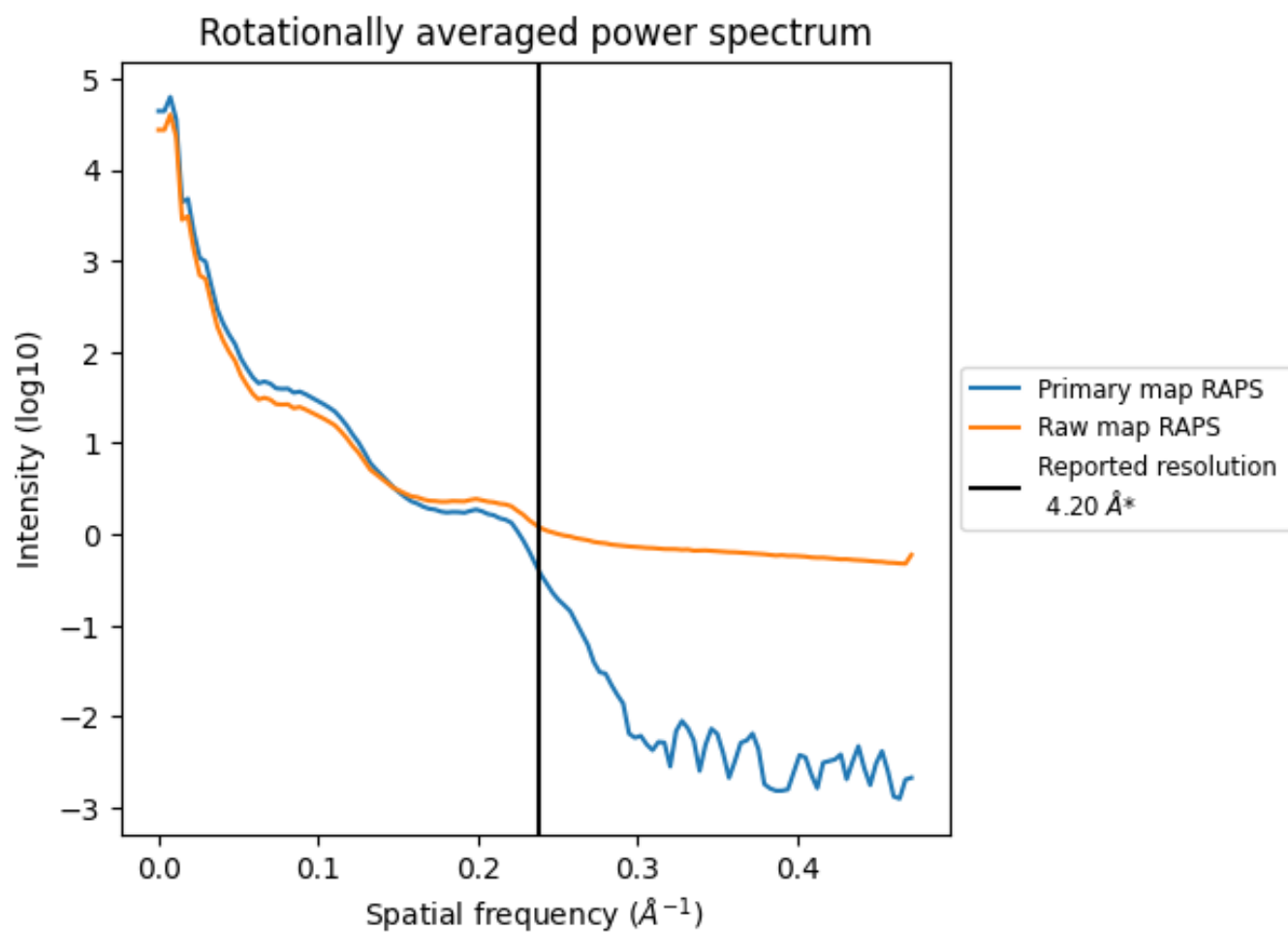
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 354 nm³; this corresponds to an approximate mass of 320 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

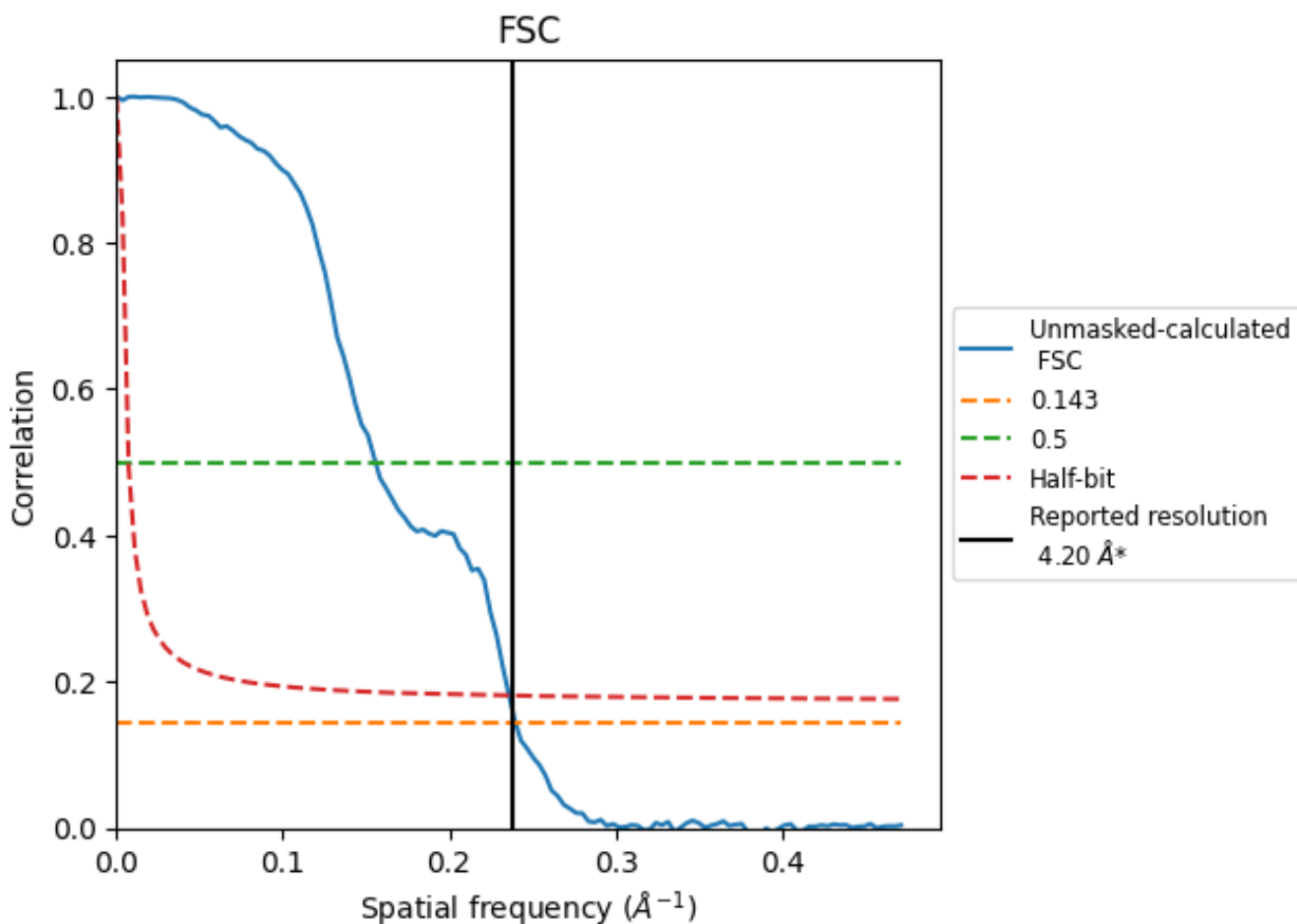


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 \AA^{-1}

8.2 Resolution estimates [i](#)

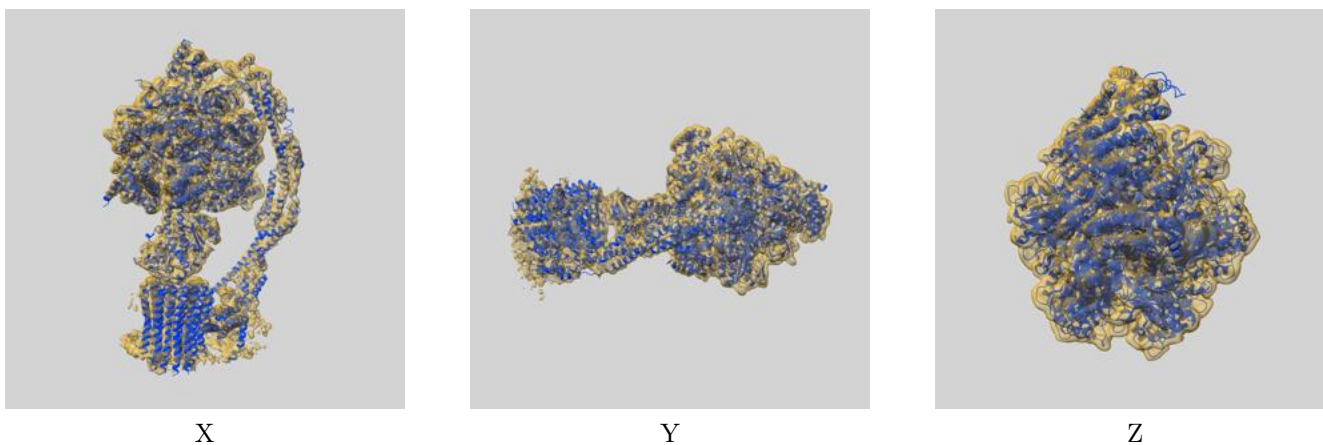
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.17	6.42	4.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

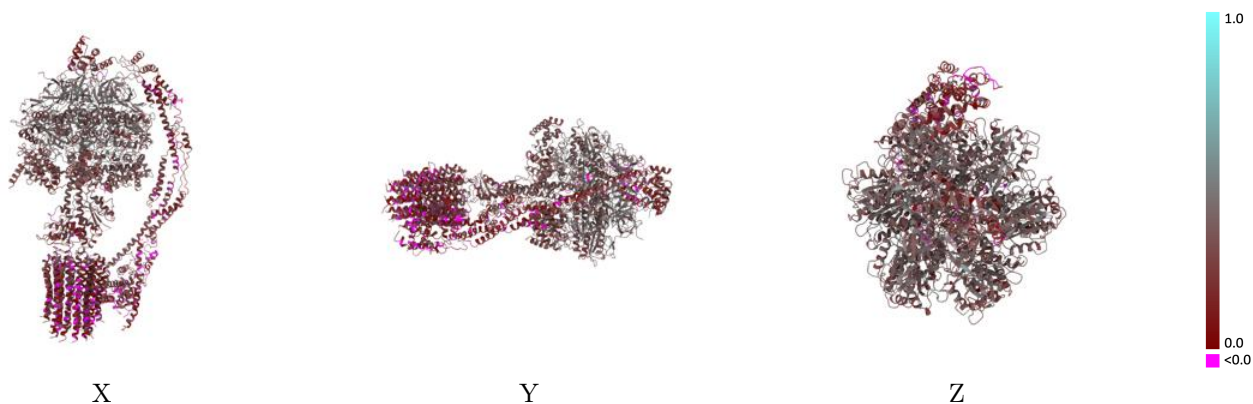
This section contains information regarding the fit between EMDB map EMD-29270 and PDB model 8FL8. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



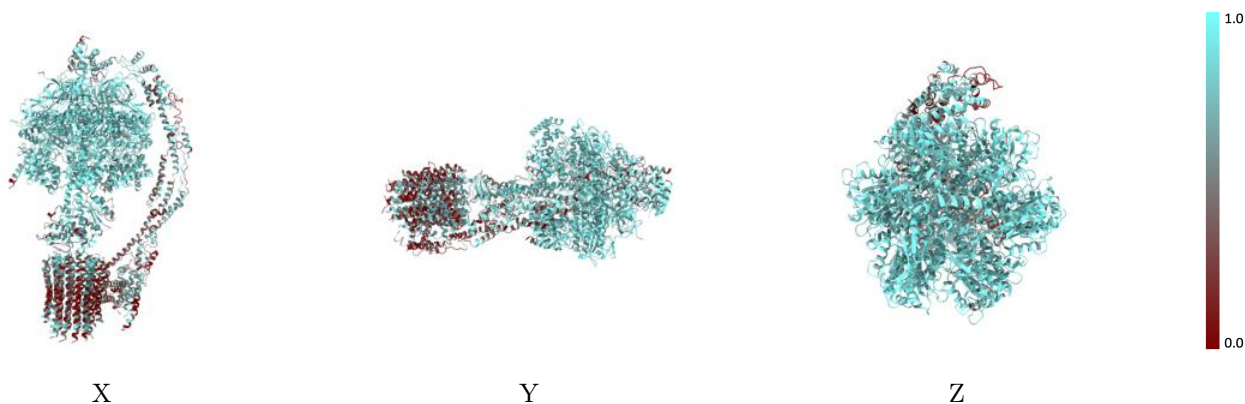
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



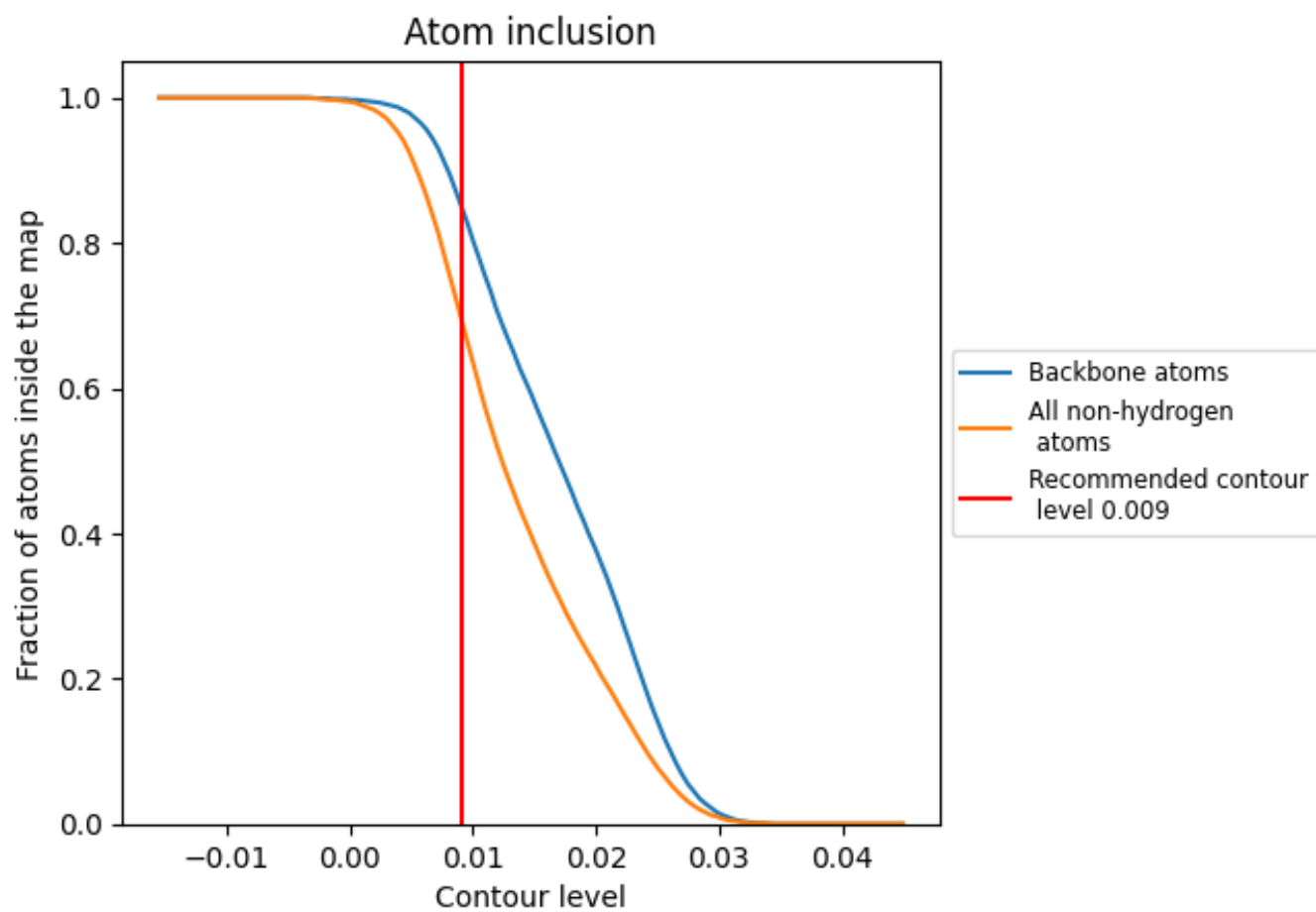
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 70% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6980	 0.2850
6	 0.4010	 0.1340
7	 0.4540	 0.1510
8	 0.5390	 0.0860
A	 0.8240	 0.3550
B	 0.8050	 0.3450
C	 0.8360	 0.3640
D	 0.8100	 0.3450
E	 0.8250	 0.3780
F	 0.8260	 0.3740
G	 0.7630	 0.2950
H	 0.6100	 0.2140
I	 0.6550	 0.2100
J	 0.3430	 0.1180
K	 0.4230	 0.1730
L	 0.5240	 0.1590
M	 0.5660	 0.1700
N	 0.4640	 0.1400
O	 0.3600	 0.1330
P	 0.3900	 0.1510
Q	 0.5600	 0.1950
R	 0.4420	 0.1630
S	 0.3700	 0.1280
T	 0.3380	 0.1130
U	 0.4520	 0.1470
X	 0.4880	 0.1570
Y	 0.7320	 0.2550
Z	 0.5160	 0.1840

