



wwPDB EM Validation Summary Report ⓘ

May 10, 2026 – 12:26 AM JST

PDB ID : 9W2R / pdb_00009w2r
EMDB ID : EMD-65577
Title : Cryo-EM structure of FoF1-ATPase monomer state 1 on the bovine heart submitochondrial particles (FoF1-1)
Authors : Nakano, A.; Masuya, T.; Akisada, S.; Ishikawa-Fukuda, M.; Mitsuoka, K.; Miyoshi, H.; Murai, M.; Yokoyama, K.
Deposited on : 2025-07-28
Resolution : 3.40 Å (reported)
Based on initial model : 6ZPO

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 : 1.8.5 (274361), CSD as541be (2020)
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

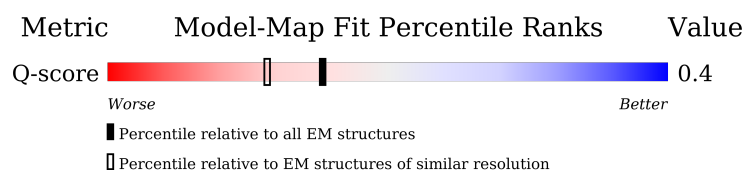
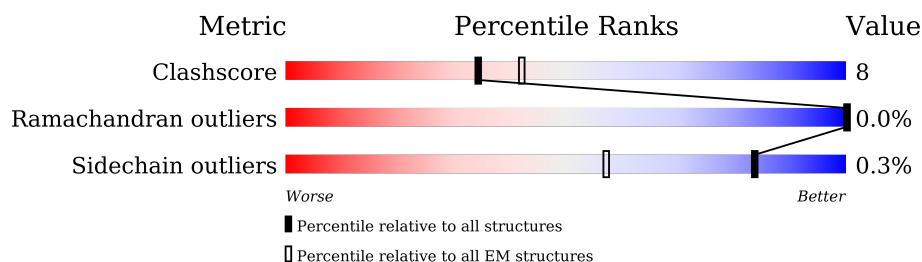
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.



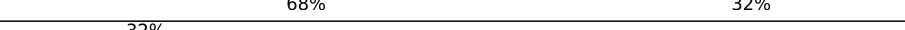
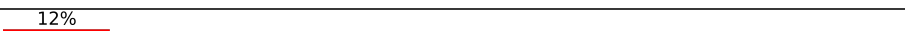
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	66	
2	A	510	
2	B	510	
2	C	510	

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Mol	Chain	Length	Quality of chain
3	D	482	
3	E	482	
3	F	482	
4	G	273	
5	H	146	
6	I	50	
7	J	60	
8	K	75	
8	L	75	
8	M	75	
8	N	75	
8	O	75	
8	P	75	
8	Q	75	
8	R	75	
9	S	190	
10	a	226	
11	b	214	
12	d	160	
13	e	70	
14	f	87	
15	g	102	
16	h	76	
17	j	60	
18	k	57	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	ATP	B	601	-	-	X	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 39088 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 F(0) complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	8	35	Total	C	N	O	S	0	0
			298	202	45	48	3		

- Molecule 2 is a protein called ATP synthase F(1) complex subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	508	Total	C	N	O	S	0	0
			3870	2435	681	742	12		
2	B	486	Total	C	N	O	S	0	0
			3710	2339	655	704	12		
2	C	503	Total	C	N	O	S	0	0
			3834	2414	675	733	12		

- Molecule 3 is a protein called ATP synthase F(1) complex catalytic subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	469	Total	C	N	O	S	0	0
			3558	2254	605	688	11		
3	E	467	Total	C	N	O	S	0	0
			3539	2243	601	684	11		
3	F	467	Total	C	N	O	S	0	0
			3539	2243	601	684	11		

- Molecule 4 is a protein called ATP synthase F(1) complex subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	272	Total	C	N	O	S	0	0
			2115	1330	368	409	8		

- Molecule 5 is a protein called ATP synthase F(1) complex subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	131	Total	C	N	O	S	0	0
			970	609	164	195	2		

- Molecule 6 is a protein called ATP synthase F(1) complex subunit epsilon, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	47	Total	C	N	O	S	0	0
			369	237	66	64	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	47	Total	C	N	O	S	0	0
			370	224	76	70			

- Molecule 8 is a protein called ATP synthase F(0) complex subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	74	Total	C	N	O	S	0	0
			529	351	82	93	3		
8	L	74	Total	C	N	O	S	0	0
			529	351	82	93	3		
8	M	75	Total	C	N	O	S	0	0
			525	349	79	93	4		
8	N	75	Total	C	N	O	S	0	0
			528	352	79	93	4		
8	O	75	Total	C	N	O	S	0	0
			528	352	79	93	4		
8	P	75	Total	C	N	O	S	0	0
			537	356	83	94	4		
8	Q	75	Total	C	N	O	S	0	0
			534	353	83	94	4		
8	R	75	Total	C	N	O	S	0	0
			538	356	83	95	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	188	Total	C	N	O	S	0	0
			1447	920	249	269	9		

- Molecule 10 is a protein called ATP synthase F(0) complex subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	a	226	Total	C	N	O	S	0	0
			1694	1122	271	289	12		

- Molecule 11 is a protein called ATP synthase peripheral stalk subunit b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	b	205	Total	C	N	O	S	0	0
			1619	1031	287	295	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	154	Total	C	N	O	S	0	0
			1224	790	201	232	1		

- Molecule 13 is a protein called ATP synthase F(0) complex subunit e, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	e	30	Total	C	N	O	0	0
			207	133	40	34		

- Molecule 14 is a protein called ATP synthase F(0) complex subunit f, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	79	Total	C	N	O	S	0	0
			624	402	114	106	2		

- Molecule 15 is a protein called ATP synthase F(0) complex subunit g, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	g	79	Total	C	N	O	0	0
			570	370	98	102		

- Molecule 16 is a protein called ATP synthase peripheral stalk subunit F6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	62	Total	C	N	O	S	0	0
			514	326	87	99	2		

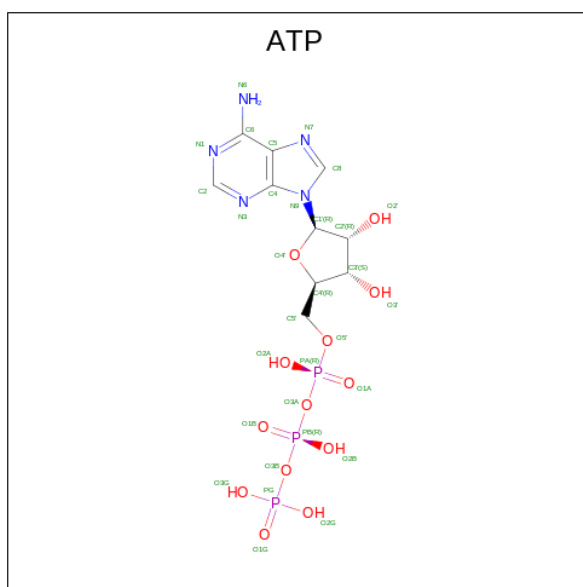
- Molecule 17 is a protein called ATP synthase F(0) complex subunit j, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	j	48	Total	C	N	O	S	0	0
			352	230	63	58	1		

- Molecule 18 is a protein called ATP synthase F(0) complex subunit k, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	k	34	Total	C	N	O	S	0	0
			261	171	45	43	2		

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

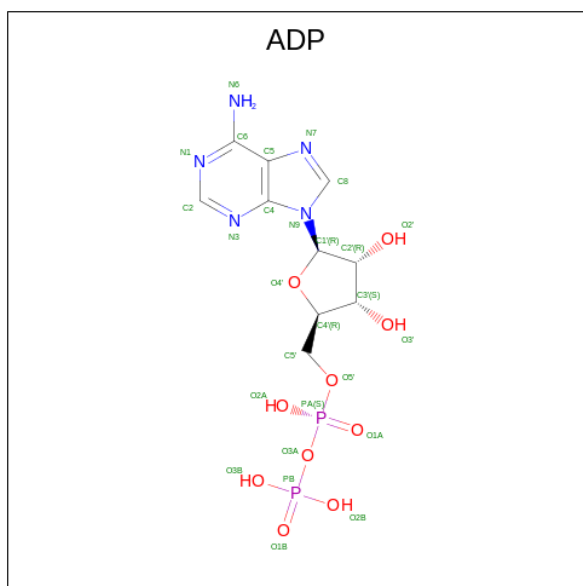


Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
19	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
19	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
19	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 21 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

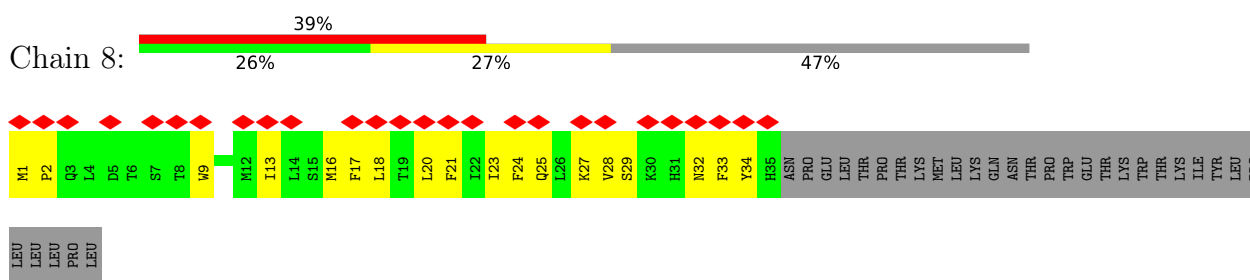


Mol	Chain	Residues	Atoms					AltConf
21	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

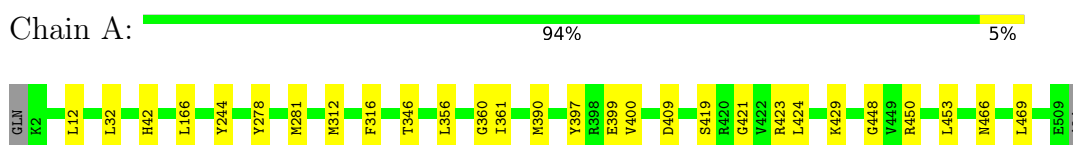
3 Residue-property plots [i](#)

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.

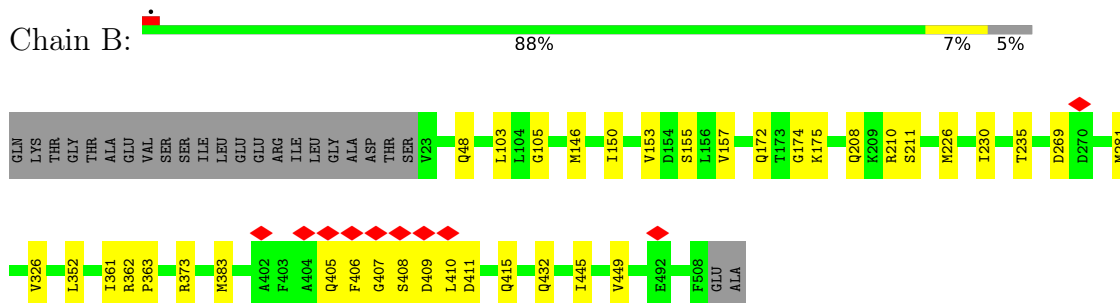
- Molecule 1: ATP synthase F(0) complex subunit 8



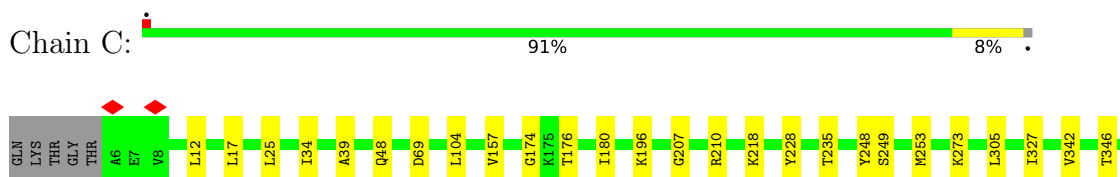
- Molecule 2: ATP synthase F(1) complex subunit alpha, mitochondrial



- Molecule 2: ATP synthase F(1) complex subunit alpha, mitochondrial



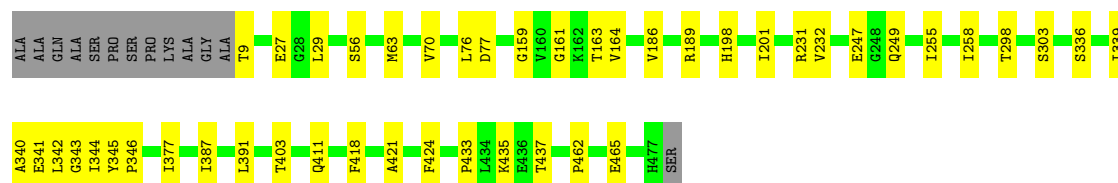
- Molecule 2: ATP synthase F(1) complex subunit alpha, mitochondrial





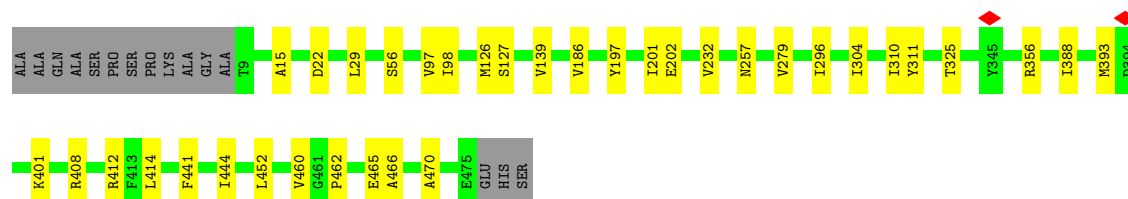
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

Chain D: 88% 10% .



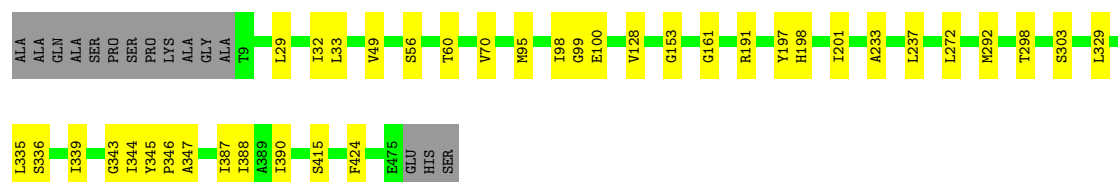
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

Chain E: 89% 7% .



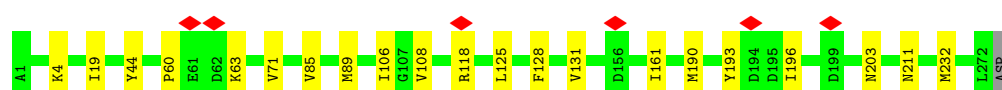
- Molecule 3: ATP synthase F(1) complex catalytic subunit beta, mitochondrial

Chain F: 89% 8% .



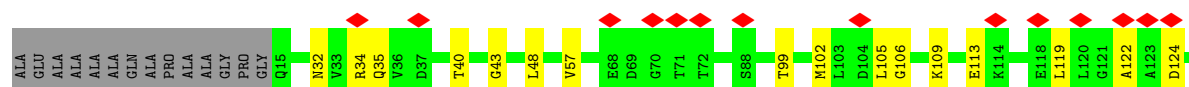
- Molecule 4: ATP synthase F(1) complex subunit gamma, mitochondrial

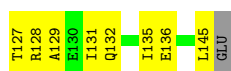
Chain G: 92% 8% .



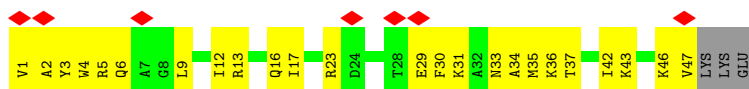
- Molecule 5: ATP synthase F(1) complex subunit delta, mitochondrial

Chain H: 10% 73% 16% 10%

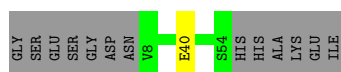
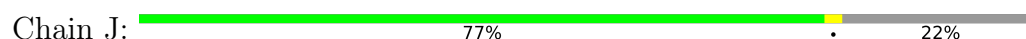




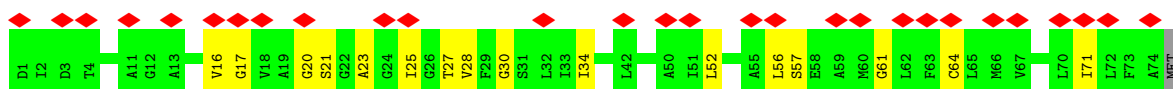
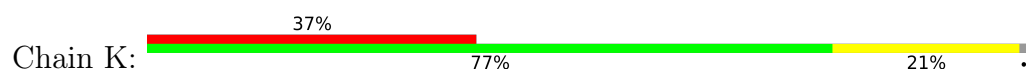
- Molecule 6: ATP synthase F(1) complex subunit epsilon, mitochondrial



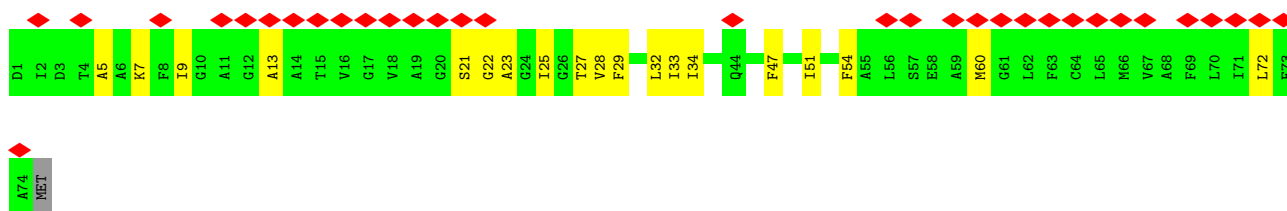
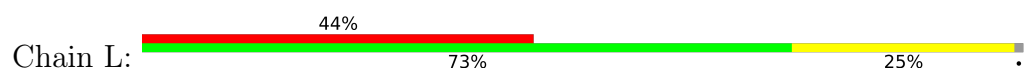
- Molecule 7: ATPase inhibitor, mitochondrial



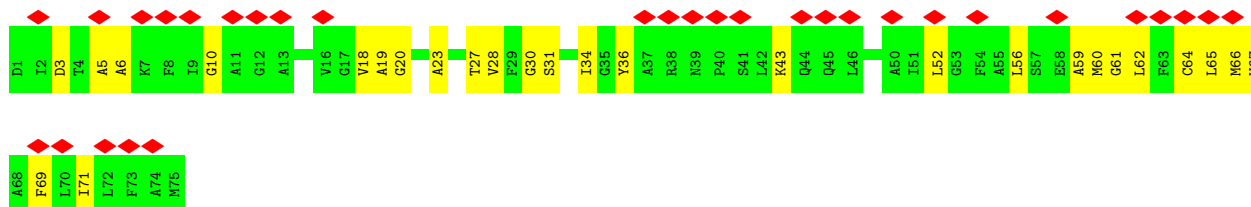
- Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial



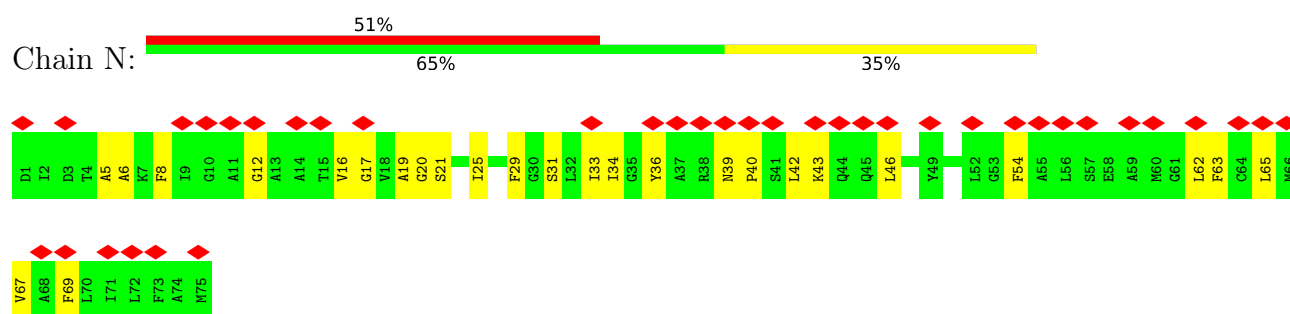
- Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial



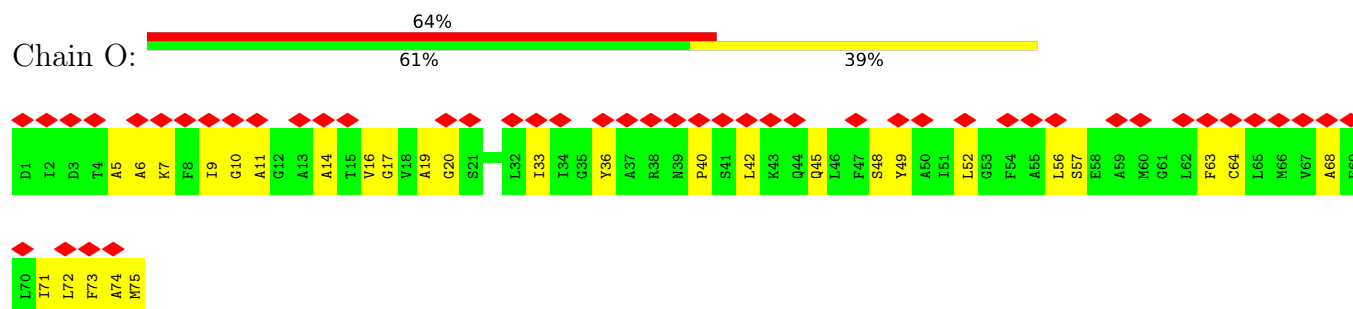
- Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial



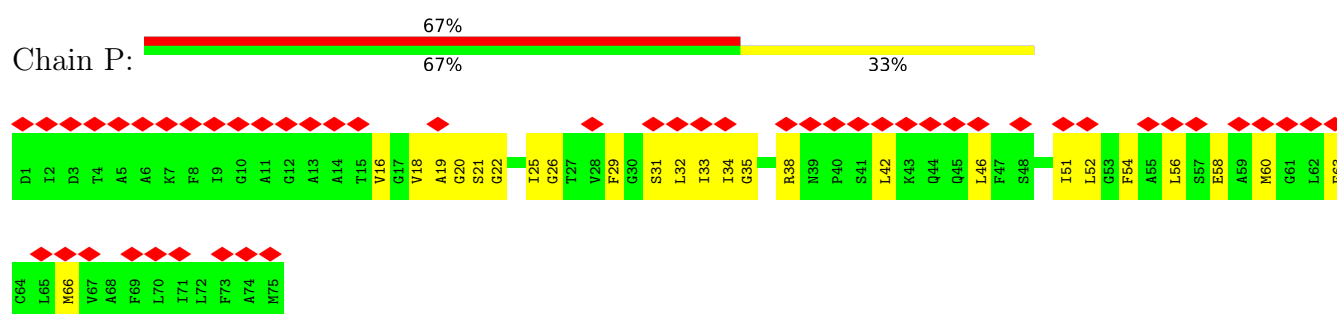
- Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial



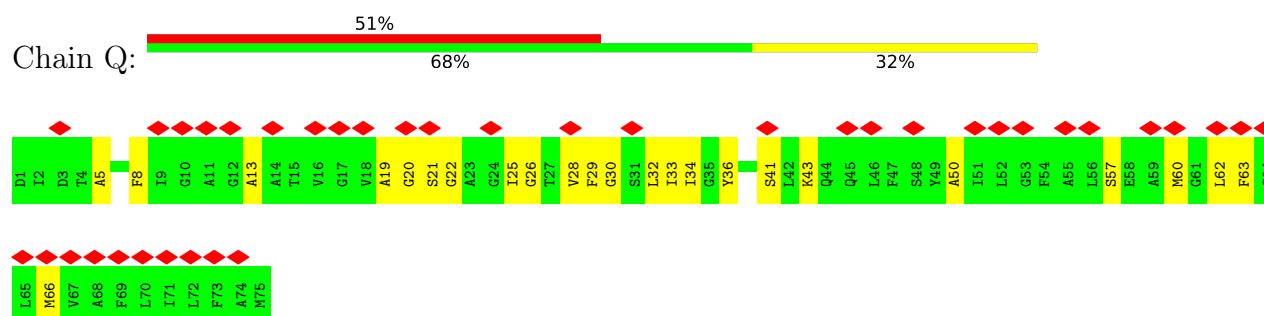
- Molecule 8: ATP synthase F(0) complex subunit C1, mitochondrial



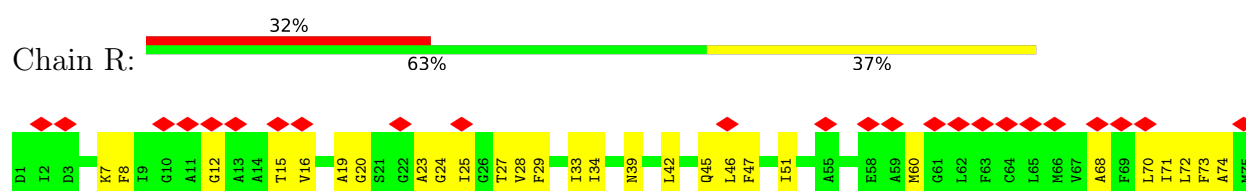
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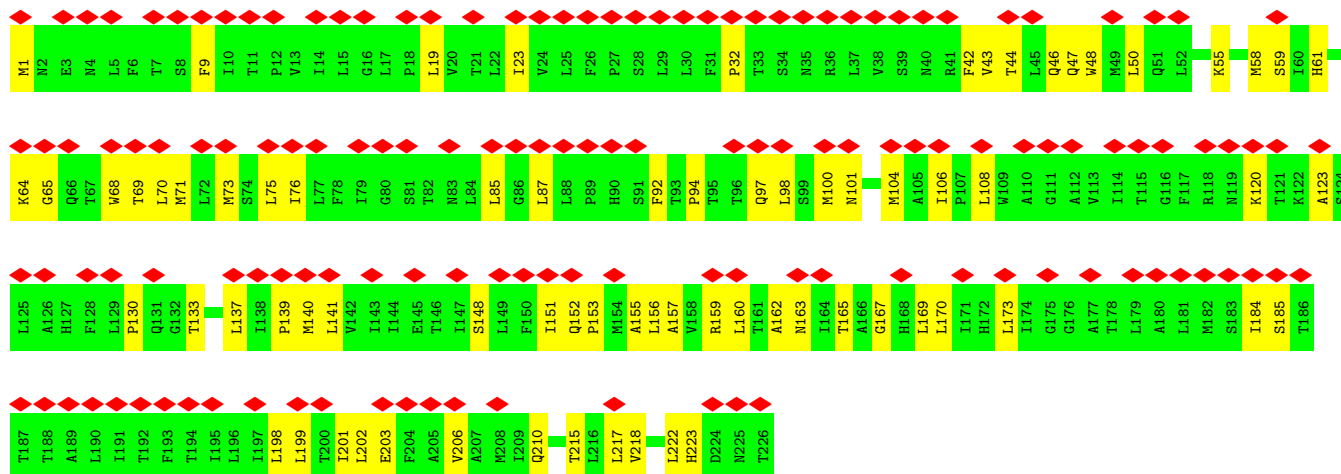
- Molecule 9: ATP synthase peripheral stalk subunit OSCP, mitochondrial

Chain S:  88% 11% .



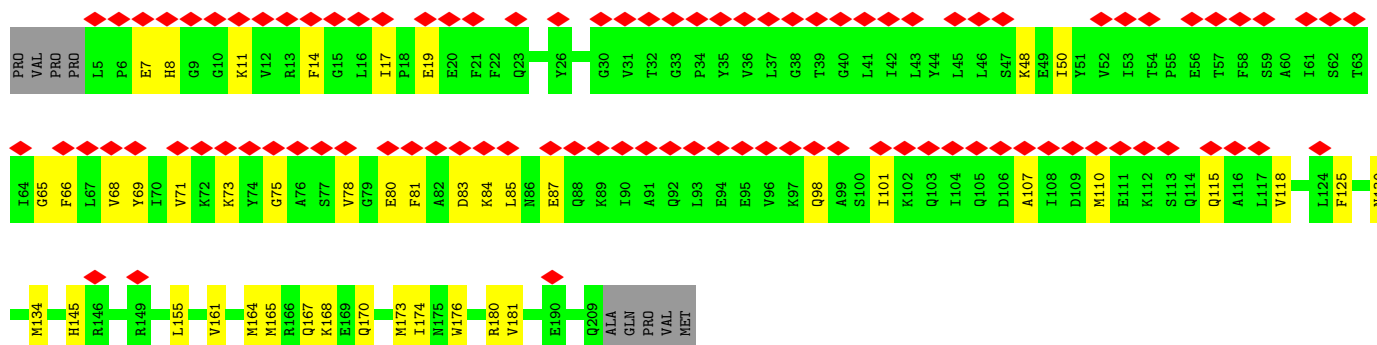
- Molecule 10: ATP synthase F(0) complex subunit a

Chain a:  62% 67% 33%



- Molecule 11: ATP synthase peripheral stalk subunit b, mitochondrial

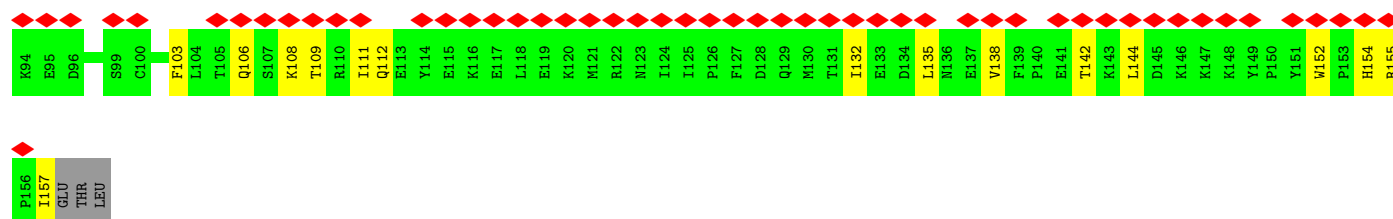
Chain b:  45% 75% 21% .



- Molecule 12: ATP synthase peripheral stalk subunit d, mitochondrial

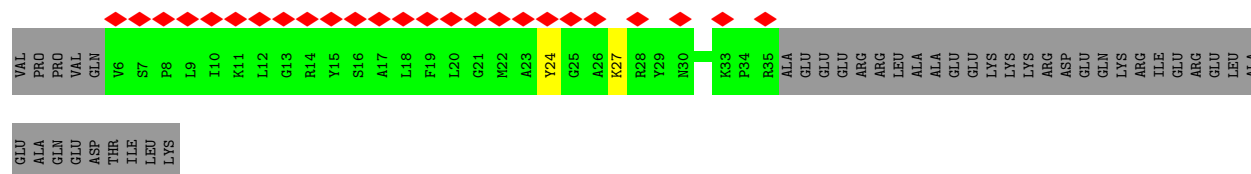
Chain d:  45% 76% 21% .





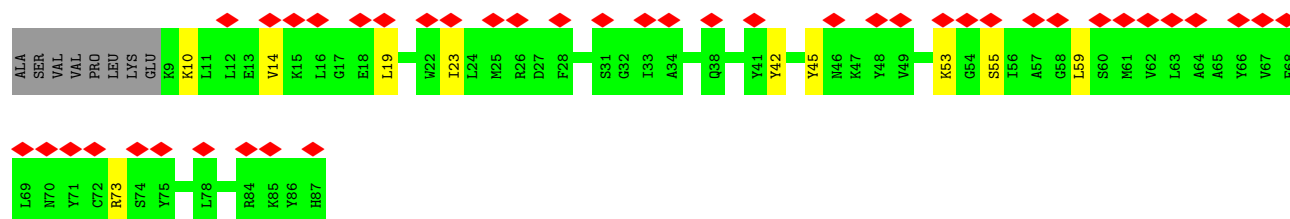
- Molecule 13: ATP synthase F(0) complex subunit e, mitochondrial

Chain e:



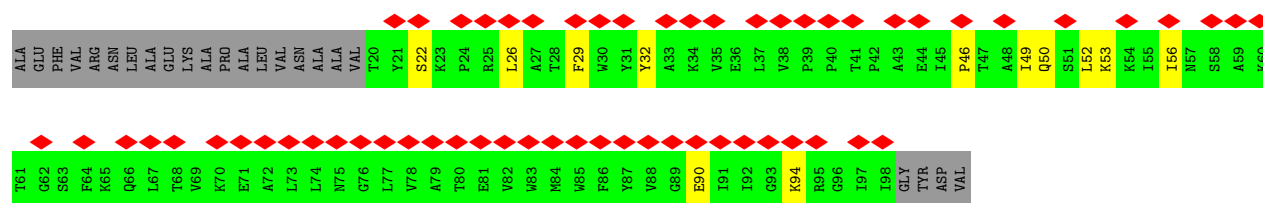
- Molecule 14: ATP synthase F(0) complex subunit f, mitochondrial

Chain f:



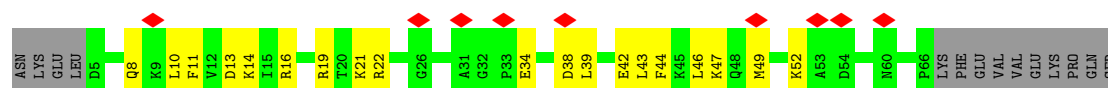
- Molecule 15: ATP synthase F(0) complex subunit g, mitochondrial

Chain g:



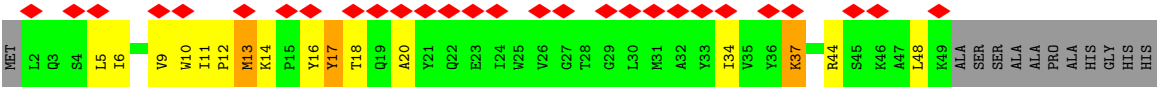
- Molecule 16: ATP synthase peripheral stalk subunit F6, mitochondrial

Chain h:

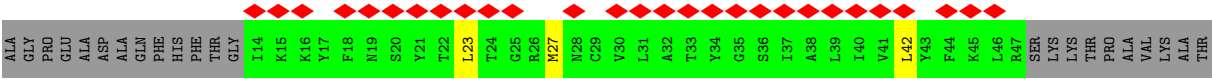


- Molecule 17: ATP synthase F(0) complex subunit j, mitochondrial

Chain j:



• Molecule 18: ATP synthase F(0) complex subunit k, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	328822	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.956	Depositor
Minimum map value	-1.382	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	654.0, 654.0, 654.0	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4533334, 1.4533334, 1.4533334	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, ATP, M3L

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	0.15	0/307	0.56	0/415
2	A	0.27	0/3921	0.53	0/5290
2	B	0.17	0/3761	0.42	0/5074
2	C	0.20	0/3885	0.43	0/5242
3	D	0.24	0/3616	0.47	0/4906
3	E	0.21	0/3596	0.46	0/4879
3	F	0.18	0/3596	0.40	0/4879
4	G	0.15	0/2141	0.38	0/2876
5	H	0.18	0/982	0.58	0/1337
6	I	0.17	0/374	0.51	0/501
7	J	0.22	0/374	0.63	0/495
8	K	0.14	0/526	0.41	0/711
8	L	0.15	0/526	0.41	0/711
8	M	0.19	0/522	0.60	0/705
8	N	0.14	0/525	0.38	0/709
8	O	0.42	0/525	0.60	0/709
8	P	0.17	0/534	0.48	0/720
8	Q	0.19	0/531	0.54	0/716
8	R	0.13	0/535	0.36	0/721
9	S	0.12	0/1464	0.36	0/1969
10	a	0.16	0/1731	0.47	0/2369
11	b	0.16	0/1646	0.45	0/2214
12	d	0.13	0/1254	0.38	0/1705
13	e	0.13	0/210	0.40	0/283
14	f	0.13	0/639	0.40	0/857
15	g	0.13	0/581	0.43	0/790
16	h	0.19	0/526	0.63	0/707
17	j	0.71	0/358	1.03	1/482 (0.2%)
18	k	0.09	0/265	0.34	0/356
All	All	0.21	0/39451	0.47	1/53328 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
17	j	13	MET	CA-CB-CG	7.17	128.44	114.10

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	298	0	308	24	0
2	A	3870	0	3973	20	0
2	B	3710	0	3814	72	0
2	C	3834	0	3937	46	0
3	D	3558	0	3606	41	0
3	E	3539	0	3593	24	0
3	F	3539	0	3592	43	0
4	G	2115	0	2185	19	0
5	H	970	0	972	25	0
6	I	369	0	395	21	0
7	J	370	0	361	1	0
8	K	529	0	550	13	0
8	L	529	0	550	18	0
8	M	525	0	532	20	0
8	N	528	0	541	42	0
8	O	528	0	541	49	0
8	P	537	0	556	28	0
8	Q	534	0	547	38	0
8	R	538	0	559	29	0
9	S	1447	0	1557	20	0
10	a	1694	0	1755	66	0
11	b	1619	0	1609	35	0
12	d	1224	0	1198	35	0
13	e	207	0	200	1	0
14	f	624	0	603	8	0
15	g	570	0	564	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	h	514	0	495	19	0
17	j	352	0	353	13	0
18	k	261	0	260	2	0
19	A	31	0	12	0	0
19	B	31	0	11	28	0
19	C	31	0	12	6	0
19	D	31	0	12	6	0
20	A	1	0	0	0	0
20	B	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	F	27	0	12	4	0
All	All	39088	0	39765	637	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 637 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)
2:B:373:ARG:HG3	3:F:424:PHE:CE1	1.12	1.60
8:R:47:PHE:CE1	8:R:51:ILE:HD11	1.38	1.54
2:B:373:ARG:HG3	3:F:424:PHE:CZ	1.51	1.45
8:R:47:PHE:CZ	8:R:51:ILE:HD11	1.57	1.39
2:B:174:GLY:CA	19:B:601:ATP:H5'2	1.49	1.37

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8	33/66 (50%)	31 (94%)	2 (6%)	0	100	100
2	A	506/510 (99%)	489 (97%)	17 (3%)	0	100	100
2	B	484/510 (95%)	473 (98%)	10 (2%)	1 (0%)	43	71
2	C	501/510 (98%)	486 (97%)	15 (3%)	0	100	100
3	D	467/482 (97%)	450 (96%)	17 (4%)	0	100	100
3	E	465/482 (96%)	450 (97%)	15 (3%)	0	100	100
3	F	465/482 (96%)	452 (97%)	13 (3%)	0	100	100
4	G	270/273 (99%)	266 (98%)	4 (2%)	0	100	100
5	H	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
6	I	45/50 (90%)	44 (98%)	1 (2%)	0	100	100
7	J	45/60 (75%)	44 (98%)	1 (2%)	0	100	100
8	K	71/75 (95%)	70 (99%)	1 (1%)	0	100	100
8	L	71/75 (95%)	68 (96%)	3 (4%)	0	100	100
8	M	72/75 (96%)	71 (99%)	1 (1%)	0	100	100
8	N	72/75 (96%)	71 (99%)	1 (1%)	0	100	100
8	O	72/75 (96%)	68 (94%)	4 (6%)	0	100	100
8	P	72/75 (96%)	71 (99%)	1 (1%)	0	100	100
8	Q	72/75 (96%)	70 (97%)	2 (3%)	0	100	100
8	R	72/75 (96%)	72 (100%)	0	0	100	100
9	S	186/190 (98%)	184 (99%)	2 (1%)	0	100	100
10	a	224/226 (99%)	214 (96%)	10 (4%)	0	100	100
11	b	203/214 (95%)	199 (98%)	4 (2%)	0	100	100
12	d	152/160 (95%)	148 (97%)	4 (3%)	0	100	100
13	e	28/70 (40%)	28 (100%)	0	0	100	100
14	f	77/87 (88%)	75 (97%)	2 (3%)	0	100	100
15	g	77/102 (76%)	74 (96%)	3 (4%)	0	100	100
16	h	60/76 (79%)	59 (98%)	1 (2%)	0	100	100
17	j	46/60 (77%)	39 (85%)	7 (15%)	0	100	100
18	k	32/57 (56%)	32 (100%)	0	0	100	100
All	All	5069/5413 (94%)	4924 (97%)	144 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	407	GLY

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	35/66 (53%)	35 (100%)	0	100	100
2	A	412/413 (100%)	411 (100%)	1 (0%)	87	85
2	B	394/413 (95%)	391 (99%)	3 (1%)	73	77
2	C	408/413 (99%)	406 (100%)	2 (0%)	81	81
3	D	379/386 (98%)	379 (100%)	0	100	100
3	E	377/386 (98%)	376 (100%)	1 (0%)	86	84
3	F	377/386 (98%)	376 (100%)	1 (0%)	86	84
4	G	230/231 (100%)	230 (100%)	0	100	100
5	H	104/109 (95%)	104 (100%)	0	100	100
6	I	38/41 (93%)	38 (100%)	0	100	100
7	J	34/44 (77%)	34 (100%)	0	100	100
8	K	49/50 (98%)	49 (100%)	0	100	100
8	L	49/50 (98%)	49 (100%)	0	100	100
8	M	46/50 (92%)	46 (100%)	0	100	100
8	N	47/50 (94%)	47 (100%)	0	100	100
8	O	47/50 (94%)	47 (100%)	0	100	100
8	P	49/50 (98%)	49 (100%)	0	100	100
8	Q	48/50 (96%)	48 (100%)	0	100	100
8	R	50/50 (100%)	50 (100%)	0	100	100
9	S	163/165 (99%)	163 (100%)	0	100	100
10	a	182/200 (91%)	182 (100%)	0	100	100
11	b	166/190 (87%)	166 (100%)	0	100	100
12	d	127/142 (89%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	e	16/59 (27%)	16 (100%)	0	100	100
14	f	58/75 (77%)	58 (100%)	0	100	100
15	g	53/83 (64%)	53 (100%)	0	100	100
16	h	56/70 (80%)	56 (100%)	0	100	100
17	j	31/49 (63%)	28 (90%)	3 (10%)	8	28
18	k	25/46 (54%)	25 (100%)	0	100	100
All	All	4050/4367 (93%)	4039 (100%)	11 (0%)	84	84

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	345	TYR
17	j	17	TYR
17	j	37	LYS
17	j	34	ILE
2	C	409	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	411	GLN
3	F	198	HIS
12	d	112	GLN
10	a	172	HIS
11	b	103	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
8	M3L	M	43	8	10,11,12	0.36	0	9,14,16	0.25	0
8	M3L	R	43	8	10,11,12	0.35	0	9,14,16	0.32	0
8	M3L	K	43	8	10,11,12	0.37	0	9,14,16	0.34	0
8	M3L	L	43	8	10,11,12	0.38	0	9,14,16	0.32	0
8	M3L	O	43	8	10,11,12	0.35	0	9,14,16	0.31	0
8	M3L	Q	43	8	10,11,12	0.31	0	9,14,16	0.25	0
8	M3L	P	43	8	10,11,12	0.31	0	9,14,16	0.31	0
8	M3L	N	43	8	10,11,12	0.32	0	9,14,16	0.29	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
8	M3L	M	43	8	-	0/9/10/12	-
8	M3L	R	43	8	-	0/9/10/12	-
8	M3L	K	43	8	-	0/9/10/12	-
8	M3L	L	43	8	-	1/9/10/12	-
8	M3L	O	43	8	-	6/9/10/12	-
8	M3L	Q	43	8	-	3/9/10/12	-
8	M3L	P	43	8	-	1/9/10/12	-
8	M3L	N	43	8	-	2/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	N	43	M3L	C-CA-CB-CG
8	P	43	M3L	C-CA-CB-CG
8	Q	43	M3L	O-C-CA-CB
8	L	43	M3L	CG-CD-CE-NZ
8	O	43	M3L	CA-CB-CG-CD

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	43	M3L	1	0
8	Q	43	M3L	4	0
8	N	43	M3L	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
21	ADP	F	501	20	27,29,29	0.63	0	42,45,45	0.75	0
19	ATP	B	601	20	29,33,33	0.50	0	44,52,52	0.72	0
19	ATP	A	601	20	29,33,33	1.08	2 (6%)	44,52,52	1.40	7 (15%)
19	ATP	C	601	20	29,33,33	0.82	1 (3%)	44,52,52	1.19	3 (6%)
19	ATP	D	501	20	29,33,33	0.50	0	44,52,52	0.71	1 (2%)

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
21	ADP	F	501	20	-	2/16/32/32	0/3/3/3
19	ATP	B	601	20	-	4/22/38/38	0/3/3/3
19	ATP	A	601	20	-	1/22/38/38	0/3/3/3
19	ATP	C	601	20	-	3/22/38/38	0/3/3/3
19	ATP	D	501	20	-	5/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	601	ATP	O5'-C5'	-2.80	1.34	1.44
19	A	601	ATP	C5-C4	-2.10	1.35	1.39
19	A	601	ATP	PG-O3G	-2.02	1.47	1.54

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	C	601	ATP	O5'-C5'-C4'	-5.77	89.12	108.99
19	A	601	ATP	O3G-PG-O3B	3.31	115.74	104.64
19	A	601	ATP	C5-C4-N3	-2.82	123.06	126.75
19	A	601	ATP	PA-O3A-PB	-2.79	123.26	132.83
19	A	601	ATP	C4-C5-N7	2.74	113.95	110.62

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	B	601	ATP	C5'-O5'-PA-O1A
21	F	501	ADP	O4'-C4'-C5'-O5'
21	F	501	ADP	C3'-C4'-C5'-O5'
19	D	501	ATP	C3'-C4'-C5'-O5'
19	C	601	ATP	O4'-C4'-C5'-O5'

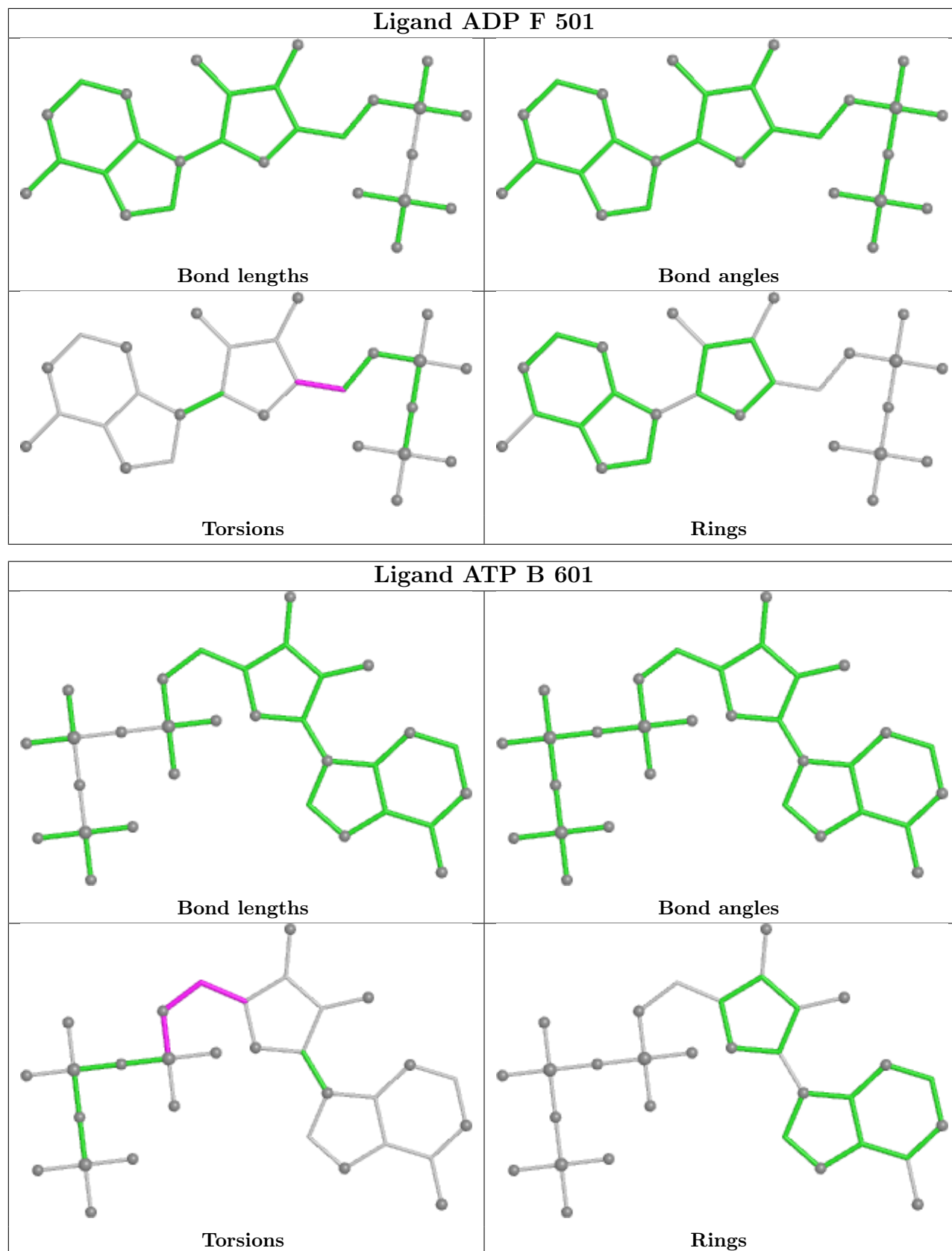
There are no ring outliers.

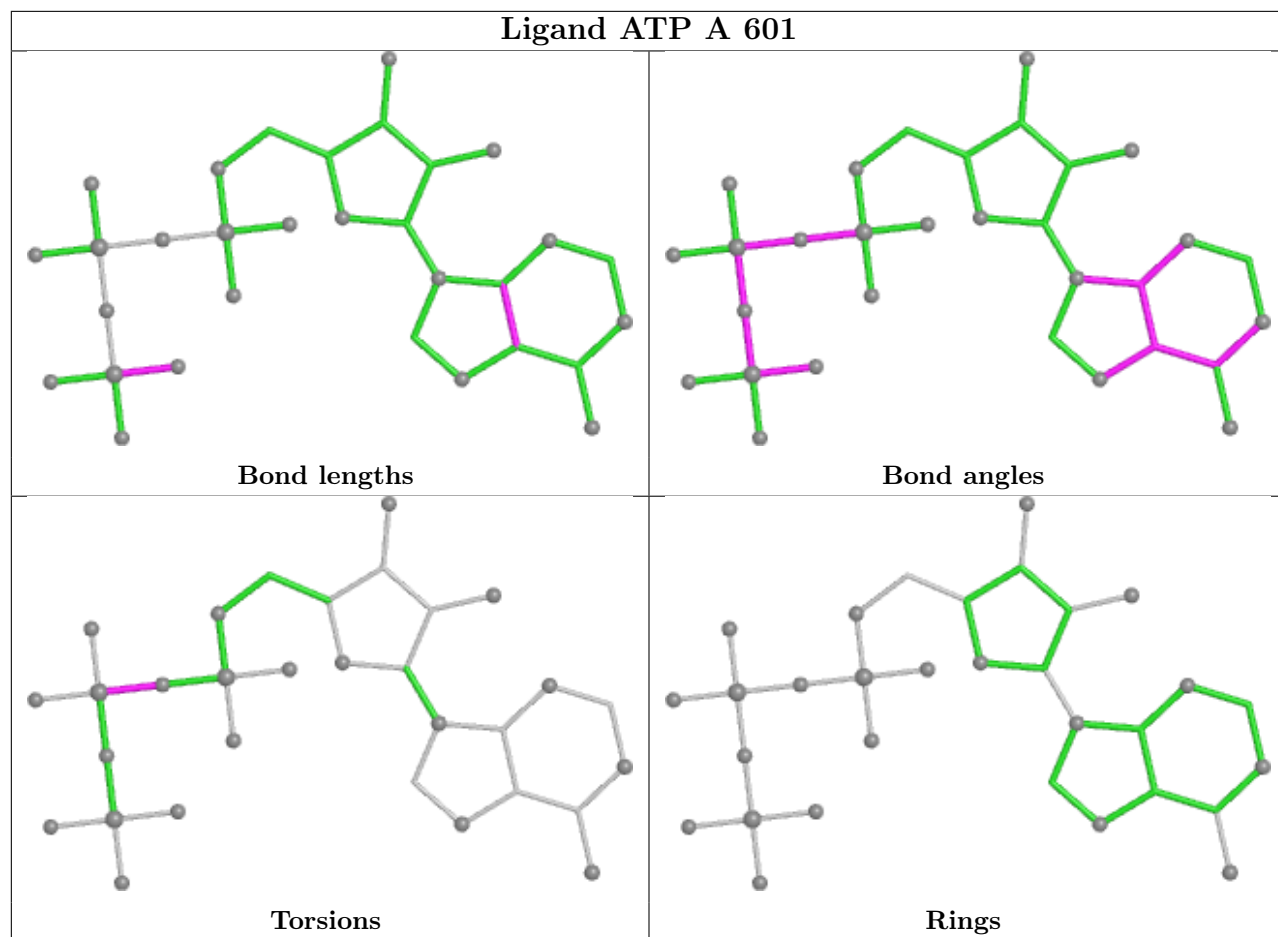
4 monomers are involved in 44 short contacts:

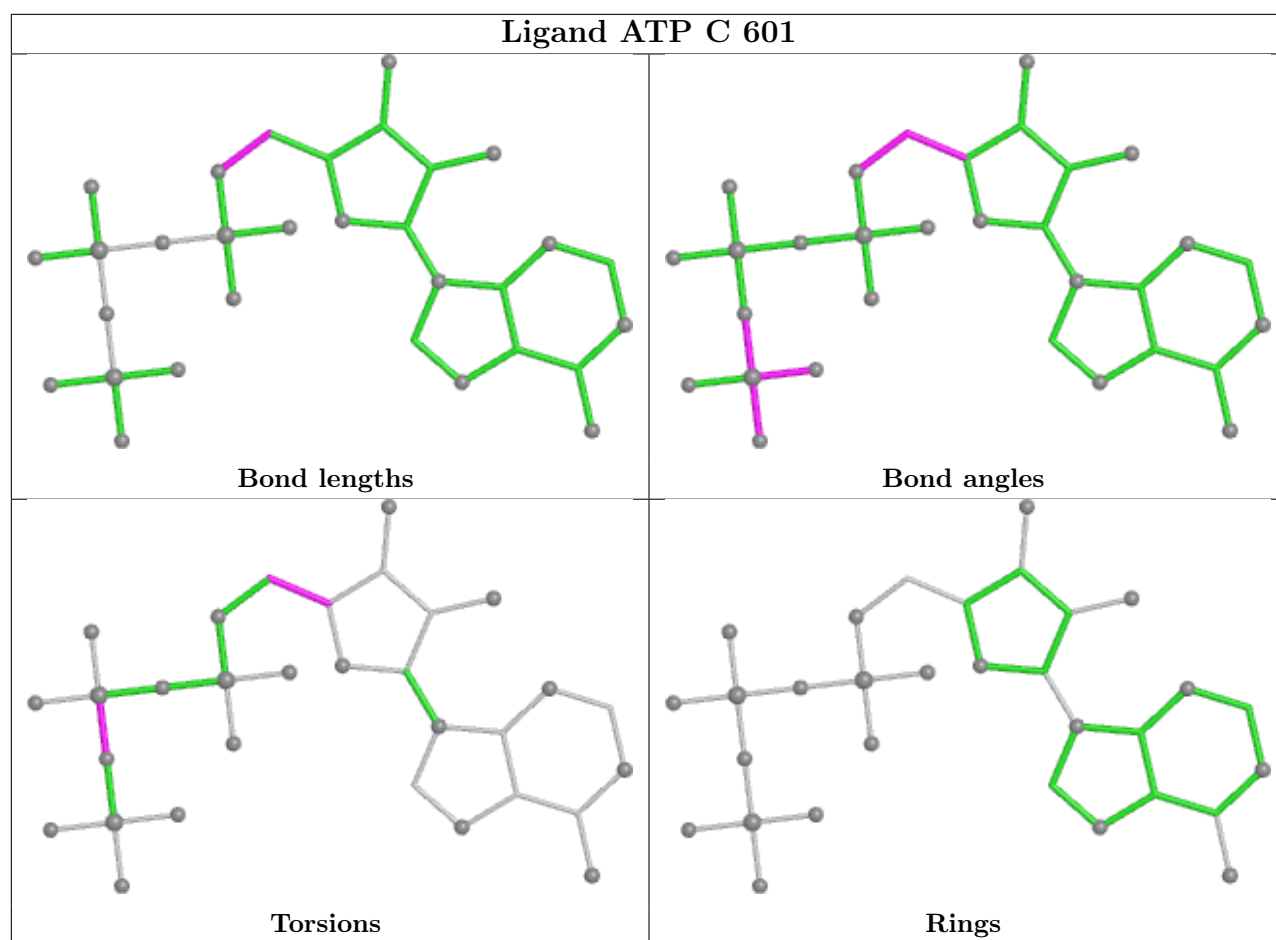
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	F	501	ADP	4	0
19	B	601	ATP	28	0
19	C	601	ATP	6	0
19	D	501	ATP	6	0

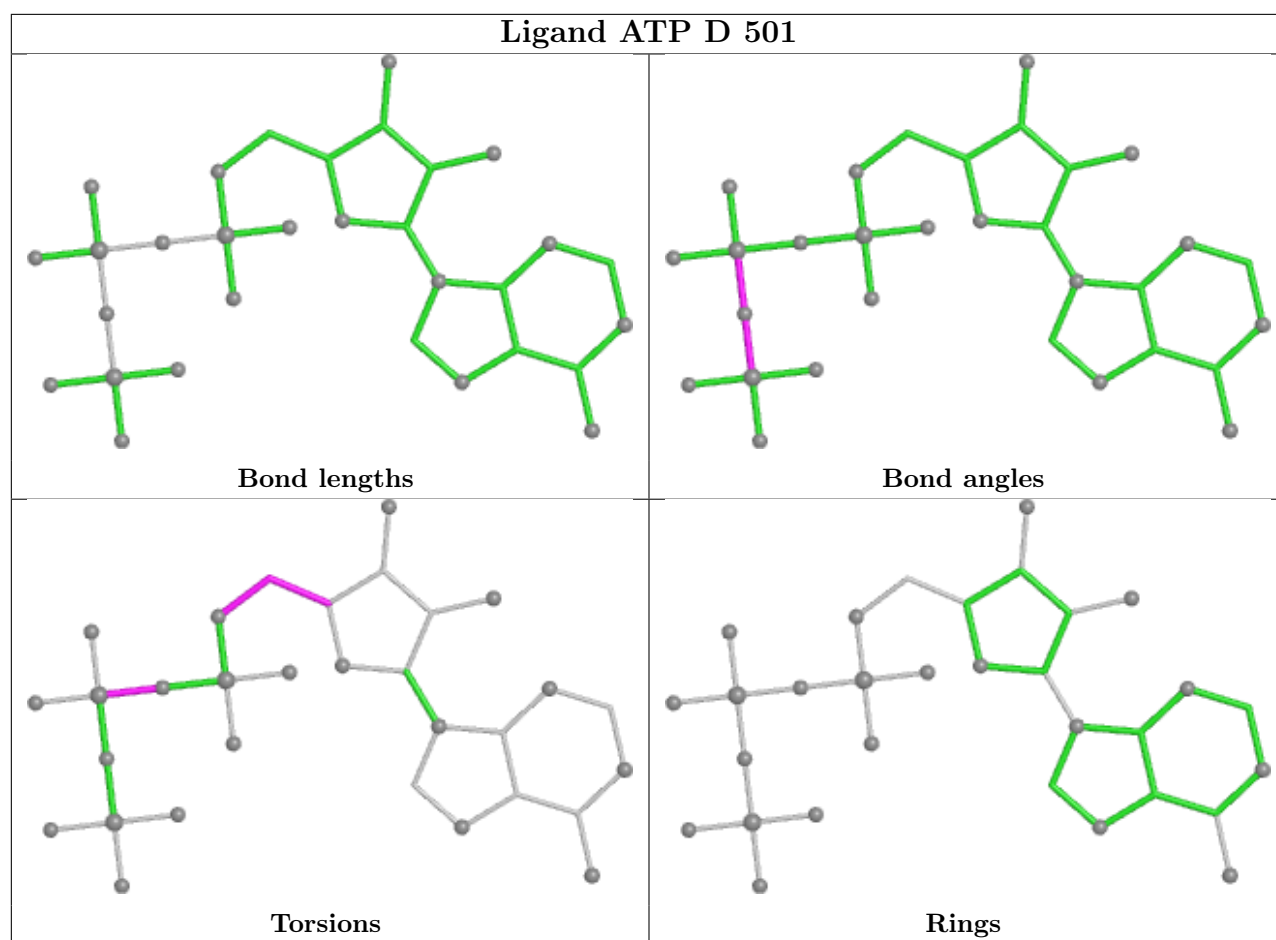
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

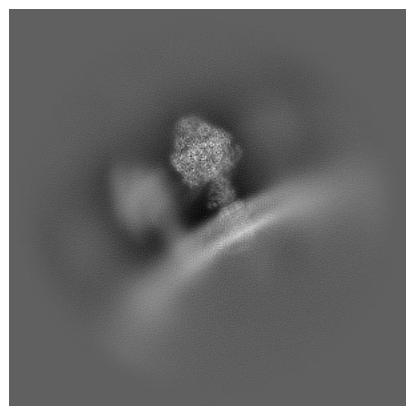
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65577. These allow visual inspection of the internal detail of the map and identification of artifacts.

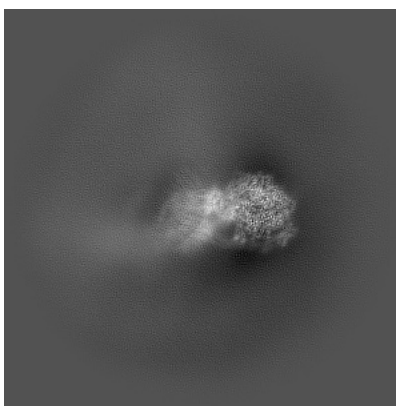
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

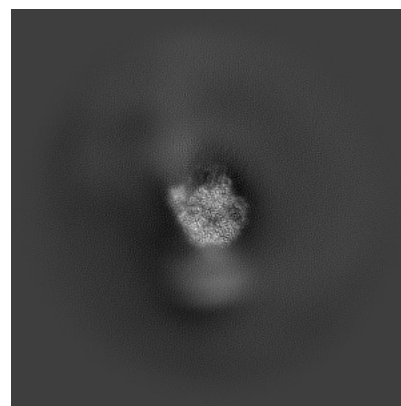
6.1.1 Primary map



X

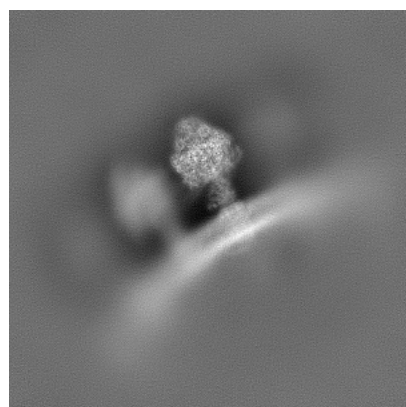


Y

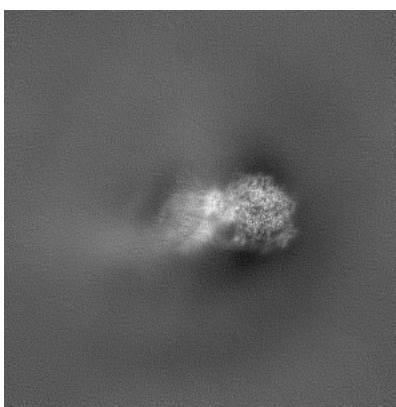


Z

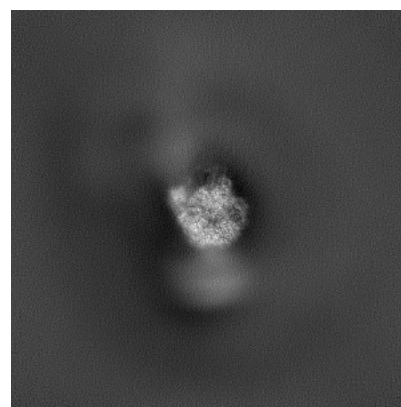
6.1.2 Raw map



X



Y

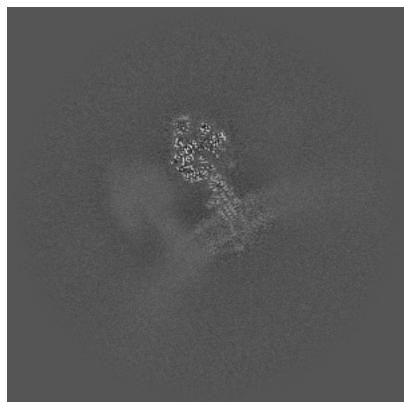


Z

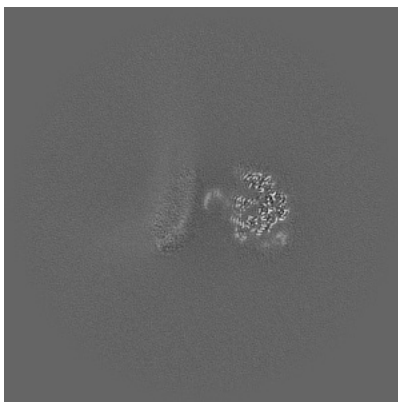
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

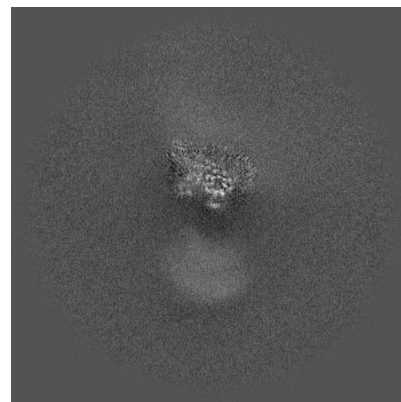
6.2.1 Primary map



X Index: 225

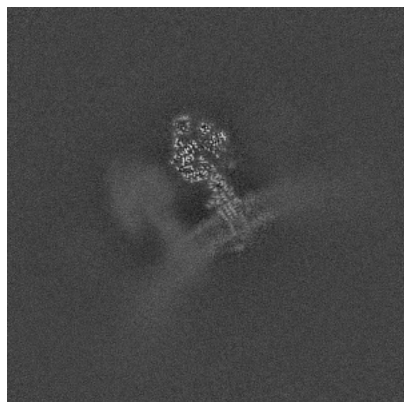


Y Index: 225

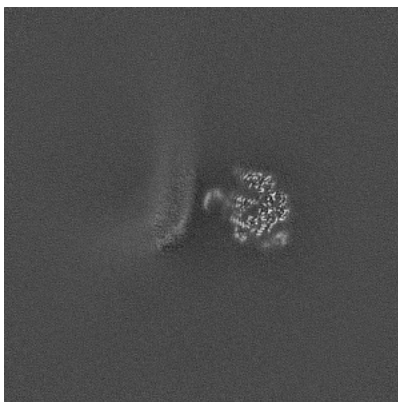


Z Index: 225

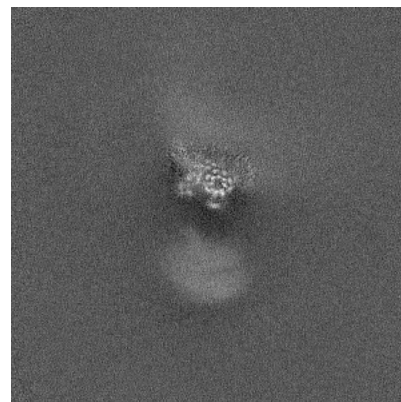
6.2.2 Raw map



X Index: 225



Y Index: 225

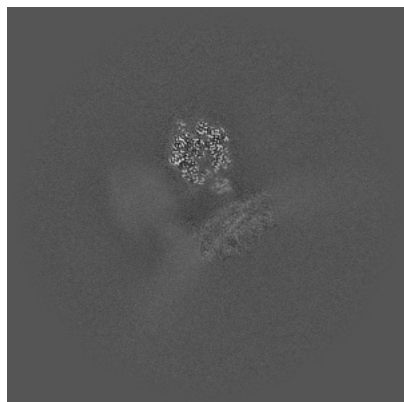


Z Index: 225

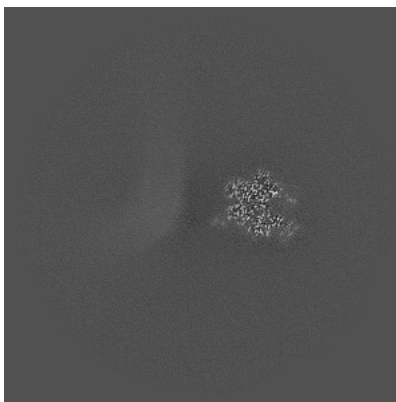
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

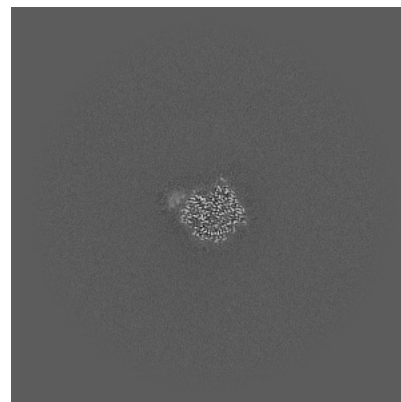
6.3.1 Primary map



X Index: 216

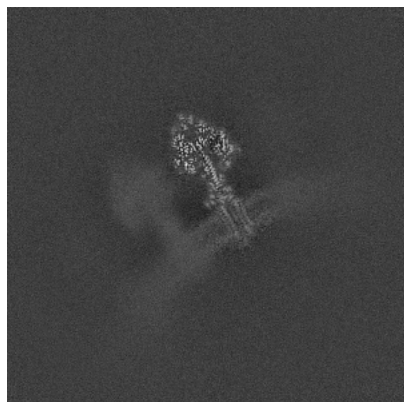


Y Index: 207

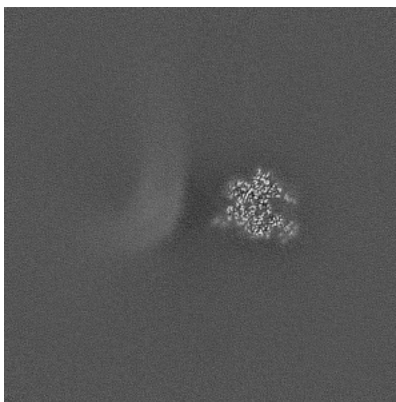


Z Index: 297

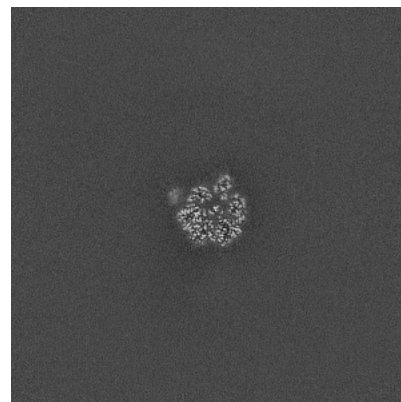
6.3.2 Raw map



X Index: 232



Y Index: 208

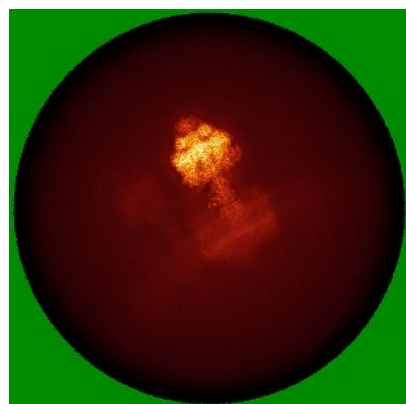


Z Index: 281

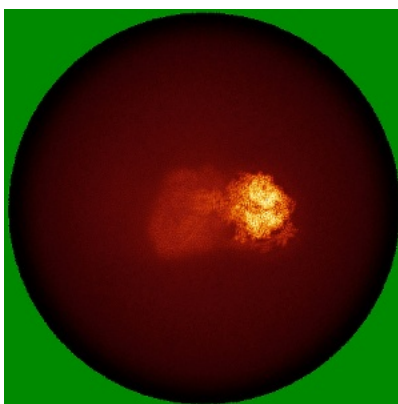
The images above show the largest variance slices of the map in three orthogonal directions.

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

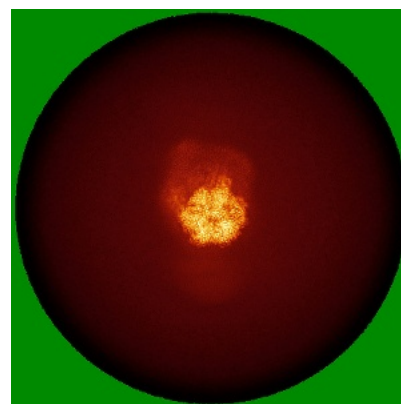
6.4.1 Primary map



X

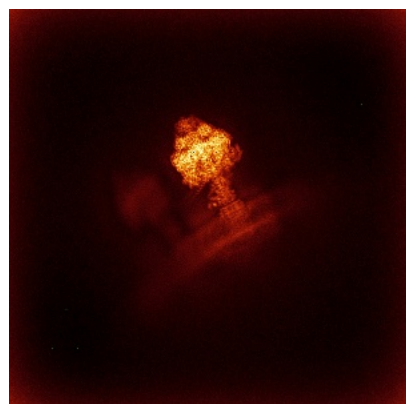


Y

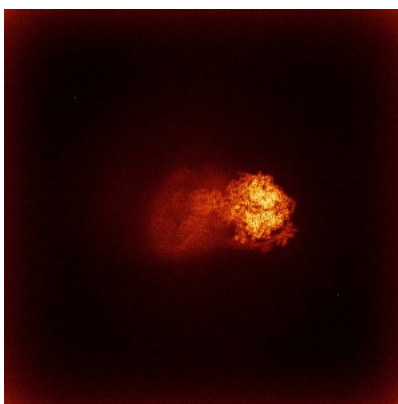


Z

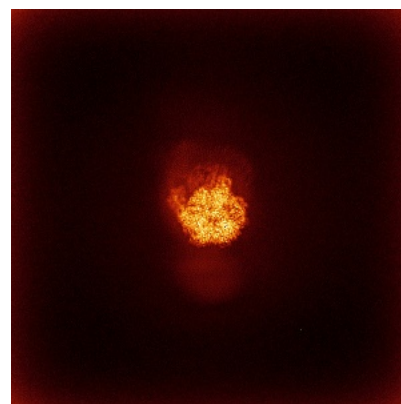
6.4.2 Raw map



X



Y

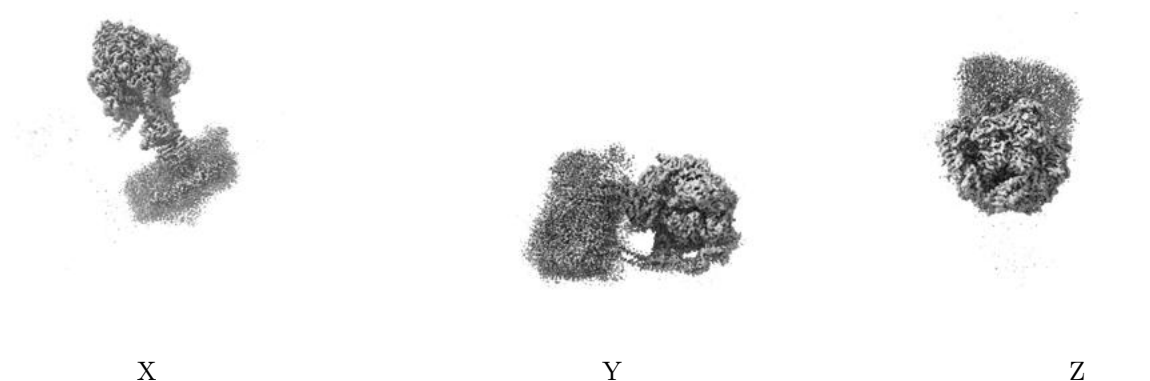


Z

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.

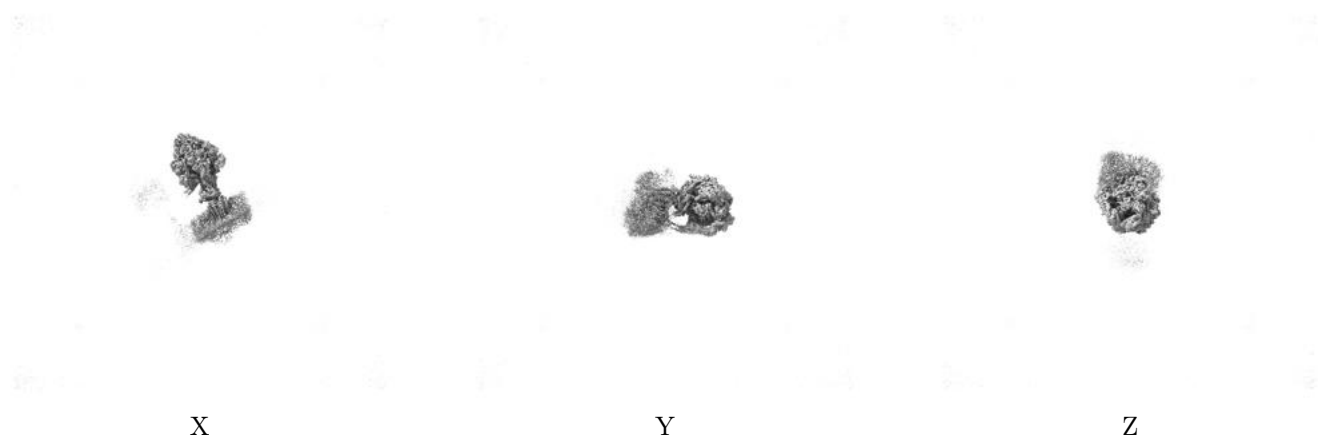
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

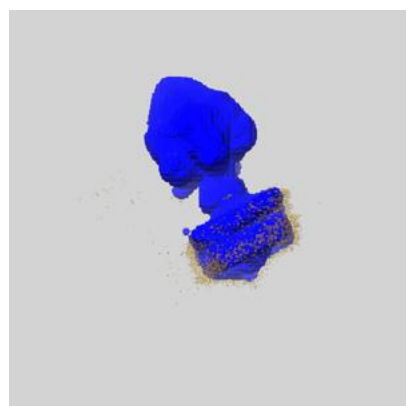
6.6 Mask visualisation [i](#)

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

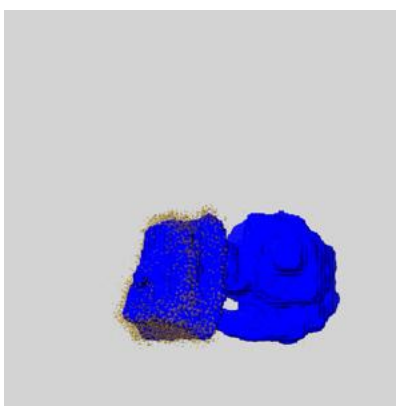
A mask typically either:

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

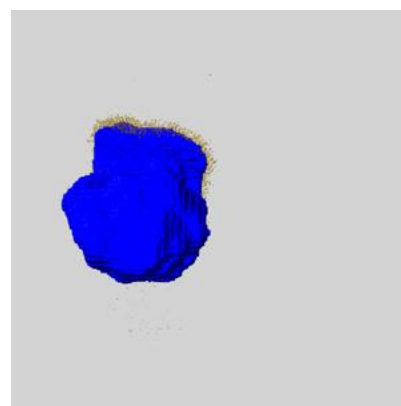
6.6.1 emd_65577_msk_1.map [i](#)



X



Y

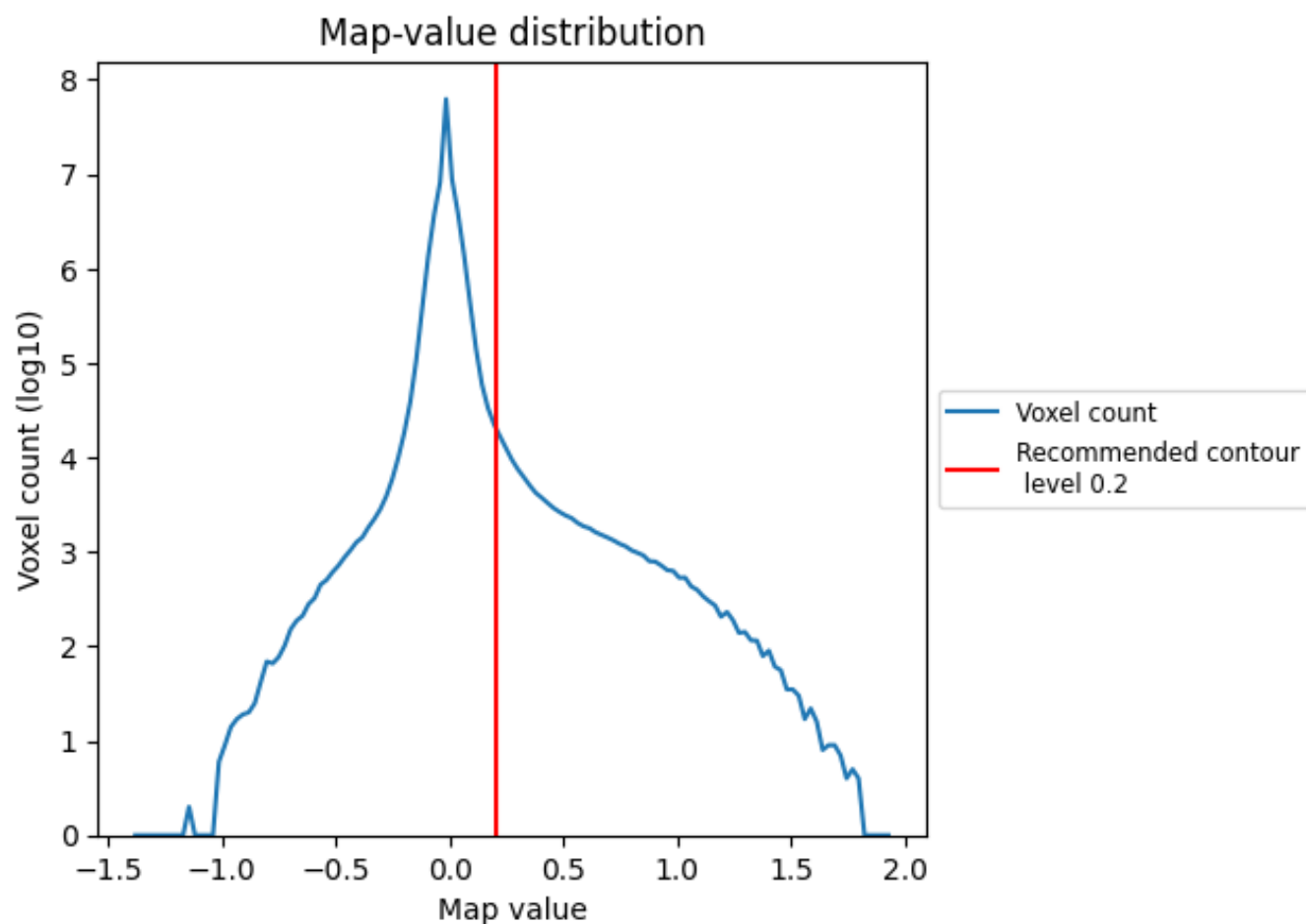


Z

7 Map analysis [i](#)

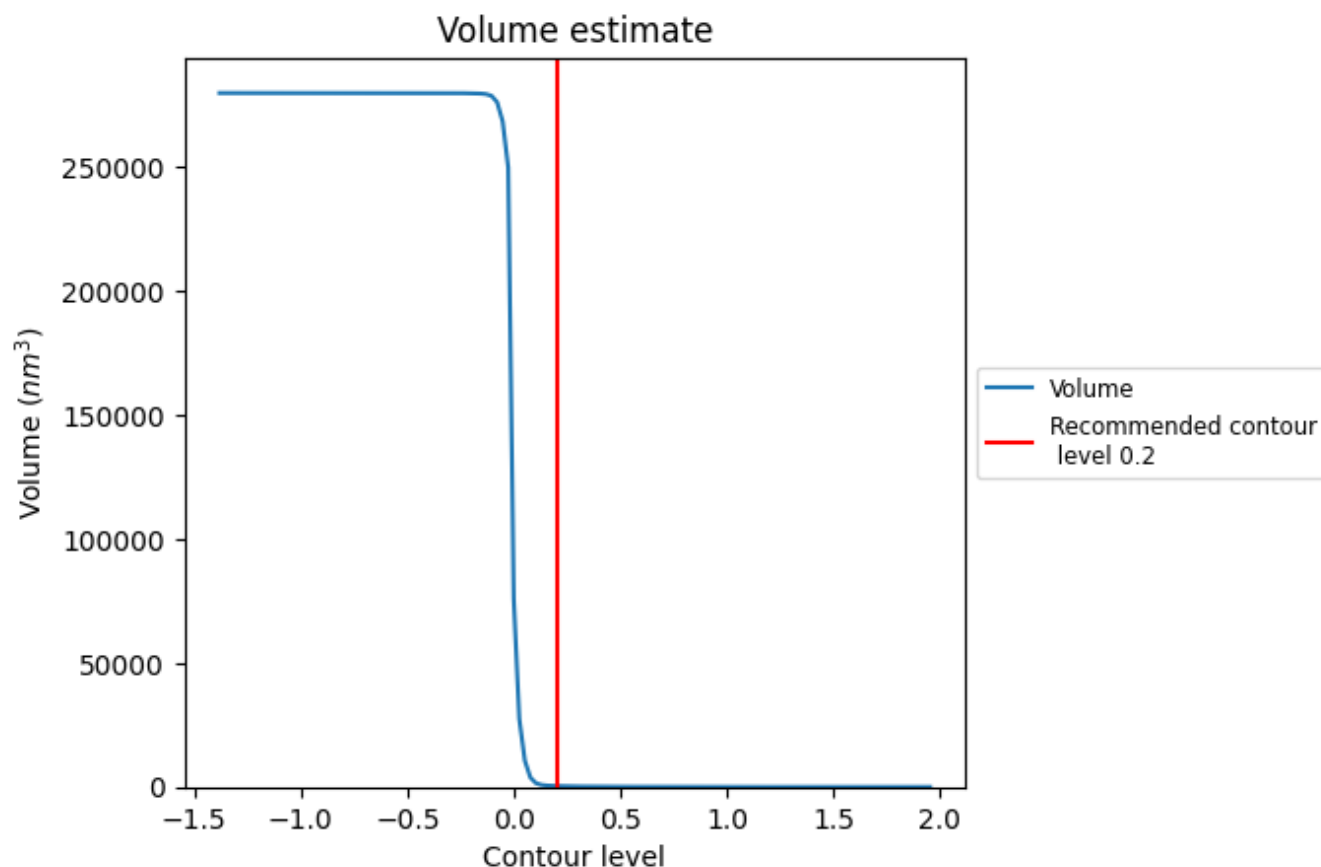
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

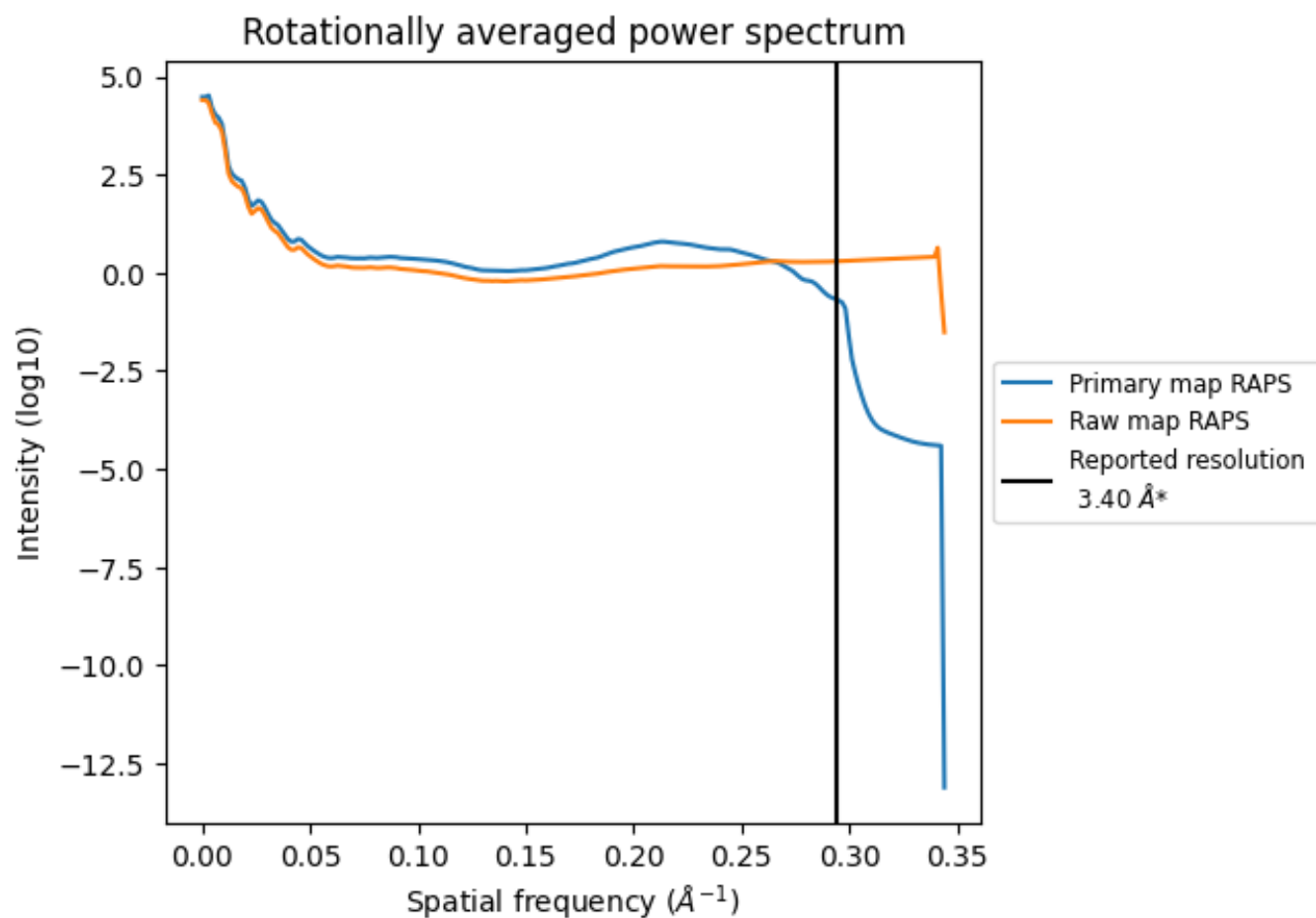
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 377 nm³; this corresponds to an approximate mass of 341 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 ⓘ

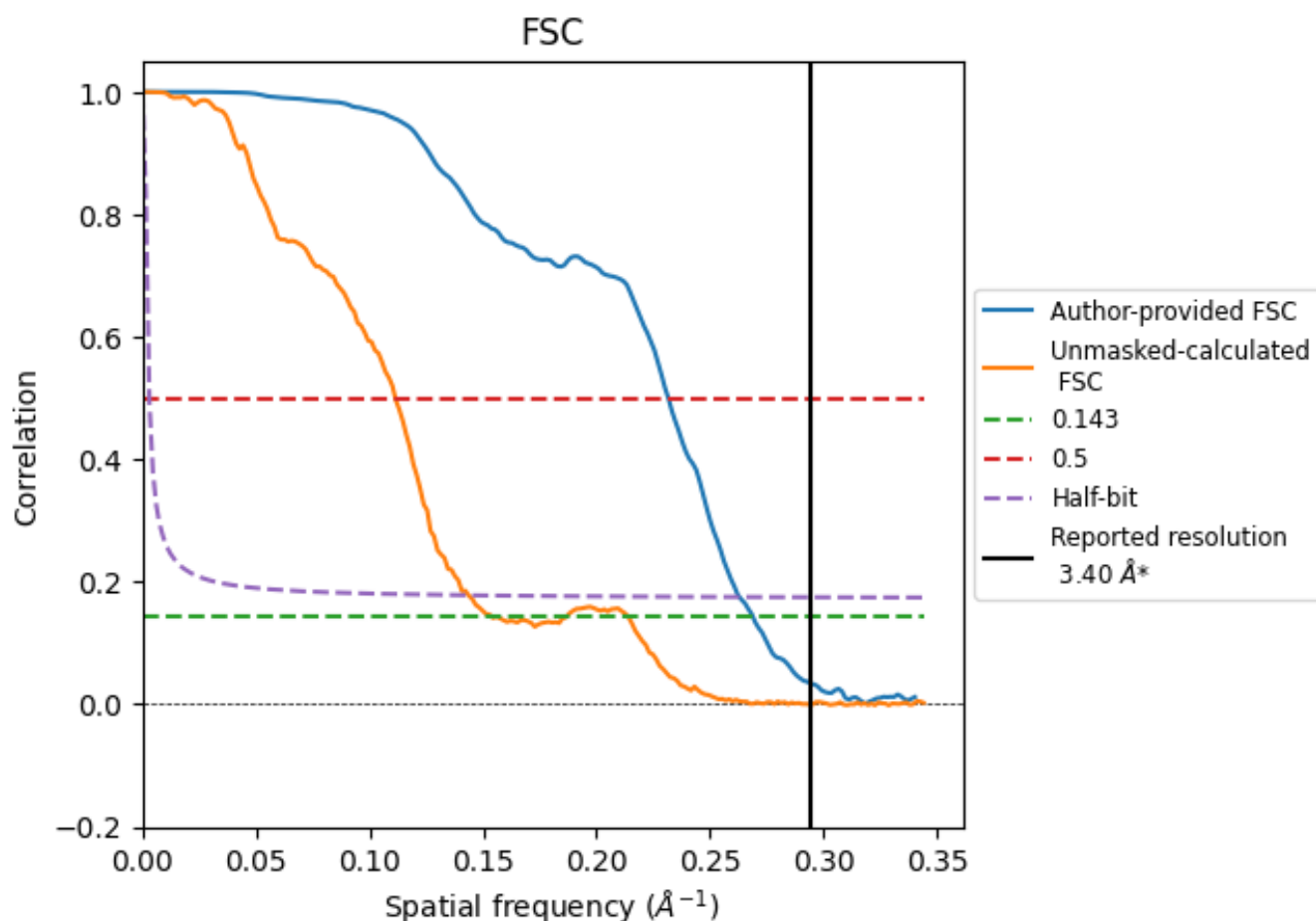


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

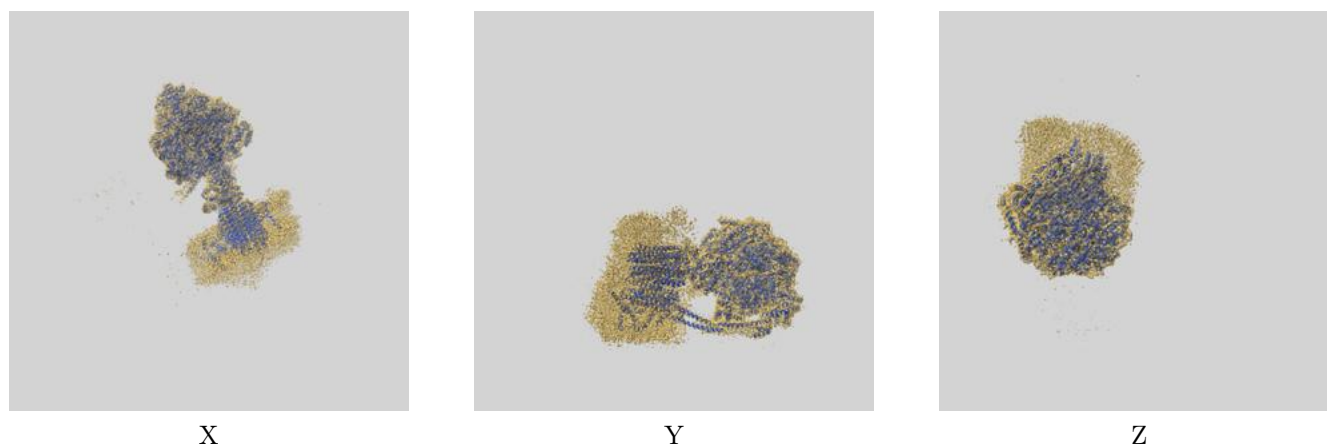
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.72	4.32	3.80
Unmasked-calculated*	6.50	8.98	6.96

*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 6.50 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

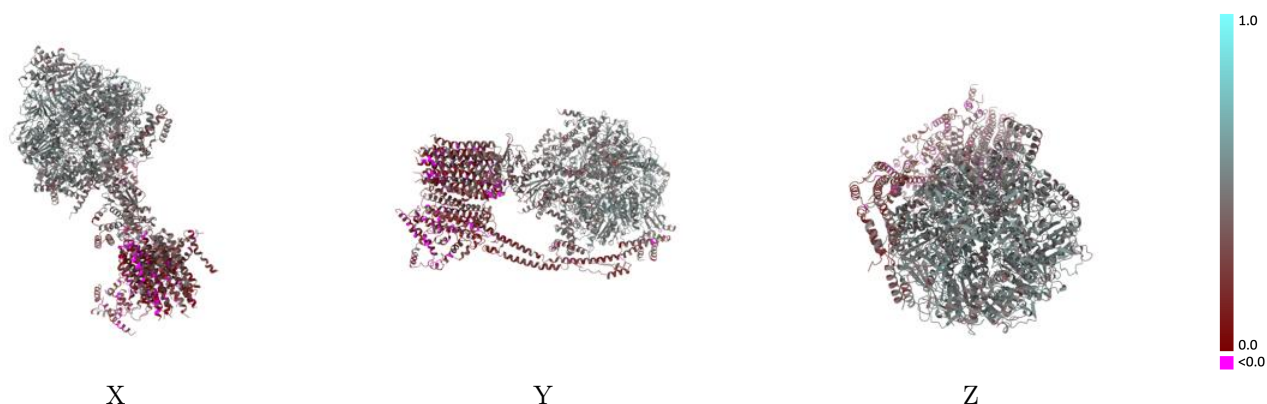
This section contains information regarding the fit between EMDB map EMD-65577 and PDB model 9W2R. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



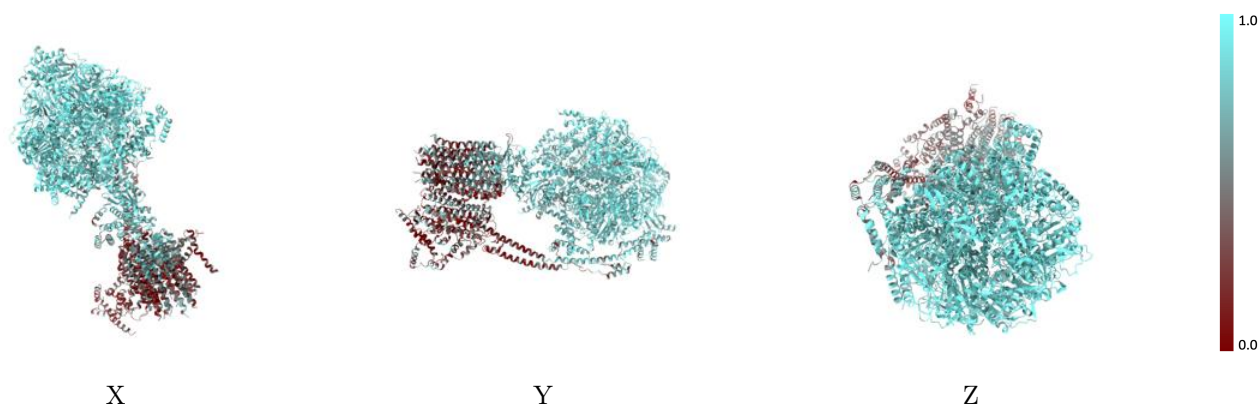
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



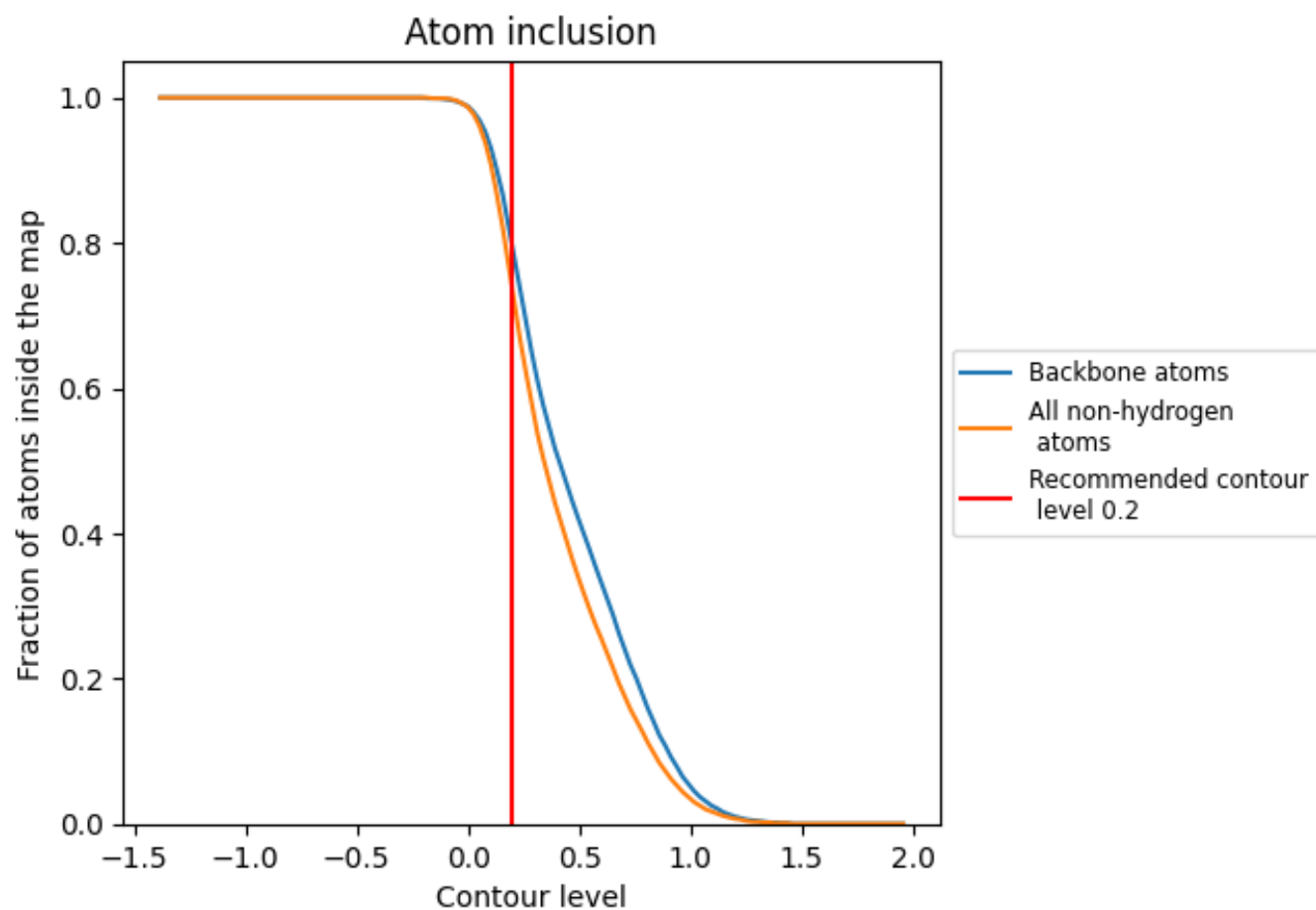
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion ⓘ



At the recommended contour level, 79% of all backbone atoms, 74% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7350	 0.4000
8	 0.2940	 0.1550
A	 0.8950	 0.4930
B	 0.8830	 0.4800
C	 0.8750	 0.4820
D	 0.8850	 0.4970
E	 0.8960	 0.4870
F	 0.8870	 0.4990
G	 0.8220	 0.4240
H	 0.7020	 0.3560
I	 0.7270	 0.3520
J	 0.8120	 0.4430
K	 0.5120	 0.3200
L	 0.4690	 0.2760
M	 0.4720	 0.2190
N	 0.3990	 0.1570
O	 0.3440	 0.1590
P	 0.3270	 0.1270
Q	 0.4090	 0.1400
R	 0.5260	 0.3130
S	 0.8460	 0.4540
a	 0.3740	 0.2350
b	 0.4760	 0.2410
d	 0.4240	 0.2330
e	 0.2440	 0.1350
f	 0.3800	 0.1920
g	 0.2860	 0.2020
h	 0.6680	 0.2900
j	 0.3690	 0.2050
k	 0.2480	 0.2390

