



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 11:30 pm GMT

PDB ID : 6FKI
EMDB ID : EMD-4272
Title : Chloroplast F1Fo conformation 3
Authors : Hahn, A.; Vonck, J.; Mills, D.J.; Meier, T.; Kuehlbrandt, W.
Deposited on : 2018-01-24
Resolution : 4.30 Å (reported)

This is a Full wwPDB EM Validation 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:

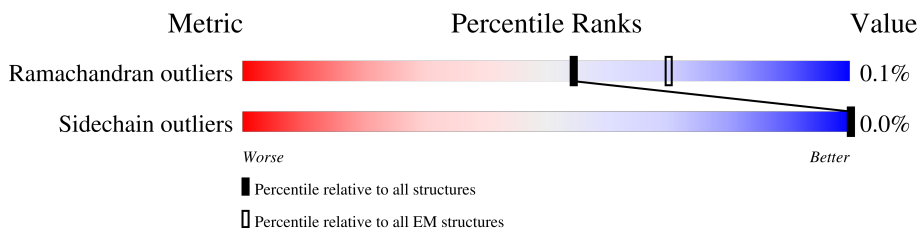
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.30 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	247	
2	b	184	
3	d	257	
4	p	222	
5	e	134	
6	g	364	
7	G	81	
7	H	81	
7	I	81	

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Mol	Chain	Length	Quality of chain
7	J	81	53% 96%
7	K	81	57% 96%
7	L	81	60% 96%
7	M	81	63% 96%
7	N	81	64% 96%
7	O	81	58% 96%
7	P	81	43% 96%
7	Q	81	57% 96%
7	R	81	74% 96%
7	S	81	69% 96%
7	T	81	69% 96%
8	A	507	11% 98%
8	C	507	7% 98%
8	E	507	5% 97%
9	B	498	• 95%
9	D	498	• 96%
9	F	498	5% 95%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 39231 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 a, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	223	Total	C	N	O	S	0	0
			1741	1172	268	299	2		

- Molecule 2 is a protein called ATP synthase subunit b, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	161	Total	C	N	O	S	0	0
			1299	812	236	246	5		

- Molecule 3 is a protein called ATP synthase delta chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	d	179	Total	C	N	O	S	0	0
			1383	876	229	277	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	p	143	Total	C	N	O	S	0	0
			1124	713	182	224	5		

- Molecule 5 is a protein called ATP synthase epsilon chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	131	Total	C	N	O	S	0	0
			1010	622	190	195	3		

- Molecule 6 is a protein called ATP synthase gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	g	321	Total	C	N	O	S	0	0
			2497	1574	429	482	12		

- Molecule 7 is a protein called ATP synthase subunit c, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
7	N	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
7	O	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
7	P	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
7	Q	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
7	R	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
7	M	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
7	T	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
7	G	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
7	H	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
7	L	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
7	K	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
7	J	79	Total	C	N	O	S	0	0
			544	355	90	98	1		
7	I	79	Total	C	N	O	S	0	0
			544	355	90	98	1		

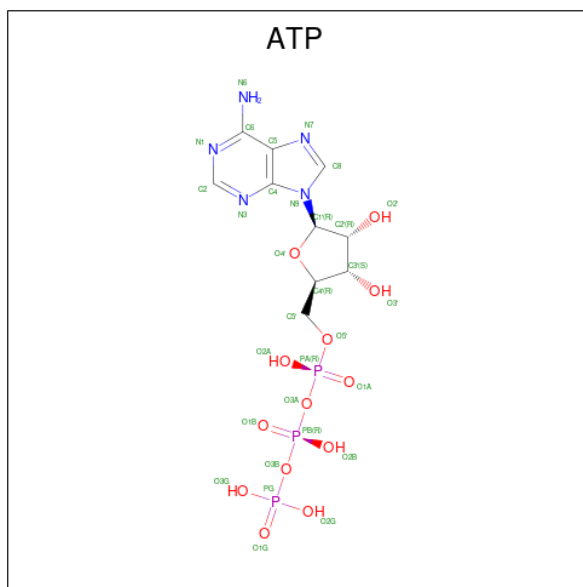
- Molecule 8 is a protein called ATP synthase subunit alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	498	Total	C	N	O	S	0	0
			3827	2408	661	745	13		
8	A	501	Total	C	N	O	S	0	0
			3849	2422	666	748	13		
8	C	501	Total	C	N	O	S	0	0
			3851	2423	667	748	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	479	Total 3627	C 2288	N 623	O 700	S 16	0	0
9	B	478	Total 3619	C 2282	N 622	O 699	S 16	0	0
9	D	480	Total 3636	C 2294	N 625	O 701	S 16	0	0

- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

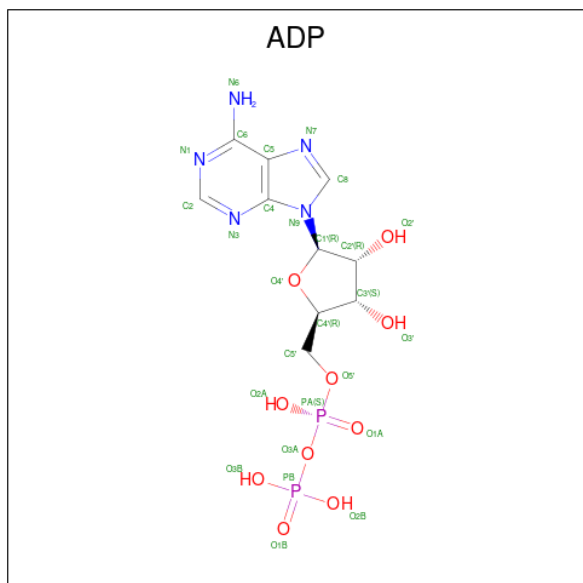
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
11	E	1	Total 1	Mg 1	0
11	A	1	Total 1	Mg 1	0
11	B	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
11	C	1	Total	Mg	0
			1	1	
11	D	1	Total	Mg	0
			1	1	

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

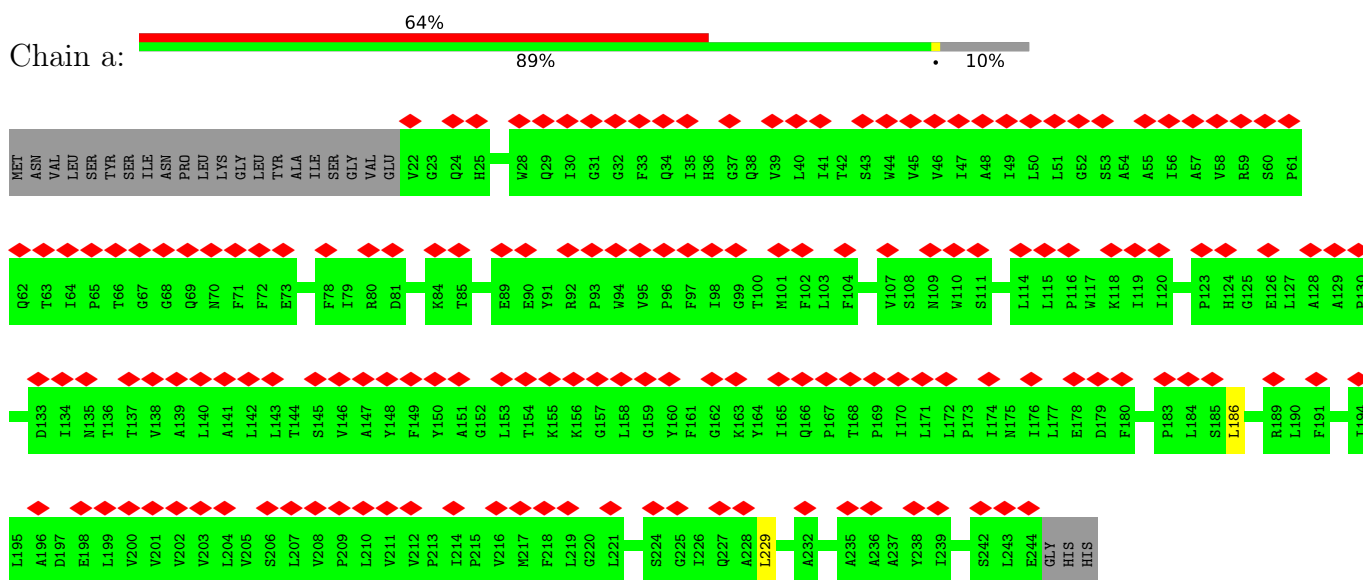


Mol	Chain	Residues	Atoms				AltConf	
12	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
12	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

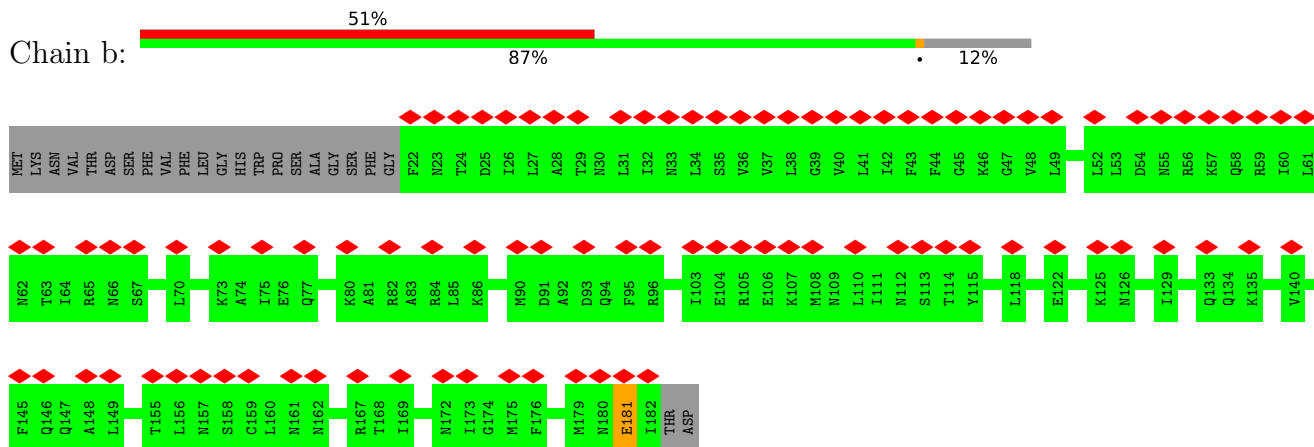
3 Residue-property plots

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 a, chloroplastic

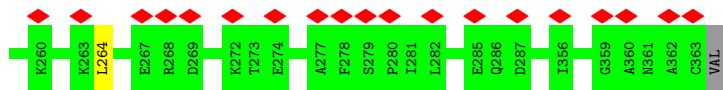


- Molecule 2: ATP synthase subunit b, chloroplastic

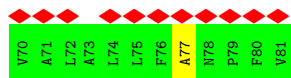
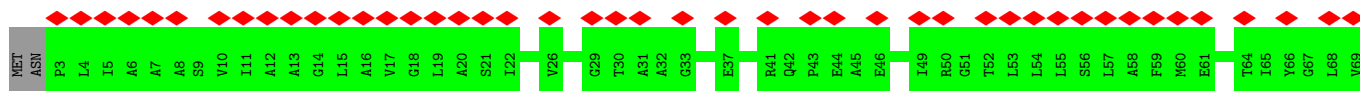


- Molecule 3: ATP synthase delta chain, chloroplastic

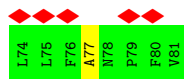
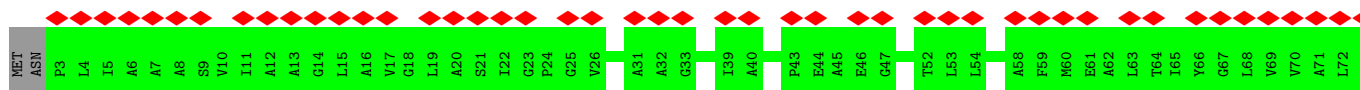




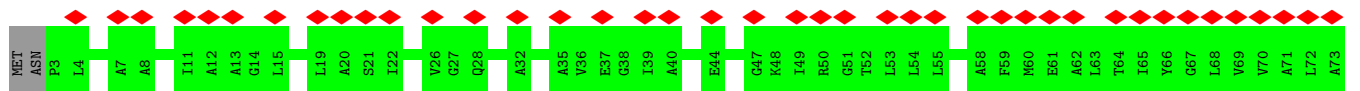
• Molecule 7: ATP synthase subunit c, chloroplastic



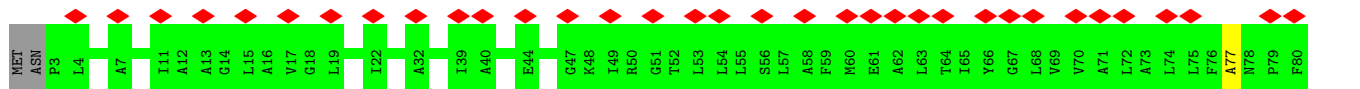
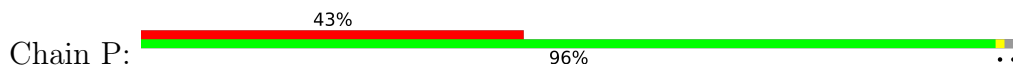
• Molecule 7: ATP synthase subunit c, chloroplastic



• Molecule 7: ATP synthase subunit c, chloroplastic

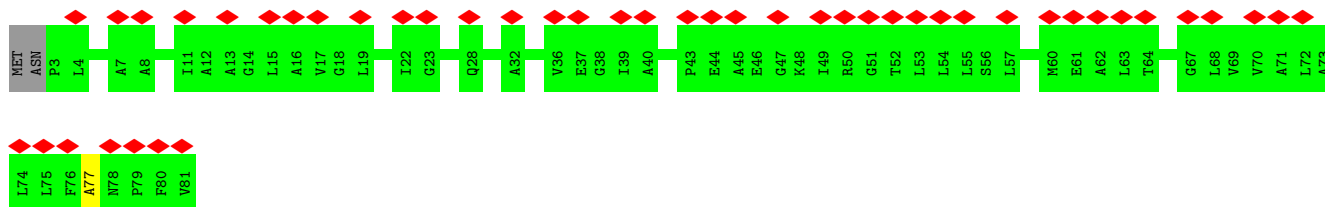


• Molecule 7: ATP synthase subunit c, chloroplastic

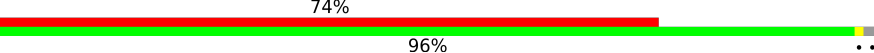


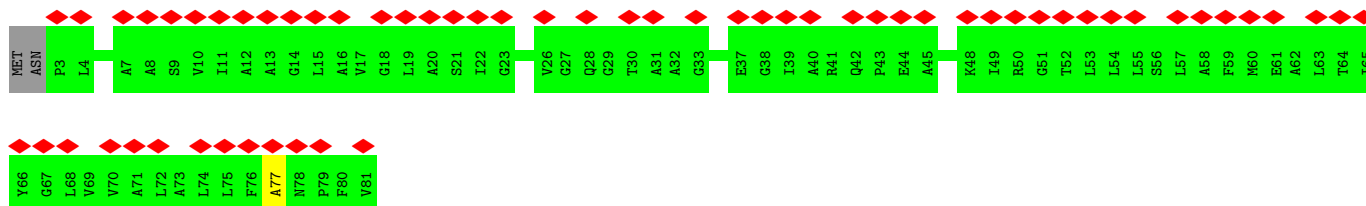
• Molecule 7: ATP synthase subunit c, chloroplastic

Chain Q: 



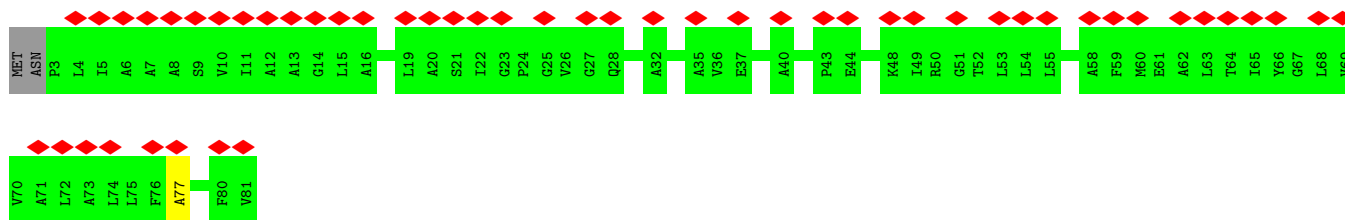
- Molecule 7: ATP synthase subunit c, chloroplastic

Chain R: 



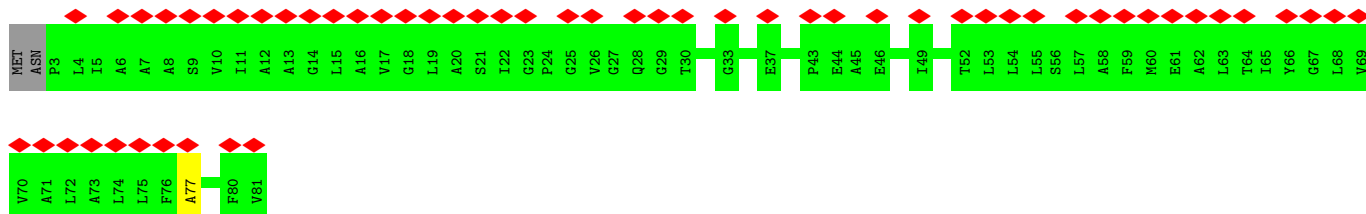
- Molecule 7: ATP synthase subunit c, chloroplastic

Chain M: 



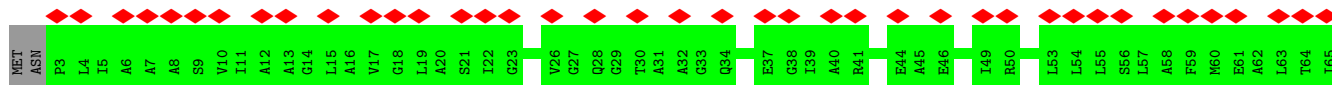
- Molecule 7: ATP synthase subunit c, chloroplastic

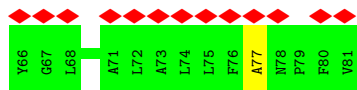
Chain T: 



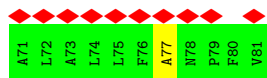
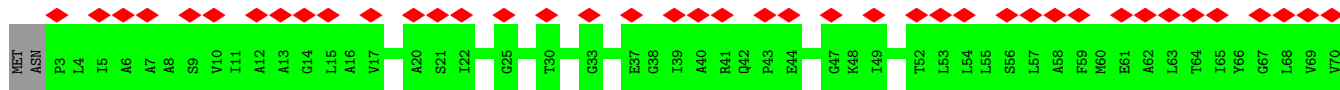
- Molecule 7: ATP synthase subunit c, chloroplastic

Chain G: 

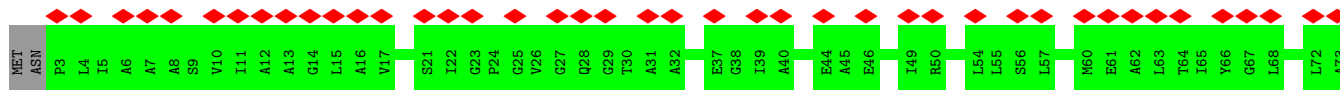




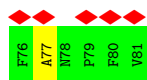
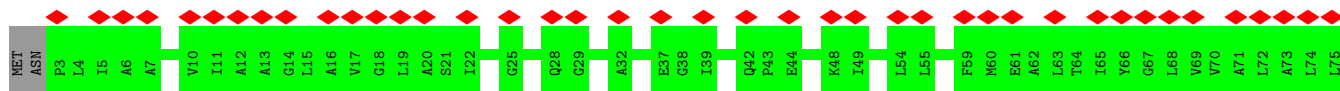
• Molecule 7: ATP synthase subunit c, chloroplastic



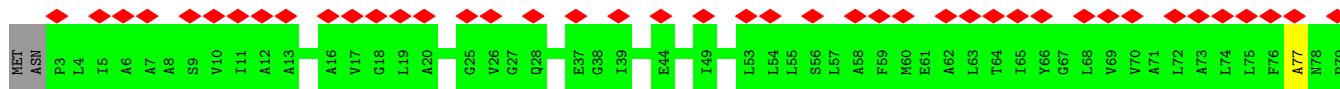
• Molecule 7: ATP synthase subunit c, chloroplastic



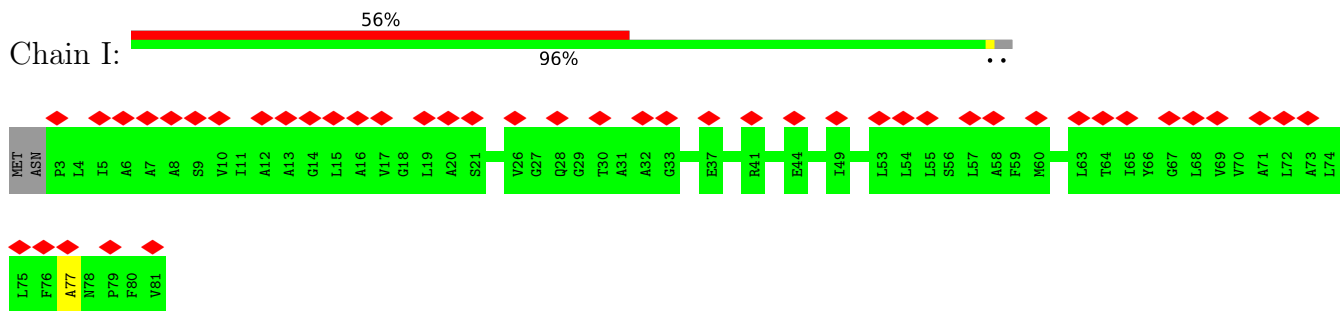
• Molecule 7: ATP synthase subunit c, chloroplastic



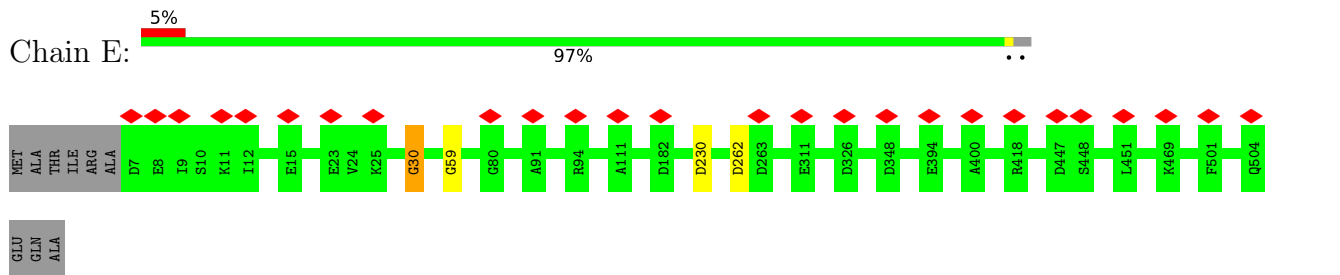
• Molecule 7: ATP synthase subunit c, chloroplastic



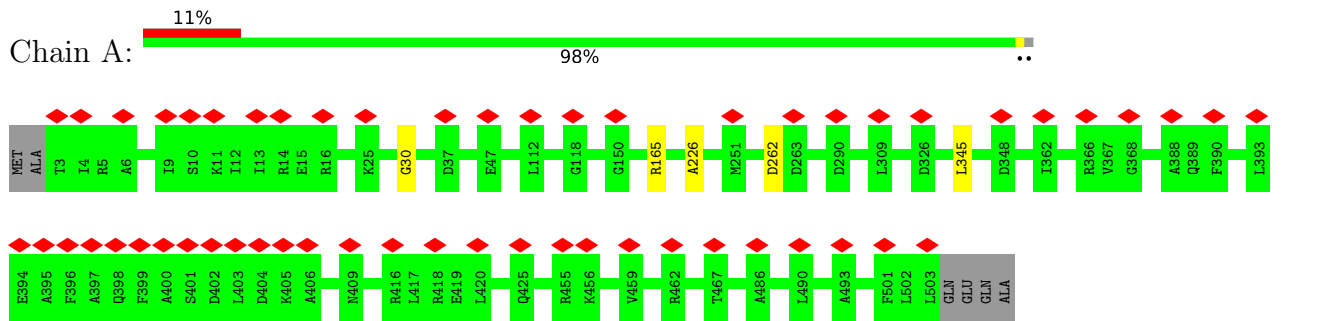
• Molecule 7: ATP synthase subunit c, chloroplastic



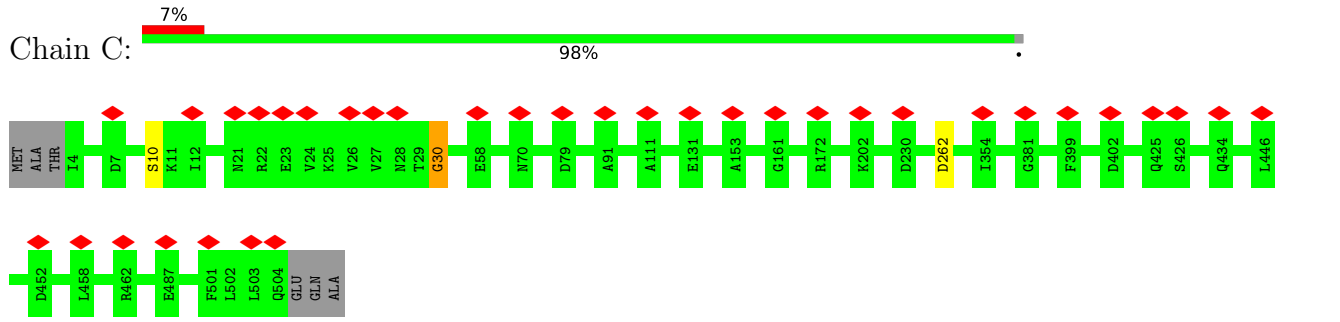
• Molecule 8: ATP synthase subunit alpha, chloroplastic



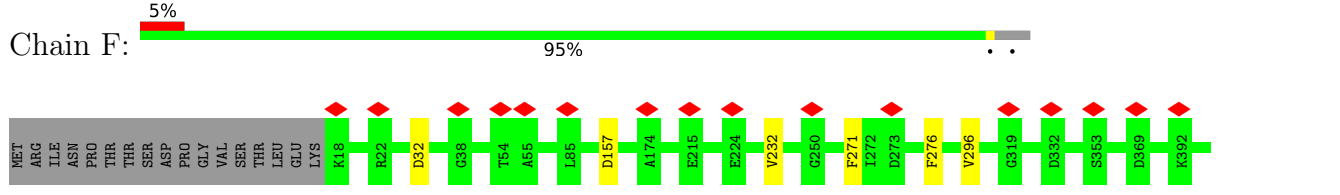
• Molecule 8: ATP synthase subunit alpha, chloroplastic

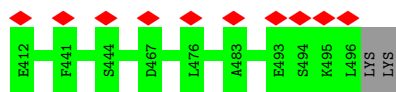


• Molecule 8: ATP synthase subunit alpha, chloroplastic



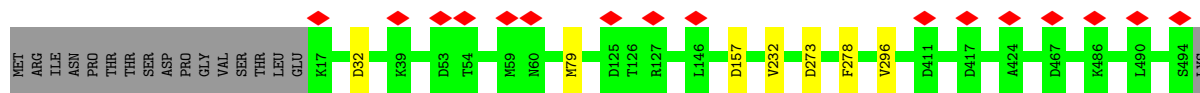
• Molecule 9: ATP synthase subunit beta, chloroplastic





- Molecule 9: ATP synthase subunit beta, chloroplastic

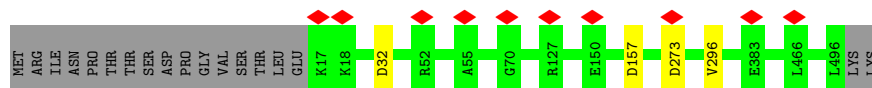
Chain B: 95%



LEU
LYS
LYS

- Molecule 9: ATP synthase subunit beta, chloroplastic

Chain D: 96%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	14409	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	132953	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.225	Depositor
Minimum map value	-0.142	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	368.55, 368.55, 368.55	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.053, 1.053, 1.053	Depositor

5 Model quality i

5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.47	0/1792	0.71	2/2454 (0.1%)
2	b	0.32	0/1309	0.55	1/1754 (0.1%)
3	d	0.43	0/1399	0.59	0/1898
4	p	0.41	1/1134 (0.1%)	0.63	2/1519 (0.1%)
5	e	0.43	0/1019	0.65	0/1381
6	g	0.56	1/2526 (0.0%)	0.69	4/3412 (0.1%)
7	G	0.36	0/551	0.59	0/750
7	H	0.36	0/551	0.59	0/750
7	I	0.36	0/551	0.59	0/750
7	J	0.36	0/551	0.59	0/750
7	K	0.36	0/551	0.59	0/750
7	L	0.36	0/551	0.59	0/750
7	M	0.36	0/551	0.59	0/750
7	N	0.36	0/551	0.59	0/750
7	O	0.36	0/551	0.59	0/750
7	P	0.36	0/551	0.59	0/750
7	Q	0.36	0/551	0.59	0/750
7	R	0.36	0/551	0.59	0/750
7	S	0.36	0/551	0.59	0/750
7	T	0.36	0/551	0.59	0/750
8	A	0.75	1/3898 (0.0%)	0.70	2/5274 (0.0%)
8	C	0.76	0/3900	0.75	2/5276 (0.0%)
8	E	0.73	0/3876	0.70	3/5244 (0.1%)
9	B	0.71	0/3676	0.71	5/4983 (0.1%)
9	D	0.74	0/3693	0.69	2/5005 (0.0%)
9	F	0.80	2/3684 (0.1%)	0.74	3/4994 (0.1%)
All	All	0.63	5/39620 (0.0%)	0.68	26/53694 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	b	0	1
4	p	0	1
7	G	0	1
7	H	0	1
7	I	0	1
7	J	0	1
7	K	0	1
7	L	0	1
7	M	0	1
7	N	0	1
7	O	0	1
7	P	0	1
7	Q	0	1
7	R	0	1
7	S	0	1
7	T	0	1
8	A	0	2
8	C	0	3
8	E	0	2
9	D	0	1
All	All	0	24

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	276	PHE	C-N	-15.92	0.97	1.34
6	g	84	PRO	N-CD	12.69	1.65	1.47
8	A	30	GLY	C-N	8.21	1.52	1.34
4	p	105	ASP	C-N	-7.20	1.17	1.34
9	F	232	VAL	CB-CG2	-6.69	1.38	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	30	GLY	O-C-N	-8.56	109.00	122.70
2	b	181	GLU	O-C-N	-8.07	109.79	122.70
8	E	30	GLY	O-C-N	-8.02	109.87	122.70
8	C	30	GLY	C-N-CA	7.37	140.12	121.70
8	A	30	GLY	O-C-N	6.64	133.32	122.70
9	B	273	ASP	CB-CG-OD1	6.54	124.19	118.30
9	B	232	VAL	CG1-CB-CG2	-5.71	101.77	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	157	ASP	CB-CG-OD2	5.27	123.04	118.30
9	B	157	ASP	CB-CG-OD2	5.24	123.01	118.30
9	F	271	PHE	O-C-N	-5.21	114.36	122.70
6	g	248	ASP	CB-CG-OD2	5.19	122.97	118.30
9	F	32	ASP	CB-CG-OD2	5.18	122.96	118.30
1	a	186	LEU	CB-CG-CD2	-5.17	102.20	111.00
9	D	32	ASP	CB-CG-OD2	5.15	122.94	118.30
9	D	157	ASP	CB-CG-OD2	5.12	122.91	118.30
1	a	229	LEU	CA-CB-CG	5.12	127.07	115.30
6	g	220	LEU	CB-CG-CD2	-5.11	102.31	111.00
8	A	345	LEU	CB-CG-CD2	-5.11	102.31	111.00
6	g	241	ASP	CB-CG-OD2	5.10	122.89	118.30
9	B	32	ASP	CB-CG-OD2	5.10	122.89	118.30
6	g	264	LEU	CA-CB-CG	5.08	126.99	115.30
8	E	230	ASP	CB-CG-OD1	5.08	122.87	118.30
4	p	104	LEU	CA-CB-CG	5.07	126.96	115.30
8	E	59	GLY	N-CA-C	5.02	125.65	113.10
4	p	105	ASP	C-N-CA	-5.01	109.17	121.70
9	B	79	MET	CG-SD-CE	-5.01	92.18	100.20

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	A	226	ALA	Peptide
8	A	262	ASP	Peptide
8	C	10	SER	Peptide
8	C	262	ASP	Peptide
8	C	30	GLY	Mainchain
9	D	273	ASP	Peptide
8	E	262	ASP	Peptide
8	E	30	GLY	Mainchain
7	G	77	ALA	Mainchain
7	H	77	ALA	Mainchain
7	I	77	ALA	Mainchain
7	J	77	ALA	Mainchain
7	K	77	ALA	Mainchain
7	L	77	ALA	Mainchain
7	M	77	ALA	Mainchain
7	N	77	ALA	Mainchain
7	O	77	ALA	Mainchain
7	P	77	ALA	Mainchain

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Mol	Chain	Res	Type	Group
7	Q	77	ALA	Mainchain
7	R	77	ALA	Mainchain
7	S	77	ALA	Mainchain
7	T	77	ALA	Mainchain
2	b	181	GLU	Mainchain
4	p	105	ASP	Mainchain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	a	221/247 (90%)	211 (96%)	10 (4%)	0	100	100
2	b	157/184 (85%)	151 (96%)	6 (4%)	0	100	100
3	d	177/257 (69%)	170 (96%)	6 (3%)	1 (1%)	25	65
4	p	141/222 (64%)	130 (92%)	11 (8%)	0	100	100
5	e	129/134 (96%)	122 (95%)	7 (5%)	0	100	100
6	g	319/364 (88%)	306 (96%)	13 (4%)	0	100	100
7	G	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
7	H	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
7	I	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
7	J	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
7	K	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
7	L	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
7	M	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
7	N	77/81 (95%)	74 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	O	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
7	P	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
7	Q	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
7	R	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
7	S	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
7	T	77/81 (95%)	74 (96%)	3 (4%)	0	100	100
8	A	499/507 (98%)	485 (97%)	14 (3%)	0	100	100
8	C	499/507 (98%)	478 (96%)	21 (4%)	0	100	100
8	E	496/507 (98%)	483 (97%)	13 (3%)	0	100	100
9	B	476/498 (96%)	444 (93%)	31 (6%)	1 (0%)	47	81
9	D	478/498 (96%)	463 (97%)	14 (3%)	1 (0%)	47	81
9	F	477/498 (96%)	463 (97%)	13 (3%)	1 (0%)	47	81
All	All	5147/5557 (93%)	4942 (96%)	201 (4%)	4 (0%)	54	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	d	217	LEU
9	B	296	VAL
9	F	296	VAL
9	D	296	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	187/207 (90%)	187 (100%)	0	100	100
2	b	142/161 (88%)	142 (100%)	0	100	100
3	d	156/220 (71%)	156 (100%)	0	100	100
4	p	124/197 (63%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	109/112 (97%)	109 (100%)	0	100	100
6	g	276/315 (88%)	276 (100%)	0	100	100
7	G	51/53 (96%)	51 (100%)	0	100	100
7	H	51/53 (96%)	51 (100%)	0	100	100
7	I	51/53 (96%)	51 (100%)	0	100	100
7	J	51/53 (96%)	51 (100%)	0	100	100
7	K	51/53 (96%)	51 (100%)	0	100	100
7	L	51/53 (96%)	51 (100%)	0	100	100
7	M	51/53 (96%)	51 (100%)	0	100	100
7	N	51/53 (96%)	51 (100%)	0	100	100
7	O	51/53 (96%)	51 (100%)	0	100	100
7	P	51/53 (96%)	51 (100%)	0	100	100
7	Q	51/53 (96%)	51 (100%)	0	100	100
7	R	51/53 (96%)	51 (100%)	0	100	100
7	S	51/53 (96%)	51 (100%)	0	100	100
7	T	51/53 (96%)	51 (100%)	0	100	100
8	A	410/414 (99%)	409 (100%)	1 (0%)	93	96
8	C	410/414 (99%)	410 (100%)	0	100	100
8	E	408/414 (99%)	408 (100%)	0	100	100
9	B	389/408 (95%)	388 (100%)	1 (0%)	92	95
9	D	391/408 (96%)	391 (100%)	0	100	100
9	F	390/408 (96%)	390 (100%)	0	100	100
All	All	4106/4420 (93%)	4104 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	A	165	ARG
9	B	278	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	70	ASN
1	a	86	GLN
1	a	135	ASN
1	a	193	ASN
2	b	33	ASN
2	b	133	GLN
3	d	141	HIS
3	d	188	ASN
3	d	199	GLN
3	d	240	GLN
4	p	167	GLN
4	p	195	GLN
6	g	56	ASN
6	g	81	ASN
6	g	228	HIS
6	g	301	ASN
6	g	303	GLN
7	S	42	GLN
7	N	42	GLN
7	O	42	GLN
7	P	42	GLN
7	Q	42	GLN
7	R	42	GLN
7	M	42	GLN
7	T	42	GLN
7	G	42	GLN
7	H	42	GLN
7	L	42	GLN
7	K	42	GLN
7	J	42	GLN
7	I	42	GLN
8	E	34	GLN
8	E	43	HIS
8	E	148	GLN
8	E	208	GLN
9	F	25	GLN
9	F	238	GLN
9	F	264	ASN
9	F	280	GLN
9	F	310	GLN
9	F	384	HIS
9	F	396	GLN
8	A	28	ASN

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Mol	Chain	Res	Type
8	A	66	ASN
8	A	186	ASN
8	A	187	GLN
8	A	214	GLN
8	A	256	HIS
8	A	409	ASN
8	A	423	GLN
8	A	497	GLN
9	B	71	ASN
9	B	112	ASN
9	B	210	ASN
9	B	238	GLN
9	B	345	HIS
9	B	389	GLN
8	C	187	GLN
8	C	423	GLN
9	D	67	GLN
9	D	389	GLN
9	D	396	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	ATP	C	601	11	26,33,33	0.95	1 (3%)	31,52,52	1.52	6 (19%)
12	ADP	D	600	11	24,29,29	1.32	3 (12%)	29,45,45	1.48	4 (13%)
10	ATP	E	600	11	26,33,33	1.19	2 (7%)	31,52,52	1.56	8 (25%)
10	ATP	A	600	11	26,33,33	1.07	1 (3%)	31,52,52	1.36	4 (12%)
12	ADP	B	501	11	24,29,29	1.08	1 (4%)	29,45,45	1.48	4 (13%)

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
10	ATP	C	601	11	-	0/18/38/38	0/3/3/3
12	ADP	D	600	11	-	5/12/32/32	0/3/3/3
10	ATP	E	600	11	-	4/18/38/38	0/3/3/3
10	ATP	A	600	11	-	3/18/38/38	0/3/3/3
12	ADP	B	501	11	-	5/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	600	ADP	C2'-C1'	-2.72	1.49	1.53
10	E	600	ATP	C2'-C1'	-2.61	1.49	1.53
12	B	501	ADP	C2'-C1'	-2.35	1.50	1.53
12	D	600	ADP	PB-O3B	-2.23	1.46	1.54
10	C	601	ATP	C2'-C1'	-2.13	1.50	1.53
12	D	600	ADP	O4'-C4'	-2.06	1.40	1.45
10	A	600	ATP	C5-C4	2.06	1.46	1.40
10	E	600	ATP	PG-O2G	-2.04	1.47	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	600	ATP	N3-C2-N1	-3.93	122.53	128.68
12	D	600	ADP	N3-C2-N1	-3.87	122.63	128.68
10	A	600	ATP	N3-C2-N1	-3.49	123.22	128.68
10	C	601	ATP	N3-C2-N1	-3.44	123.30	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	501	ADP	C3'-C2'-C1'	3.30	105.94	100.98
12	B	501	ADP	N3-C2-N1	-3.25	123.60	128.68
12	B	501	ADP	PA-O3A-PB	-3.24	121.69	132.83
10	E	600	ATP	C4-C5-N7	-3.18	106.08	109.40
10	C	601	ATP	C4-C5-N7	-2.66	106.62	109.40
10	A	600	ATP	O2B-PB-O1B	2.59	125.05	112.24
10	E	600	ATP	C2-N1-C6	2.53	123.09	118.75
10	C	601	ATP	C2-N1-C6	2.53	123.09	118.75
12	D	600	ADP	C4-C5-N7	-2.51	106.79	109.40
10	C	601	ATP	C3'-C2'-C1'	2.42	104.63	100.98
10	E	600	ATP	C3'-C2'-C1'	2.42	104.62	100.98
12	B	501	ADP	C4-C5-N7	-2.39	106.91	109.40
12	D	600	ADP	C2-N1-C6	2.33	122.75	118.75
12	D	600	ADP	O3B-PB-O2B	2.26	116.28	107.64
10	C	601	ATP	PB-O3B-PG	-2.25	125.12	132.83
10	A	600	ATP	C2-N1-C6	2.24	122.58	118.75
10	C	601	ATP	C1'-N9-C4	-2.19	122.79	126.64
10	E	600	ATP	O2B-PB-O1B	2.17	122.98	112.24
10	E	600	ATP	PB-O3B-PG	-2.11	125.59	132.83
10	E	600	ATP	C5'-C4'-C3'	-2.07	107.43	115.18
10	A	600	ATP	O4'-C1'-C2'	-2.04	103.95	106.93
10	E	600	ATP	O3B-PG-O1G	-2.00	100.09	111.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	501	ADP	C5'-O5'-PA-O2A
12	D	600	ADP	C5'-O5'-PA-O1A
12	D	600	ADP	C5'-O5'-PA-O2A
12	B	501	ADP	O4'-C4'-C5'-O5'
12	B	501	ADP	C3'-C4'-C5'-O5'
10	A	600	ATP	PB-O3B-PG-O1G
10	A	600	ATP	PB-O3B-PG-O2G
12	B	501	ADP	C5'-O5'-PA-O3A
10	E	600	ATP	PG-O3B-PB-O2B
10	E	600	ATP	PA-O3A-PB-O2B
12	D	600	ADP	PB-O3A-PA-O2A
12	B	501	ADP	C5'-O5'-PA-O1A
12	D	600	ADP	O4'-C4'-C5'-O5'
10	E	600	ATP	PA-O3A-PB-O1B
10	A	600	ATP	PA-O3A-PB-O2B

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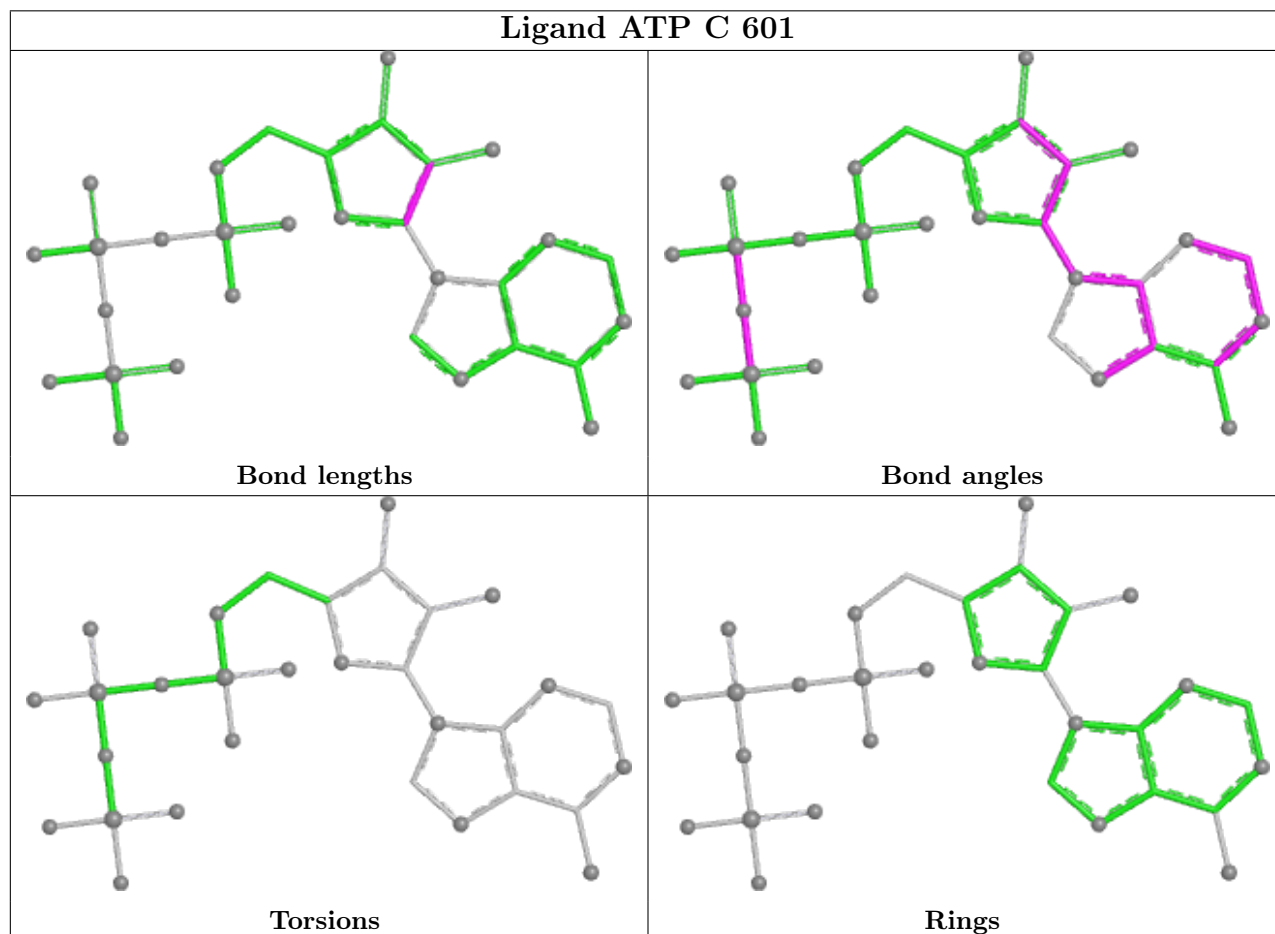
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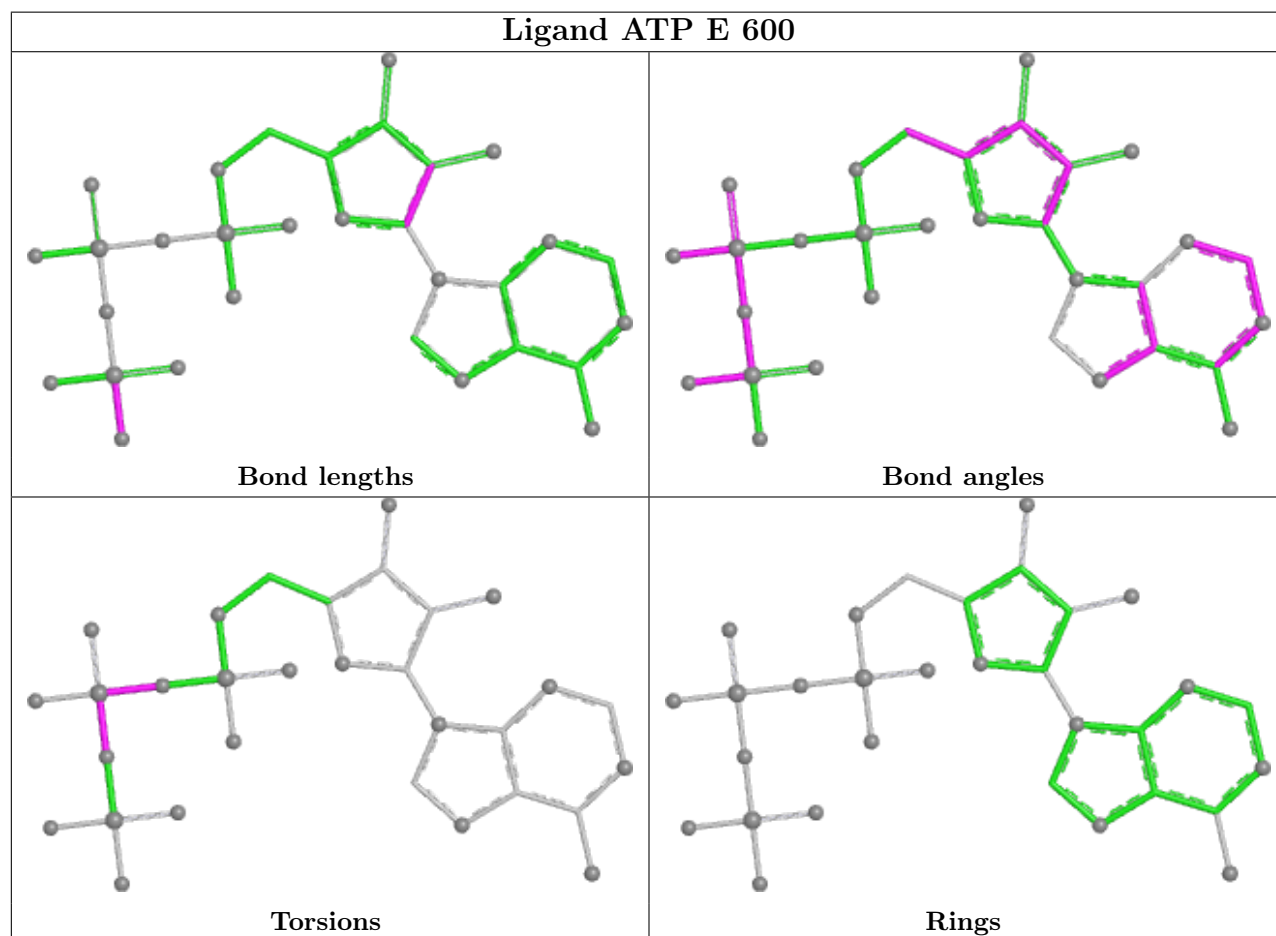
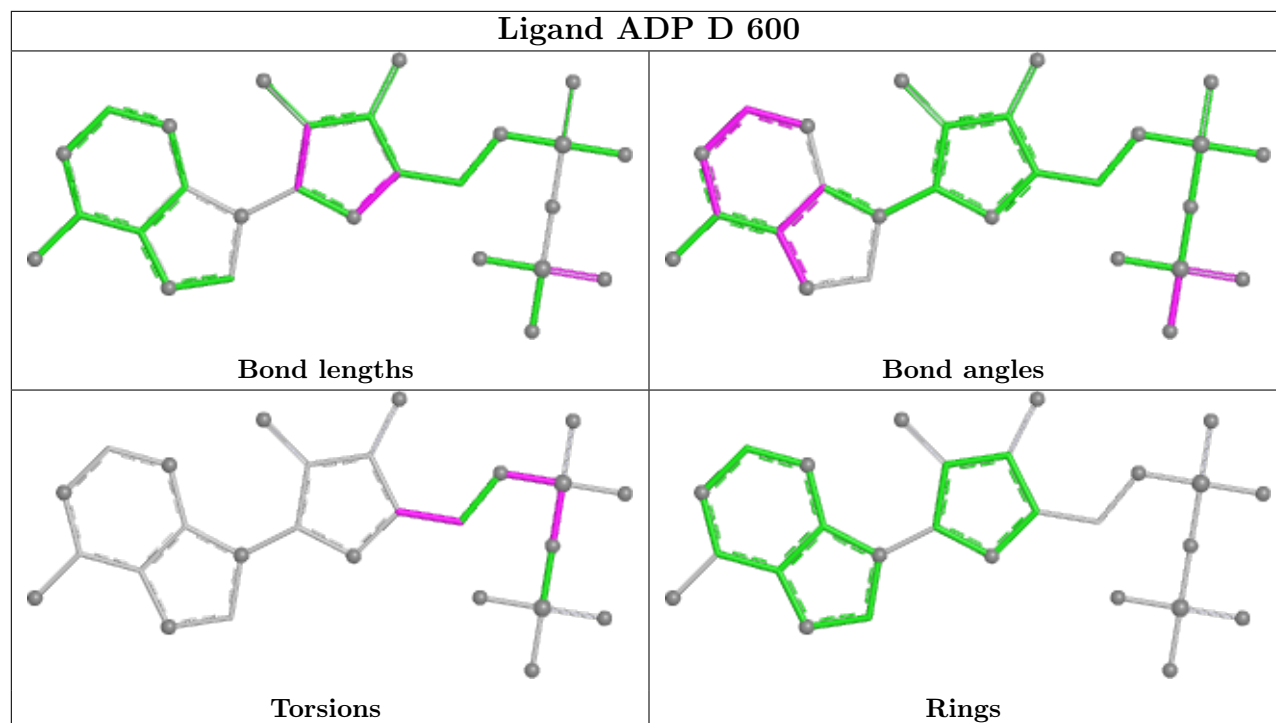
Mol	Chain	Res	Type	Atoms
12	D	600	ADP	C5'-O5'-PA-O3A
10	E	600	ATP	PG-O3B-PB-O1B

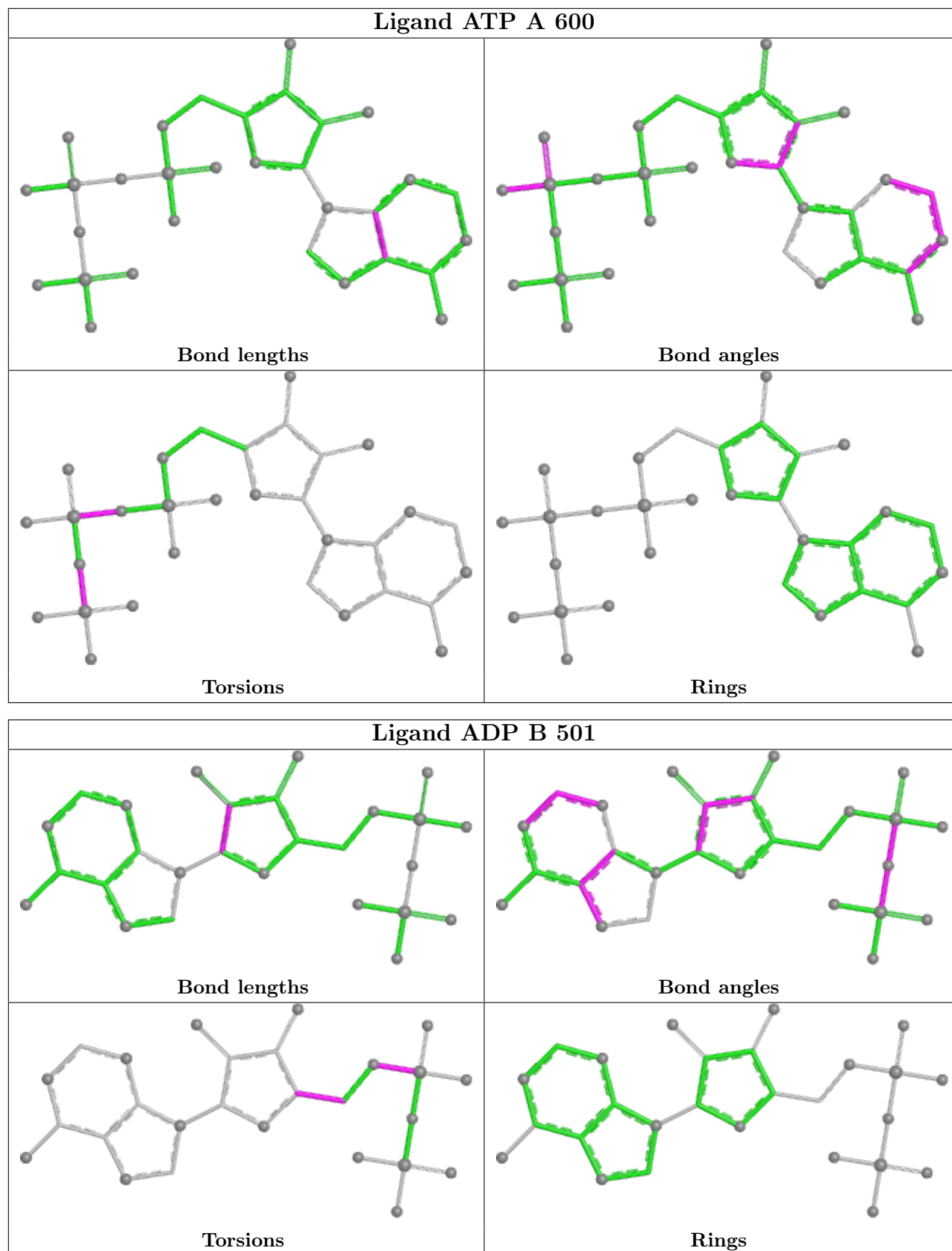
There are no ring outliers.

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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	b	1
4	p	1
9	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	77:GLN	C	78:LEU	N	2.25
1	p	105:ASP	C	106:LYS	N	1.17
1	F	276:PHE	C	277:ARG	N	0.97

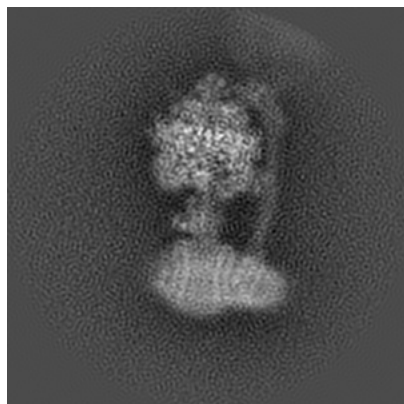
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4272. These allow visual inspection of the internal detail of the map and identification of artifacts.

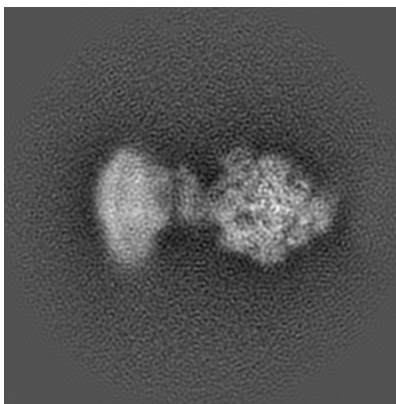
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

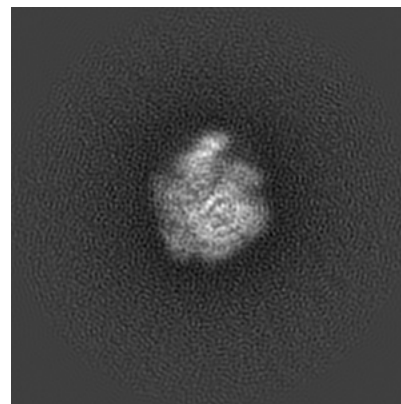
6.1.1 Primary map



X

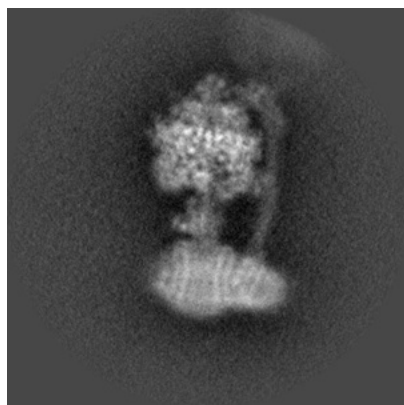


Y

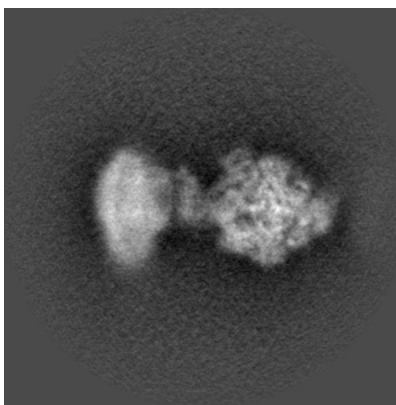


Z

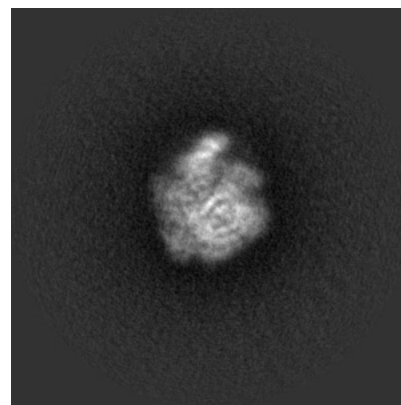
6.1.2 Raw map



X



Y

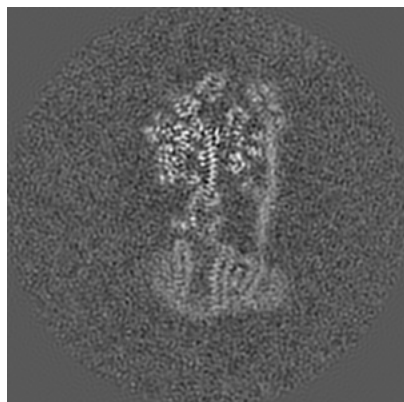


Z

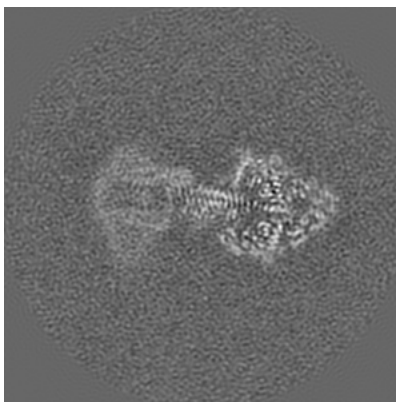
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

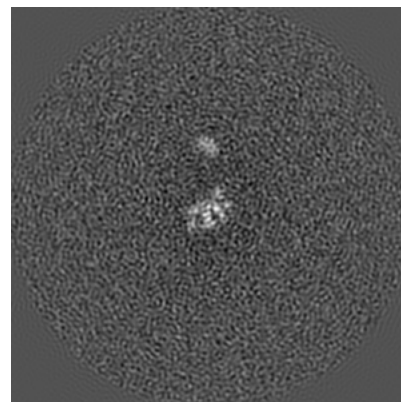
6.2.1 Primary map



X Index: 175

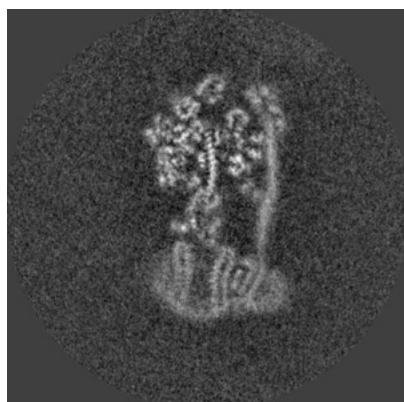


Y Index: 175

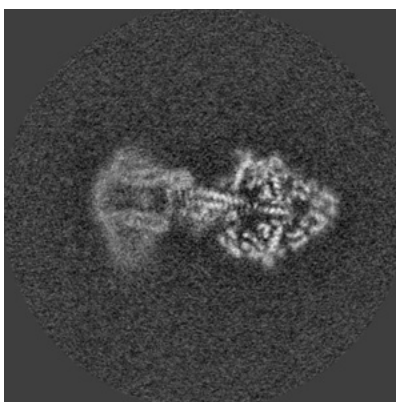


Z Index: 175

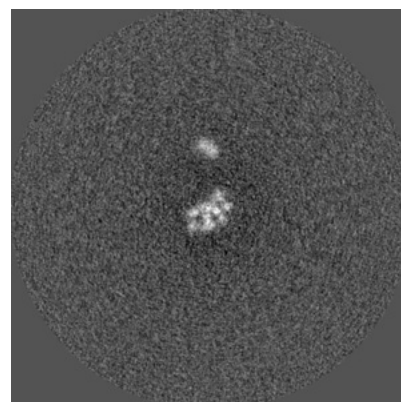
6.2.2 Raw map



X Index: 175



Y Index: 175

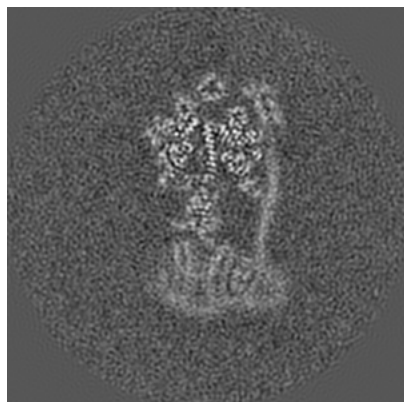


Z Index: 175

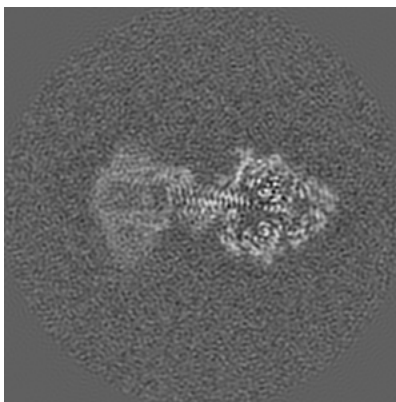
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

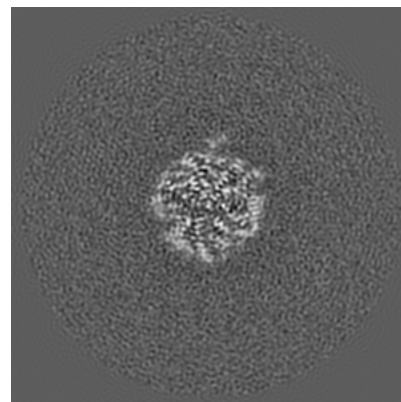
6.3.1 Primary map



X Index: 172

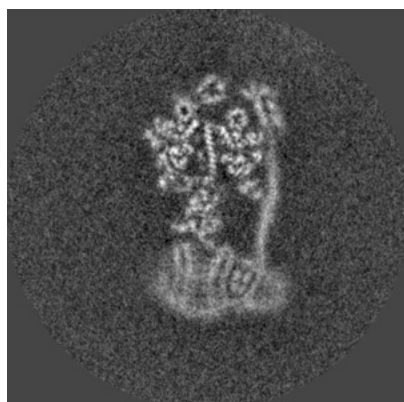


Y Index: 174

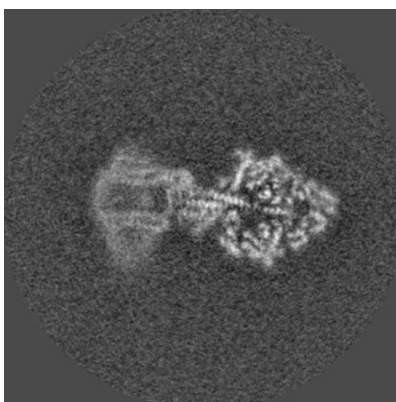


Z Index: 233

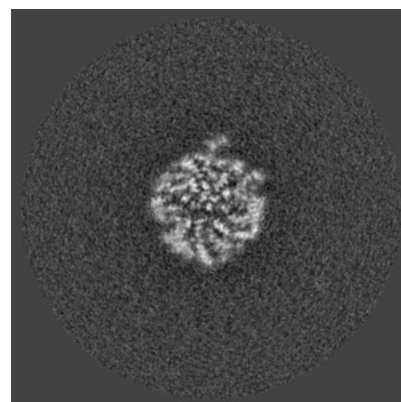
6.3.2 Raw map



X Index: 172



Y Index: 174

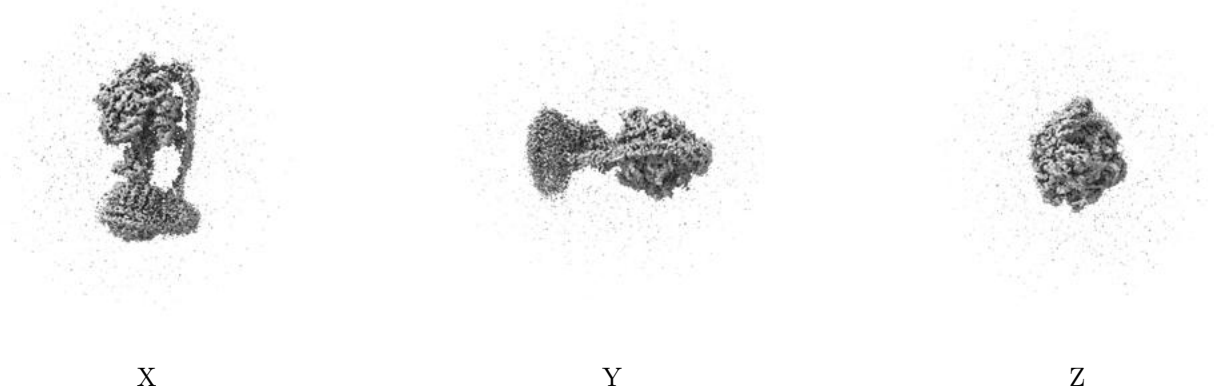


Z Index: 233

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

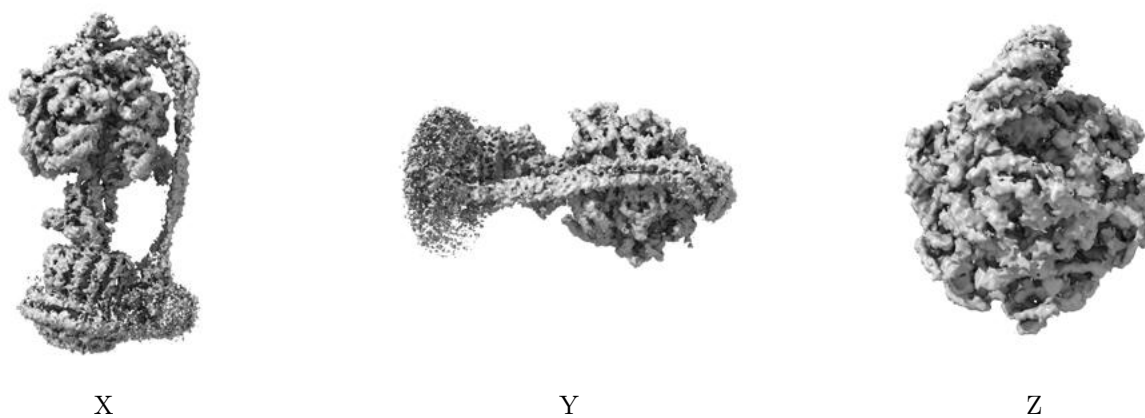
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

6.5 Mask visualisation [i](#)

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

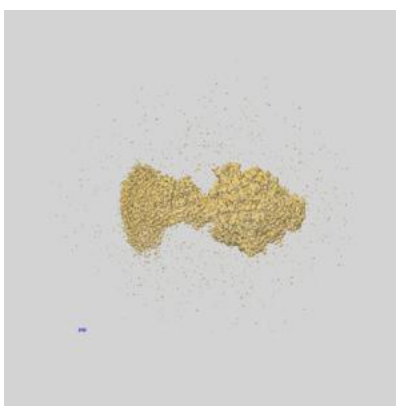
A mask typically either:

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

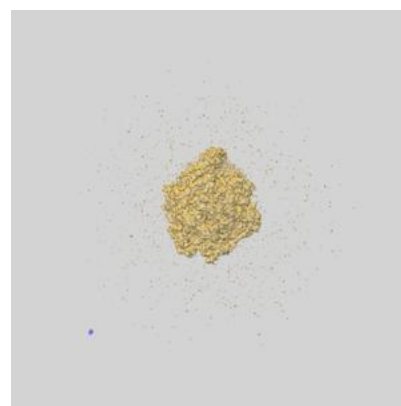
6.5.1 emd_4272_msk_1.map [i](#)



X



Y

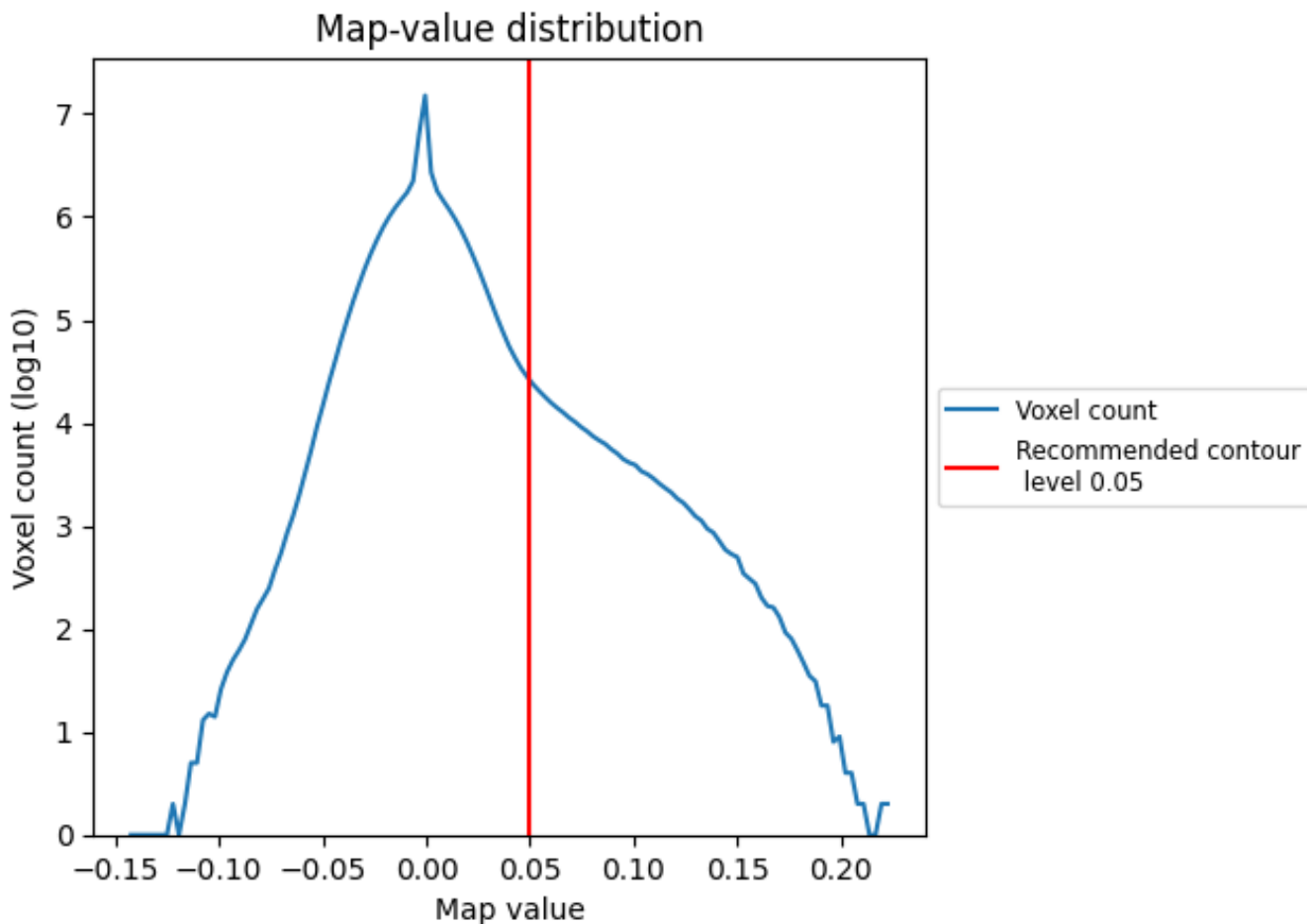


Z

7 Map analysis [i](#)

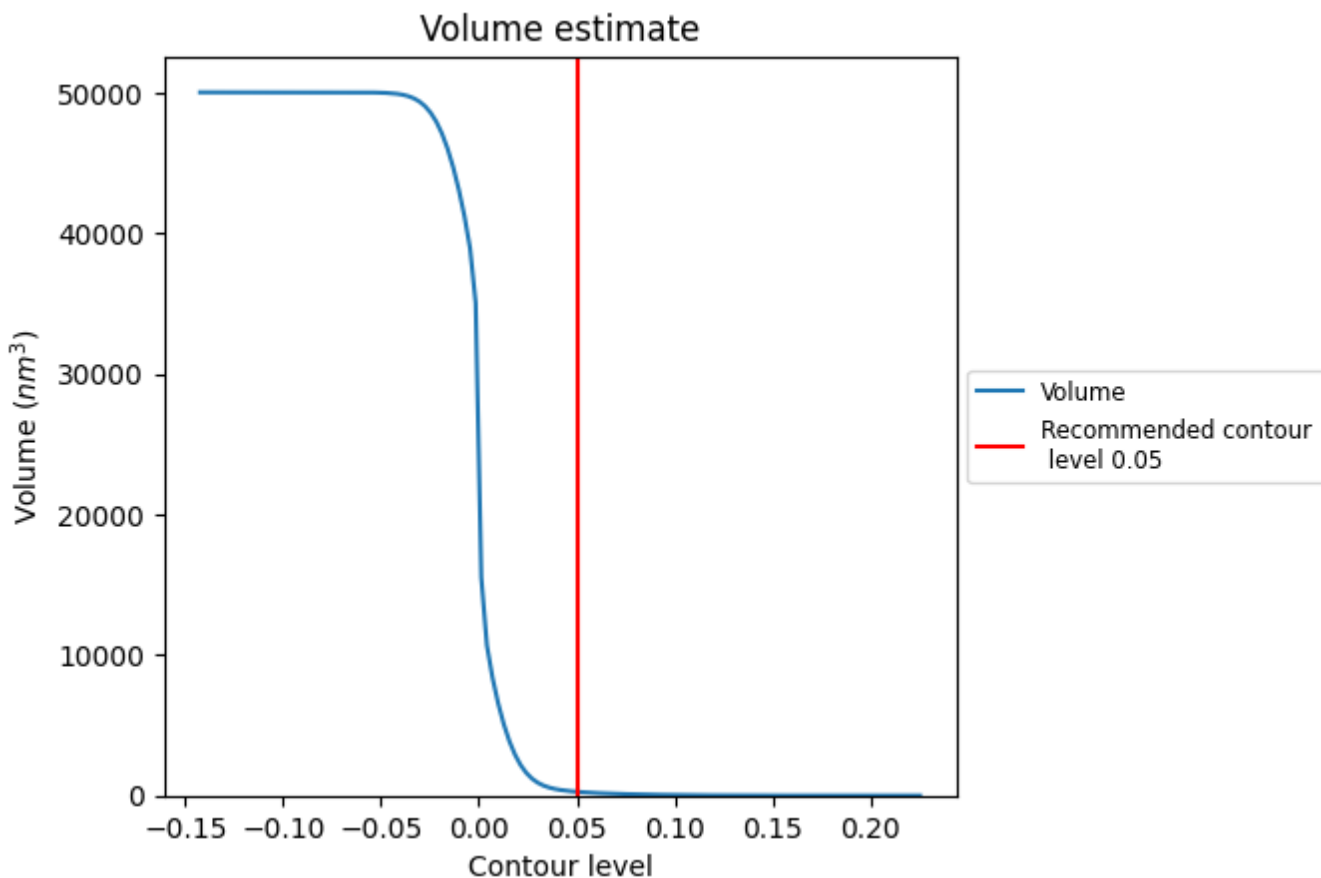
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

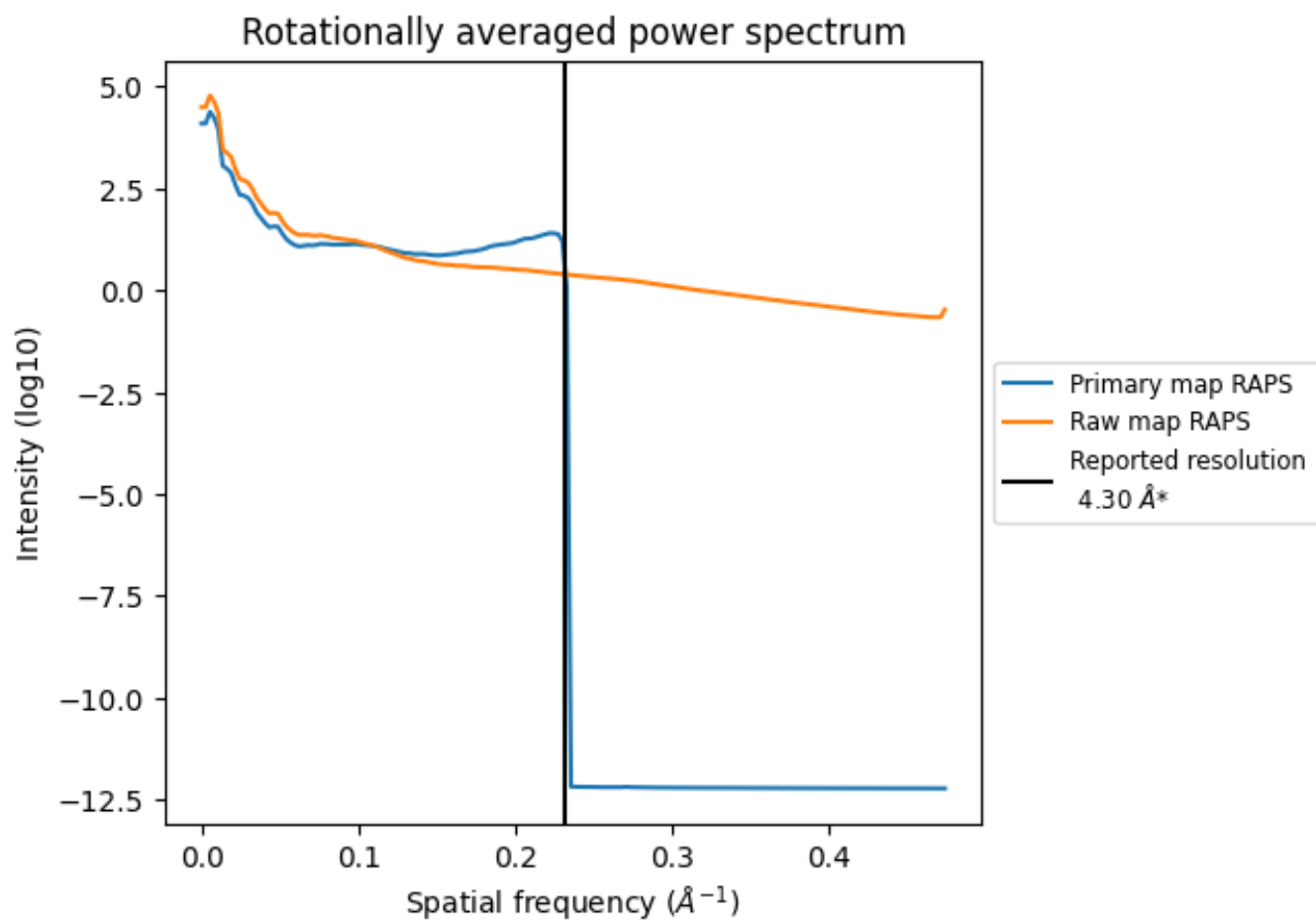
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 269 nm³; this corresponds to an approximate mass of 243 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](#)

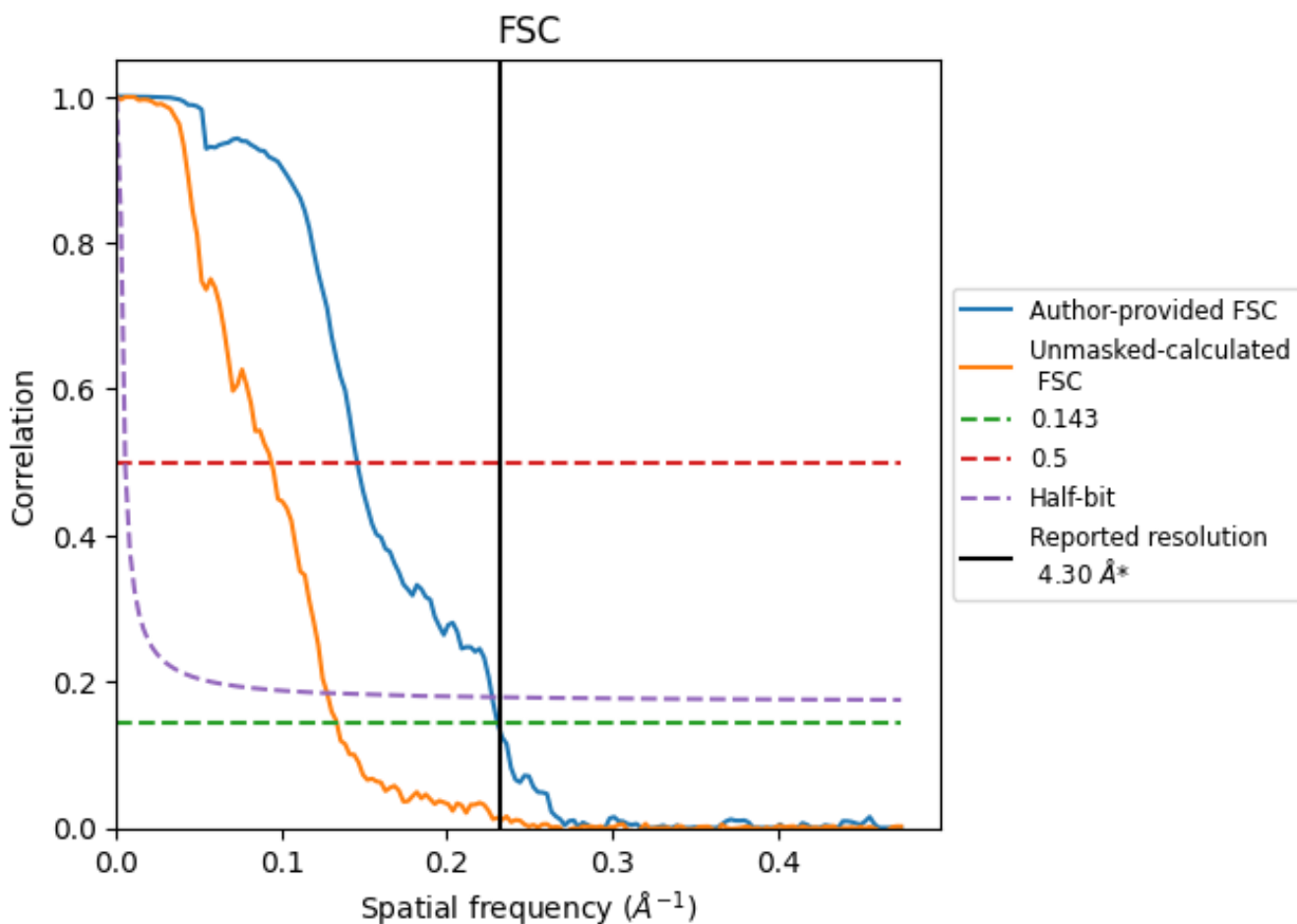


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

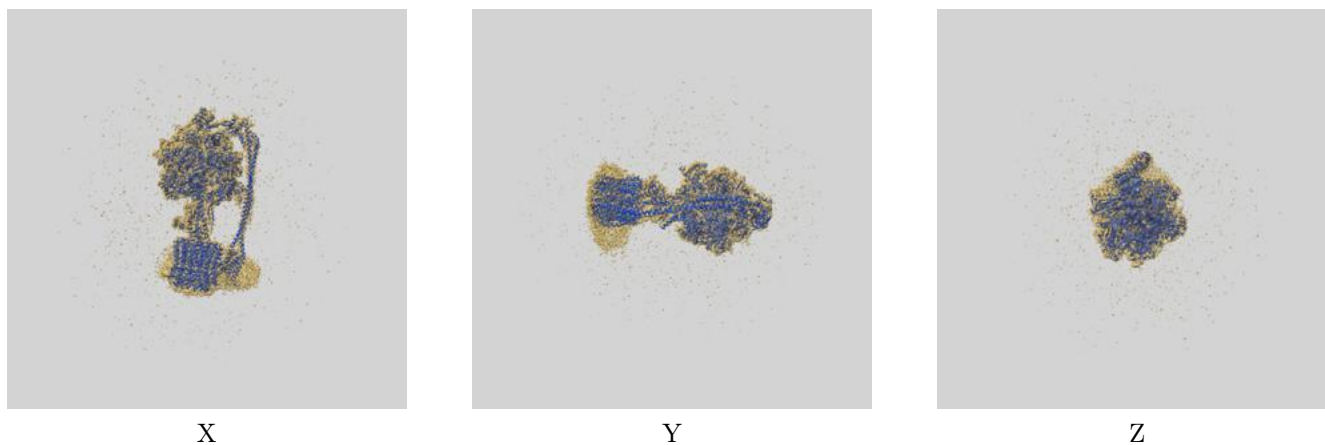
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.33	6.87	4.40
Unmasked-calculated*	7.50	10.68	7.84

*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 7.50 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

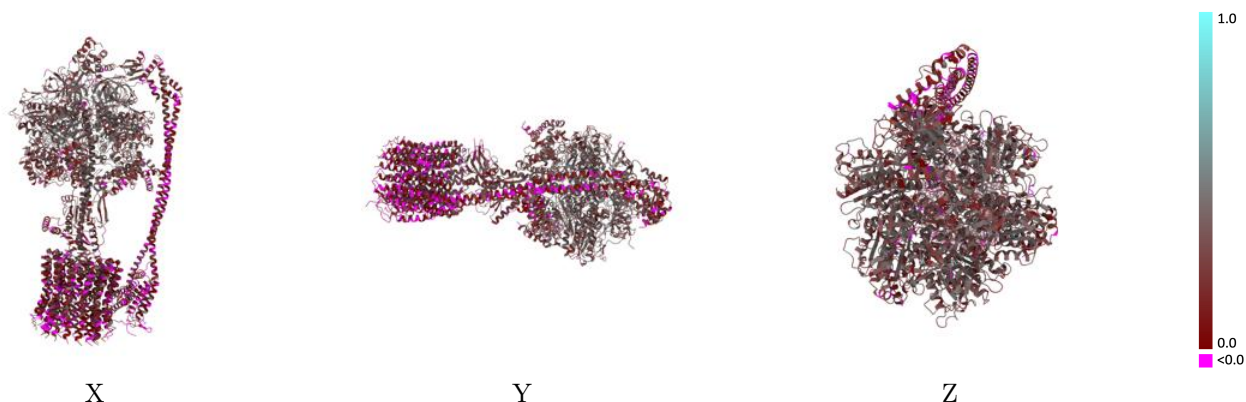
This section contains information regarding the fit between EMDB map EMD-4272 and PDB model 6FKI. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



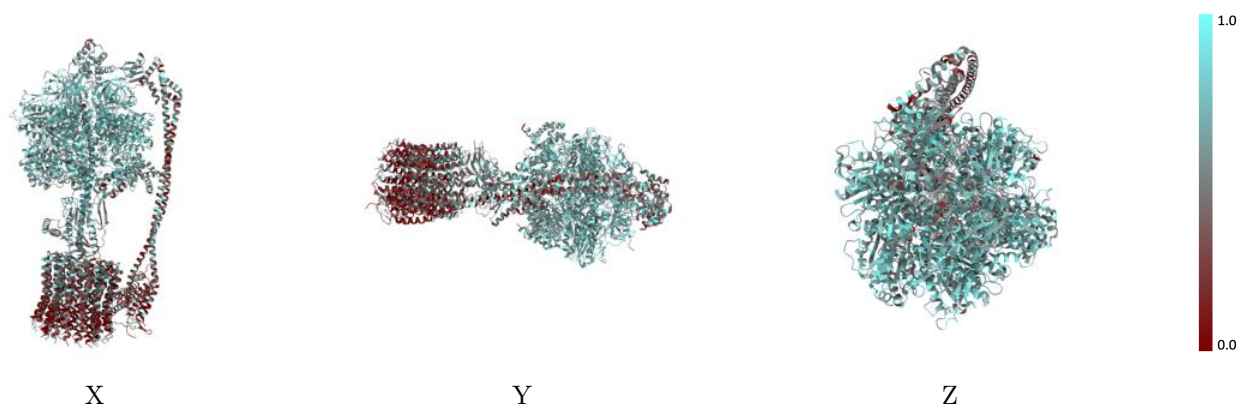
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



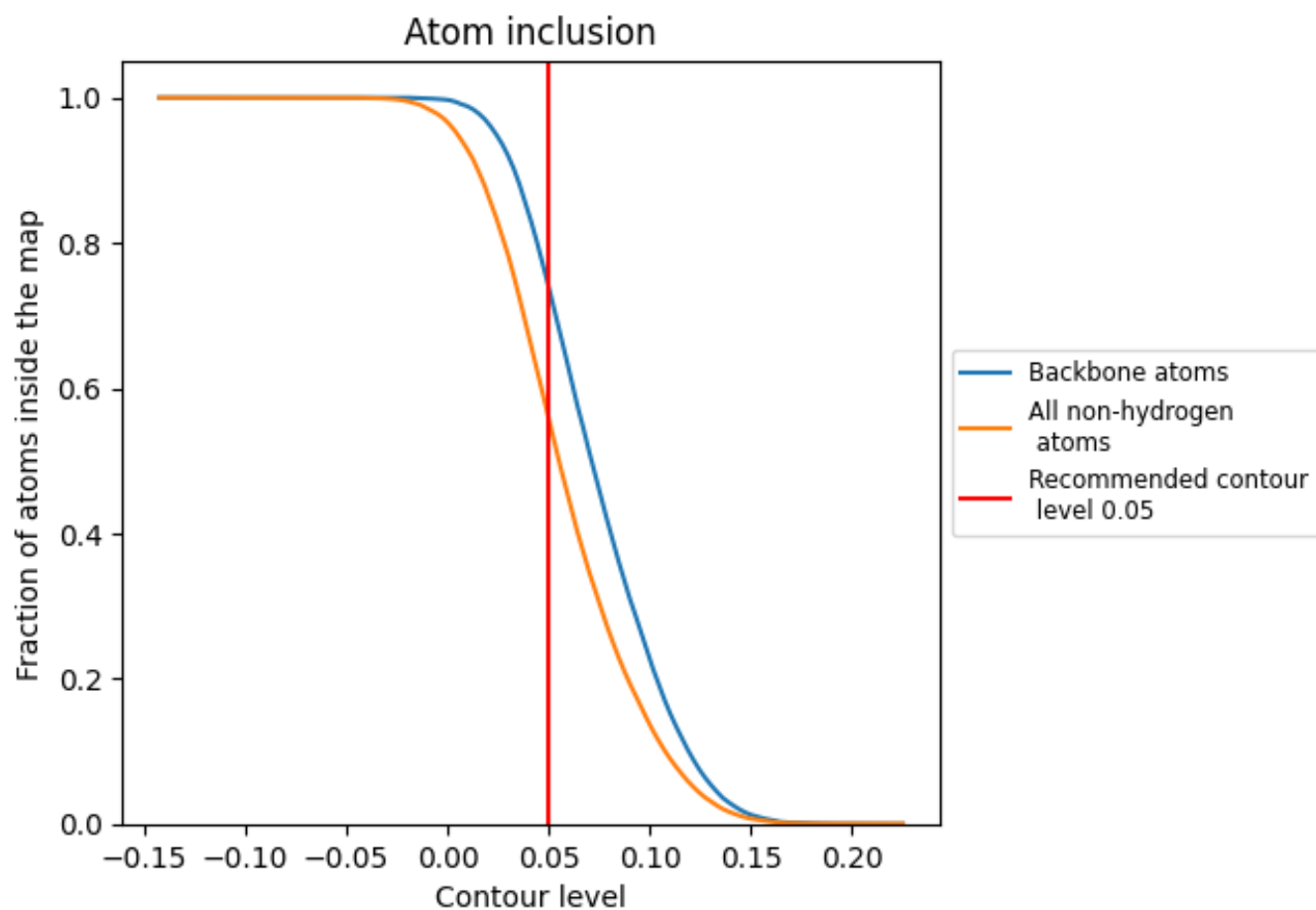
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 56% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5605	 0.2530
A	 0.6443	 0.3040
B	 0.6914	 0.3370
C	 0.6813	 0.3170
D	 0.7009	 0.3390
E	 0.6816	 0.3290
F	 0.6914	 0.3440
G	 0.3154	 0.1020
H	 0.3191	 0.1190
I	 0.3673	 0.1480
J	 0.3896	 0.1260
K	 0.3581	 0.1500
L	 0.3340	 0.1390
M	 0.3395	 0.1560
N	 0.3265	 0.1300
O	 0.3377	 0.1450
P	 0.3915	 0.1470
Q	 0.3340	 0.0960
R	 0.2412	 0.1100
S	 0.2653	 0.1010
T	 0.2672	 0.1140
a	 0.2849	 0.0850
b	 0.3611	 0.0810
d	 0.5472	 0.2520
e	 0.5375	 0.1940
g	 0.5880	 0.2630
p	 0.3654	 0.0900

