



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2025 – 03:02 PM EDT

PDB ID : 9B0X
EMDB ID : EMD-44061
Title : Artemia franciscana ATP synthase state 2 (composite structure), pH 7.0
Authors : Mnatsakanyan, N.; Mello, J.F.R.
Deposited on : 2024-03-12
Resolution : 2.60 Å(reported)
Based on initial model : .

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.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

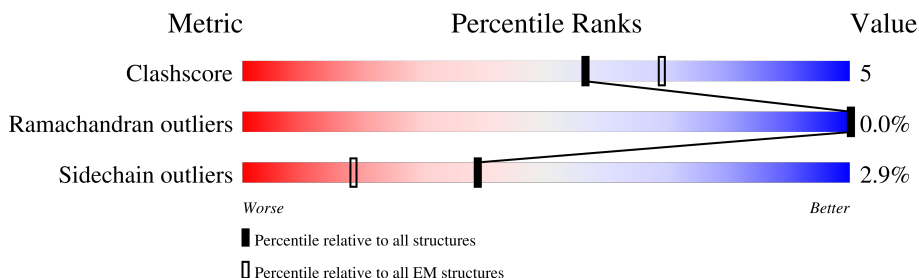
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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.





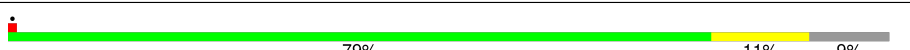
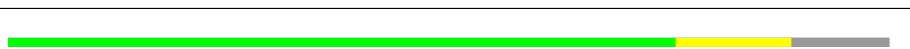

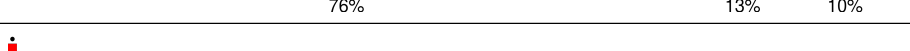
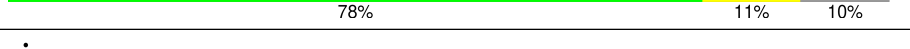

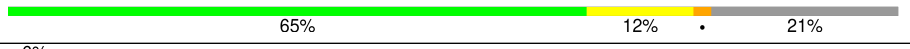
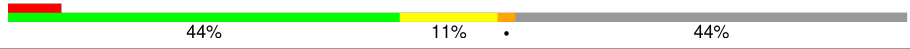


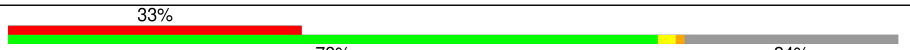


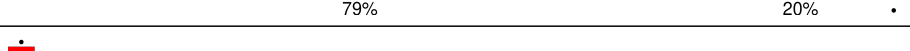

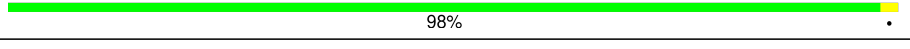


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1	128	
1	2	128	
1	3	128	
1	4	128	
1	5	128	
1	6	128	
1	7	128	
1	8	128	

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Mol	Chain	Length	Quality of chain
2	A	551	
2	B	551	
2	C	551	
3	D	524	
3	E	524	
3	F	524	
4	G	290	
5	H	169	
6	I	66	
7	J	105	
8	K	265	
9	L	99	
10	M	219	
11	N	219	
12	O	207	
13	P	44	
14	Q	53	
15	R	119	
16	S	103	
17	T	84	

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 39830 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	S	0	0
			537	355	83	95	4		
1	2	75	Total	C	N	O	S	0	0
			537	355	83	95	4		
1	3	75	Total	C	N	O	S	0	0
			537	355	83	95	4		
1	4	75	Total	C	N	O	S	0	0
			537	355	83	95	4		
1	5	75	Total	C	N	O	S	0	0
			537	355	83	95	4		
1	6	75	Total	C	N	O	S	0	0
			537	355	83	95	4		
1	7	75	Total	C	N	O	S	0	0
			537	355	83	95	4		
1	8	75	Total	C	N	O	S	0	0
			537	355	83	95	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	504	Total	C	N	O	S	0	0
			3844	2419	677	734	14		
2	B	503	Total	C	N	O	S	0	0
			3842	2419	676	733	14		
2	C	501	Total	C	N	O	S	0	0
			3828	2411	674	729	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	465	Total	C	N	O	S	0	0
			3525	2239	597	678	11		
3	E	469	Total	C	N	O	S	0	0
			3554	2255	602	686	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	469	Total	C	N	O	S	0	0
			3554	2255	602	686	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	261	Total	C	N	O	S	0	0
			2013	1258	352	389	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	134	Total	C	N	O	S	0	0
			984	620	161	201	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	37	Total	C	N	O	S	0	0
			304	185	65	52	2		

- Molecule 7 is a protein called ATP synthase inhibitory factor 1, IF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	42	Total	C	N	O	S	0	0
			292	174	58	60			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	208	Total	C	N	O	S	0	0
			1686	1081	292	306	7		

- Molecule 9 is a protein called ATP synthase coupling factor 6, F6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	75	Total	C	N	O	S	0	0
			594	380	95	117	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	161	Total	C	N	O	S	0	0
			1309	836	222	246	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	219	Total	C	N	O	S	0	0
			1716	1157	256	287	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	189	Total	C	N	O	S	0	0
			1451	928	252	266	5		

- Molecule 13 is a protein called ATP synthase subunit 6.8PL.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	P	44	Total	C	N	O	0	0
			220	132	44	44		

- Molecule 14 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	46	Total	C	N	O	S	0	0
			390	266	60	60	4		

- Molecule 15 is a protein called ATP synthase subunit f.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	104	Total	C	N	O	S	0	0
			851	555	158	136	2		

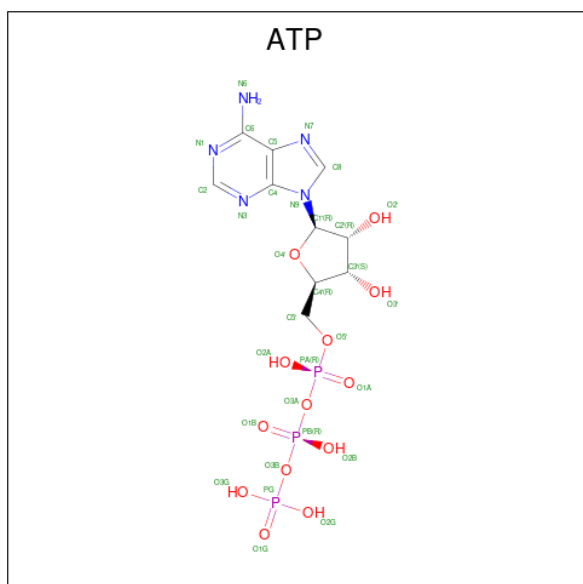
- Molecule 16 is a protein called ATP synthase subunit g.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	76	Total	C	N	O	S	0	0
			596	392	99	103	2		

- Molecule 17 is a protein called ATP synthase subunit e.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	82	Total	C	N	O	S	0	0
			658	418	122	117	1		

- Molecule 18 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 19 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

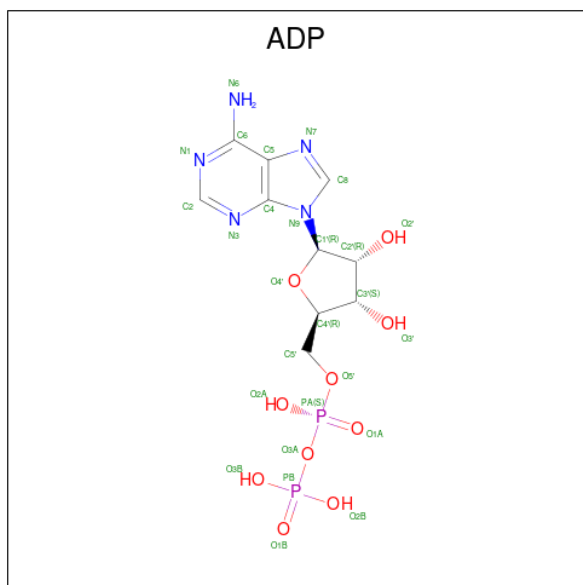
Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Mg	0
			1	1	
19	B	1	Total	Mg	0
			1	1	
19	C	1	Total	Mg	0
			1	1	
19	D	1	Total	Mg	0
			1	1	

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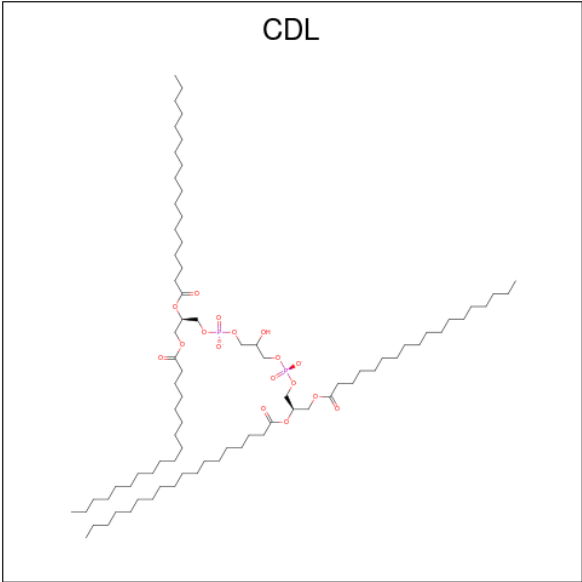
Mol	Chain	Residues	Atoms		AltConf
19	E	1	Total	Mg	0
			1	1	

- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 21 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

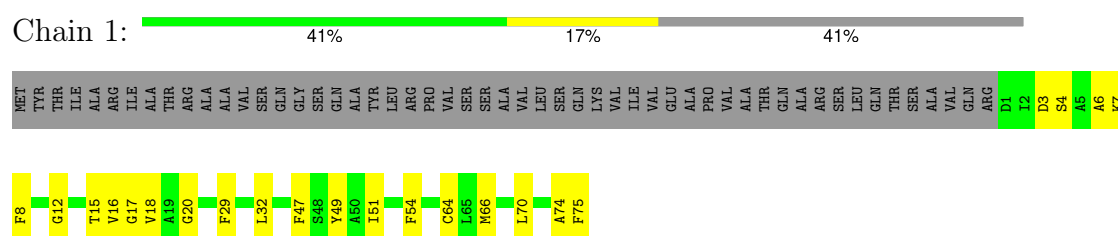


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
21	K	1	90	71	17	2	0
21	K	1	77	58	17	2	0

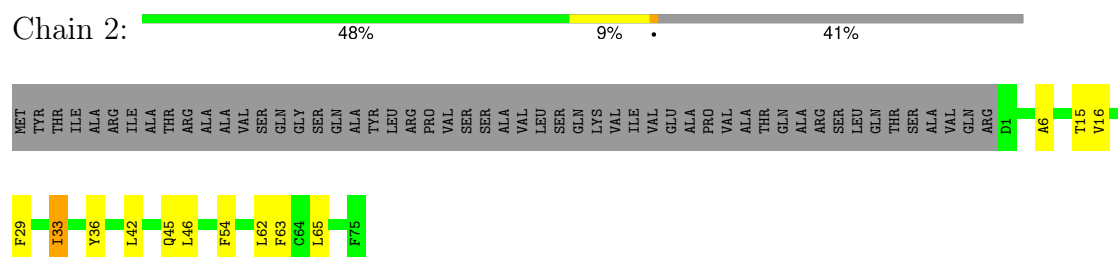
3 Residue-property plots [i](#)

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.

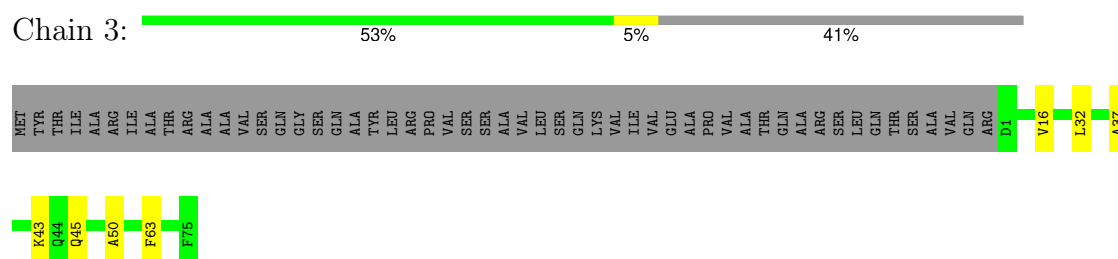
- Molecule 1: ATP synthase subunit c



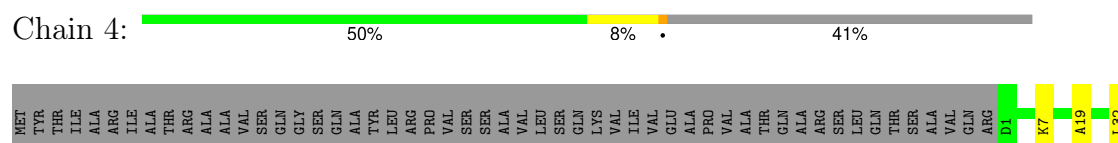
- Molecule 1: ATP synthase subunit c

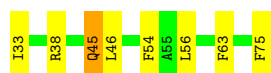


- Molecule 1: ATP synthase subunit c

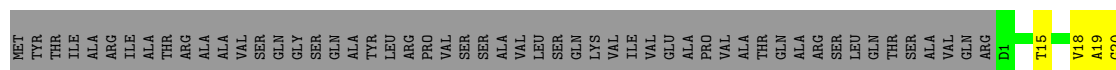


- Molecule 1: ATP synthase subunit c

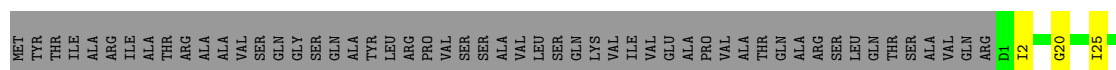




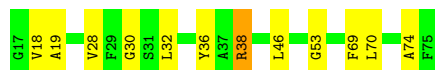
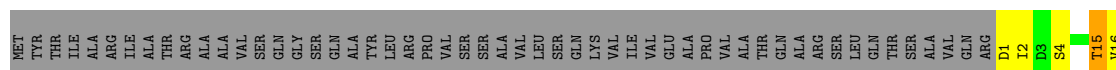
- Molecule 1: ATP synthase subunit c



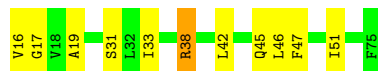
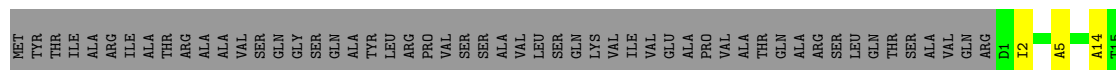
- Molecule 1: ATP synthase subunit c



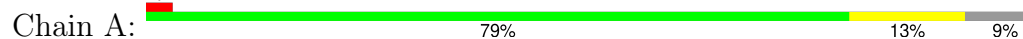
- Molecule 1: ATP synthase subunit c

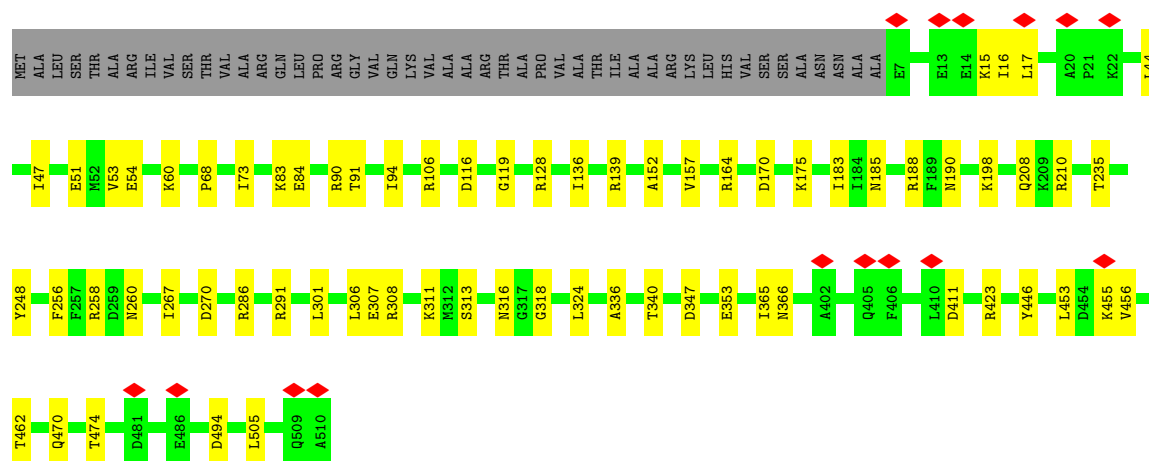


- Molecule 1: ATP synthase subunit c

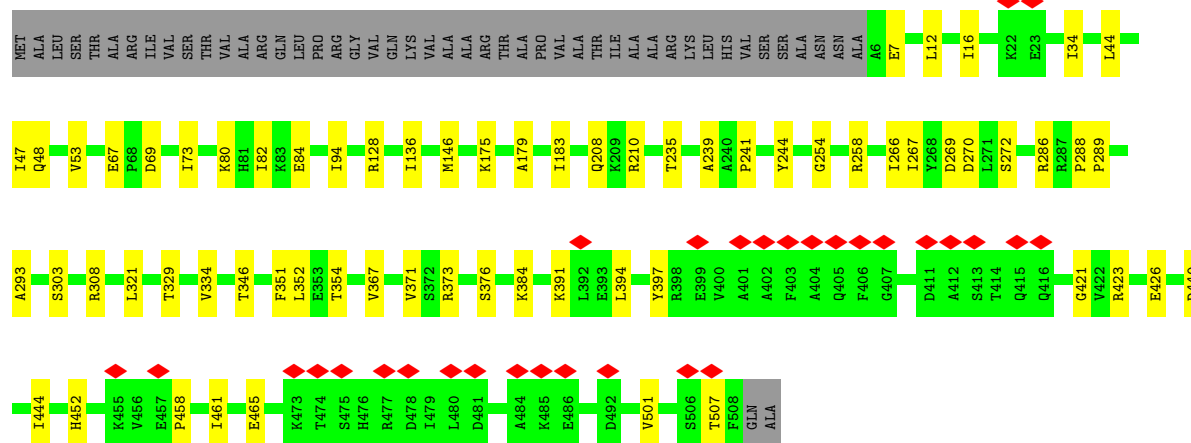
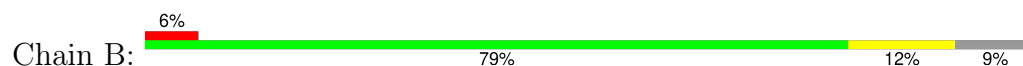


- Molecule 2: ATP synthase subunit alpha

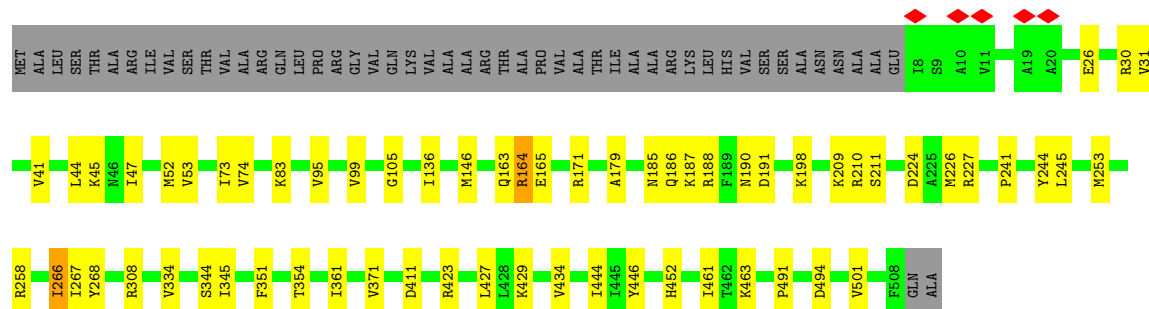
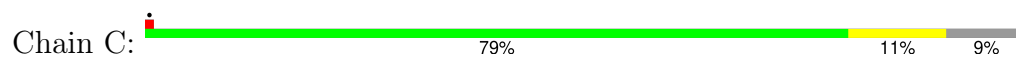




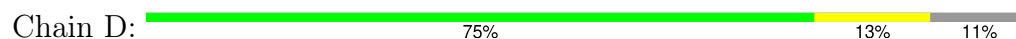
• Molecule 2: ATP synthase subunit alpha



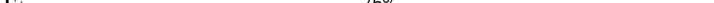
• Molecule 2: ATP synthase subunit alpha

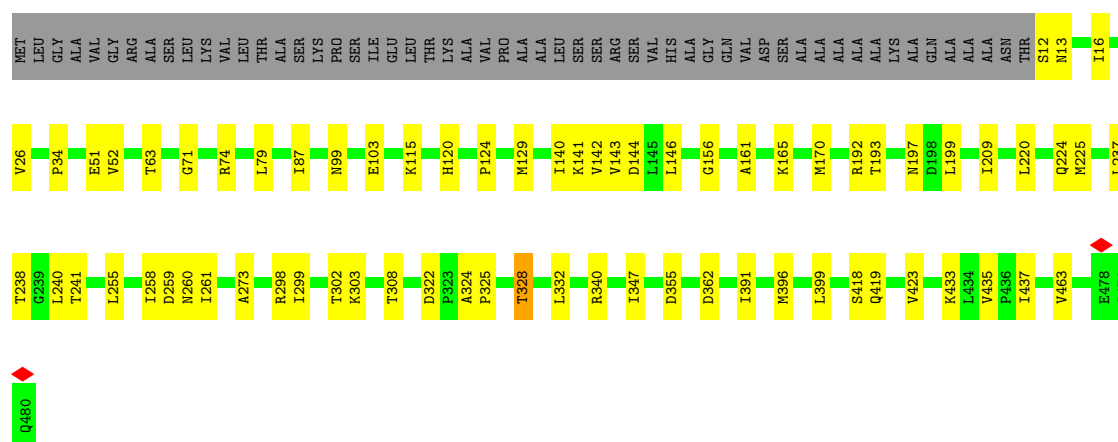


• Molecule 3: ATP synthase subunit beta

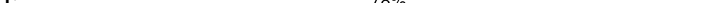


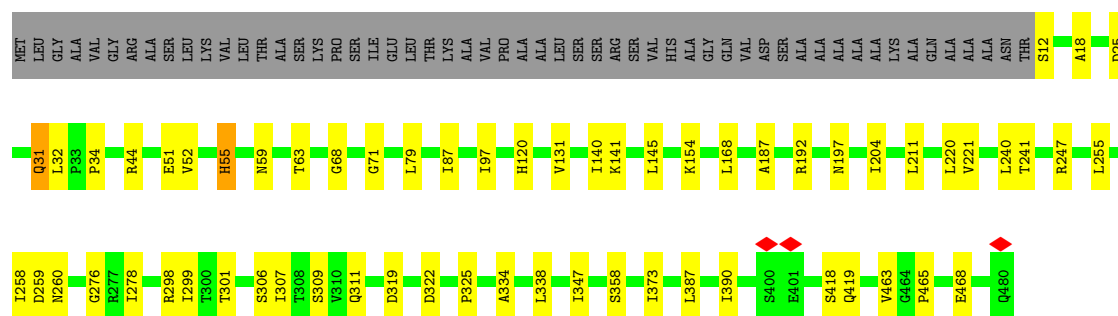
- Molecule 3: ATP synthase subunit beta

Chain E:  76% 13% 10%



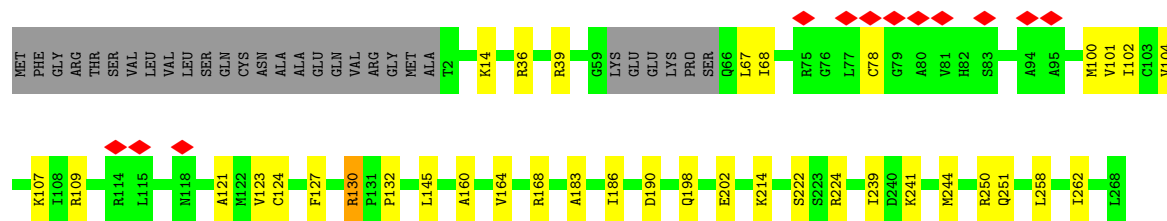
- Molecule 3: ATP synthase subunit beta

Chain F:  78% 11% 10%



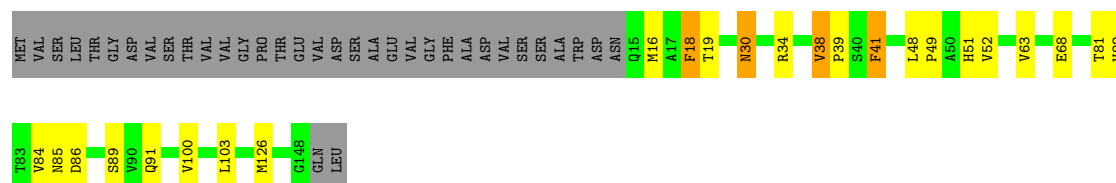
- Molecule 4: ATP synthase subunit gamma

Chain G: 77% 12% 10%



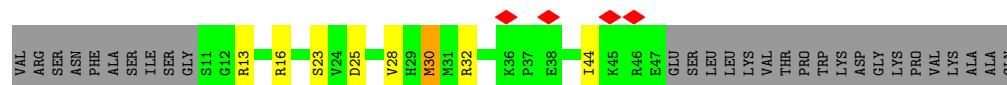
• Molecule 5: ATP synthase subunit delta

Chain H: 65% 12% 21%



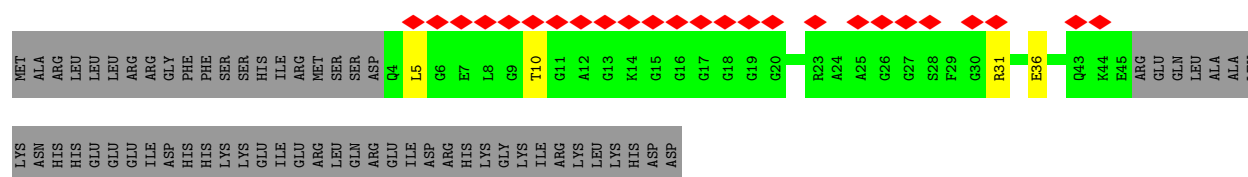
• Molecule 6: ATP synthase subunit epsilon

Chain I: 6% 44% 11% 44%



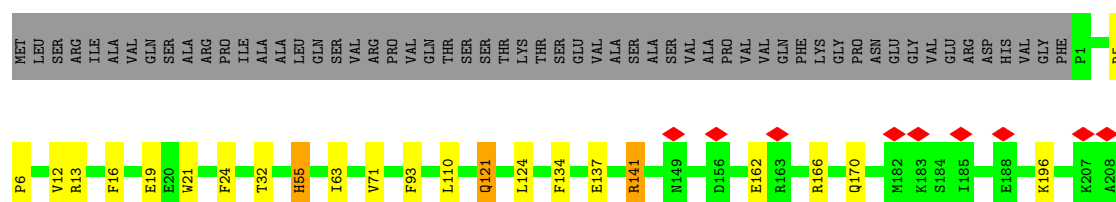
• Molecule 7: ATP synthase inhibitory factor 1, IF1

Chain J: 24% 36% 60%



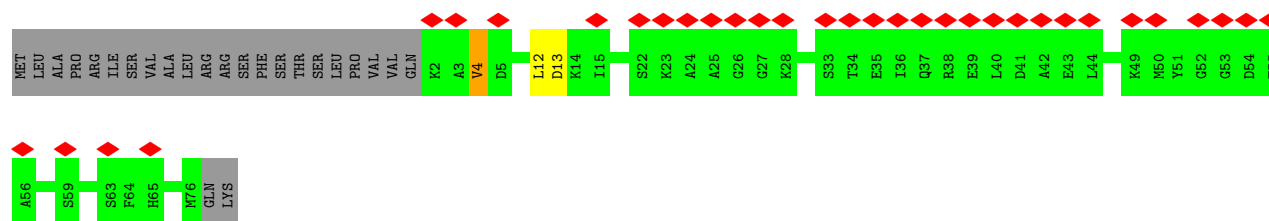
• Molecule 8: ATP synthase subunit b

Chain K: 70% 8% 22%

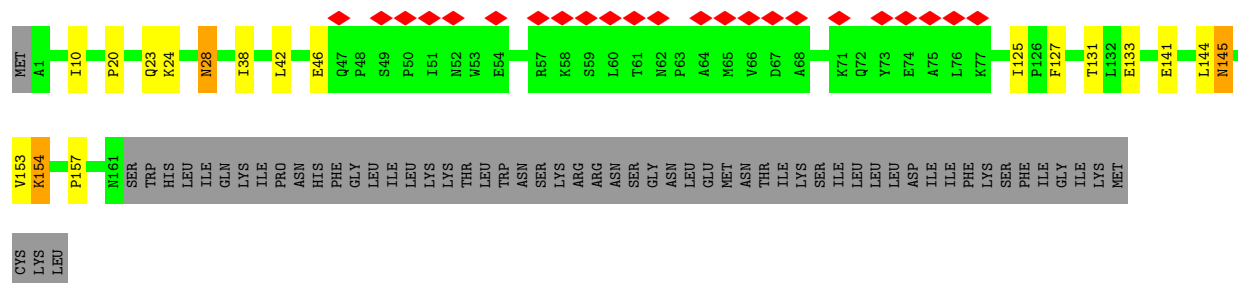


• Molecule 9: ATP synthase coupling factor 6, F6

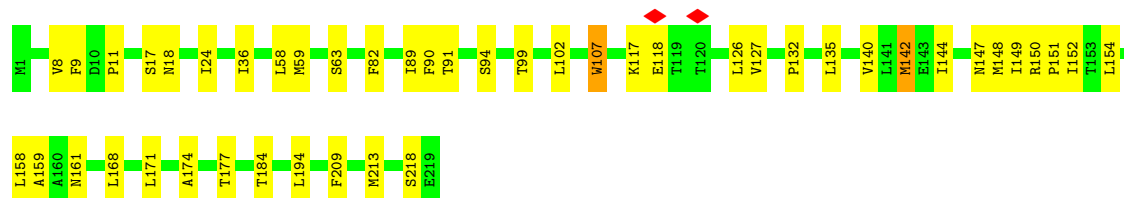
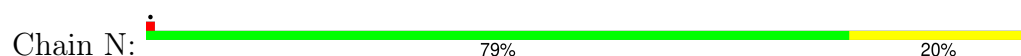
Chain L: 33% 73% 24%



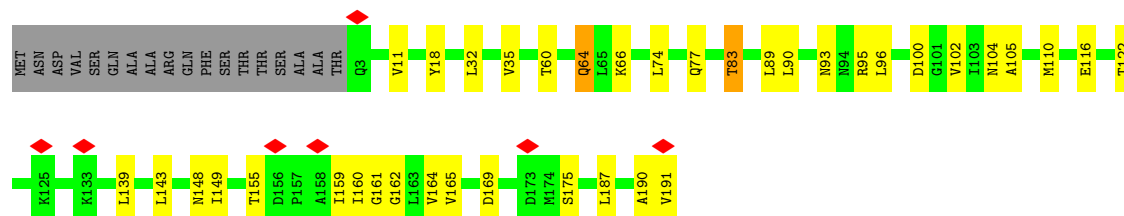
- Molecule 10: ATP synthase subunit d



- Molecule 11: ATP synthase subunit a



- Molecule 12: ATP synthase subunit OSCP



- Molecule 13: ATP synthase subunit 6.8PL




- Molecule 14: ATP synthase protein 8

Chain Q:  74% 13% 13%



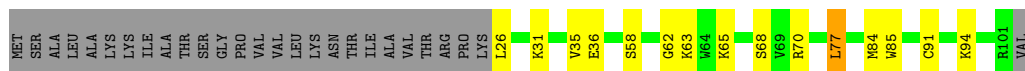
- Molecule 15: ATP synthase subunit f

Chain R:  79% 8% 13%




- Molecule 16: ATP synthase subunit g

Chain S:  59% 14% 26%



- Molecule 17: ATP synthase subunit e

Chain T:  88% 10% 2%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	232736	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 ($e^-/\text{\AA}^2$)	15.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	75.979	Depositor
Minimum map value	-49.967	Depositor
Average map value	-0.010	Depositor
Map value standard deviation	1.010	Depositor
Recommended contour level	4.51	Depositor
Map size (Å)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

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

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	1	0.27	0/547	0.39	0/734
1	2	0.27	0/547	0.41	0/734
1	3	0.27	0/547	0.40	0/734
1	4	0.27	0/547	0.39	0/734
1	5	0.28	0/547	0.40	0/734
1	6	0.28	0/547	0.41	0/734
1	7	0.29	0/547	0.41	0/734
1	8	0.28	0/547	0.40	0/734
2	A	0.27	0/3898	0.49	0/5260
2	B	0.26	0/3896	0.49	0/5257
2	C	0.27	0/3882	0.50	0/5238
3	D	0.27	0/3582	0.49	0/4862
3	E	0.27	0/3611	0.48	0/4901
3	F	0.27	0/3611	0.49	0/4901
4	G	0.27	0/2035	0.45	0/2735
5	H	0.27	0/998	0.45	0/1359
6	I	0.30	0/308	0.62	0/407
7	J	0.26	0/294	0.51	0/386
8	K	0.25	0/1720	0.42	0/2311
9	L	0.24	0/604	0.36	0/809
10	M	0.26	0/1343	0.42	0/1808
11	N	0.26	0/1761	0.44	0/2402
12	O	0.24	0/1466	0.45	0/1969
14	Q	0.28	0/405	0.41	0/549
15	R	0.30	0/882	0.48	0/1196
16	S	0.25	0/611	0.42	0/829
17	T	0.24	0/670	0.49	0/902
All	All	0.27	0/39953	0.47	0/53953

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	537	0	549	14	0
1	2	537	0	549	8	0
1	3	537	0	549	4	0
1	4	537	0	549	6	0
1	5	537	0	549	6	0
1	6	537	0	549	7	0
1	7	537	0	549	12	0
1	8	537	0	549	15	0
2	A	3844	0	3938	45	0
2	B	3842	0	3945	43	0
2	C	3828	0	3934	36	0
3	D	3525	0	3593	41	0
3	E	3554	0	3617	40	0
3	F	3554	0	3618	39	0
4	G	2013	0	2062	20	0
5	H	984	0	974	13	0
6	I	304	0	305	5	0
7	J	292	0	270	5	0
8	K	1686	0	1709	16	0
9	L	594	0	599	2	0
10	M	1309	0	1304	12	0
11	N	1716	0	1811	21	0
12	O	1451	0	1566	22	0
13	P	220	0	46	1	0
14	Q	390	0	393	4	0
15	R	851	0	840	7	0
16	S	596	0	617	9	0
17	T	658	0	672	5	0
18	A	31	0	12	0	0
18	B	31	0	12	0	0
18	C	31	0	12	0	0
18	D	31	0	12	0	0
19	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	1	0	0	0	0
19	C	1	0	0	0	0
19	D	1	0	0	0	0
19	E	1	0	0	0	0
20	E	27	0	12	1	0
21	K	167	0	231	5	0
All	All	39830	0	40496	381	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 5.

The worst 5 of 381 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:33:ILE:HG21	1:6:32:LEU:HA	1.71	0.72
1:1:16:VAL:HG13	1:2:16:VAL:HG11	1.76	0.66
8:K:6:PRO:HG2	15:R:70:PRO:HG3	1.77	0.66
1:7:16:VAL:HG13	1:8:16:VAL:HG11	1.77	0.66
3:F:44:ARG:HH12	3:F:71:GLY:H	1.45	0.65

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	1	73/128 (57%)	68 (93%)	5 (7%)	0	100	100
1	2	73/128 (57%)	70 (96%)	3 (4%)	0	100	100
1	3	73/128 (57%)	71 (97%)	2 (3%)	0	100	100
1	4	73/128 (57%)	73 (100%)	0	0	100	100
1	5	73/128 (57%)	71 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6	73/128 (57%)	71 (97%)	2 (3%)	0	100	100
1	7	73/128 (57%)	72 (99%)	1 (1%)	0	100	100
1	8	73/128 (57%)	68 (93%)	5 (7%)	0	100	100
2	A	502/551 (91%)	497 (99%)	5 (1%)	0	100	100
2	B	501/551 (91%)	495 (99%)	6 (1%)	0	100	100
2	C	499/551 (91%)	495 (99%)	4 (1%)	0	100	100
3	D	463/524 (88%)	446 (96%)	17 (4%)	0	100	100
3	E	467/524 (89%)	447 (96%)	20 (4%)	0	100	100
3	F	467/524 (89%)	449 (96%)	18 (4%)	0	100	100
4	G	257/290 (89%)	253 (98%)	4 (2%)	0	100	100
5	H	132/169 (78%)	128 (97%)	4 (3%)	0	100	100
6	I	35/66 (53%)	31 (89%)	4 (11%)	0	100	100
7	J	40/105 (38%)	36 (90%)	4 (10%)	0	100	100
8	K	206/265 (78%)	202 (98%)	4 (2%)	0	100	100
9	L	73/99 (74%)	73 (100%)	0	0	100	100
10	M	159/219 (73%)	138 (87%)	21 (13%)	0	100	100
11	N	217/219 (99%)	205 (94%)	12 (6%)	0	100	100
12	O	187/207 (90%)	176 (94%)	10 (5%)	1 (0%)	25	47
14	Q	44/53 (83%)	42 (96%)	2 (4%)	0	100	100
15	R	102/119 (86%)	93 (91%)	9 (9%)	0	100	100
16	S	74/103 (72%)	72 (97%)	2 (3%)	0	100	100
17	T	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
All	All	5089/6247 (82%)	4919 (97%)	169 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	O	160	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	51/93 (55%)	45 (88%)	6 (12%)	4	8
1	2	51/93 (55%)	47 (92%)	4 (8%)	10	22
1	3	51/93 (55%)	49 (96%)	2 (4%)	27	53
1	4	51/93 (55%)	46 (90%)	5 (10%)	6	13
1	5	51/93 (55%)	47 (92%)	4 (8%)	10	22
1	6	51/93 (55%)	47 (92%)	4 (8%)	10	22
1	7	51/93 (55%)	46 (90%)	5 (10%)	6	13
1	8	51/93 (55%)	49 (96%)	2 (4%)	27	53
2	A	410/446 (92%)	407 (99%)	3 (1%)	81	93
2	B	411/446 (92%)	406 (99%)	5 (1%)	67	85
2	C	410/446 (92%)	403 (98%)	7 (2%)	56	78
3	D	379/418 (91%)	376 (99%)	3 (1%)	79	91
3	E	382/418 (91%)	375 (98%)	7 (2%)	54	77
3	F	382/418 (91%)	377 (99%)	5 (1%)	65	84
4	G	220/244 (90%)	216 (98%)	4 (2%)	54	77
5	H	106/135 (78%)	98 (92%)	8 (8%)	11	24
6	I	31/55 (56%)	29 (94%)	2 (6%)	14	31
7	J	23/82 (28%)	23 (100%)	0	100	100
8	K	178/225 (79%)	170 (96%)	8 (4%)	23	47
9	L	65/87 (75%)	63 (97%)	2 (3%)	35	62
10	M	142/197 (72%)	135 (95%)	7 (5%)	21	43
11	N	194/194 (100%)	183 (94%)	11 (6%)	17	37
12	O	157/171 (92%)	152 (97%)	5 (3%)	34	60
14	Q	42/49 (86%)	40 (95%)	2 (5%)	21	44
15	R	83/97 (86%)	81 (98%)	2 (2%)	44	70
16	S	63/85 (74%)	59 (94%)	4 (6%)	15	32
17	T	67/69 (97%)	65 (97%)	2 (3%)	36	63
All	All	4153/5026 (83%)	4034 (97%)	119 (3%)	39	64

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	31	GLN
14	Q	26	MET
5	H	81	THR
14	Q	20	LEU
17	T	80	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	480	GLN
5	H	85	ASN
10	M	152	ASN
3	E	132	GLN
3	E	27	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	CDL	K	302	-	76,76,99	0.35	0	82,88,111	0.22	0
21	CDL	K	301	-	89,89,99	0.33	0	95,101,111	0.23	0
18	ATP	A	601	19	28,33,33	0.81	0	34,52,52	0.84	1 (2%)
20	ADP	E	601	19	24,29,29	0.86	0	29,45,45	1.25	2 (6%)
18	ATP	D	601	19	28,33,33	0.80	0	34,52,52	0.83	1 (2%)
18	ATP	B	601	19	28,33,33	0.79	0	34,52,52	0.81	1 (2%)
18	ATP	C	601	19	28,33,33	0.79	0	34,52,52	0.80	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	CDL	K	302	-	-	29/87/87/110	-
21	CDL	K	301	-	-	35/100/100/110	-
18	ATP	A	601	19	-	2/18/38/38	0/3/3/3
20	ADP	E	601	19	-	4/12/32/32	0/3/3/3
18	ATP	D	601	19	-	11/18/38/38	0/3/3/3
18	ATP	B	601	19	-	0/18/38/38	0/3/3/3
18	ATP	C	601	19	-	1/18/38/38	0/3/3/3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	E	601	ADP	N3-C2-N1	-3.71	123.64	128.67
20	E	601	ADP	C4-C5-N7	-2.39	106.81	109.34
18	C	601	ATP	C5-C6-N6	2.28	123.79	120.31
18	A	601	ATP	C5-C6-N6	2.25	123.73	120.31
18	B	601	ATP	C5-C6-N6	2.22	123.69	120.31

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	601	ATP	PB-O3B-PG-O2G
18	D	601	ATP	PB-O3B-PG-O2G
18	D	601	ATP	PB-O3B-PG-O3G

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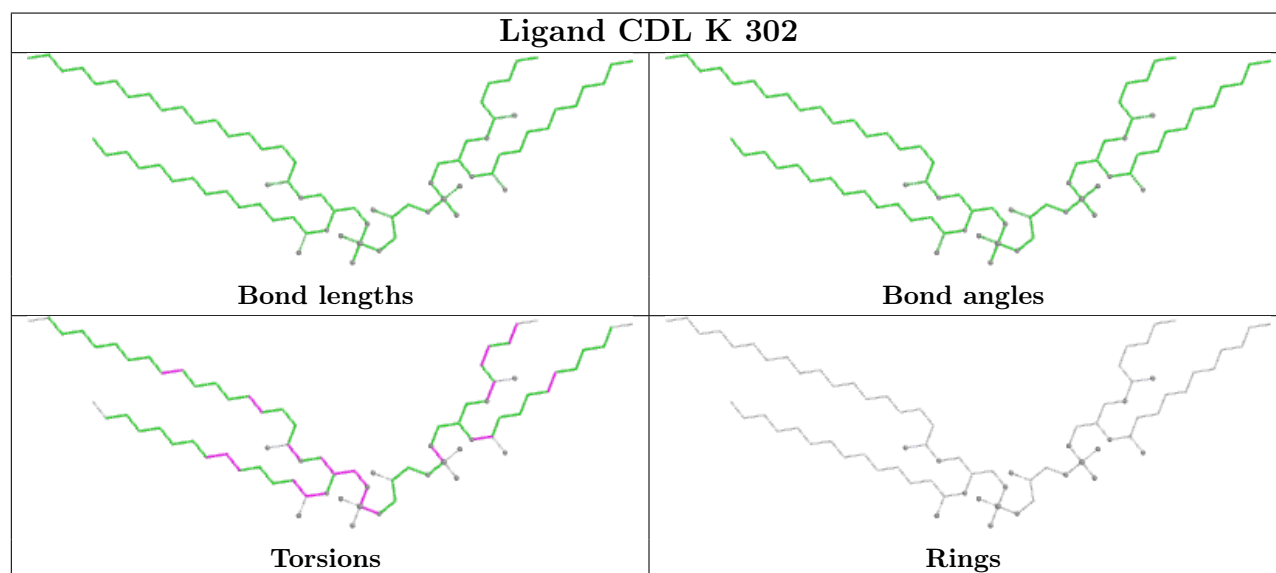
Mol	Chain	Res	Type	Atoms
18	D	601	ATP	C5'-O5'-PA-O2A
20	E	601	ADP	C5'-O5'-PA-O1A

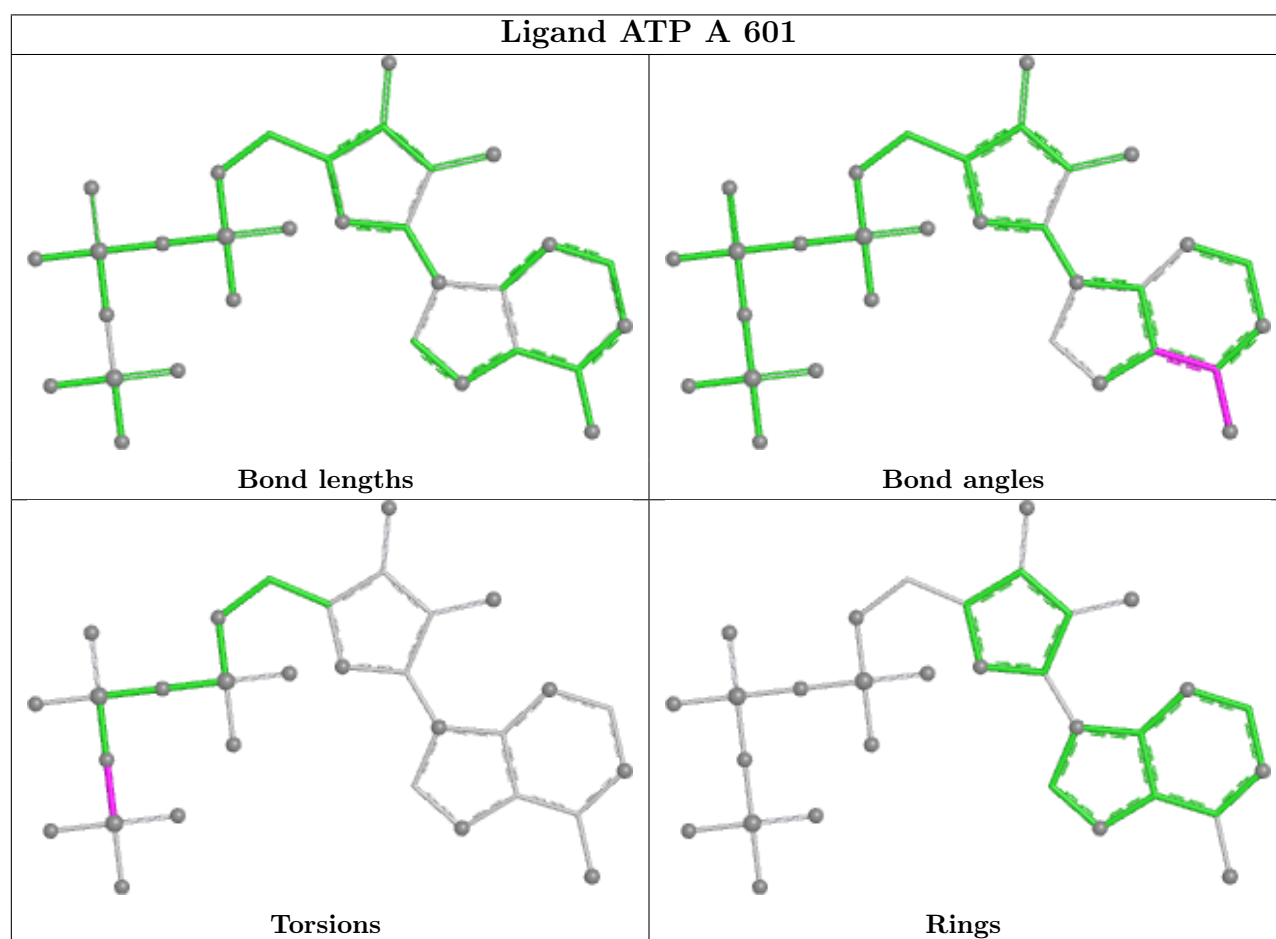
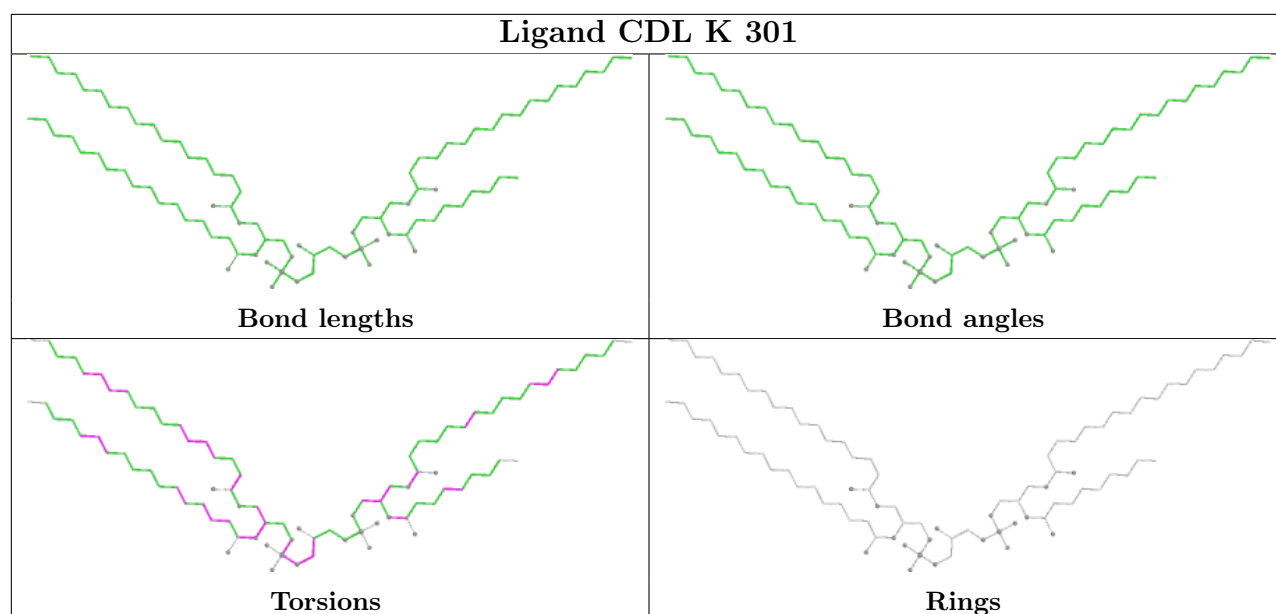
There are no ring outliers.

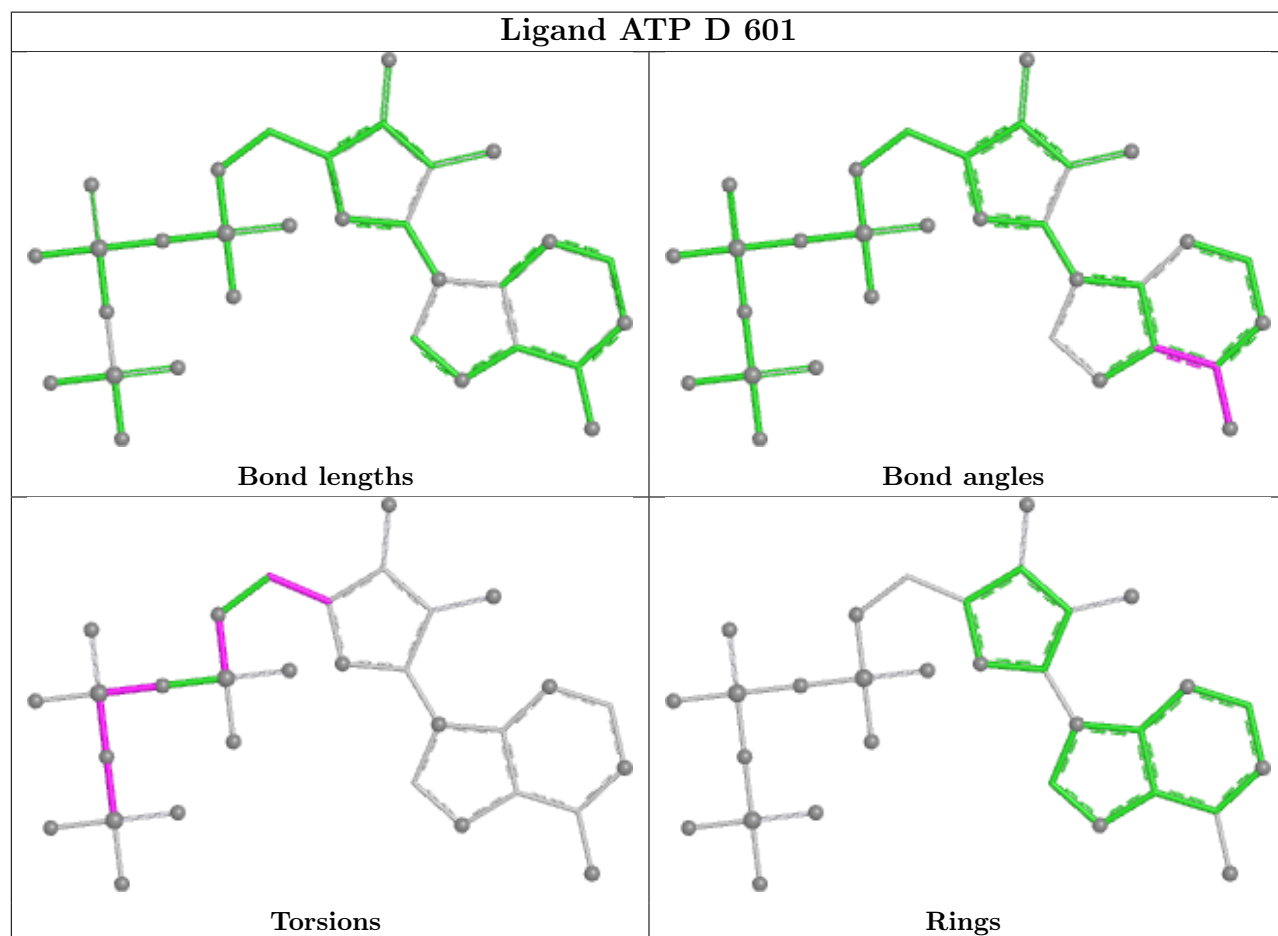
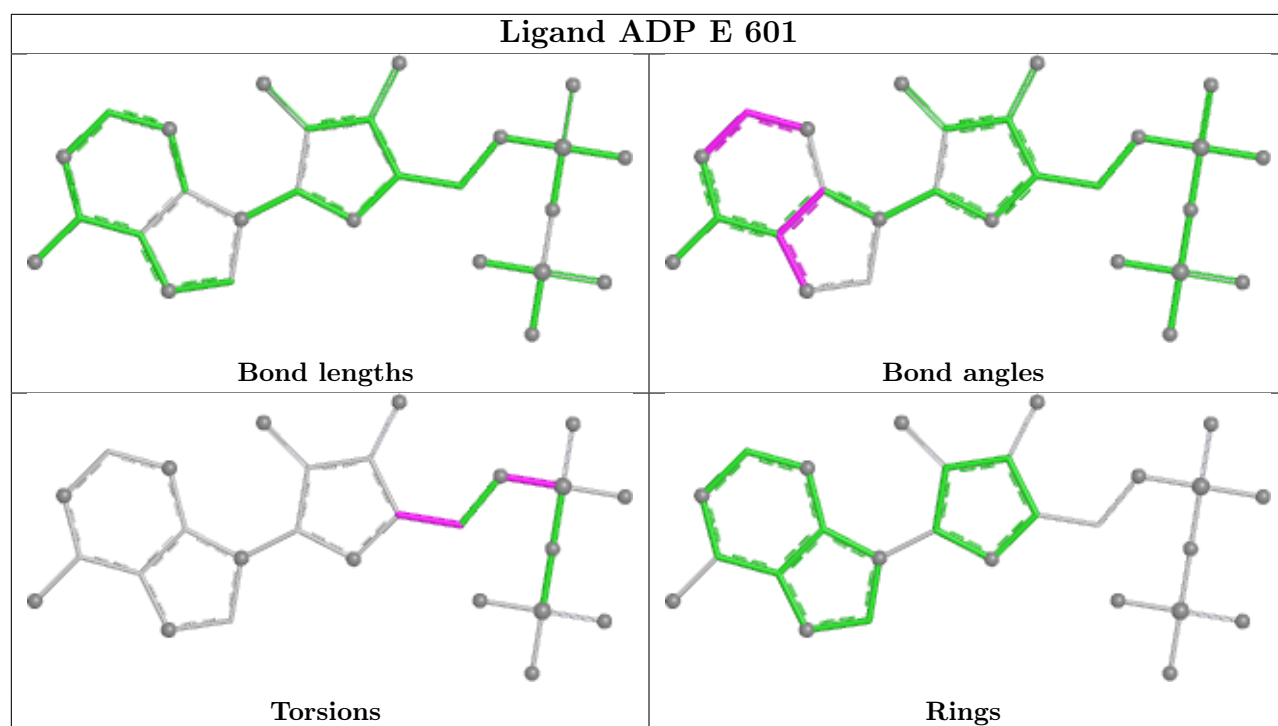
3 monomers are involved in 6 short contacts:

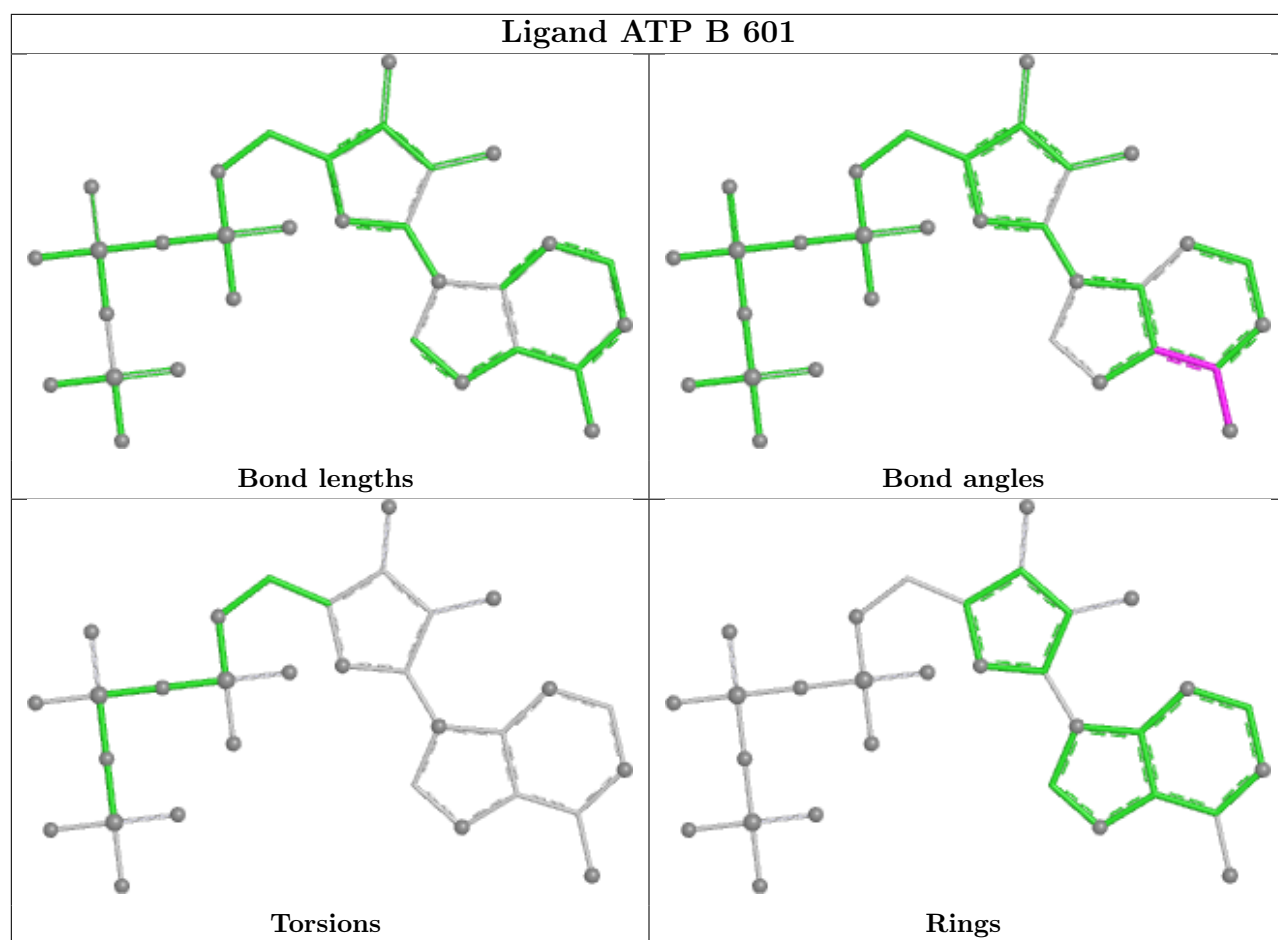
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	K	302	CDL	2	0
21	K	301	CDL	3	0
20	E	601	ADP	1	0

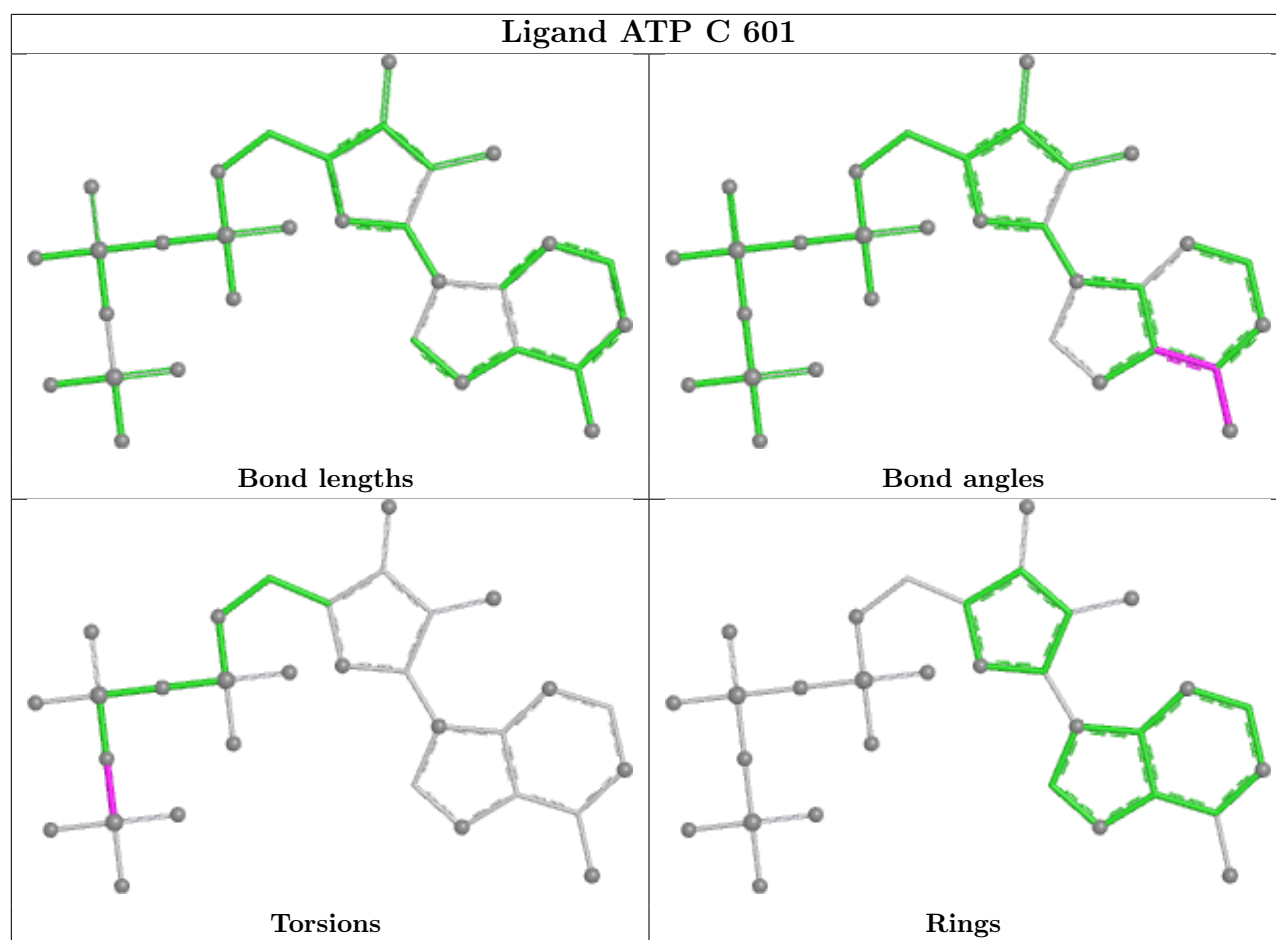
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

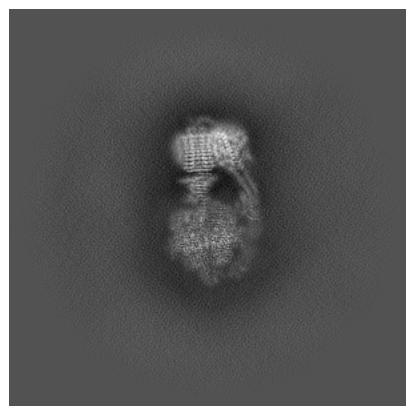
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44061. These allow visual inspection of the internal detail of the map and identification of artifacts.

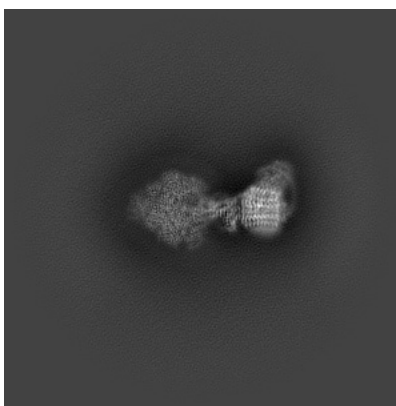
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

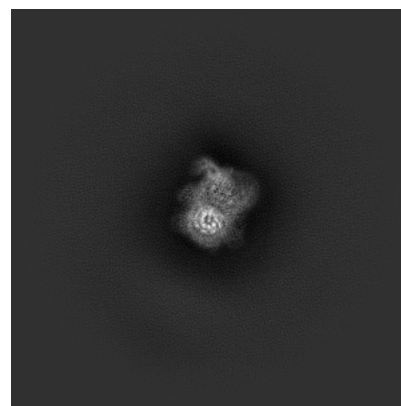
6.1.1 Primary map



X

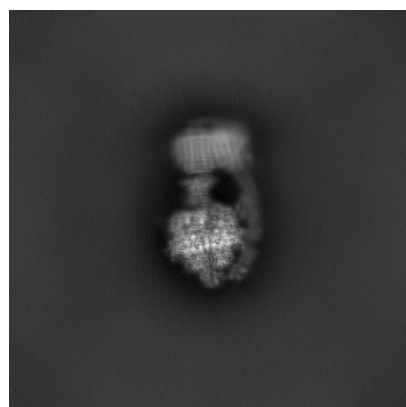


Y

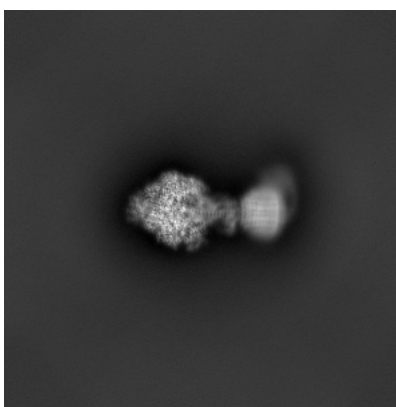


Z

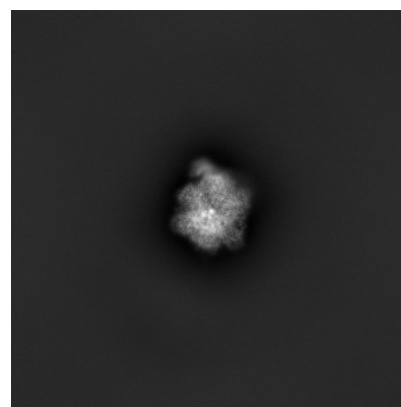
6.1.2 Raw map



X



Y

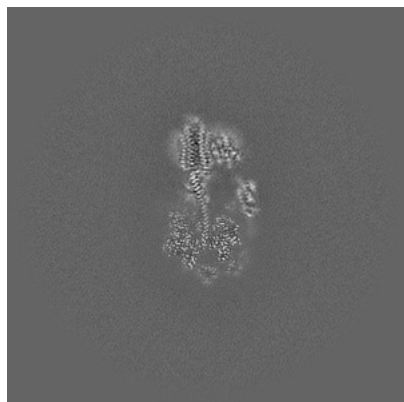


Z

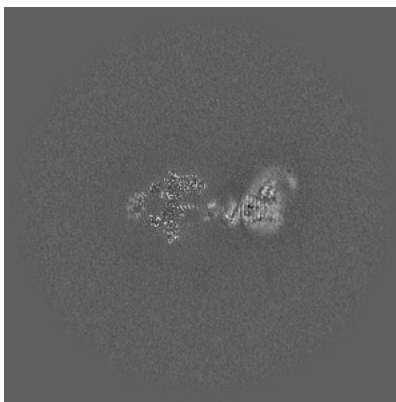
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

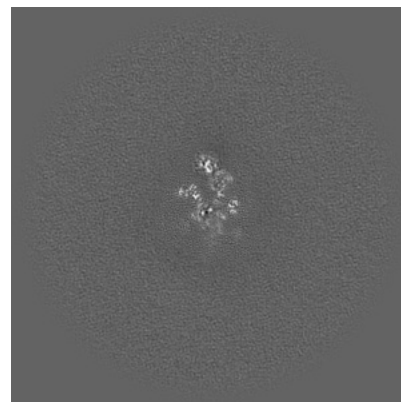
6.2.1 Primary map



X Index: 256



Y Index: 256

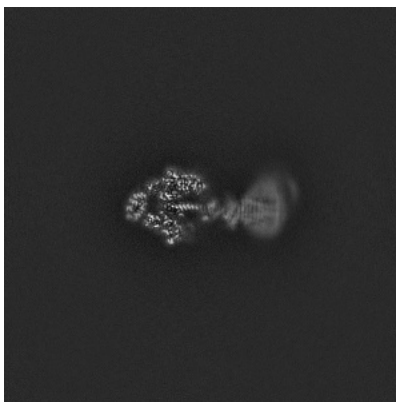


Z Index: 256

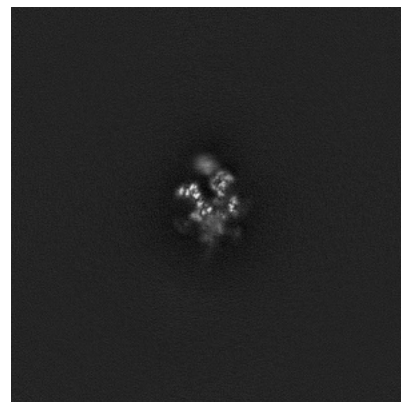
6.2.2 Raw map



X Index: 256



Y Index: 256

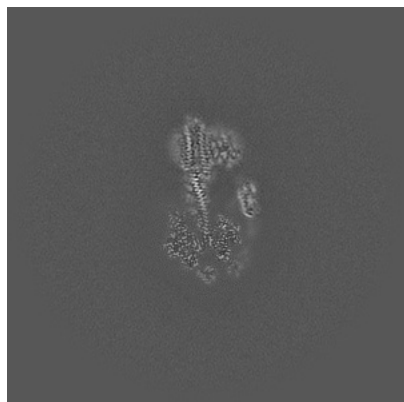


Z Index: 256

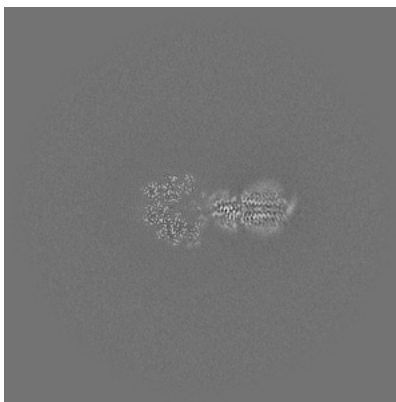
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

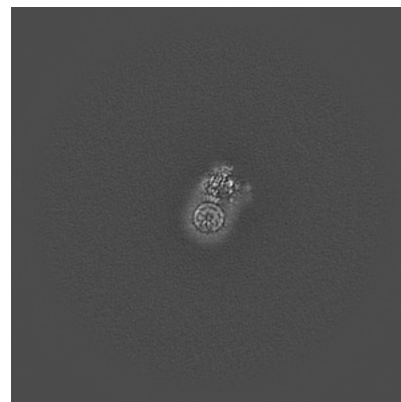
6.3.1 Primary map



X Index: 254

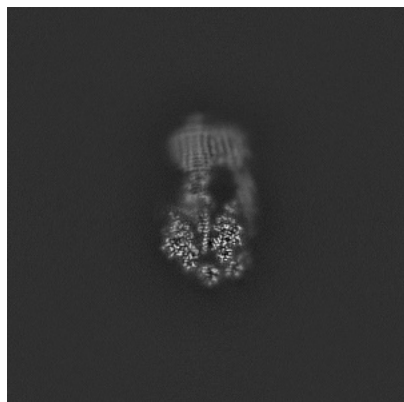


Y Index: 241

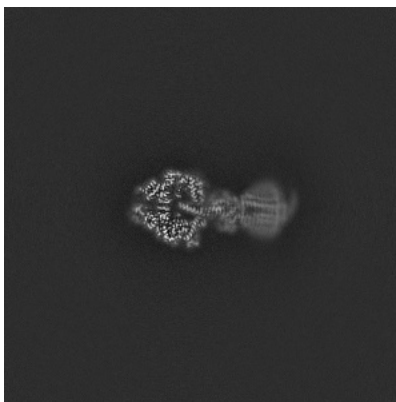


Z Index: 325

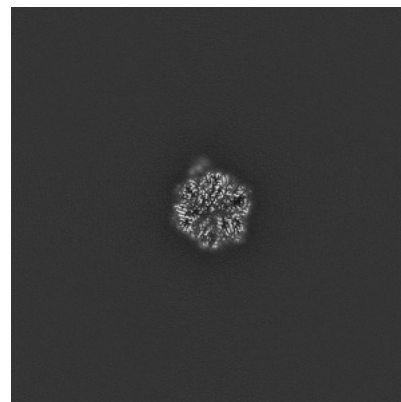
6.3.2 Raw map



X Index: 258



Y Index: 246

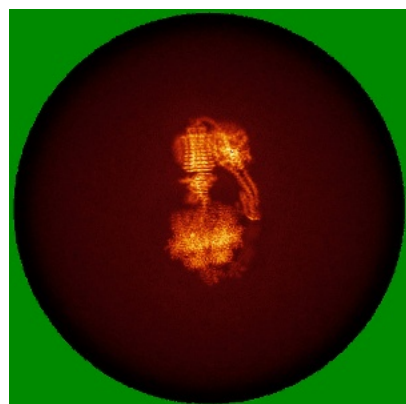


Z Index: 214

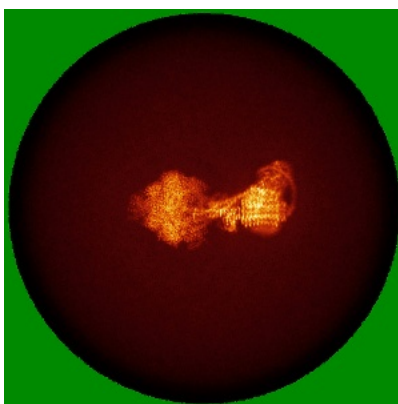
The images above show the largest variance slices of the map in three orthogonal directions.

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

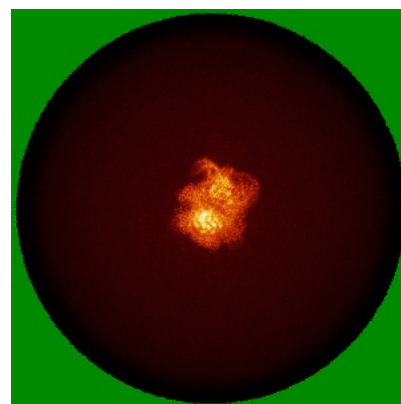
6.4.1 Primary map



X

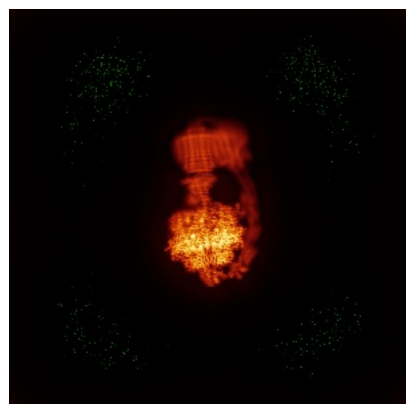


Y

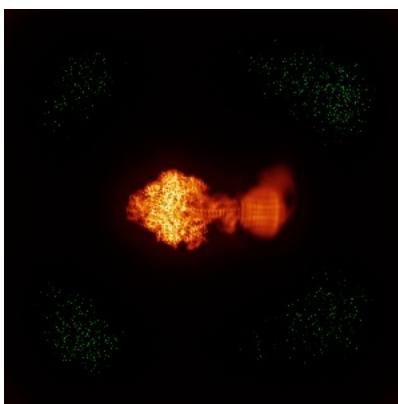


Z

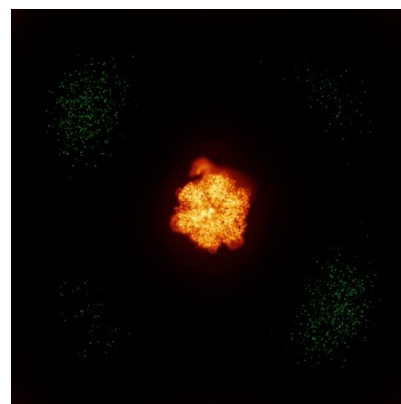
6.4.2 Raw map



X



Y

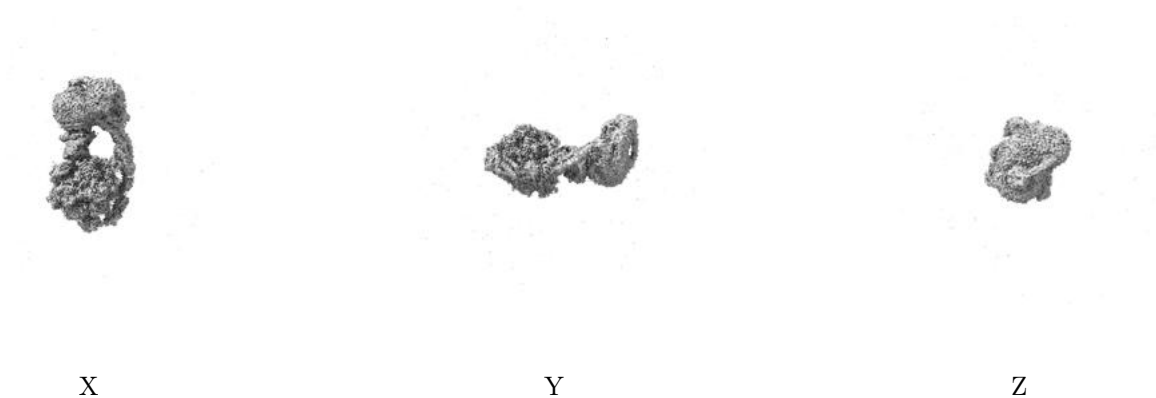


Z

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.

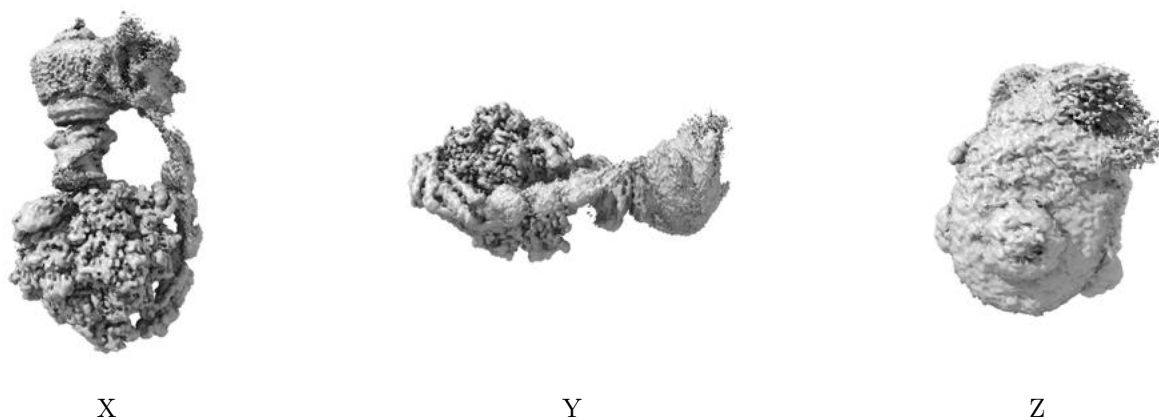
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.51. 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.

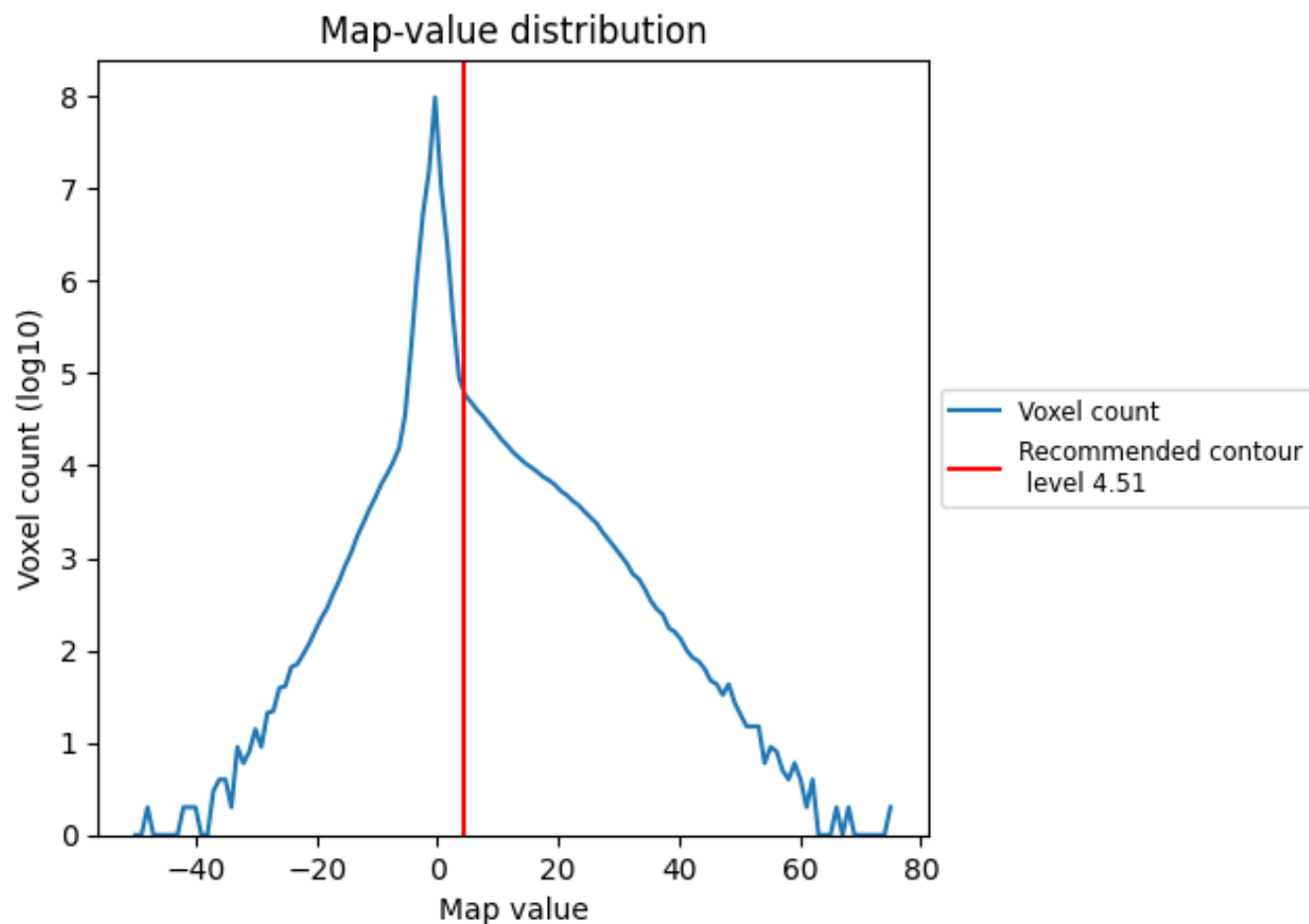
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

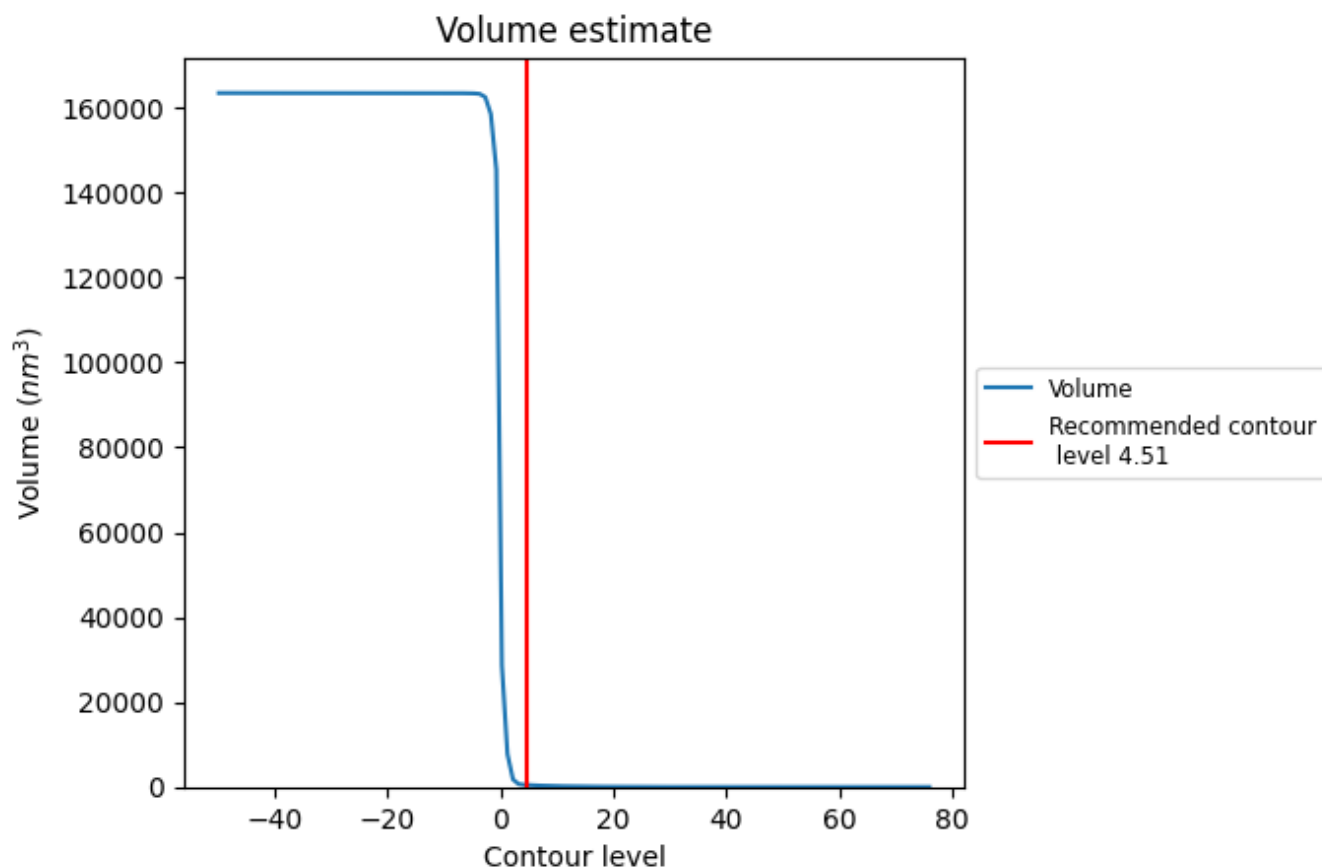
This section contains the results of statistical analysis of the map.

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.

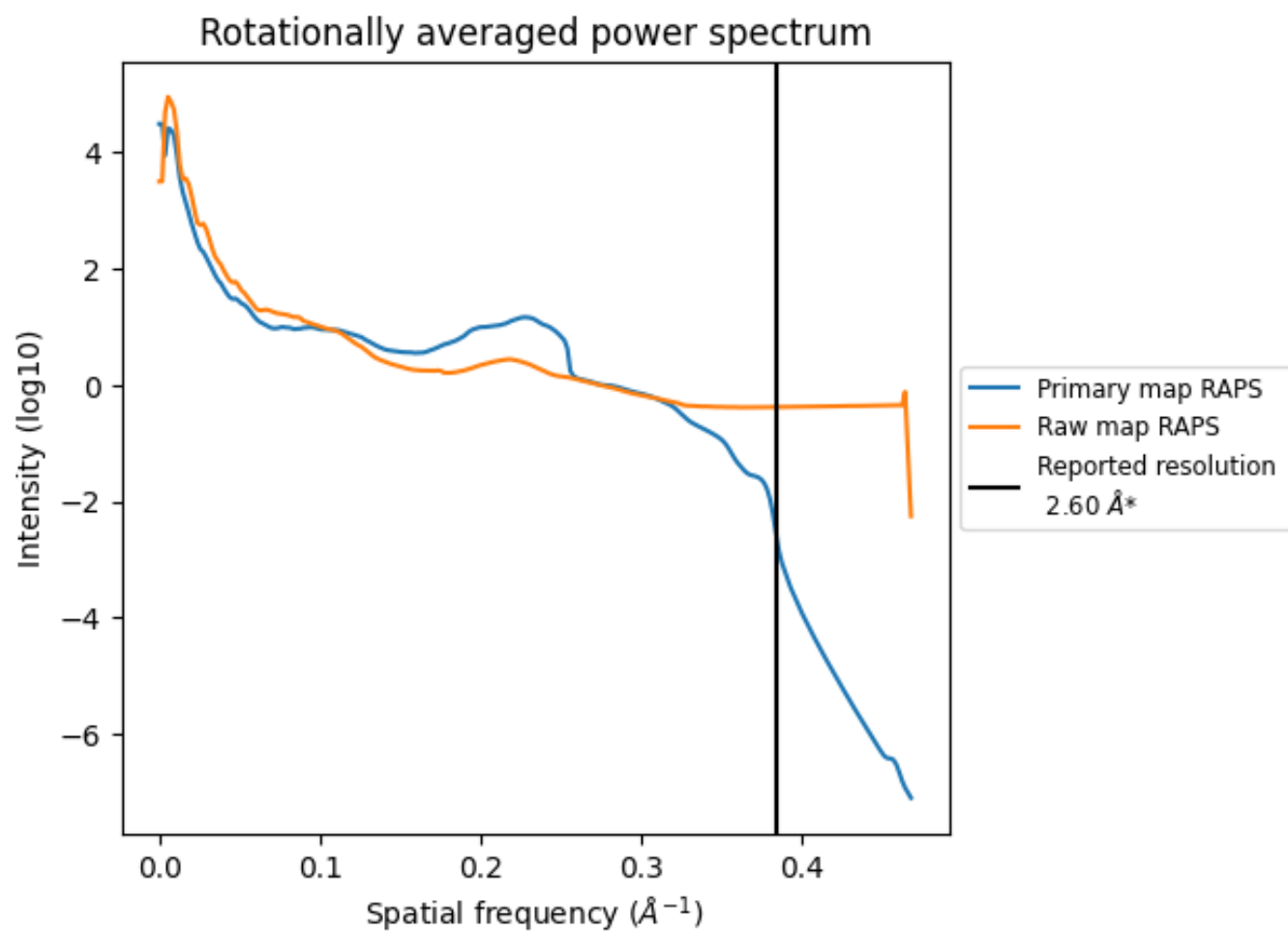
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 474 nm^3 ; this corresponds to an approximate mass of 428 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 ⓘ

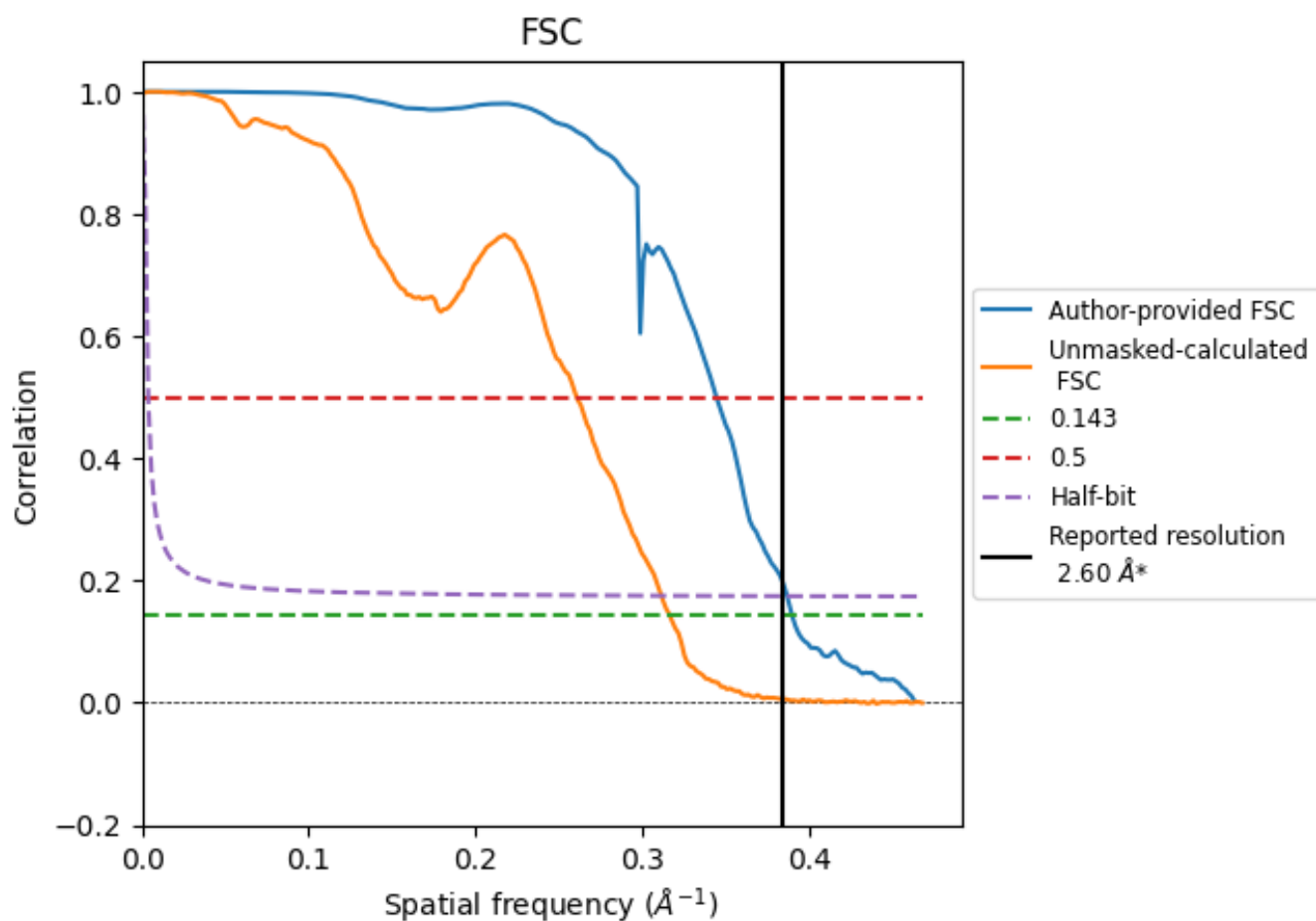


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.56	2.90	2.58
Unmasked-calculated*	3.16	3.83	3.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.16 differs from the reported value 2.6 by more than 10 %

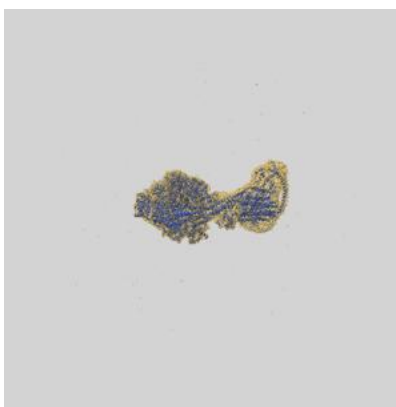
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44061 and PDB model 9B0X. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

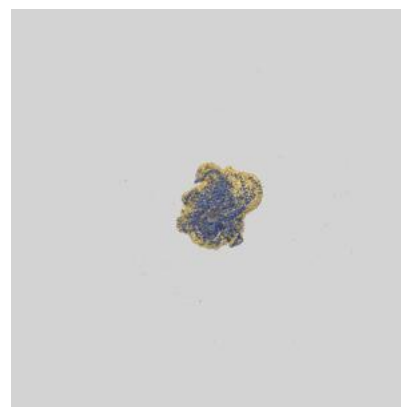
9.1 Map-model overlay [i](#)



X



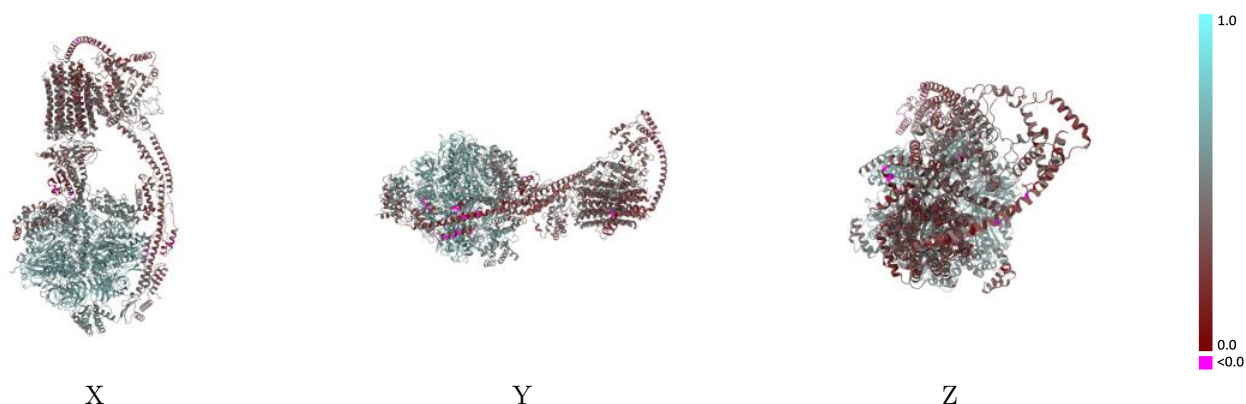
Y



Z

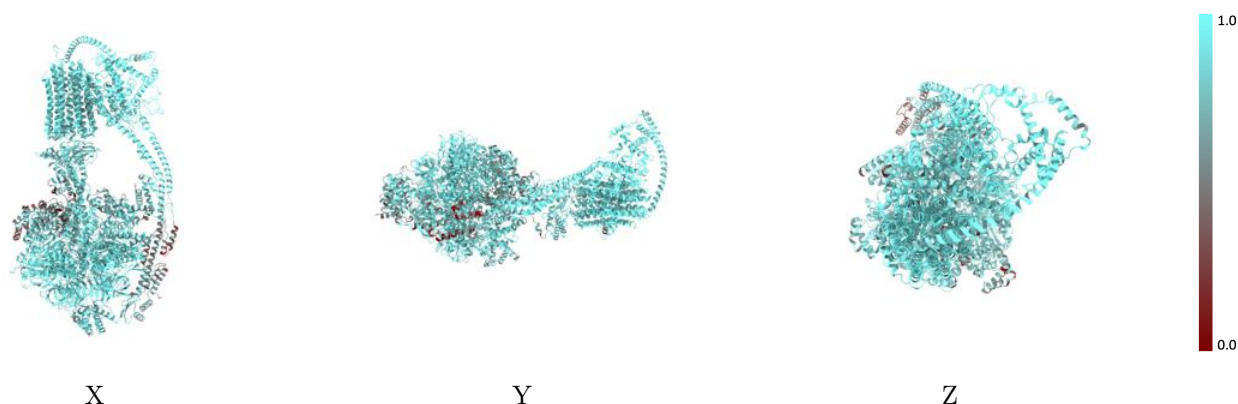
The images above show the 3D surface view of the map at the recommended contour level 4.51 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



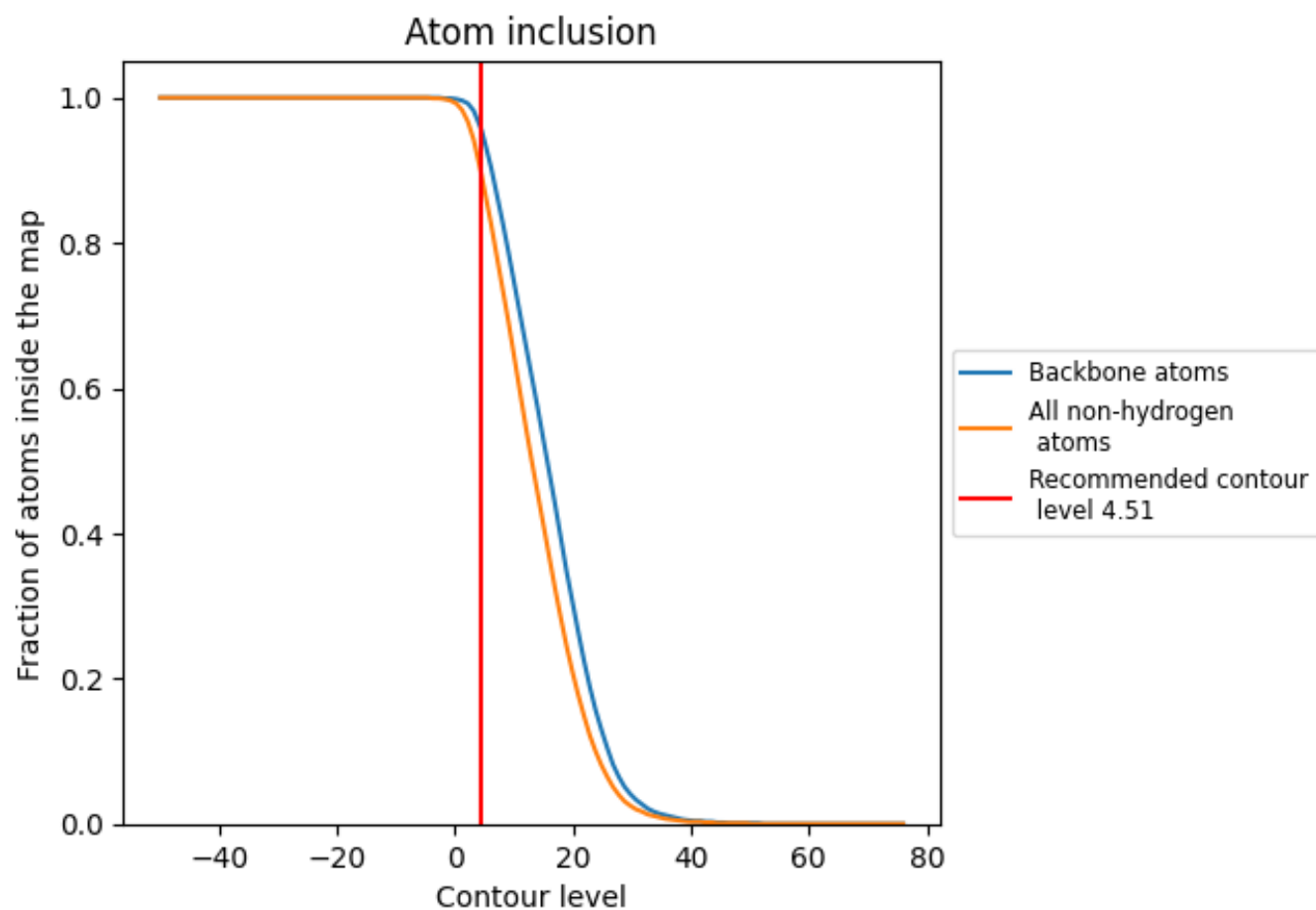
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.51).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (4.51) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8930	 0.4890
1	 0.9140	 0.3160
2	 0.9360	 0.3480
3	 0.9320	 0.3890
4	 0.9510	 0.3820
5	 0.9550	 0.3860
6	 0.9400	 0.3880
7	 0.9420	 0.3540
8	 0.9230	 0.3090
A	 0.8860	 0.5710
B	 0.8630	 0.5570
C	 0.9190	 0.5910
D	 0.9470	 0.6120
E	 0.9350	 0.6070
F	 0.9320	 0.6070
G	 0.8560	 0.3800
H	 0.9320	 0.3560
I	 0.8000	 0.3160
J	 0.4130	 0.4540
K	 0.8530	 0.3610
L	 0.4930	 0.2710
M	 0.7930	 0.2940
N	 0.9360	 0.3450
O	 0.7760	 0.4840
P	 1.0000	 0.3620
Q	 0.9420	 0.3640
R	 0.9650	 0.4070
S	 0.9200	 0.3040
T	 0.8990	 0.2760

