wwPDB EM Validation Summary Report (i)

Mar 9, 2026 – 05:19 AM UTC

PDB ID	:	5LQZ / pdb_00005lqz
EMDB ID	:	EMD-4102
Title	:	Structure of F-ATPase from Pichia angusta, state1
Authors	:	Vinothkumar, K.R.; Montgomery, M.G.; Liu, S.; Walker, J.E.
Deposited on	:	2016-08-17
Resolution	:	7.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

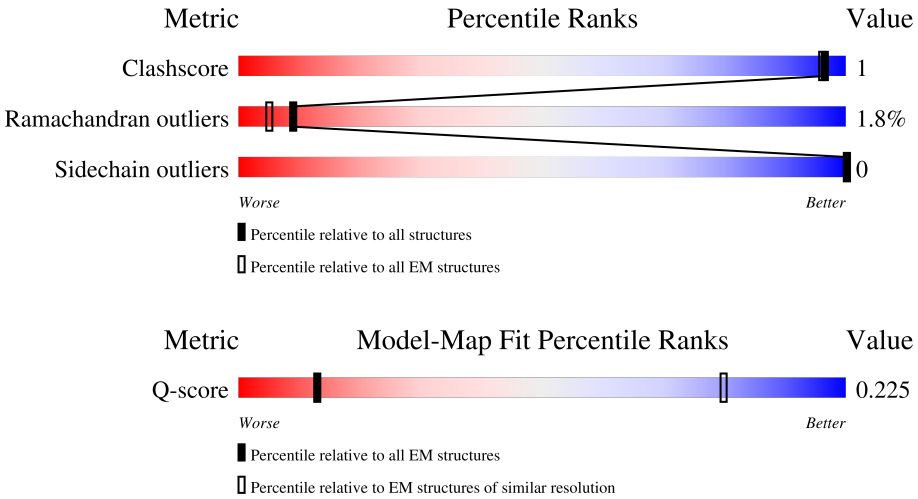
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.00 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	483 (6.50 - 7.50)

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 <=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	30	10% 100%
2	2	25	100%
3	3	17	12% 100%
4	4	27	15% 100%

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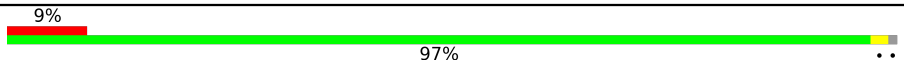
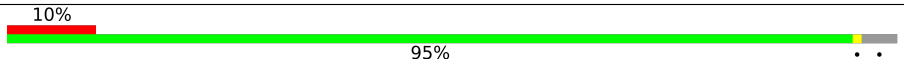
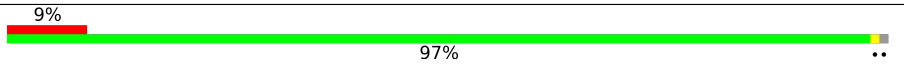
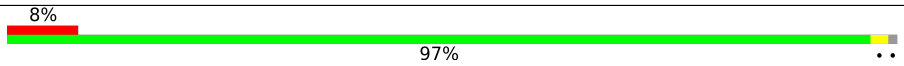
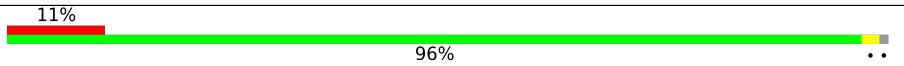
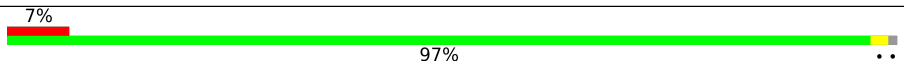
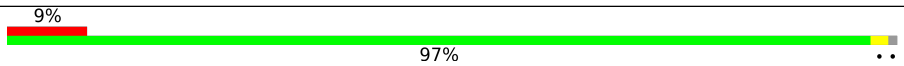
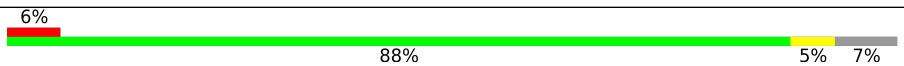
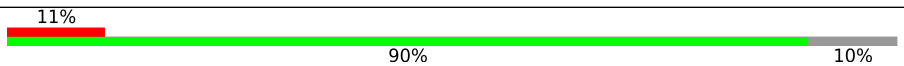
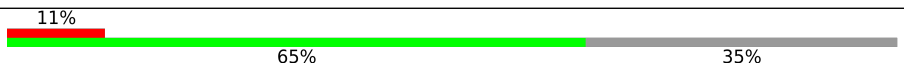
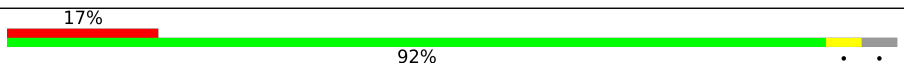
Mol	Chain	Length	Quality of chain
5	A	510	
5	B	510	
5	C	510	
6	D	476	
6	E	476	
6	F	476	
7	G	269	
8	H	138	
9	I	63	
10	J	66	
11	K	76	
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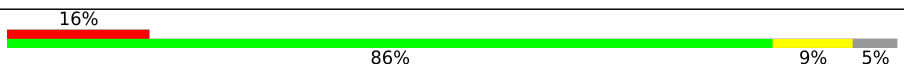
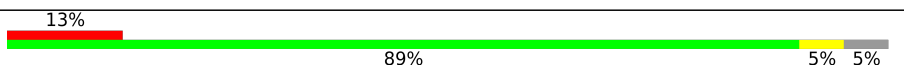
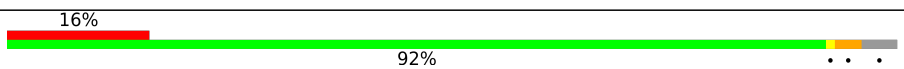
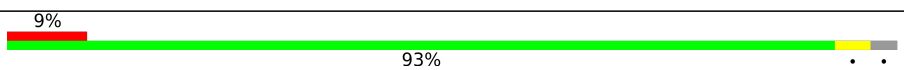
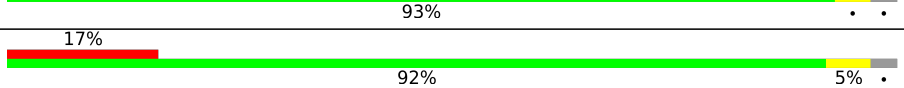
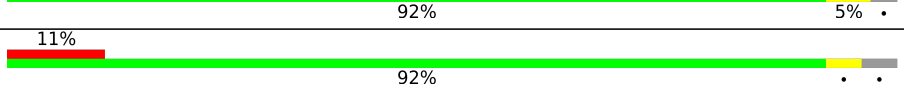
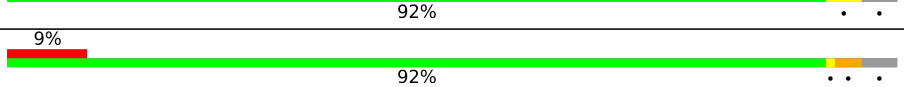
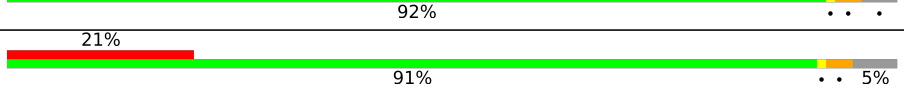
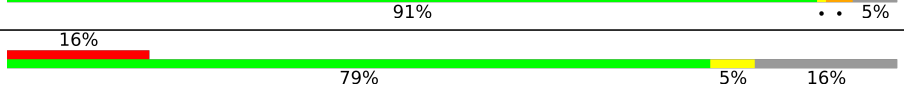
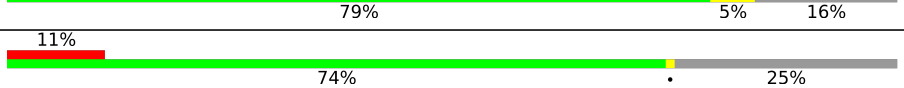
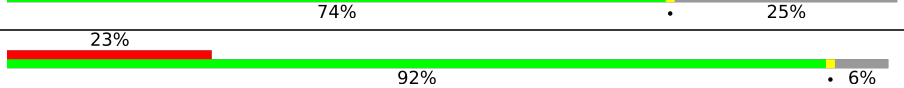
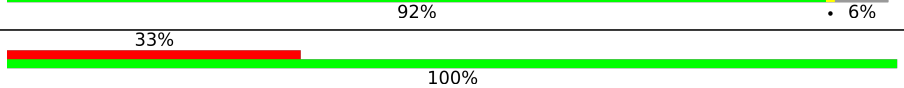
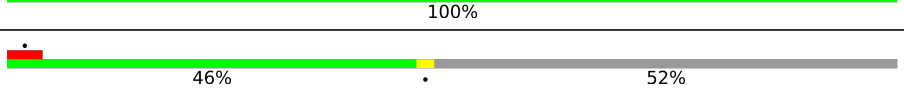
11	M	76	
11	N	76	
11	O	76	
11	P	76	
11	Q	76	
11	R	76	
11	S	76	
11	T	76	
12	U	194	
13	V	204	
14	W	155	
15	X	21	
16	Y	252	

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Mol	Chain	Length	Quality of chain
17	Z	44	

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 24199 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 f.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 2 is a protein called ATP synthase subunit AAP1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	2	25	Total	C	N	O	0	0
			125	75	25	25		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	17	Total	C	N	O	0	0
			85	51	17	17		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	4	27	Total	C	N	O	0	0
			135	81	27	27		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	A	506	Total	C	N	O	0	0
			2484	1472	506	506		
5	B	492	Total	C	N	O	0	0
			2415	1431	492	492		
5	C	503	Total	C	N	O	0	0
			2469	1463	503	503		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	D	471	Total 2306	C 1364	N 471	O 471	0	0
6	E	469	Total 2297	C 1359	N 469	O 469	0	0
6	F	470	Total 2301	C 1361	N 470	O 470	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	267	Total 1323	C 789	N 267	O 267	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	128	Total 633	C 377	N 128	O 128	0	0

- Molecule 9 is a protein called ATP synthase epsilon subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	57	Total 284	C 170	N 57	O 57	0	0

- Molecule 10 is a protein called ATP synthase inhibitor protein IF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	43	Total 211	C 125	N 43	O 43	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	73	Total 359	C 213	N 73	O 73	0	0
11	L	71	Total 350	C 208	N 71	O 71	0	0
11	M	72	Total 355	C 211	N 72	O 72	0	0
11	N	72	Total 355	C 211	N 72	O 72	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
11	O	73	Total 360	C 214	N 73	O 73	0	0
11	P	74	Total 365	C 217	N 74	O 74	0	0
11	Q	74	Total 365	C 217	N 74	O 74	0	0
11	R	73	Total 360	C 214	N 73	O 73	0	0
11	S	73	Total 360	C 214	N 73	O 73	0	0
11	T	72	Total 355	C 211	N 72	O 72	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	U	163	Total 810	C 484	N 163	O 163	0	0

- Molecule 13 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	V	154	Total 767	C 459	N 154	O 154	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	W	145	Total 723	C 433	N 145	O 145	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	X	21	Total 105	C 63	N 21	O 21	0	0

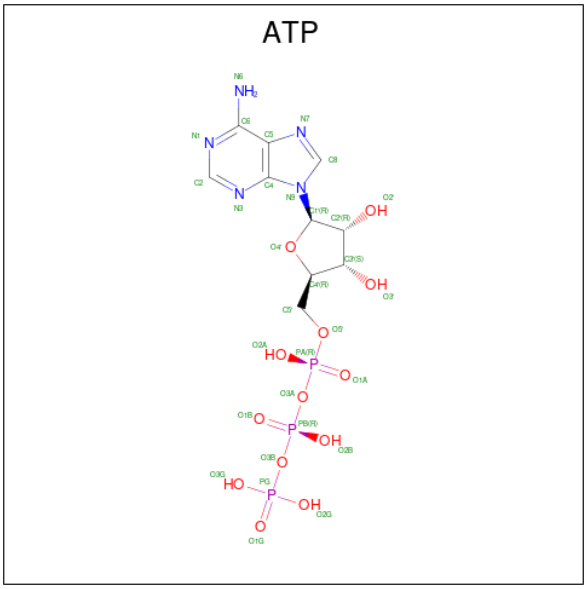
- Molecule 16 is a protein called ATP synthase subunit a.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Y	122	Total 601	C 357	N 122	O 122	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Z	44	Total 220	C 132	N 44	O 44	0	0

- Molecule 18 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

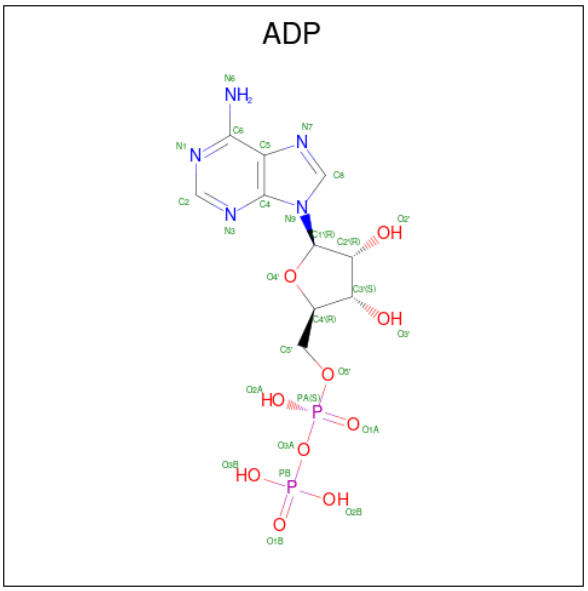


Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 19 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 20 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

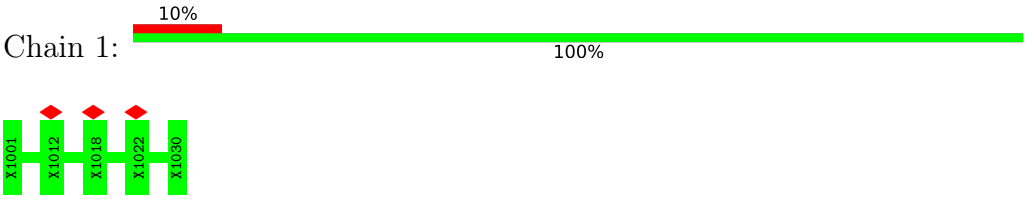


Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
20	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

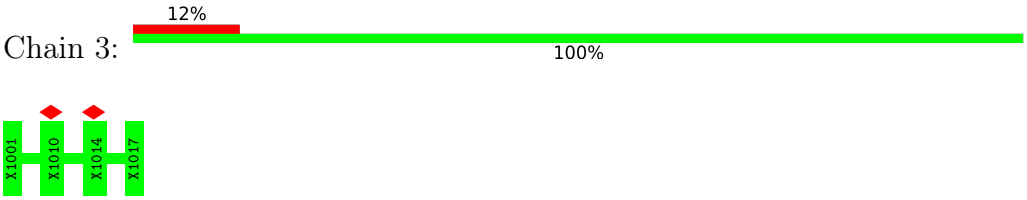
- Molecule 1: ATP synthase subunit f



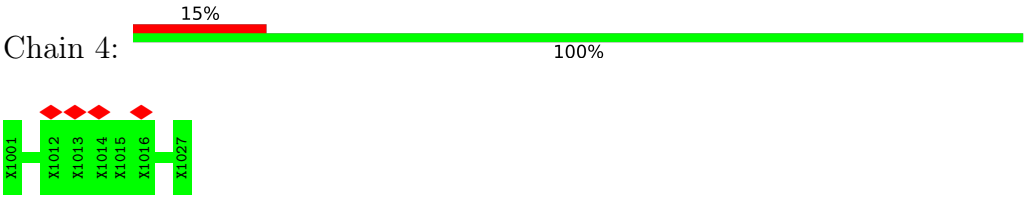
- Molecule 2: ATP synthase subunit AAP1

There are no outlier residues recorded for this chain.

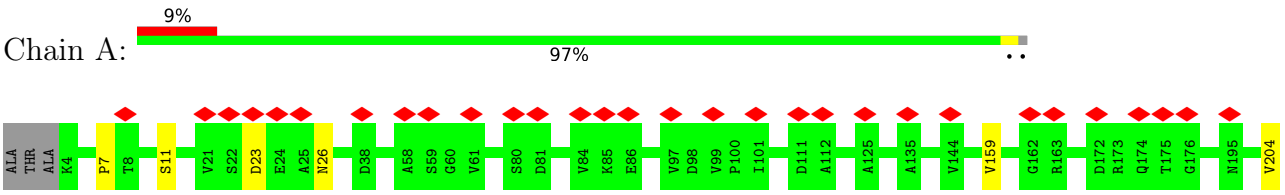
- Molecule 3: ATP synthase subunit a

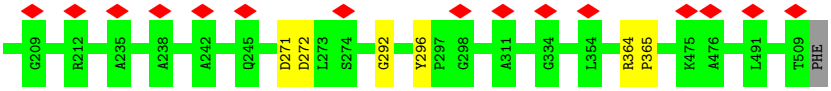


- Molecule 4: ATP synthase subunit b

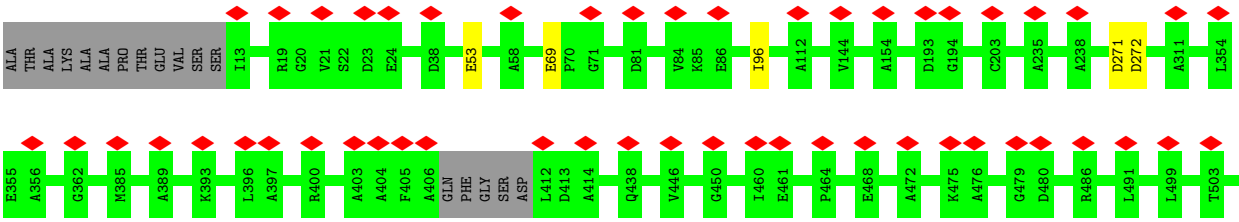


- Molecule 5: ATP synthase alpha subunit

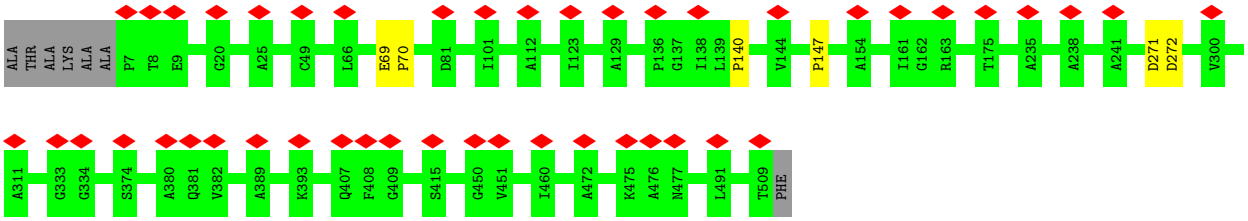




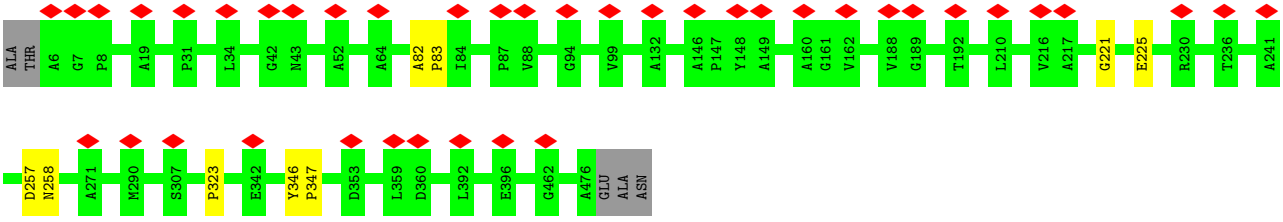
• Molecule 5: ATP synthase alpha subunit



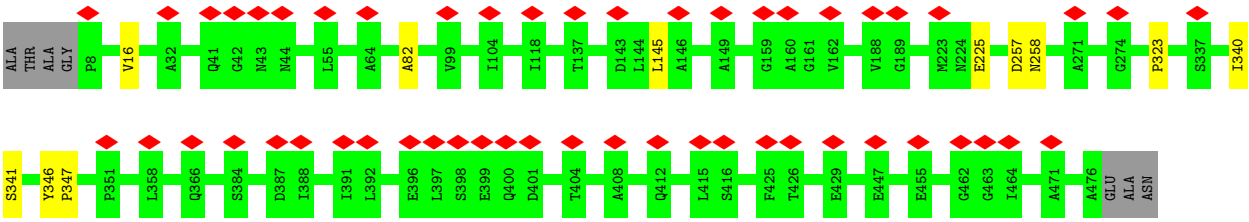
• Molecule 5: ATP synthase alpha subunit



• Molecule 6: ATP synthase beta subunit

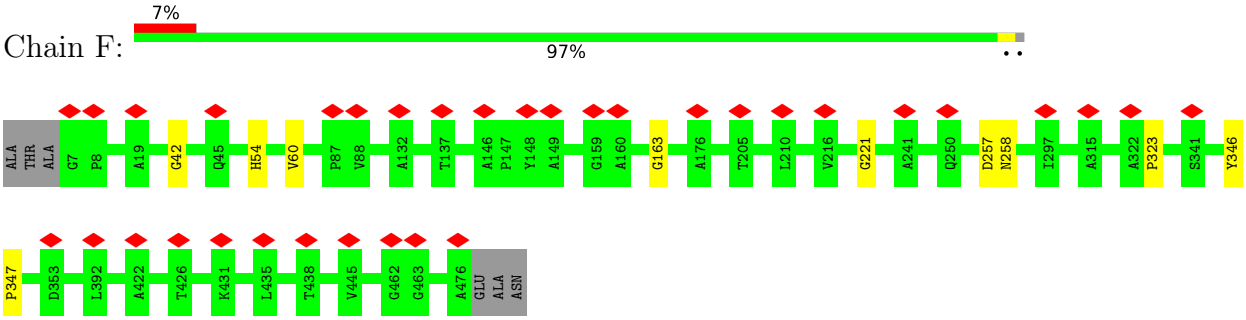


• Molecule 6: ATP synthase beta subunit



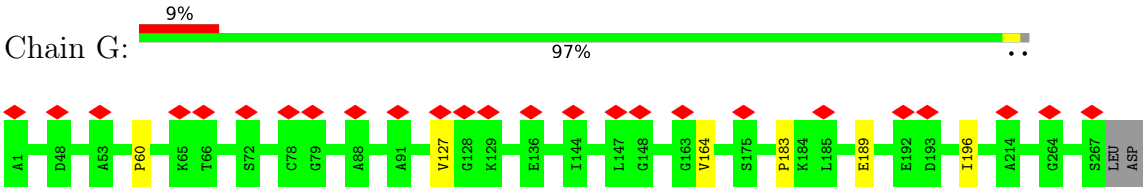
• Molecule 6: ATP synthase beta subunit

Chain F:



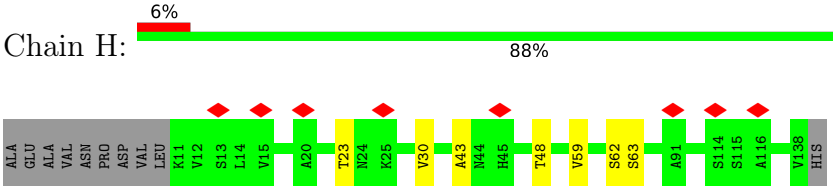
• Molecule 7: ATP synthase gamma subunit

Chain G:



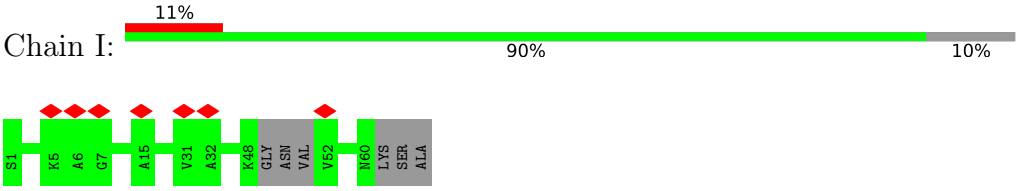
• Molecule 8: ATP synthase delta subunit

Chain H:



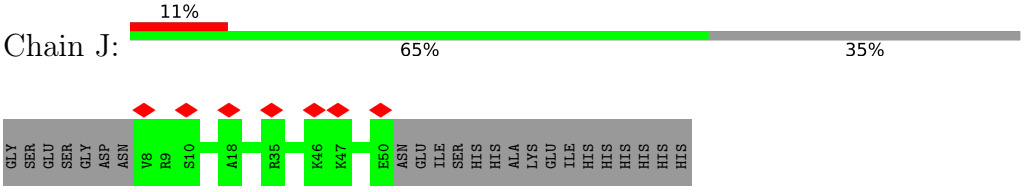
• Molecule 9: ATP synthase epsilon subunit

Chain I:



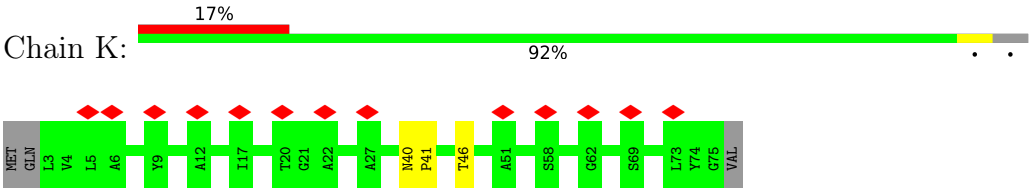
• Molecule 10: ATP synthase inhibitor protein IF1

Chain J:



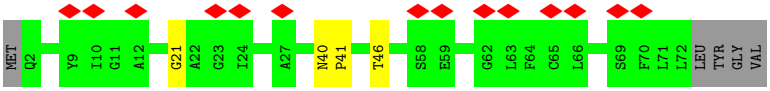
• Molecule 11: ATP synthase subunit c

Chain K:

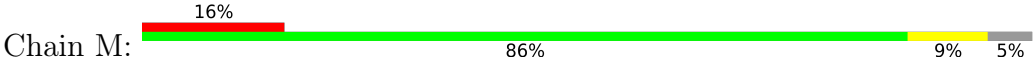


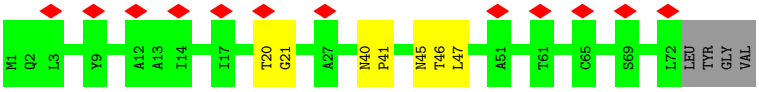
• Molecule 11: ATP synthase subunit c

Chain L:

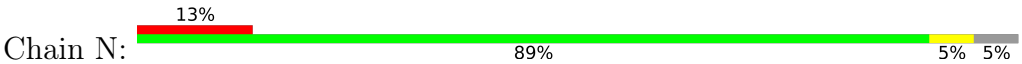


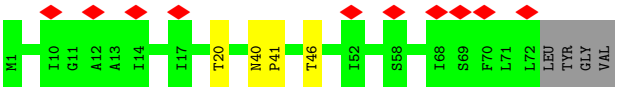
• Molecule 11: ATP synthase subunit c



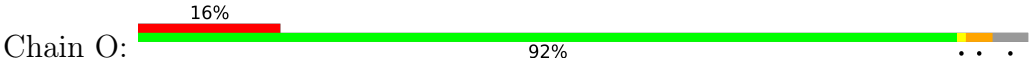


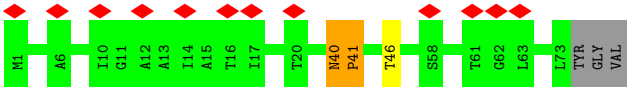
• Molecule 11: ATP synthase subunit c



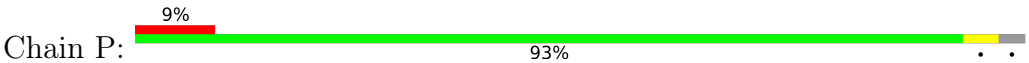


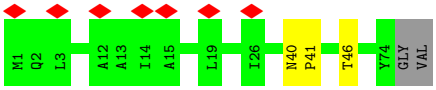
• Molecule 11: ATP synthase subunit c



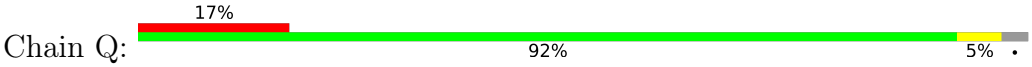


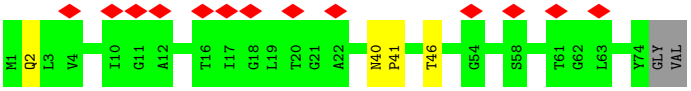
• Molecule 11: ATP synthase subunit c



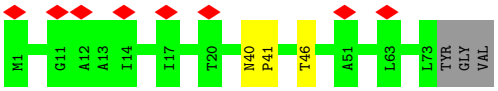


• Molecule 11: ATP synthase subunit c



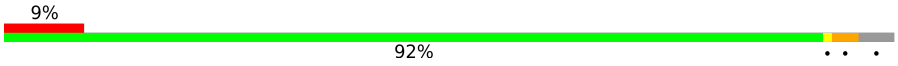


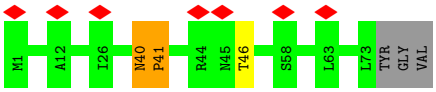
• Molecule 11: ATP synthase subunit c



• Molecule 11: ATP synthase subunit c

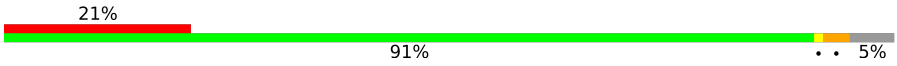
Chain S:

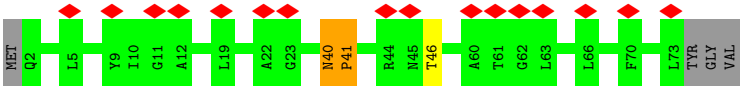




• Molecule 11: ATP synthase subunit c

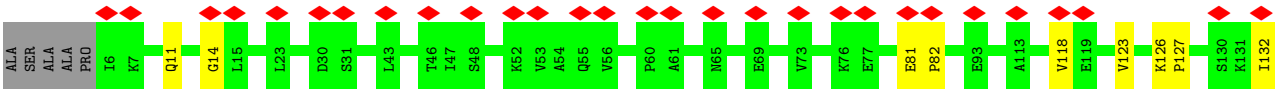
Chain T:

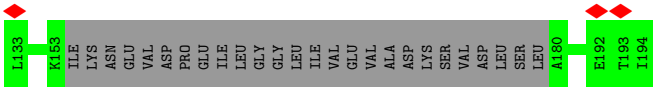




• Molecule 12: ATP synthase OSCP subunit

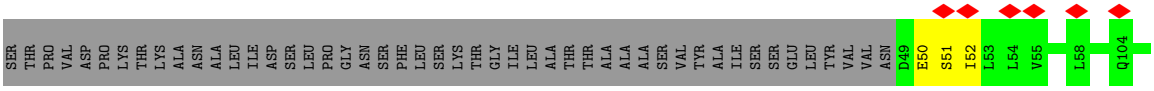
Chain U:

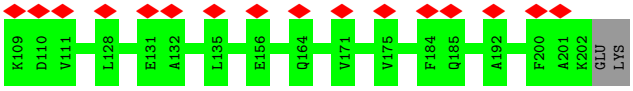




• Molecule 13: ATP synthase subunit b

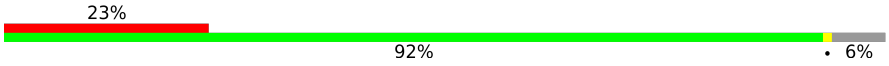
Chain V:

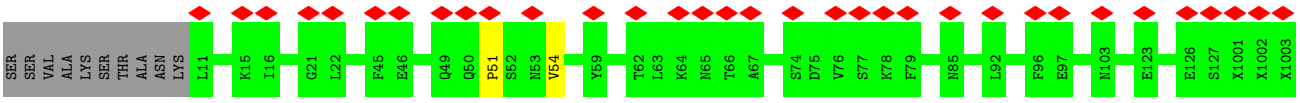


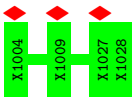


• Molecule 14: ATP synthase subunit d

Chain W:

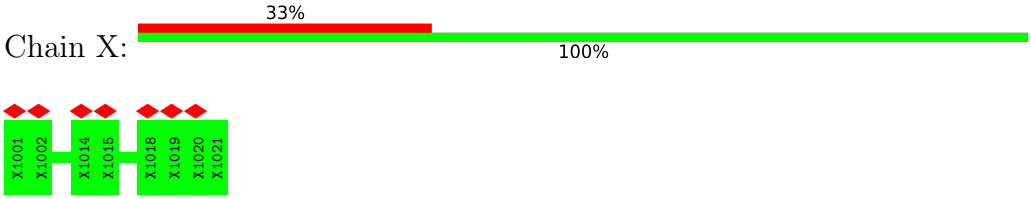






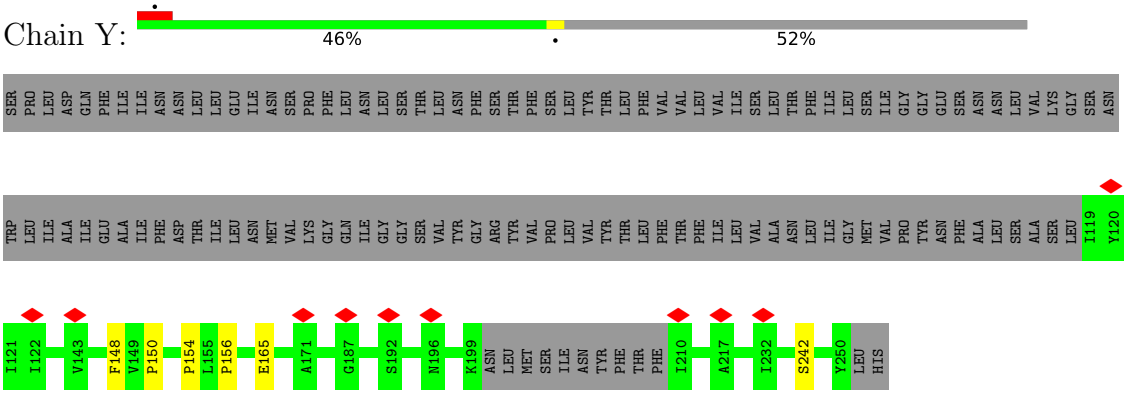
• Molecule 15: ATP synthase subunit h

Chain X:



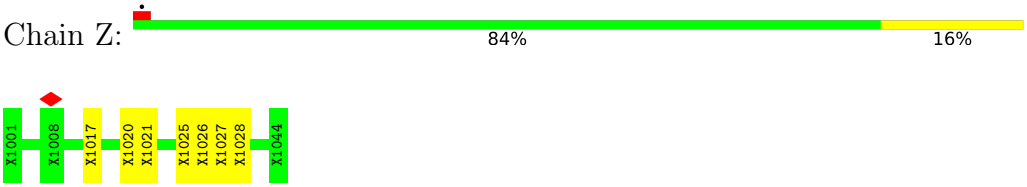
• Molecule 16: ATP synthase subunit a

Chain Y:



• Molecule 17: ATP synthase subunit a

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	42771	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF was estimated using the whole micrograph using all the frames. CTF was corrected per particle in RELION.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	64	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81395	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.599	Depositor
Minimum map value	-0.246	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.145	Depositor
Map size (Å)	525.0, 525.0, 525.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.75, 1.75, 1.75	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, ADP, ATP

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
5	A	0.06	0/2483	0.22	0/3447
5	B	0.06	0/2413	0.21	0/3348
5	C	0.06	0/2468	0.21	0/3426
6	D	0.07	0/2305	0.22	0/3196
6	E	0.06	0/2296	0.20	0/3184
6	F	0.06	0/2300	0.21	0/3189
7	G	0.05	0/1322	0.19	0/1842
8	H	0.12	0/632	0.25	0/879
9	I	0.06	0/282	0.22	0/391
10	J	0.05	0/210	0.19	0/290
11	K	0.06	0/358	0.25	0/494
11	L	0.06	0/349	0.26	0/482
11	M	0.08	0/354	0.24	0/489
11	N	0.06	0/354	0.23	0/489
11	O	0.06	0/359	0.28	0/496
11	P	0.07	0/364	0.27	0/503
11	Q	0.06	0/364	0.26	0/503
11	R	0.07	0/359	0.27	0/496
11	S	0.06	0/359	0.24	0/496
11	T	0.07	0/354	0.27	0/489
12	U	0.09	0/808	0.30	0/1125
13	V	0.06	0/766	0.22	0/1069
14	W	0.06	0/582	0.23	0/812
16	Y	0.07	0/599	0.24	0/830
All	All	0.06	0/23040	0.23	0/31965

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 (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	1	150	0	32	0	0
2	2	125	0	27	0	0
3	3	85	0	19	0	0
4	4	135	0	29	0	0
5	A	2484	0	1200	3	0
5	B	2415	0	1165	2	0
5	C	2469	0	1189	1	0
6	D	2306	0	1110	2	0
6	E	2297	0	1103	2	0
6	F	2301	0	1105	3	0
7	G	1323	0	630	1	0
8	H	633	0	316	2	0
9	I	284	0	140	0	0
10	J	211	0	116	0	0
11	K	359	0	197	0	0
11	L	350	0	192	1	0
11	M	355	0	197	3	0
11	N	355	0	197	1	0
11	O	360	0	199	1	0
11	P	365	0	201	0	0
11	Q	365	0	201	0	0
11	R	360	0	199	0	0
11	S	360	0	199	1	0
11	T	355	0	194	1	0
12	U	810	0	362	0	0
13	V	767	0	369	1	0
14	W	723	0	296	0	0
15	X	105	0	23	0	0
16	Y	601	0	279	1	0
17	Z	220	0	47	6	0
18	A	31	0	12	0	0
19	A	1	0	0	0	0
19	B	1	0	0	0	0
19	C	1	0	0	0	0
19	D	1	0	0	0	0
19	F	1	0	0	0	0
20	B	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	C	27	0	12	0	0
20	D	27	0	12	0	0
20	E	27	0	12	0	0
20	F	27	0	12	0	0
All	All	24199	0	11605	28	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 1.

The worst 5 of 28 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)
17:Z:1017:UNK:O	17:Z:1021:UNK:CB	2.37	0.73
16:Y:242:SER:CB	17:Z:1020:UNK:CB	2.77	0.63
17:Z:1025:UNK:O	17:Z:1027:UNK:N	2.37	0.58
17:Z:1025:UNK:C	17:Z:1027:UNK:N	2.67	0.56
17:Z:1025:UNK:O	17:Z:1026:UNK:C	2.59	0.50

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
5	A	504/510 (99%)	447 (89%)	51 (10%)	6 (1%)	10 44
5	B	488/510 (96%)	446 (91%)	41 (8%)	1 (0%)	43 78
5	C	501/510 (98%)	449 (90%)	48 (10%)	4 (1%)	16 54
6	D	469/476 (98%)	433 (92%)	31 (7%)	5 (1%)	11 46
6	E	467/476 (98%)	426 (91%)	34 (7%)	7 (2%)	8 40
6	F	468/476 (98%)	428 (92%)	36 (8%)	4 (1%)	14 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	G	265/269 (98%)	241 (91%)	19 (7%)	5 (2%)	6 32
8	H	126/138 (91%)	102 (81%)	20 (16%)	4 (3%)	3 21
9	I	53/63 (84%)	46 (87%)	7 (13%)	0	100 100
10	J	41/66 (62%)	40 (98%)	1 (2%)	0	100 100
11	K	71/76 (93%)	66 (93%)	2 (3%)	3 (4%)	2 17
11	L	69/76 (91%)	63 (91%)	3 (4%)	3 (4%)	2 17
11	M	70/76 (92%)	67 (96%)	0	3 (4%)	2 17
11	N	70/76 (92%)	66 (94%)	1 (1%)	3 (4%)	2 17
11	O	71/76 (93%)	65 (92%)	3 (4%)	3 (4%)	2 17
11	P	72/76 (95%)	66 (92%)	3 (4%)	3 (4%)	2 17
11	Q	72/76 (95%)	66 (92%)	2 (3%)	4 (6%)	1 14
11	R	71/76 (93%)	65 (92%)	3 (4%)	3 (4%)	2 17
11	S	71/76 (93%)	66 (93%)	2 (3%)	3 (4%)	2 17
11	T	70/76 (92%)	63 (90%)	4 (6%)	3 (4%)	2 17
12	U	159/194 (82%)	122 (77%)	28 (18%)	9 (6%)	1 14
13	V	152/204 (74%)	147 (97%)	4 (3%)	1 (1%)	18 56
14	W	115/155 (74%)	111 (96%)	2 (2%)	2 (2%)	7 36
16	Y	118/252 (47%)	104 (88%)	9 (8%)	5 (4%)	2 17
All	All	4633/5059 (92%)	4195 (90%)	354 (8%)	84 (2%)	9 34

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	60	PRO
11	K	41	PRO
11	L	41	PRO
11	M	41	PRO
11	Q	41	PRO

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	1/55 (2%)	1 (100%)	0	100	100
11	L	1/55 (2%)	1 (100%)	0	100	100
11	M	1/55 (2%)	1 (100%)	0	100	100
11	N	1/55 (2%)	1 (100%)	0	100	100
11	O	1/55 (2%)	1 (100%)	0	100	100
11	P	1/55 (2%)	1 (100%)	0	100	100
11	Q	1/55 (2%)	1 (100%)	0	100	100
11	R	1/55 (2%)	1 (100%)	0	100	100
11	S	1/55 (2%)	1 (100%)	0	100	100
11	T	1/55 (2%)	1 (100%)	0	100	100
All	All	10/550 (2%)	10 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
20	ADP	E	600	-	28,29,29	1.43	5 (17%)	43,45,45	1.83	9 (20%)
20	ADP	C	600	19	28,29,29	1.42	4 (14%)	43,45,45	1.81	9 (20%)
20	ADP	B	600	19	28,29,29	1.43	4 (14%)	43,45,45	1.82	9 (20%)
20	ADP	D	600	19	28,29,29	1.43	4 (14%)	43,45,45	1.81	9 (20%)
18	ATP	A	600	19	32,33,33	1.43	5 (15%)	48,52,52	1.75	9 (18%)
20	ADP	F	600	19	28,29,29	1.42	4 (14%)	43,45,45	1.81	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	ADP	E	600	-	-	3/16/32/32	0/3/3/3
20	ADP	C	600	19	-	3/16/32/32	0/3/3/3
20	ADP	B	600	19	-	3/16/32/32	0/3/3/3
20	ADP	D	600	19	-	3/16/32/32	0/3/3/3
18	ATP	A	600	19	-	2/22/38/38	0/3/3/3
20	ADP	F	600	19	-	3/16/32/32	0/3/3/3

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	600	ADP	C5-C4	4.75	1.47	1.39
20	B	600	ADP	C5-C4	4.75	1.47	1.39
18	A	600	ATP	C5-C4	4.75	1.47	1.39
20	E	600	ADP	C5-C4	4.74	1.47	1.39
20	F	600	ADP	C5-C4	4.73	1.47	1.39

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	600	ADP	C5-C4-N3	-5.87	118.64	126.72
20	C	600	ADP	C5-C4-N3	-5.85	118.67	126.72
20	D	600	ADP	C5-C4-N3	-5.84	118.68	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	E	600	ADP	C5-C4-N3	-5.83	118.69	126.72
18	A	600	ATP	C5-C4-N3	-5.83	118.69	126.72

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

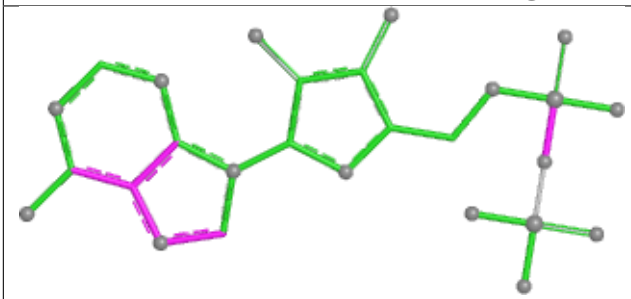
Mol	Chain	Res	Type	Atoms
18	A	600	ATP	PB-O3A-PA-O1A
18	A	600	ATP	PB-O3A-PA-O2A
20	E	600	ADP	PB-O3A-PA-O1A
20	E	600	ADP	PB-O3A-PA-O2A
20	B	600	ADP	PB-O3A-PA-O1A

There are no ring outliers.

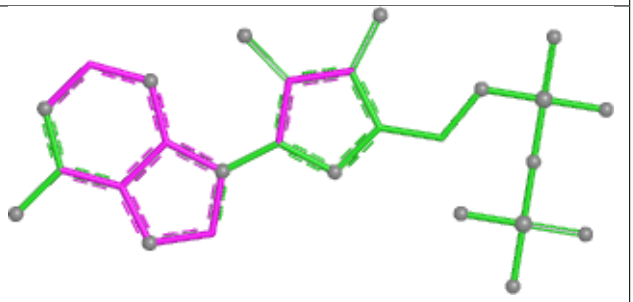
No monomer is involved in short contacts.

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 then 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.

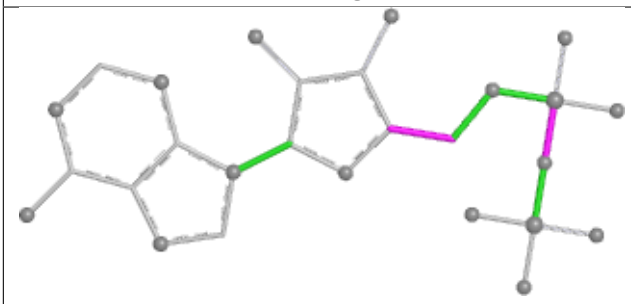
Ligand ADP E 600



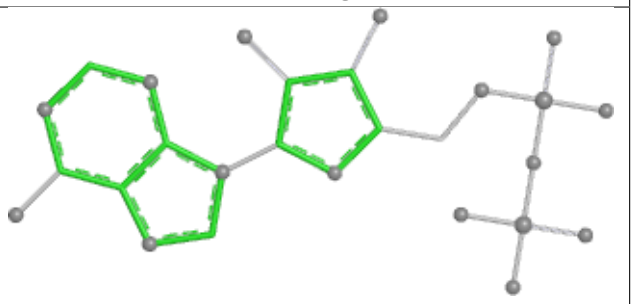
Bond lengths



Bond angles

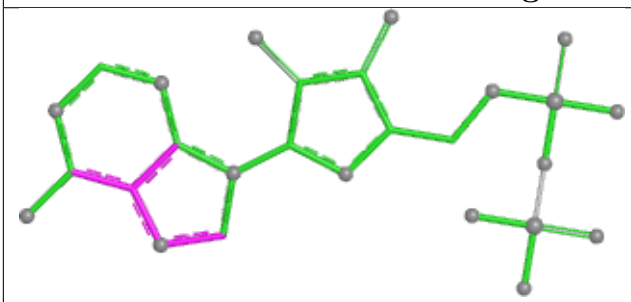


Torsions

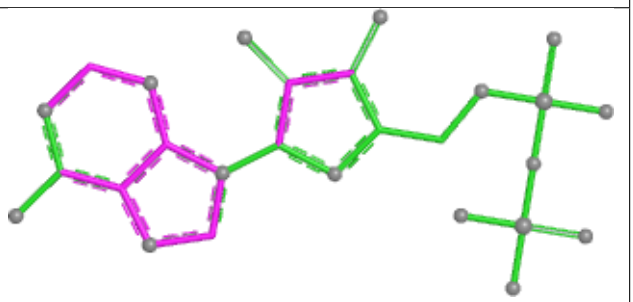


Rings

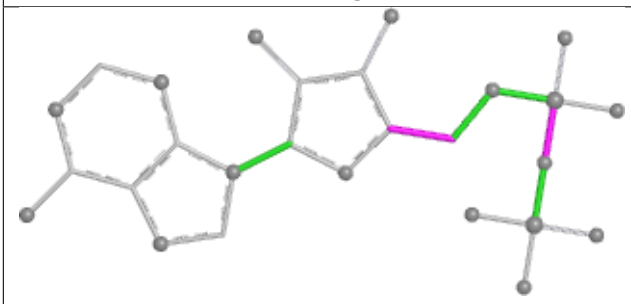
Ligand ADP C 600



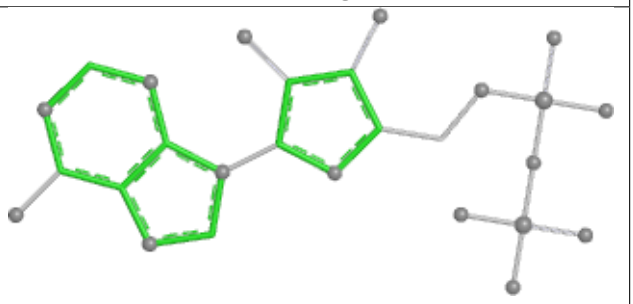
Bond lengths



Bond angles

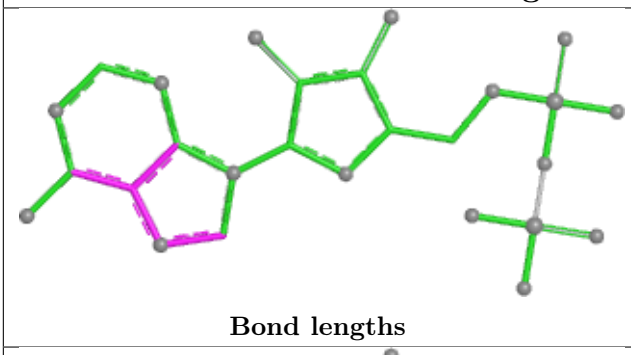


Torsions

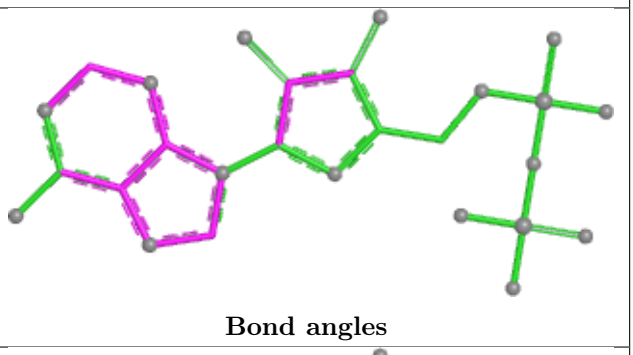


Rings

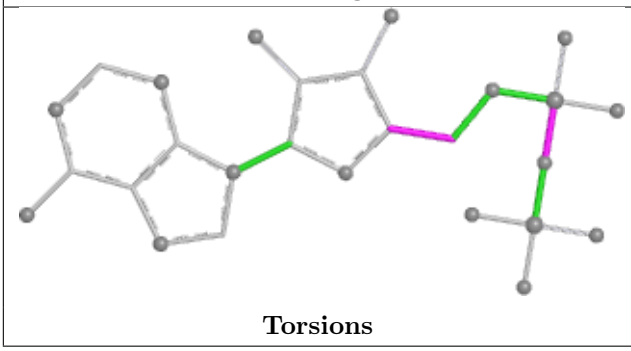
Ligand ADP B 600



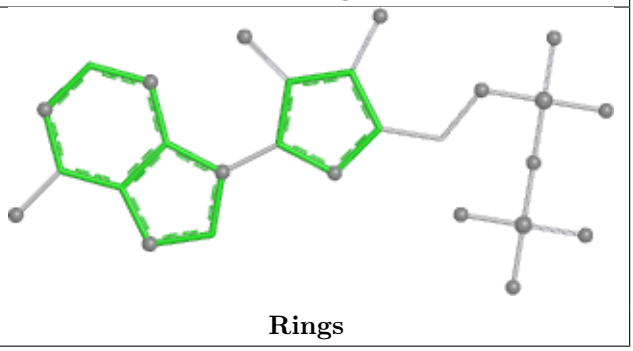
Bond lengths



Bond angles

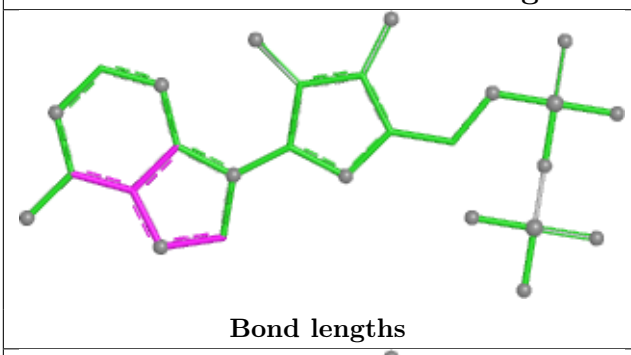


Torsions

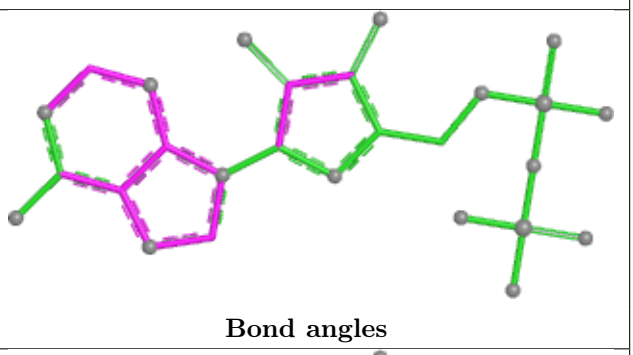


Rings

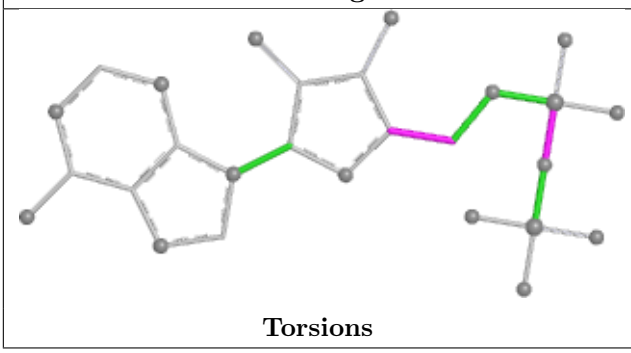
Ligand ADP D 600



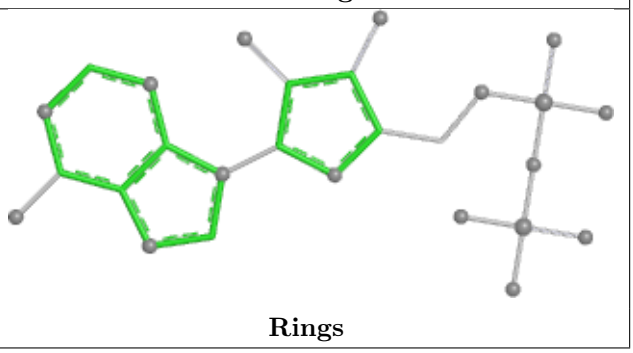
Bond lengths



Bond angles

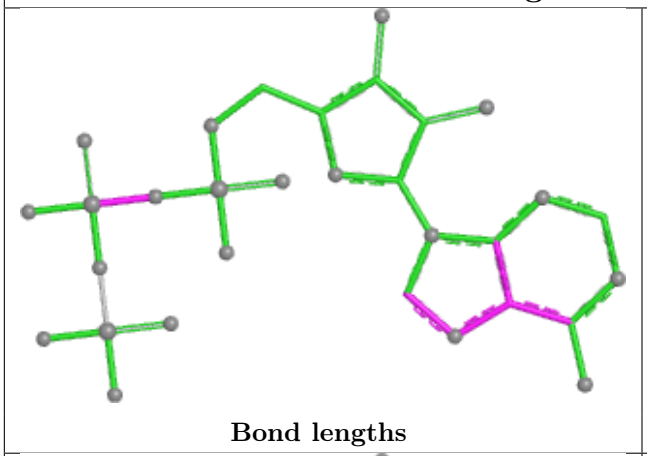


Torsions

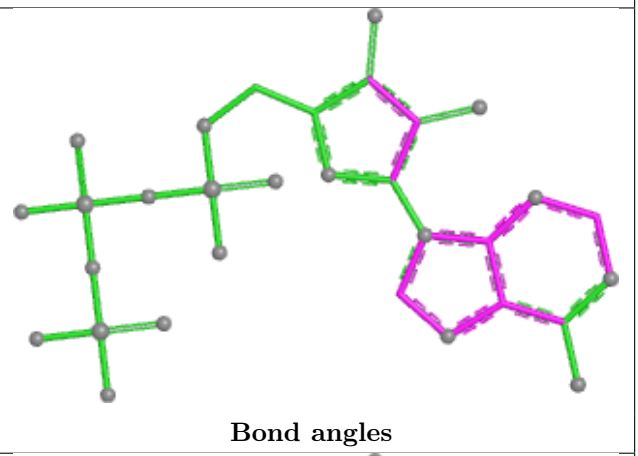


Rings

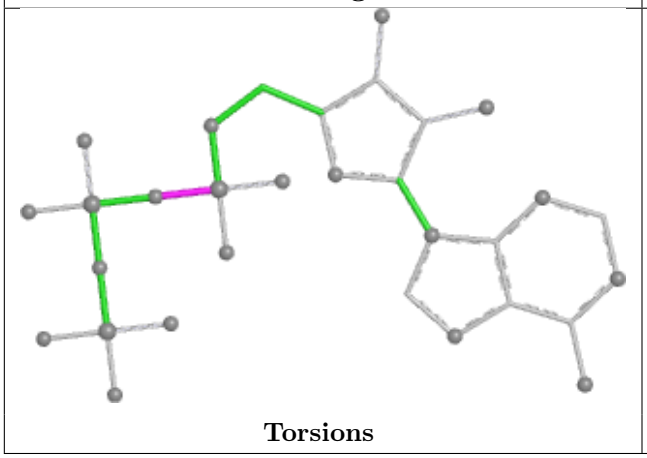
Ligand ATP A 600



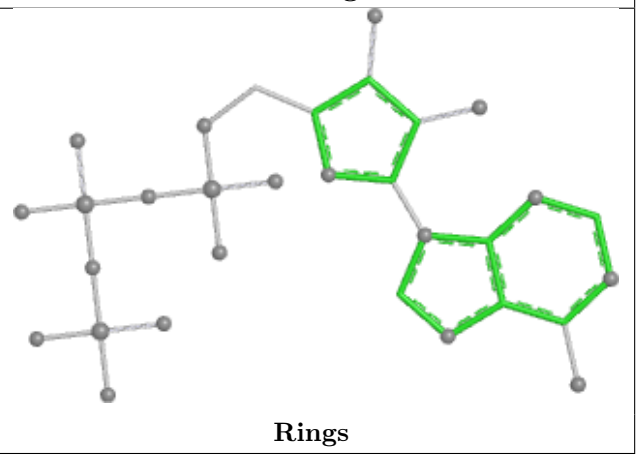
Bond lengths



Bond angles

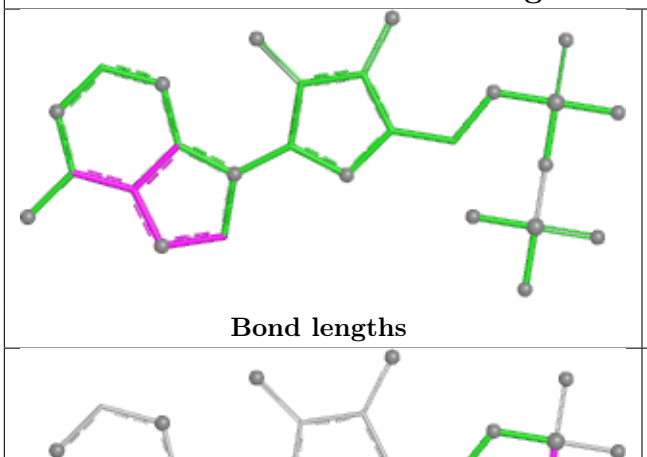


Torsions

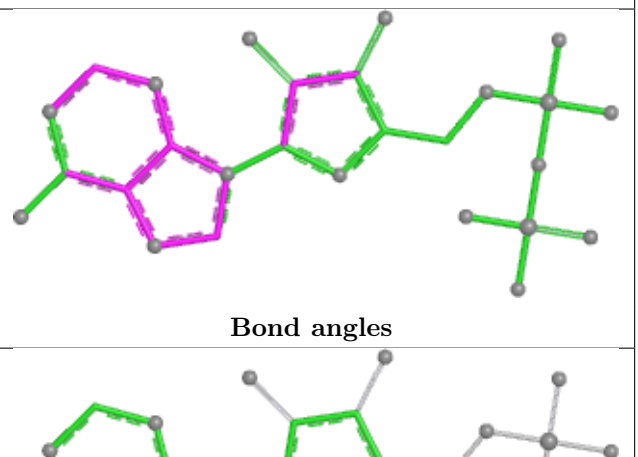


Rings

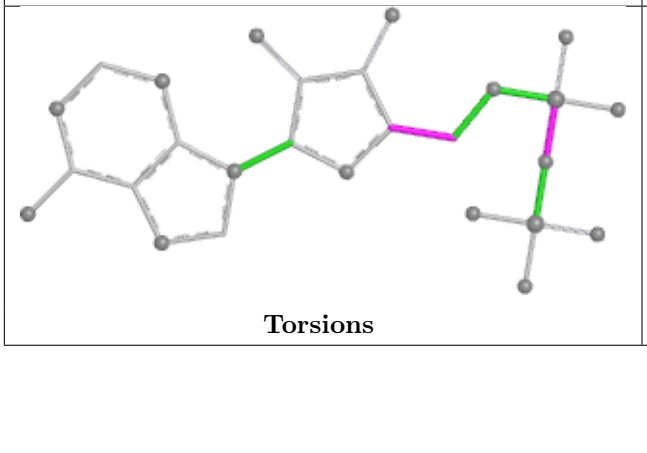
Ligand ADP F 600



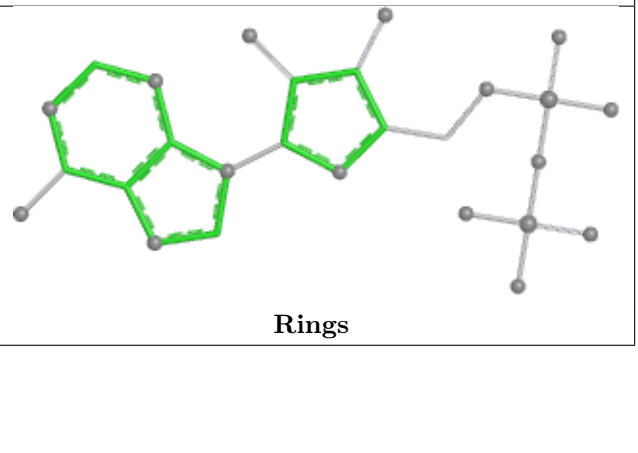
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
14	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	127:SER	C	1001:UNK	N	5.36

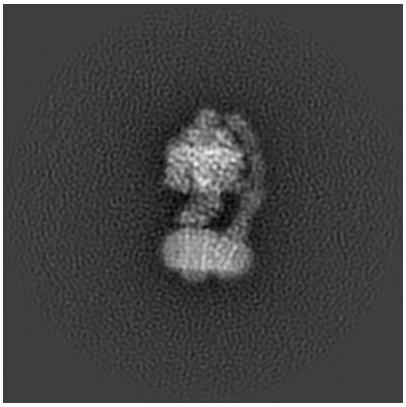
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4102. These allow visual inspection of the internal detail of the map and identification of artifacts.

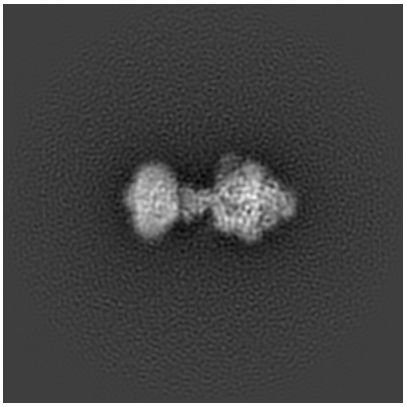
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

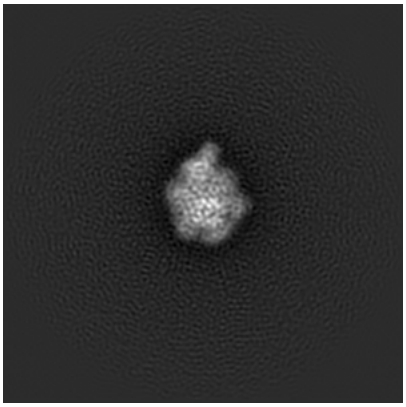
6.1.1 Primary map



X



Y



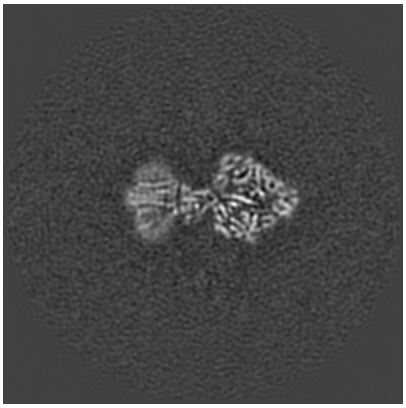
Z

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

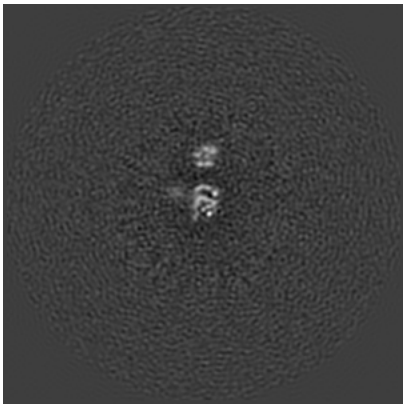
6.2 Central slices

6.2.1 Primary map

X Index: 150



Y Index: 150



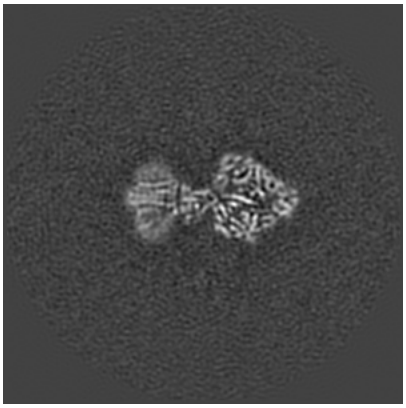
Z Index: 150

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

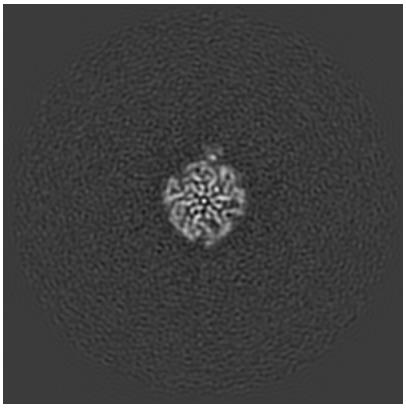
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 153



Y Index: 150

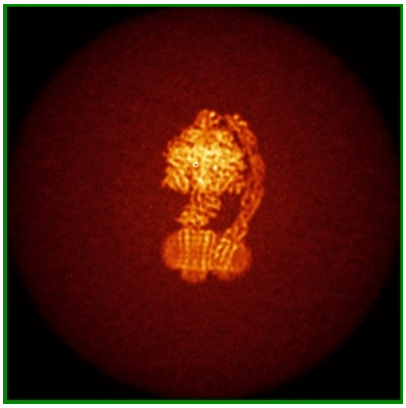


Z Index: 188

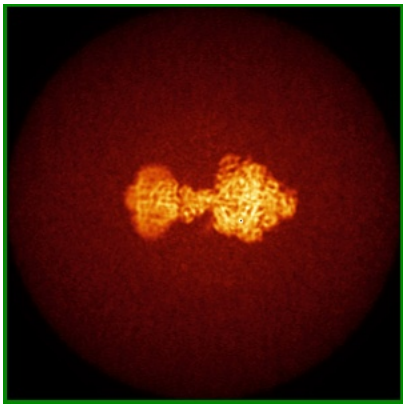
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

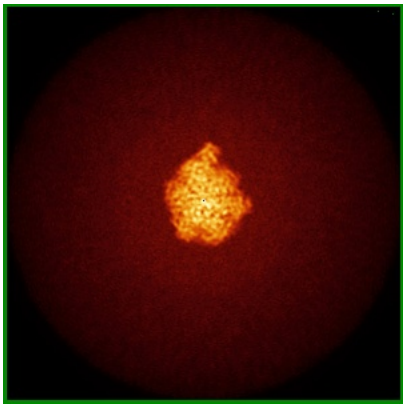
6.4.1 Primary map



X



Y

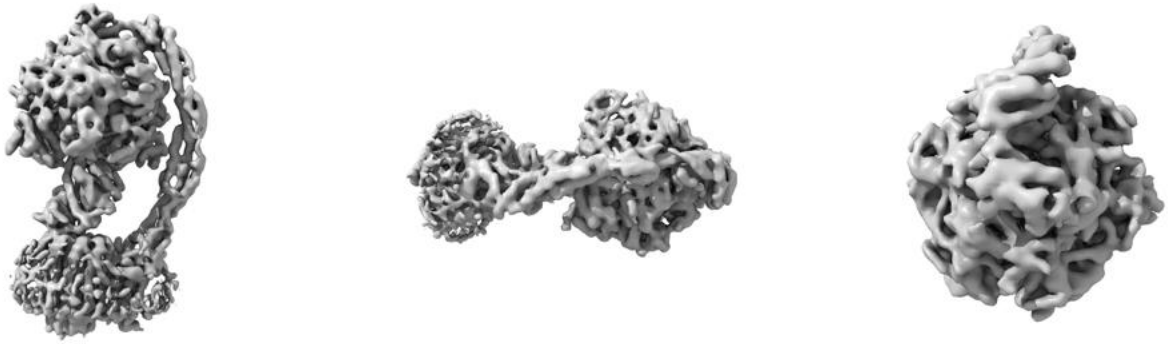


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.145. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

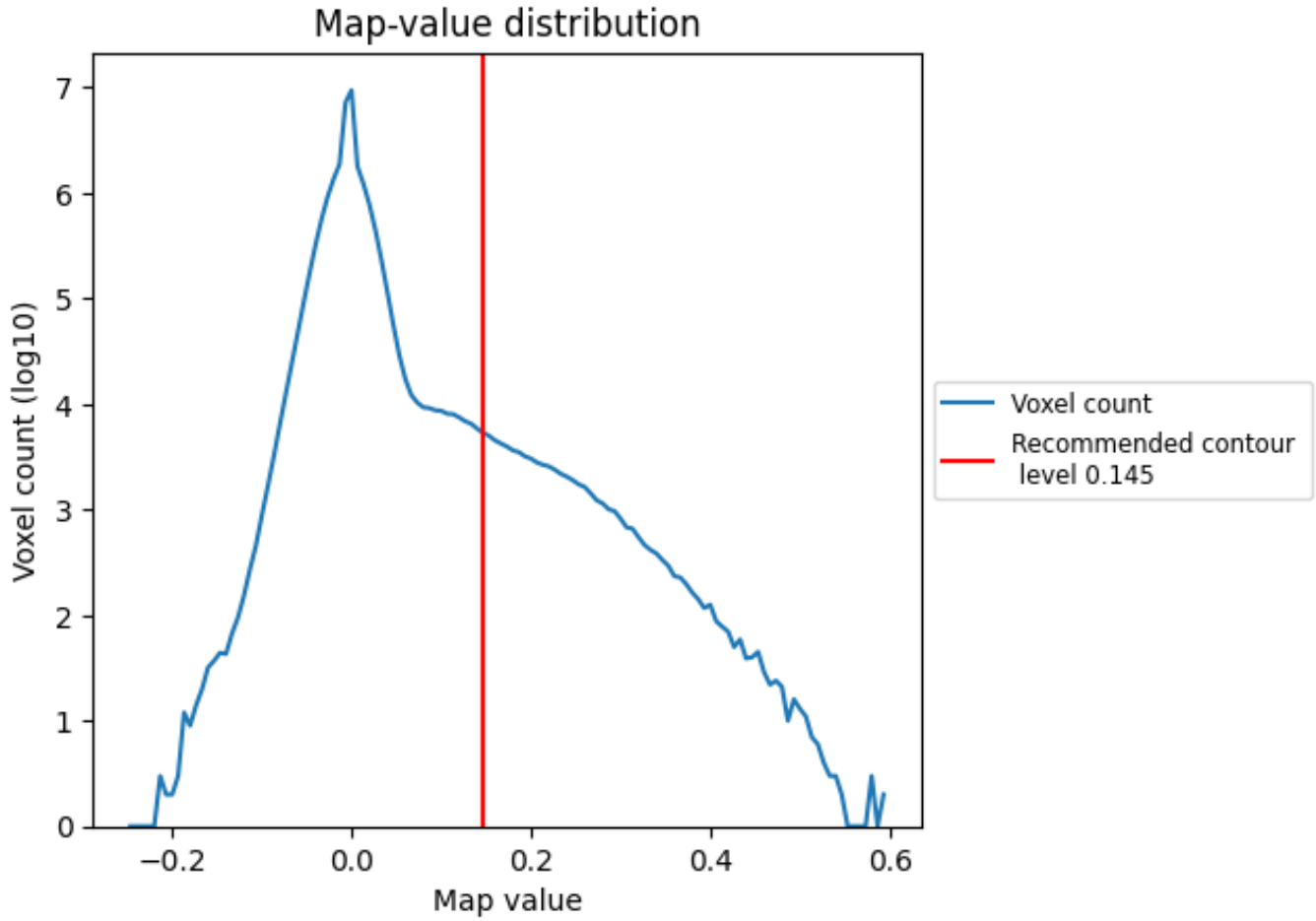
6.6 Mask visualisation (i)

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

7 Map analysis

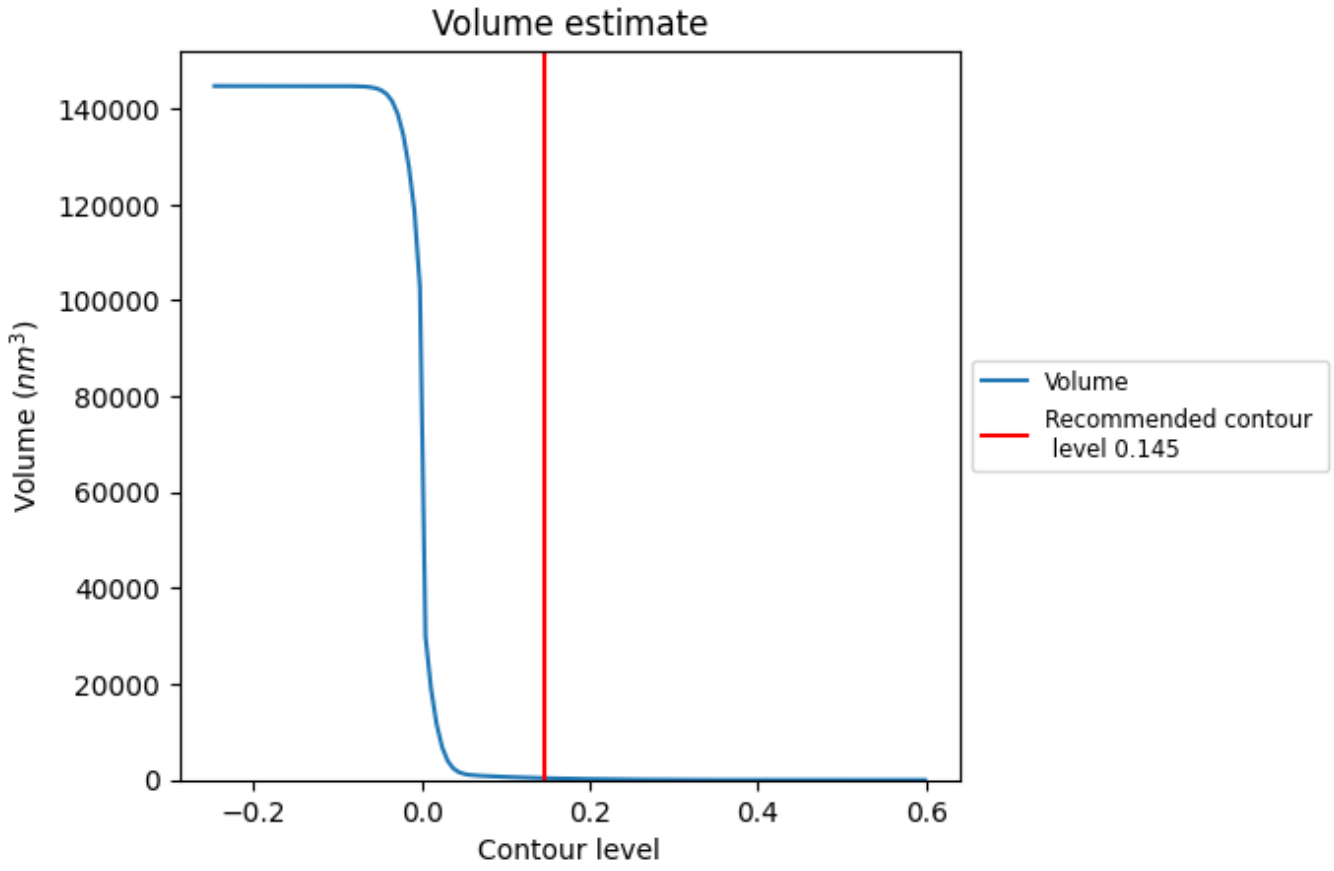
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

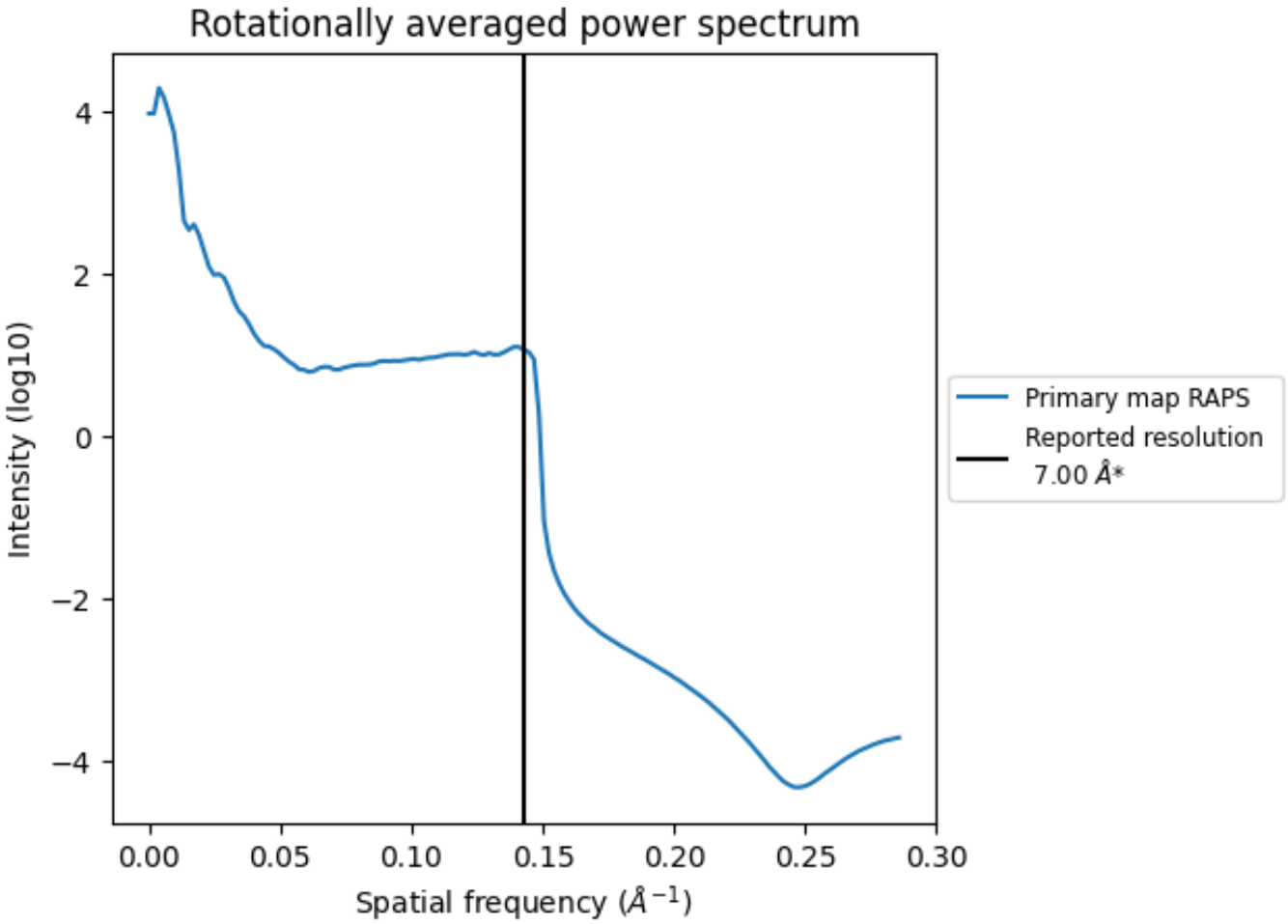
7.2 Volume estimate (i)



The volume at the recommended contour level is 375 nm^3; this corresponds to an approximate mass of 339 kDa.

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

7.3 Rotationally averaged power spectrum (i)

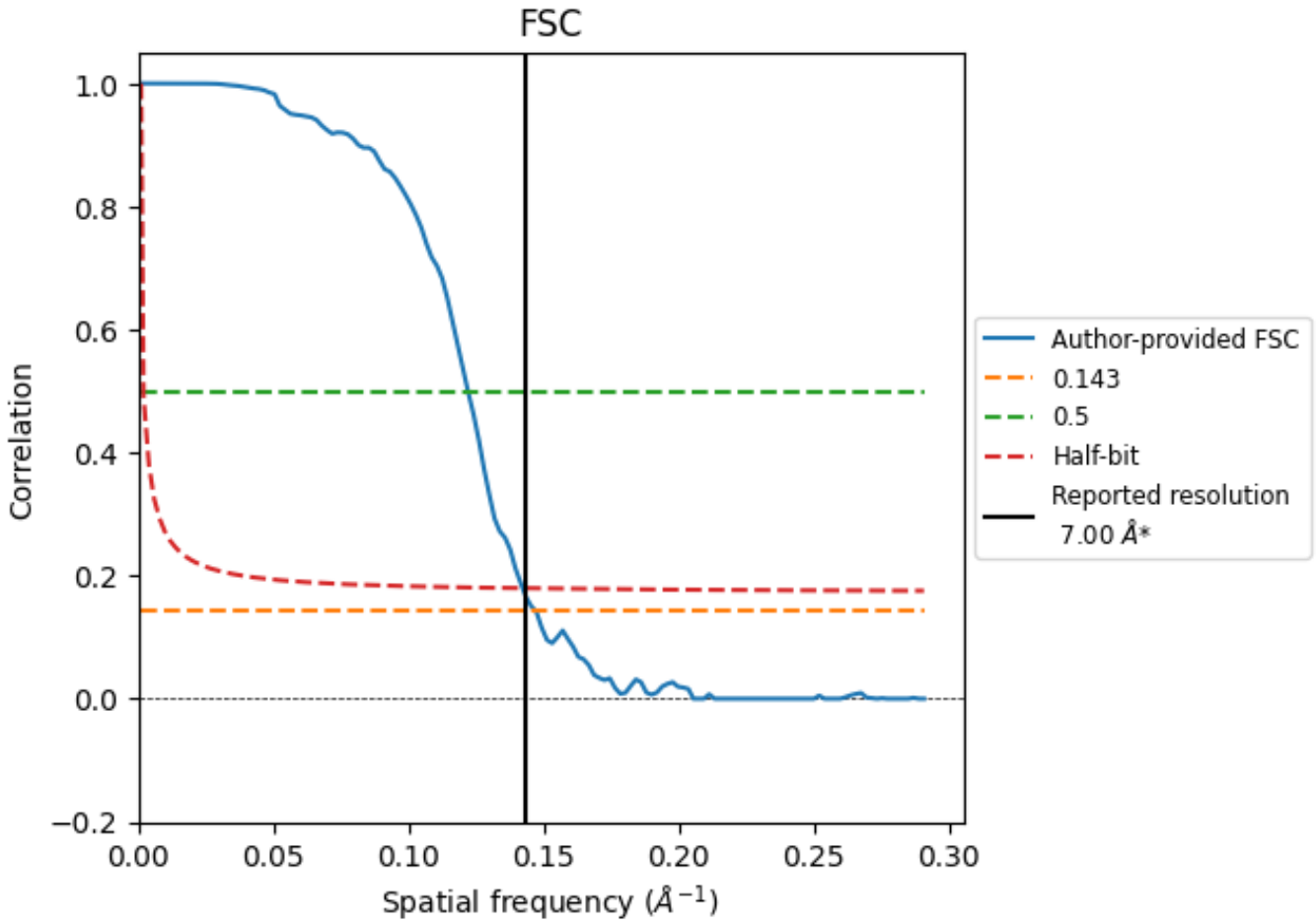


*Reported resolution corresponds to spatial frequency of 0.143 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.143 Å^{-1}

8.2 Resolution estimates (i)

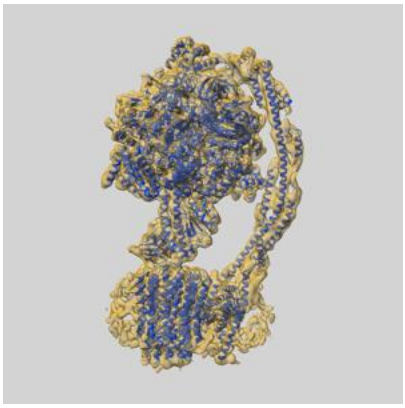
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.00	-	-
Author-provided FSC curve	6.81	8.20	7.03
Unmasked-calculated*	-	-	-

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

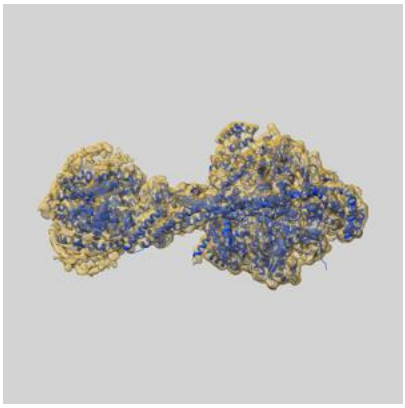
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4102 and PDB model 5LQZ. Per-residue inclusion information can be found in section 3 on page 10.

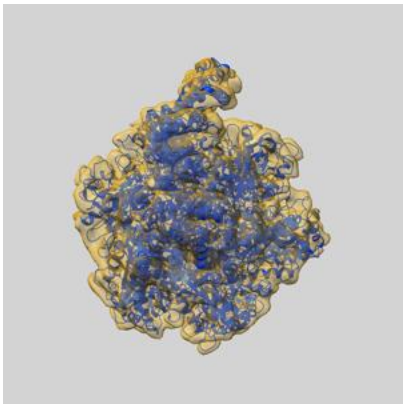
9.1 Map-model overlay



X



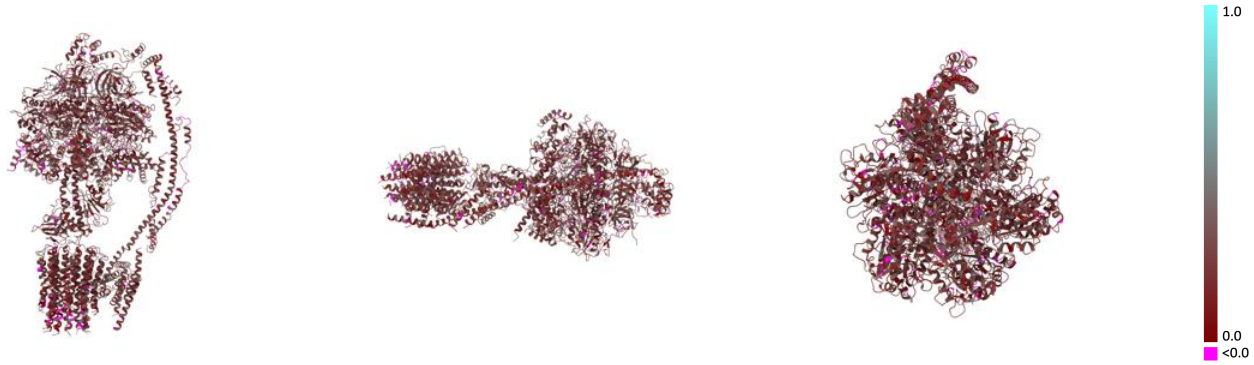
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.145 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.

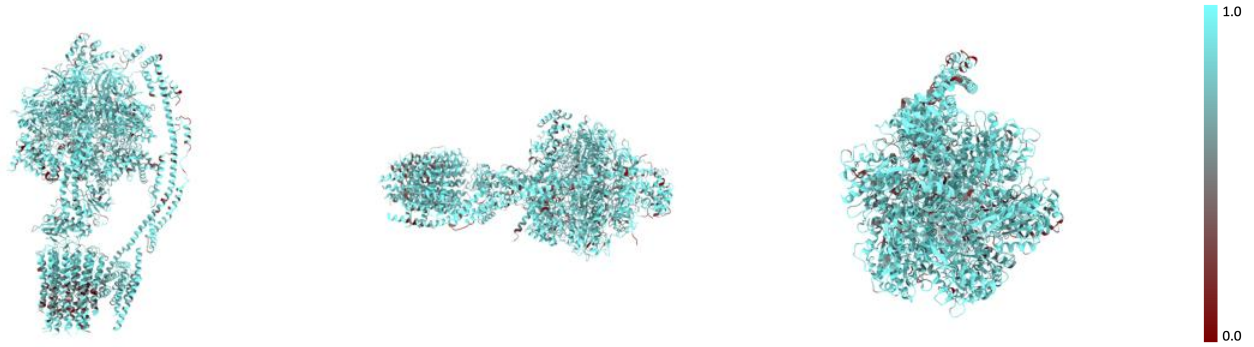
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

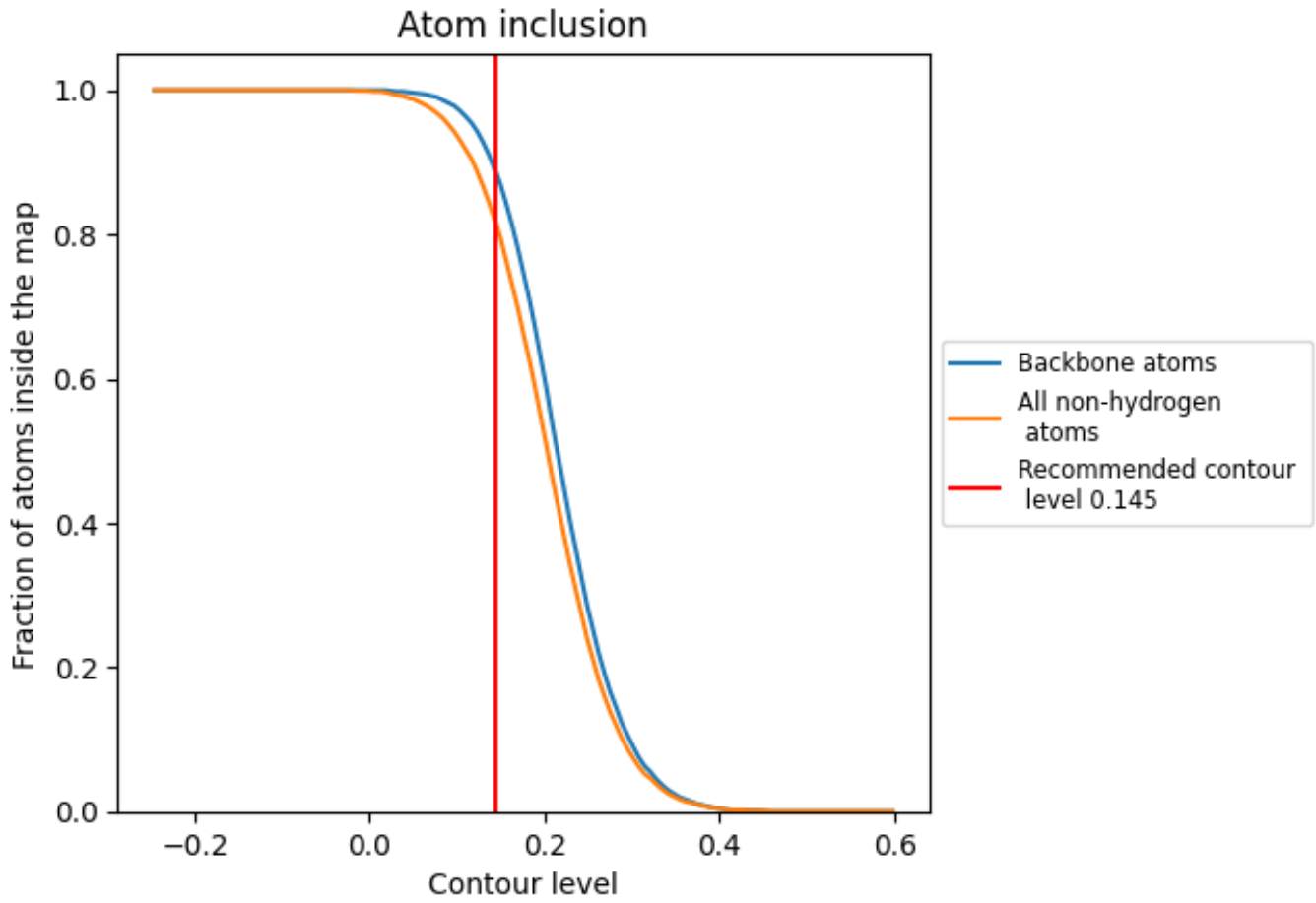
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.145).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 81% 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 (0.145) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8140	0.2250
1	0.8130	0.2120
2	0.8800	0.2320
3	0.7760	0.2550
4	0.7480	0.1900
A	0.8450	0.2300
B	0.8270	0.2310
C	0.8230	0.2360
D	0.8350	0.2340
E	0.8210	0.2290
F	0.8420	0.2390
G	0.8360	0.2300
H	0.8260	0.2250
I	0.8130	0.2370
J	0.7200	0.2400
K	0.7240	0.2010
L	0.7430	0.1960
M	0.7300	0.1930
N	0.7750	0.1810
O	0.7830	0.1980
P	0.7780	0.2040
Q	0.7290	0.2090
R	0.7860	0.2110
S	0.7780	0.2040
T	0.7270	0.2180
U	0.7740	0.2030
V	0.8190	0.2140
W	0.7370	0.1880
X	0.6760	0.2030
Y	0.8200	0.2490
Z	0.8860	0.2600