



wwPDB EM Validation Summary Report ⓘ

Oct 5, 2024 – 06:58 PM EDT

PDB ID : 6CP6
EMDB ID : EMD-7548
Title : Monomer yeast ATP synthase (F1Fo) reconstituted in nanodisc.
Authors : Srivastava, A.P.; Luo, M.; Symersky, J.; Liao, M.F.; Mueller, D.M.
Deposited on : 2018-03-13
Resolution : 3.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

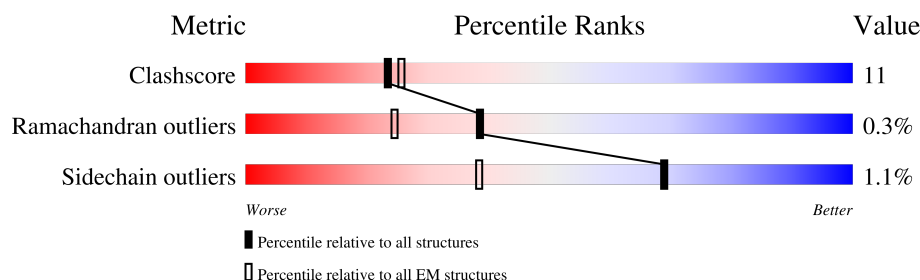
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





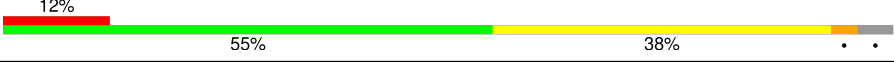

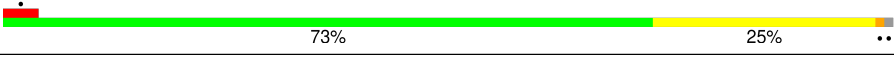
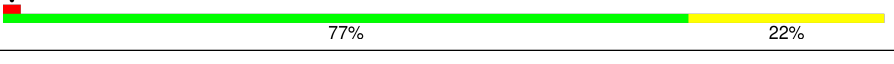
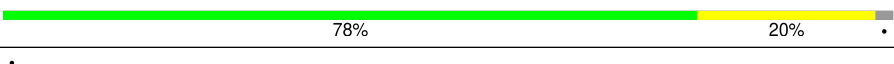

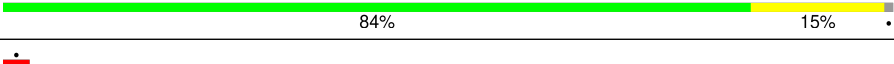

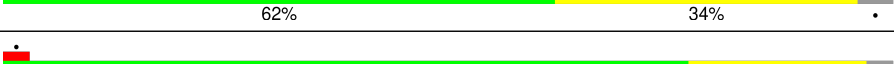
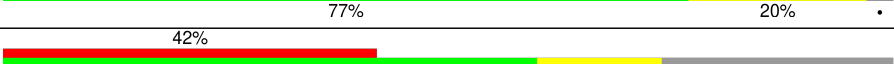



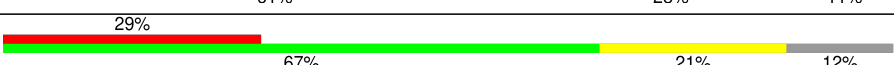

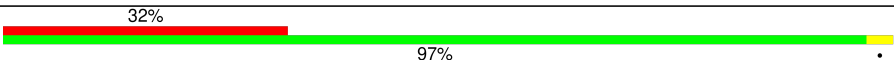

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	K	76	<div> <div>26%</div> <div>57%</div> <div>41%</div> <div>.</div> </div>
1	L	76	<div> <div>25%</div> <div>53%</div> <div>45%</div> <div>.</div> </div>
1	M	76	<div> <div>21%</div> <div>55%</div> <div>43%</div> <div>.</div> </div>
1	N	76	<div> <div>20%</div> <div>70%</div> <div>28%</div> <div>.</div> </div>
1	O	76	<div> <div>21%</div> <div>54%</div> <div>41%</div> <div>..</div> </div>
1	P	76	<div> <div>13%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
1	Q	76	<div> <div>28%</div> <div>74%</div> <div>24%</div> <div>.</div> </div>
1	R	76	<div> <div>57%</div> <div>51%</div> <div>45%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	S	76	
1	T	76	
2	Y	195	
3	A	510	
3	B	510	
3	C	510	
4	D	478	
4	E	478	
4	F	478	
5	G	278	
6	H	138	
7	I	61	
8	Z	209	
9	7	173	
10	6	92	
11	U	95	
12	8	48	
13	X	249	
14	J	37	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 38853 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 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	74	Total	C	N	O	S	0	0
			535	358	82	91	4		
1	L	74	Total	C	N	O	S	0	0
			532	356	82	91	3		
1	M	75	Total	C	N	O	S	0	0
			537	359	83	92	3		
1	N	74	Total	C	N	O	S	0	0
			529	353	82	91	3		
1	O	74	Total	C	N	O	S	0	0
			533	357	82	91	3		
1	P	74	Total	C	N	O	S	0	0
			535	358	82	91	4		
1	Q	74	Total	C	N	O	S	0	0
			523	347	82	91	3		
1	R	75	Total	C	N	O	S	0	0
			537	359	83	92	3		
1	S	74	Total	C	N	O	S	0	0
			532	356	82	91	3		
1	T	74	Total	C	N	O	S	0	0
			533	357	82	91	3		

- Molecule 2 is a protein called ATP synthase subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Y	188	Total	C	N	O	S	0	0
			1333	842	233	257	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	507	Total	C	N	O	S	0	0
			3858	2435	679	741	3		
3	B	505	Total	C	N	O	S	0	0
			3830	2417	676	734	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	508	Total	C	N	O	S	0	0
			3861	2437	680	741	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	470	Total	C	N	O	S	0	0
			3549	2250	604	689	6		
4	E	473	Total	C	N	O	S	0	0
			3572	2262	608	696	6		
4	F	472	Total	C	N	O	S	0	0
			3566	2259	607	694	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	269	Total	C	N	O	S	0	0
			2086	1309	362	405	10		

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

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

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

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

- Molecule 8 is a protein called ATP synthase subunit 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	155	Total	C	N	O	S	0	0
			1221	770	209	241	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	7	171	Total	C	N	O	S	0	0
			1357	852	235	267	3		

- Molecule 10 is a protein called ATP synthase subunit H, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	6	89	Total	C	N	O		0	0
			710	441	114	155			

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

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

- Molecule 12 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	8	42	Total	C	N	O	S	0	0
			364	256	52	53	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	X	224	Total	C	N	O	S	0	0
			1760	1203	261	286	10		

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

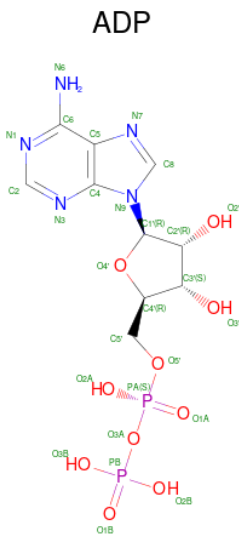
Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	37	Total	C	N	O	S	0	0
			292	197	45	48	2		

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 16 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).

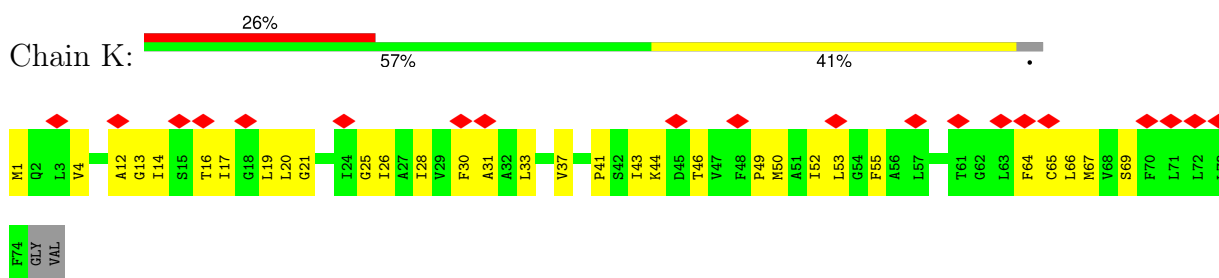


Mol	Chain	Residues	Atoms					AltConf
16	D	1	Total 27	C 10	N 5	O 10	P 2	0
16	F	1	Total 27	C 10	N 5	O 10	P 2	0

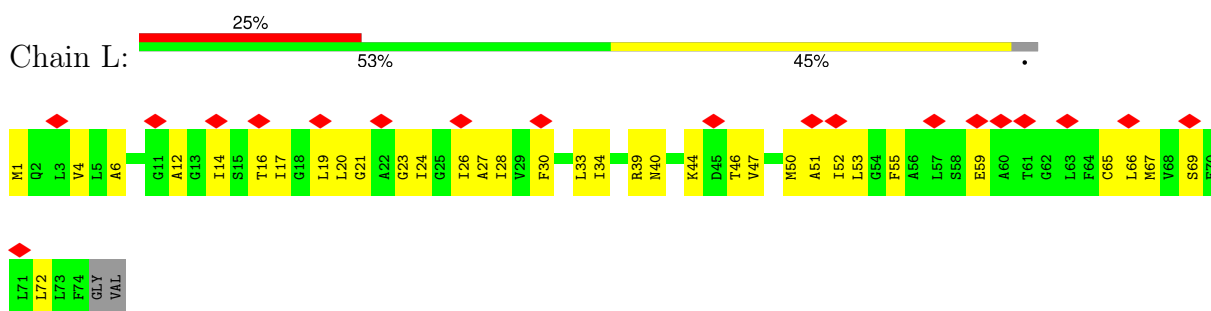
3 Residue-property plots [i](#)

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

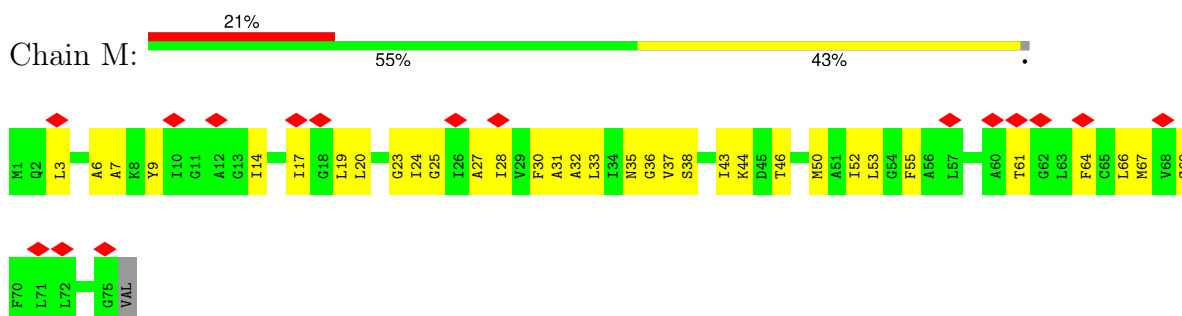
- Molecule 1: ATP synthase subunit 9, mitochondrial



- Molecule 1: ATP synthase subunit 9, mitochondrial

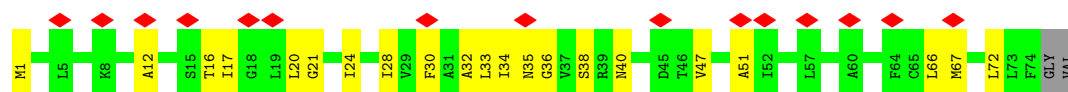


- Molecule 1: ATP synthase subunit 9, mitochondrial

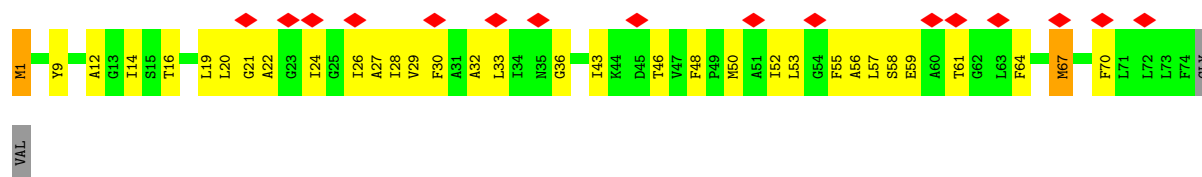


- Molecule 1: ATP synthase subunit 9, mitochondrial

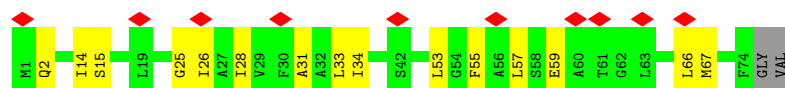
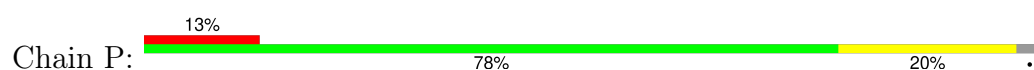




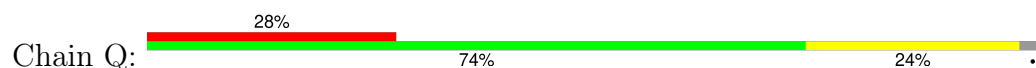
- Molecule 1: ATP synthase subunit 9, mitochondrial



- Molecule 1: ATP synthase subunit 9, mitochondrial



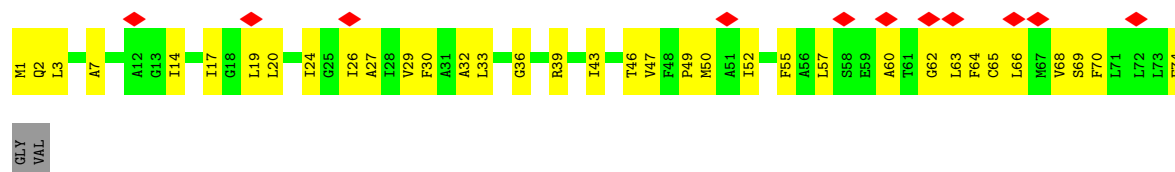
- Molecule 1: ATP synthase subunit 9, mitochondrial



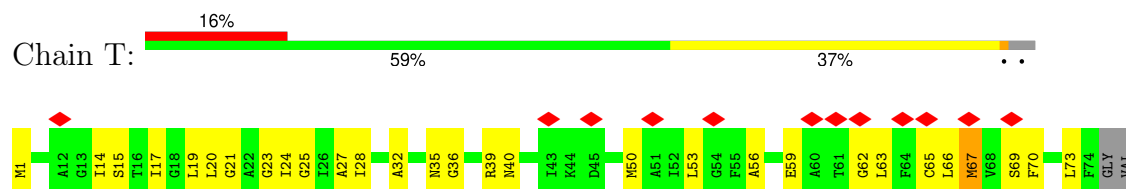
- Molecule 1: ATP synthase subunit 9, mitochondrial



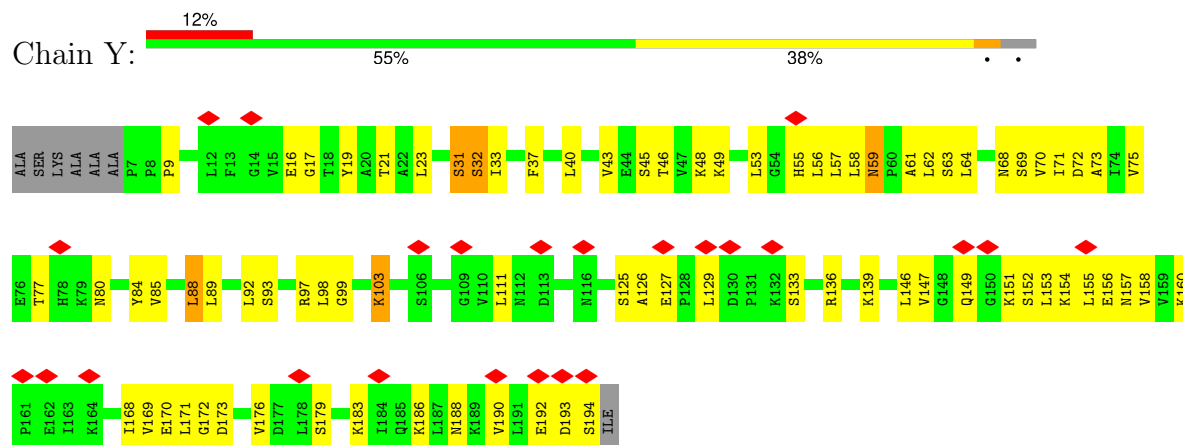
- Molecule 1: ATP synthase subunit 9, mitochondrial



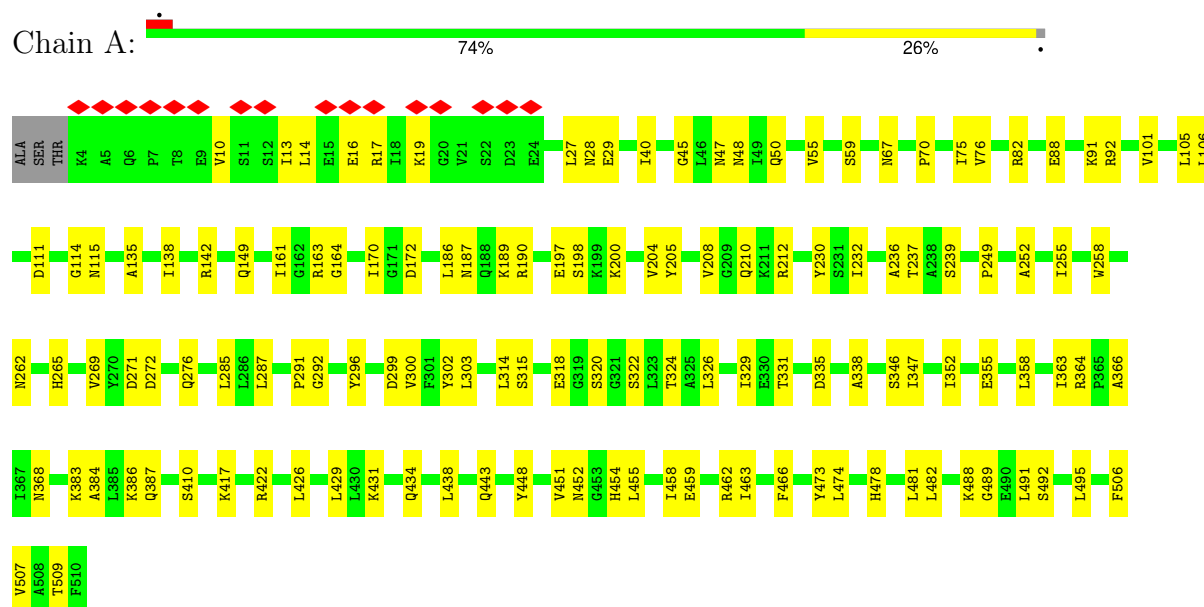
- Molecule 1: ATP synthase subunit 9, mitochondrial



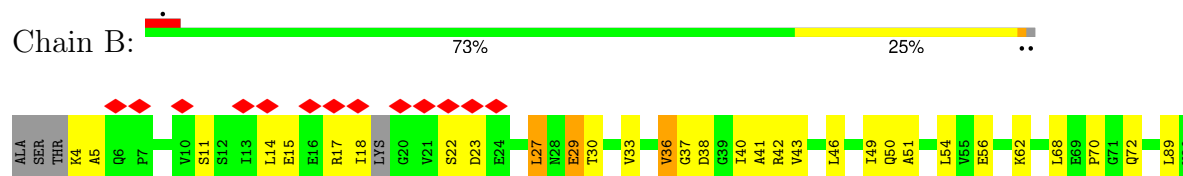
- Molecule 2: ATP synthase subunit 5, mitochondrial

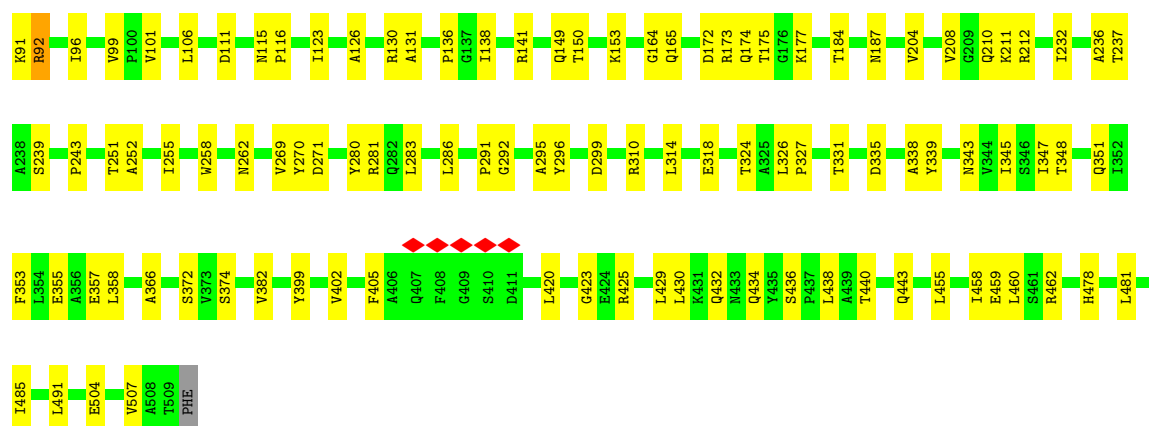


- Molecule 3: ATP synthase subunit alpha, mitochondrial

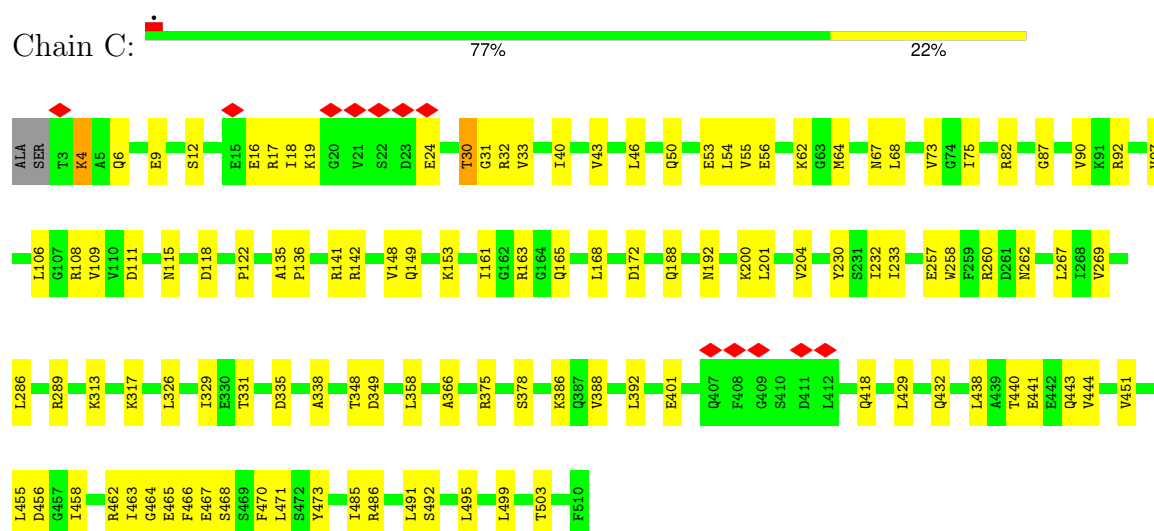


- Molecule 3: ATP synthase subunit alpha, mitochondrial

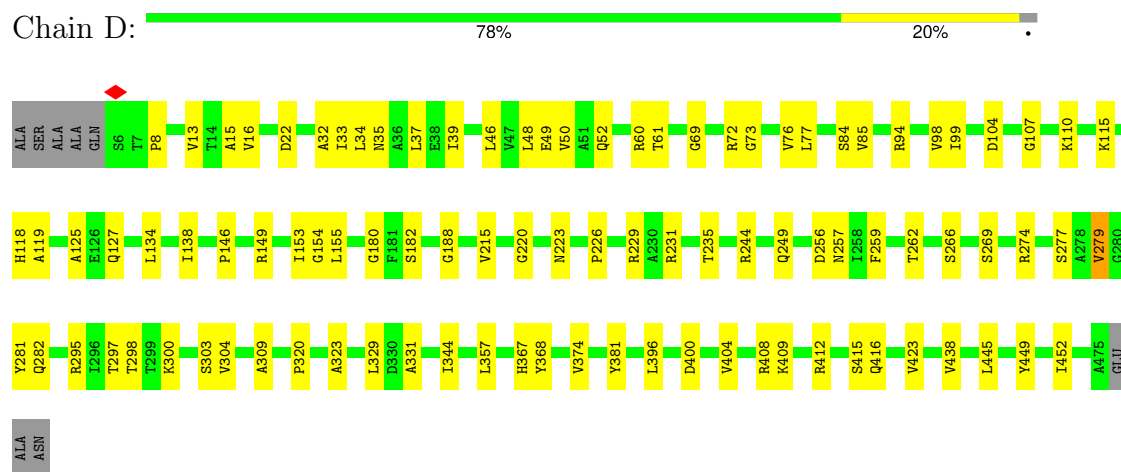




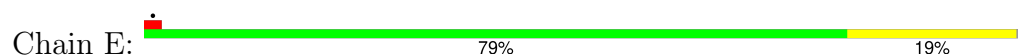
- Molecule 3: ATP synthase subunit alpha, mitochondrial

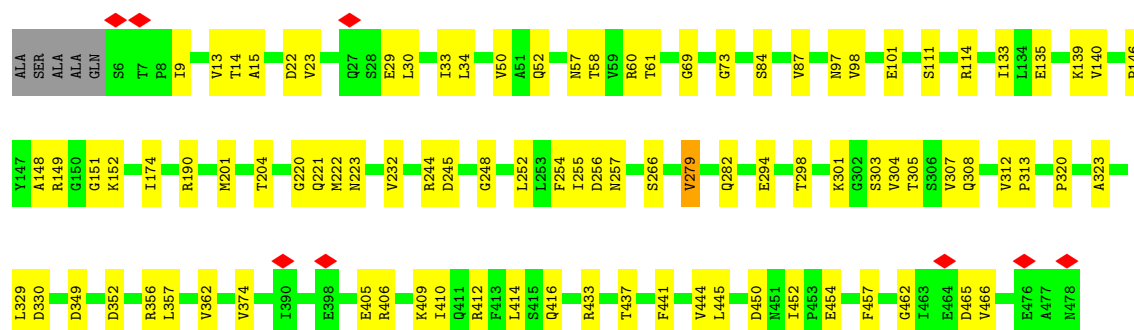


- Molecule 4: ATP synthase subunit beta, mitochondrial



- Molecule 4: ATP synthase subunit beta, mitochondrial





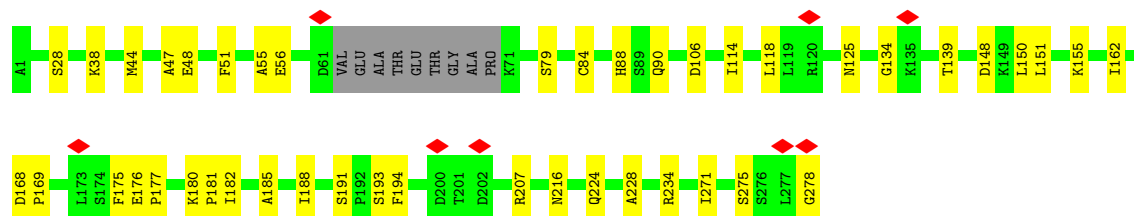
• Molecule 4: ATP synthase subunit beta, mitochondrial

Chain F: 84% 15%



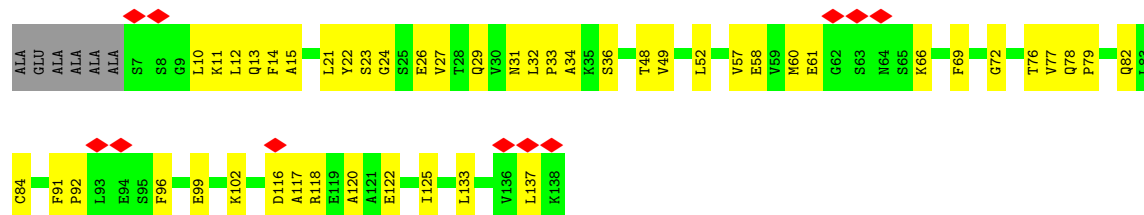
• Molecule 5: ATP synthase subunit gamma, mitochondrial

Chain G: 81% 16%



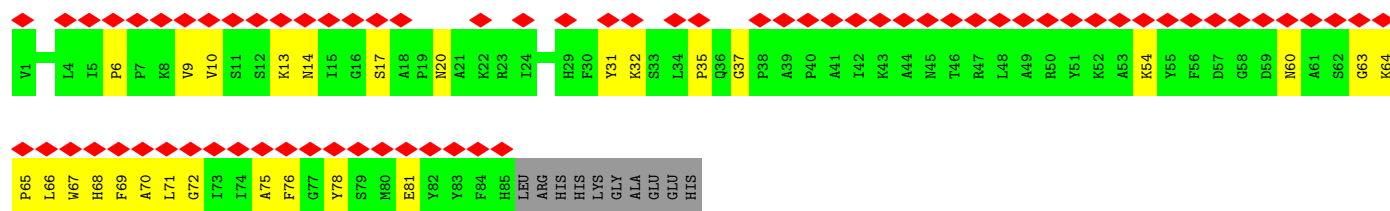
• Molecule 6: ATP synthase subunit delta, mitochondrial

Chain H: 8% 62% 34%

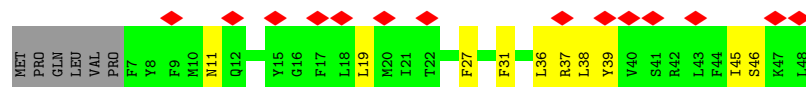


• Molecule 7: ATP synthase subunit epsilon, mitochondrial

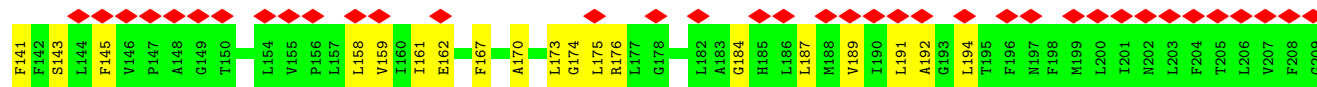
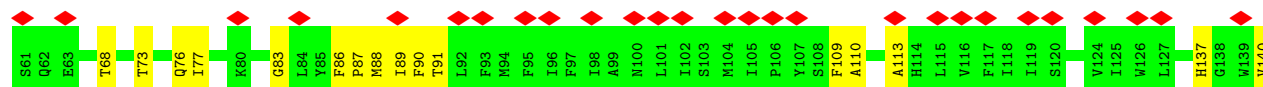
Chain I: 77% 20%



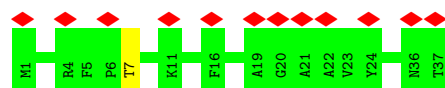
• Molecule 12: ATP synthase protein 8



• Molecule 13: ATP synthase subunit a



• Molecule 14: ATP synthase subunit J, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	160937	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.157	Depositor
Minimum map value	-0.065	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0218	Depositor
Map size (Å)	393.6, 393.6, 393.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.23, 1.23, 1.23	Depositor

5 Model quality

5.1 Standard geometry

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

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	K	0.32	0/533	0.62	0/722
1	L	0.35	0/533	0.72	0/722
1	M	0.34	0/537	0.71	0/727
1	N	0.32	0/530	0.68	0/718
1	O	0.34	0/533	0.69	0/722
1	P	0.33	0/533	0.69	0/722
1	Q	0.32	0/524	0.63	0/710
1	R	0.34	0/537	0.68	0/727
1	S	0.33	0/533	0.65	0/722
1	T	0.34	0/533	0.69	0/722
2	Y	0.35	0/1350	0.54	0/1833
3	A	0.40	0/3916	0.55	0/5298
3	B	0.40	0/3886	0.56	0/5259
3	C	0.40	0/3919	0.54	0/5303
4	D	0.41	0/3605	0.55	0/4889
4	E	0.38	0/3628	0.52	0/4919
4	F	0.41	0/3622	0.54	0/4911
5	G	0.34	0/2111	0.49	0/2838
6	H	0.32	0/1004	0.52	0/1359
7	I	0.30	0/398	0.47	0/547
8	Z	0.30	0/1235	0.51	0/1665
9	7	0.28	0/1376	0.57	0/1850
10	6	0.35	0/725	0.68	0/988
11	U	0.32	0/659	0.59	0/895
12	8	0.34	0/374	0.62	0/503
13	X	0.31	0/1808	0.58	0/2468
14	J	0.32	0/302	0.56	0/410
All	All	0.37	0/39244	0.56	0/53149

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	535	0	578	28	0
1	L	532	0	571	27	0
1	M	537	0	576	26	0
1	N	529	0	562	15	0
1	O	533	0	573	27	0
1	P	535	0	578	19	0
1	Q	523	0	544	18	0
1	R	537	0	576	30	0
1	S	532	0	571	33	0
1	T	533	0	573	25	0
2	Y	1333	0	1313	98	0
3	A	3858	0	3941	86	0
3	B	3830	0	3912	101	0
3	C	3861	0	3944	87	0
4	D	3549	0	3621	59	0
4	E	3572	0	3638	60	0
4	F	3566	0	3633	46	0
5	G	2086	0	2156	26	0
6	H	990	0	999	31	0
7	I	392	0	306	9	0
8	Z	1221	0	1230	33	0
9	7	1357	0	1376	27	0
10	6	710	0	668	34	0
11	U	639	0	615	17	0
12	8	364	0	390	8	0
13	X	1760	0	1849	38	0
14	J	292	0	298	1	0
15	A	31	0	12	1	0
15	B	31	0	12	4	0
15	C	31	0	12	0	0
16	D	27	0	12	2	0
16	F	27	0	12	0	0
All	All	38853	0	39651	848	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 11.

The worst 5 of 848 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)
3:B:29:GLU:CB	3:B:92:ARG:HG3	1.58	1.32
2:Y:57:LEU:HD11	2:Y:62:LEU:HD11	1.25	1.18
3:B:29:GLU:CB	3:B:92:ARG:CG	2.25	1.13
1:R:57:LEU:HD12	1:S:55:PHE:CZ	1.85	1.10
1:R:57:LEU:HD12	1:S:55:PHE:CE1	1.85	1.09

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	72/76 (95%)	66 (92%)	6 (8%)	0	100	100
1	L	72/76 (95%)	66 (92%)	6 (8%)	0	100	100
1	M	73/76 (96%)	68 (93%)	5 (7%)	0	100	100
1	N	72/76 (95%)	68 (94%)	4 (6%)	0	100	100
1	O	72/76 (95%)	67 (93%)	4 (6%)	1 (1%)	9	40
1	P	72/76 (95%)	69 (96%)	3 (4%)	0	100	100
1	Q	72/76 (95%)	71 (99%)	1 (1%)	0	100	100
1	R	73/76 (96%)	70 (96%)	3 (4%)	0	100	100
1	S	72/76 (95%)	67 (93%)	5 (7%)	0	100	100
1	T	72/76 (95%)	66 (92%)	6 (8%)	0	100	100
2	Y	186/195 (95%)	160 (86%)	25 (13%)	1 (0%)	25	59
3	A	505/510 (99%)	484 (96%)	21 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	501/510 (98%)	474 (95%)	25 (5%)	2 (0%)	30	63
3	C	506/510 (99%)	484 (96%)	22 (4%)	0	100	100
4	D	468/478 (98%)	449 (96%)	17 (4%)	2 (0%)	30	63
4	E	471/478 (98%)	449 (95%)	21 (4%)	1 (0%)	44	73
4	F	470/478 (98%)	452 (96%)	15 (3%)	3 (1%)	22	55
5	G	265/278 (95%)	253 (96%)	12 (4%)	0	100	100
6	H	130/138 (94%)	119 (92%)	10 (8%)	1 (1%)	16	51
7	I	57/61 (93%)	55 (96%)	2 (4%)	0	100	100
8	Z	153/209 (73%)	150 (98%)	3 (2%)	0	100	100
9	7	169/173 (98%)	154 (91%)	13 (8%)	2 (1%)	11	43
10	6	87/92 (95%)	68 (78%)	17 (20%)	2 (2%)	5	31
11	U	83/95 (87%)	74 (89%)	8 (10%)	1 (1%)	11	43
12	8	40/48 (83%)	38 (95%)	2 (5%)	0	100	100
13	X	222/249 (89%)	202 (91%)	20 (9%)	0	100	100
14	J	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
All	All	5070/5299 (96%)	4775 (94%)	279 (6%)	16 (0%)	38	67

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	279	VAL
4	E	279	VAL
1	O	57	LEU
9	7	170	LEU
2	Y	32	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	54/55 (98%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	54/55 (98%)	53 (98%)	1 (2%)	52	73
1	M	54/55 (98%)	53 (98%)	1 (2%)	52	73
1	N	53/55 (96%)	51 (96%)	2 (4%)	28	57
1	O	54/55 (98%)	53 (98%)	1 (2%)	52	73
1	P	54/55 (98%)	52 (96%)	2 (4%)	29	58
1	Q	51/55 (93%)	49 (96%)	2 (4%)	27	57
1	R	54/55 (98%)	52 (96%)	2 (4%)	29	58
1	S	54/55 (98%)	53 (98%)	1 (2%)	52	73
1	T	54/55 (98%)	53 (98%)	1 (2%)	52	73
2	Y	135/164 (82%)	128 (95%)	7 (5%)	19	49
3	A	410/412 (100%)	409 (100%)	1 (0%)	92	96
3	B	406/412 (98%)	401 (99%)	5 (1%)	67	82
3	C	410/412 (100%)	400 (98%)	10 (2%)	44	67
4	D	380/384 (99%)	379 (100%)	1 (0%)	91	96
4	E	382/384 (100%)	381 (100%)	1 (0%)	91	96
4	F	381/384 (99%)	380 (100%)	1 (0%)	91	96
5	G	230/236 (98%)	230 (100%)	0	100	100
6	H	111/112 (99%)	111 (100%)	0	100	100
7	I	25/48 (52%)	25 (100%)	0	100	100
8	Z	134/182 (74%)	133 (99%)	1 (1%)	81	90
9	7	152/158 (96%)	150 (99%)	2 (1%)	65	81
10	6	79/82 (96%)	77 (98%)	2 (2%)	42	66
11	U	60/76 (79%)	60 (100%)	0	100	100
12	8	41/47 (87%)	41 (100%)	0	100	100
13	X	190/217 (88%)	190 (100%)	0	100	100
14	J	30/30 (100%)	30 (100%)	0	100	100
All	All	4092/4290 (95%)	4048 (99%)	44 (1%)	69	83

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	9	GLU
3	C	317	LYS

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Mol	Chain	Res	Type
3	C	12	SER
3	C	24	GLU
4	E	149	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
4	F	379	GLN
9	7	123	ASN
5	G	100	ASN
6	H	51	GLN
10	6	27	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	FME	M	1	1	6,7,10	1.06	0	7,7,11	1.07	0
1	FME	Q	1	1	5,6,10	1.31	0	4,6,11	1.45	1 (25%)
1	FME	L	1	1	5,6,10	1.38	1 (20%)	4,6,11	1.30	1 (25%)
1	FME	S	1	1	5,6,10	1.36	1 (20%)	4,6,11	1.52	1 (25%)
1	FME	T	1	1	6,7,10	1.05	0	7,7,11	1.28	1 (14%)
1	FME	N	1	1	5,6,10	1.36	1 (20%)	4,6,11	1.60	1 (25%)
1	FME	K	1	1	8,9,10	0.95	0	8,9,11	0.85	0
1	FME	O	1	1	6,7,10	1.04	0	7,7,11	1.22	1 (14%)
1	FME	R	1	1	6,7,10	1.02	0	7,7,11	1.30	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	P	1	1	8,9,10	0.98	0	8,9,11	0.89	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	M	1	1	-	2/5/7/11	-
1	FME	Q	1	1	-	1/3/5/11	-
1	FME	L	1	1	-	0/3/5/11	-
1	FME	S	1	1	-	0/3/5/11	-
1	FME	T	1	1	-	3/5/7/11	-
1	FME	N	1	1	-	0/3/5/11	-
1	FME	K	1	1	-	3/7/9/11	-
1	FME	O	1	1	-	2/5/7/11	-
1	FME	R	1	1	-	3/5/7/11	-
1	FME	P	1	1	-	2/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	1	FME	CA-N	-2.28	1.44	1.46
1	S	1	FME	CA-N	-2.27	1.44	1.46
1	N	1	FME	CA-N	-2.27	1.44	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	CB-CA-N	3.03	113.10	109.68
1	S	1	FME	CB-CA-N	2.83	112.87	109.68
1	Q	1	FME	CB-CA-N	2.56	112.56	109.68
1	L	1	FME	CB-CA-N	2.43	112.43	109.68
1	R	1	FME	CB-CA-C	-2.21	107.29	112.62

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	M	1	FME	CB-CA-N-CN

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Mol	Chain	Res	Type	Atoms
1	O	1	FME	C-CA-CB-CG
1	P	1	FME	N-CA-CB-CG
1	Q	1	FME	O-C-CA-CB
1	R	1	FME	N-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	K	1	FME	1	0
1	O	1	FME	1	0
1	R	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	ATP	A	600	-	28,33,33	0.79	0	34,52,52	1.23	2 (5%)
16	ADP	D	600	-	24,29,29	0.81	0	29,45,45	1.22	1 (3%)
15	ATP	C	600	-	28,33,33	0.78	0	34,52,52	1.26	2 (5%)
15	ATP	B	600	-	28,33,33	0.76	0	34,52,52	1.22	2 (5%)
16	ADP	F	600	-	24,29,29	0.81	0	29,45,45	1.23	1 (3%)

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
15	ATP	A	600	-	-	2/18/38/38	0/3/3/3
16	ADP	D	600	-	-	5/12/32/32	0/3/3/3
15	ATP	C	600	-	-	2/18/38/38	0/3/3/3
15	ATP	B	600	-	-	2/18/38/38	0/3/3/3
16	ADP	F	600	-	-	5/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	600	ATP	N3-C2-N1	-3.87	123.42	128.67
16	D	600	ADP	N3-C2-N1	-3.85	123.44	128.67
15	A	600	ATP	N3-C2-N1	-3.66	123.71	128.67
16	F	600	ADP	N3-C2-N1	-3.61	123.77	128.67
15	C	600	ATP	N3-C2-N1	-3.57	123.83	128.67

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	B	600	ATP	C5'-O5'-PA-O3A
16	D	600	ADP	C5'-O5'-PA-O1A
16	D	600	ADP	C5'-O5'-PA-O3A
16	F	600	ADP	C5'-O5'-PA-O1A
16	F	600	ADP	C5'-O5'-PA-O3A

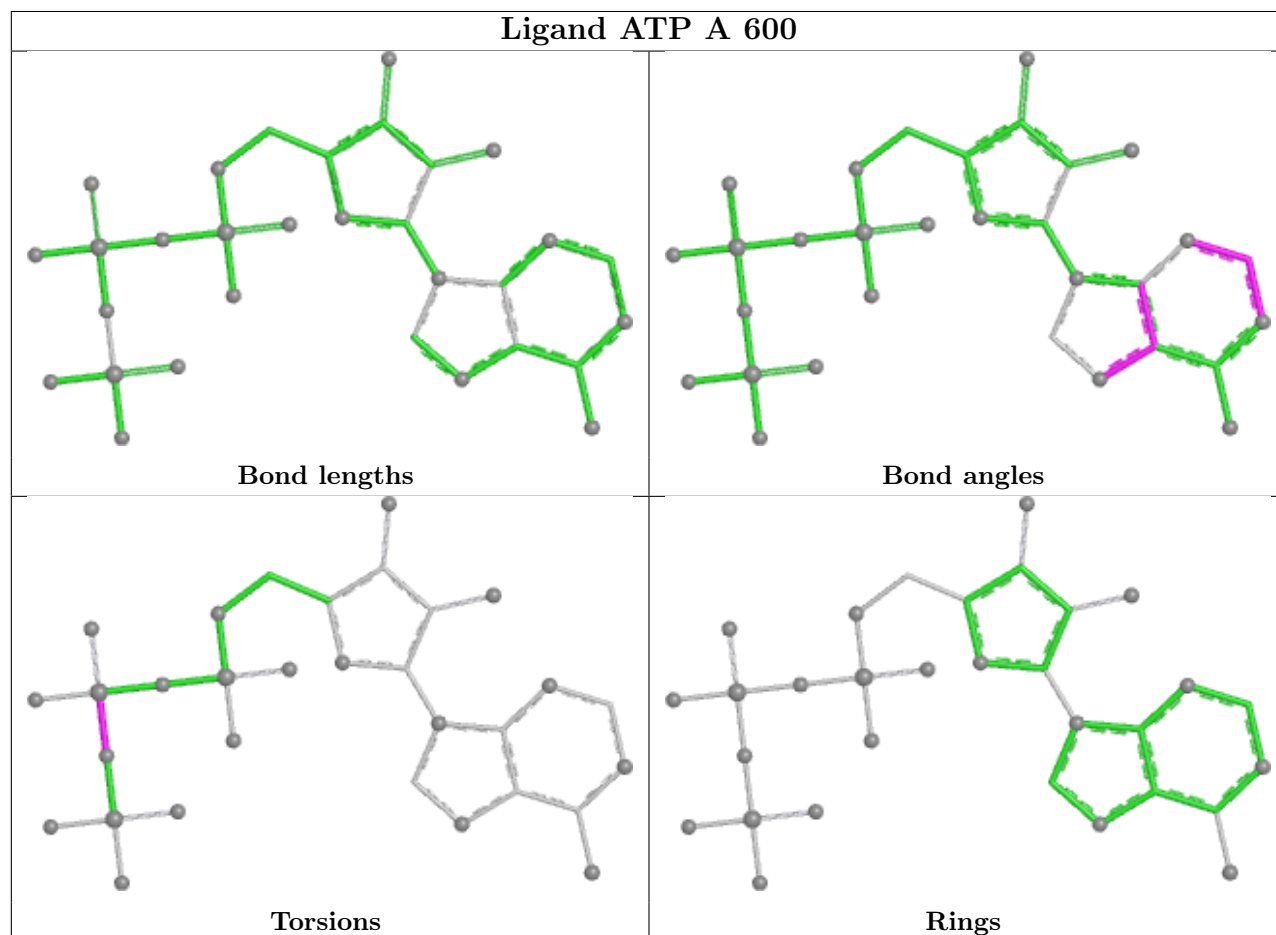
There are no ring outliers.

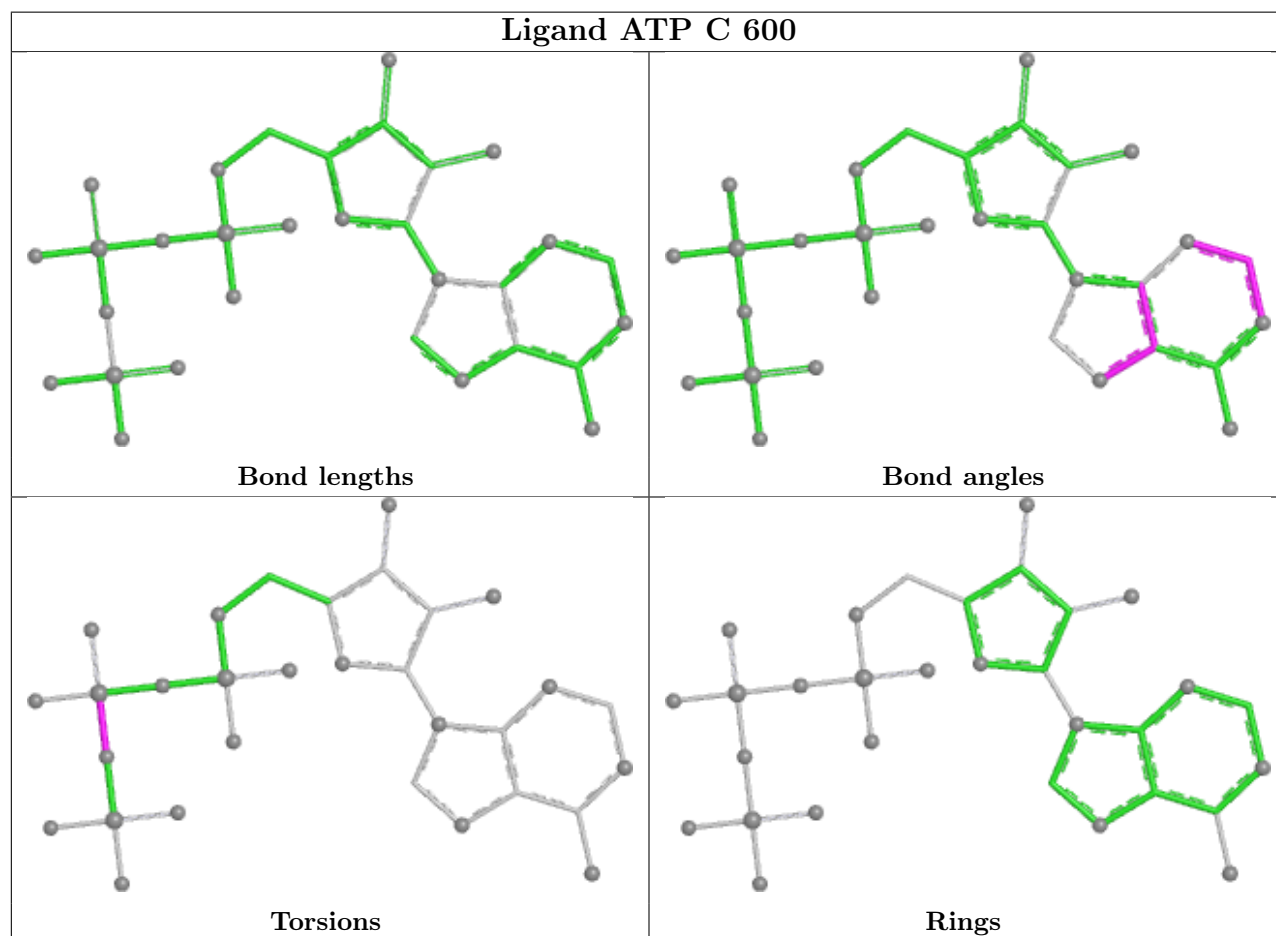
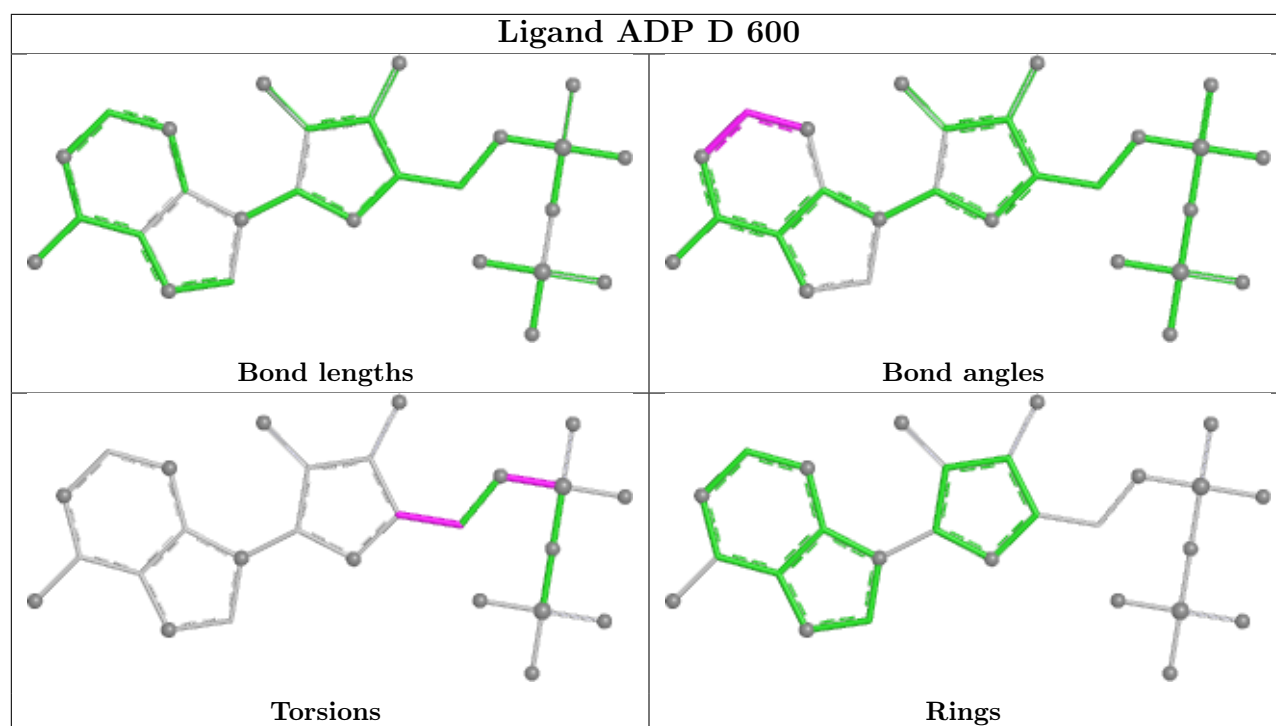
3 monomers are involved in 7 short contacts:

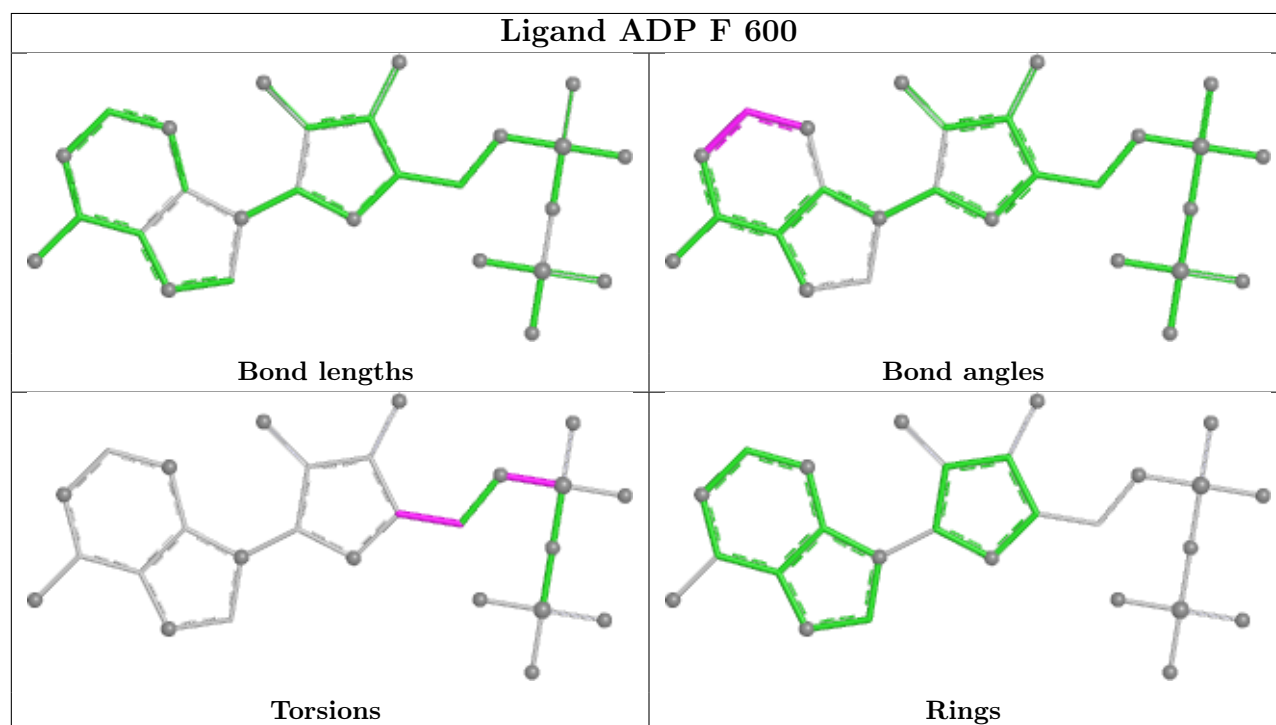
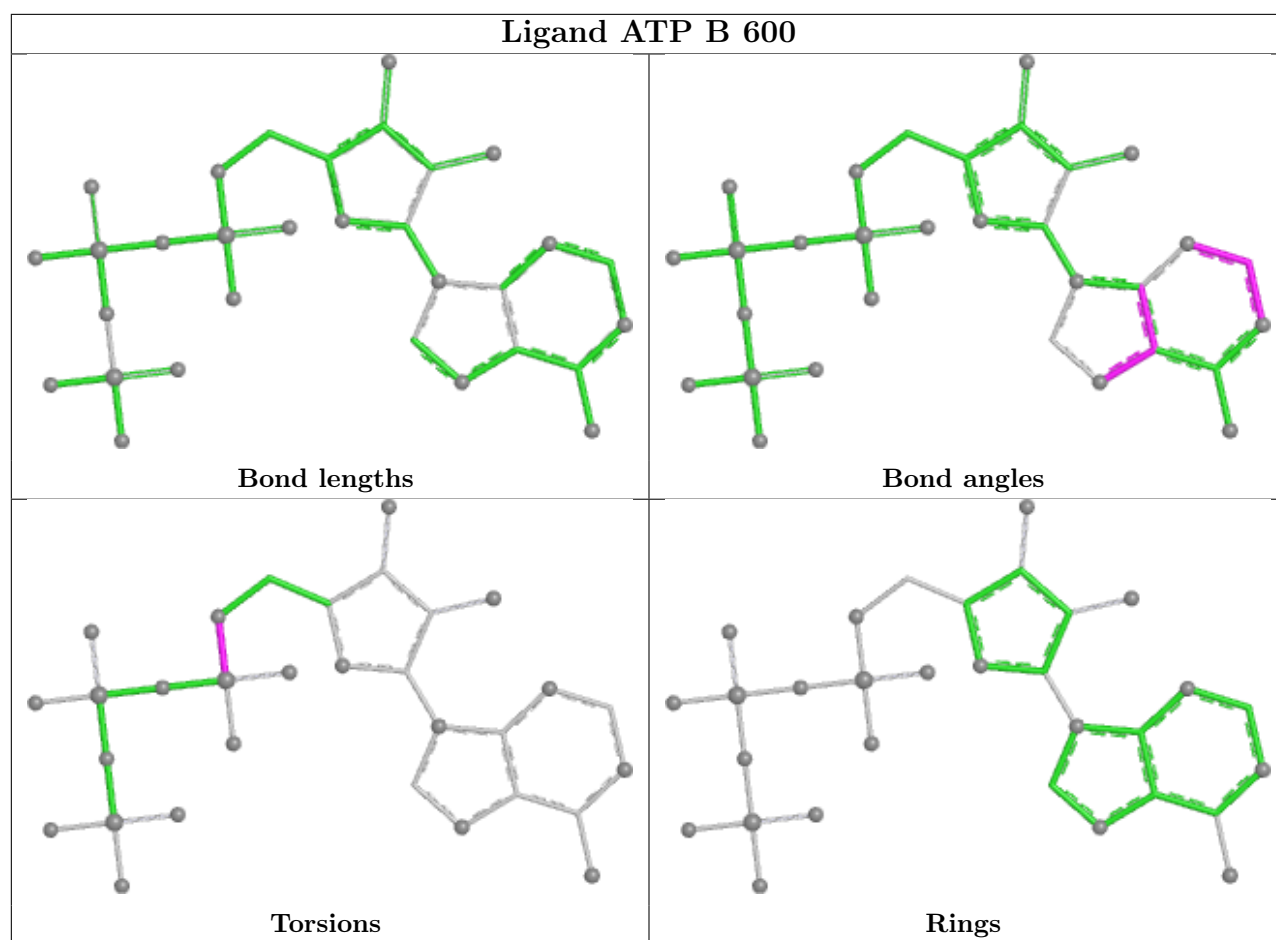
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	600	ATP	1	0
16	D	600	ADP	2	0
15	B	600	ATP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

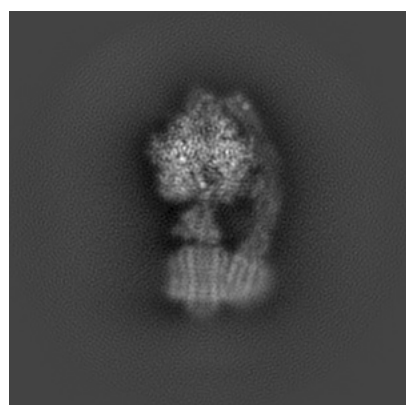
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7548. These allow visual inspection of the internal detail of the map and identification of artifacts.

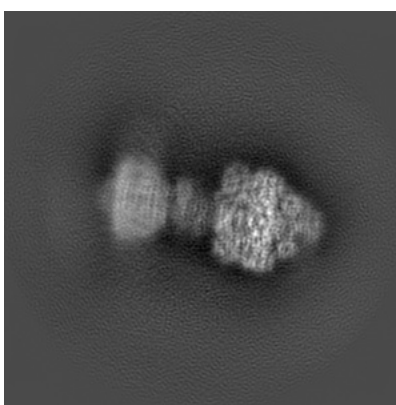
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

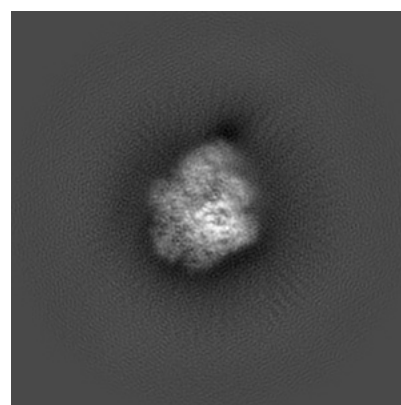
6.1.1 Primary map



X



Y

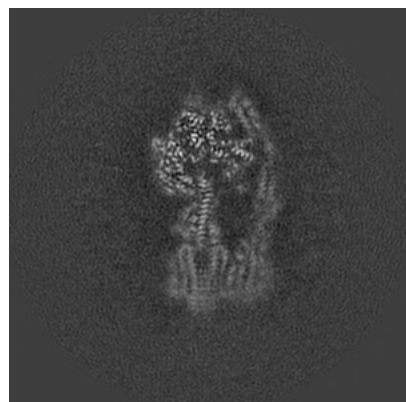


Z

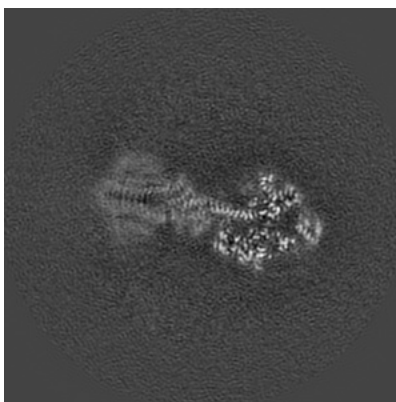
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

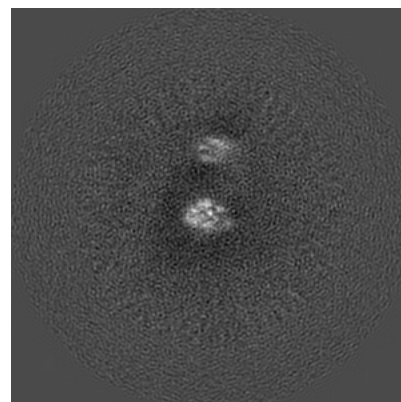
6.2.1 Primary map



X Index: 160



Y Index: 160

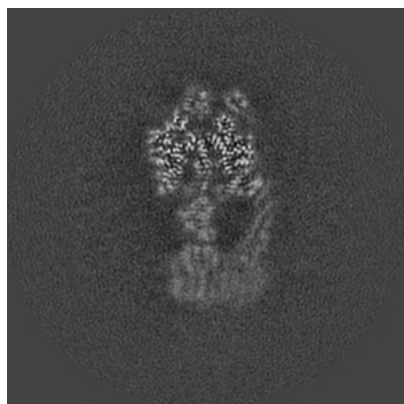


Z Index: 160

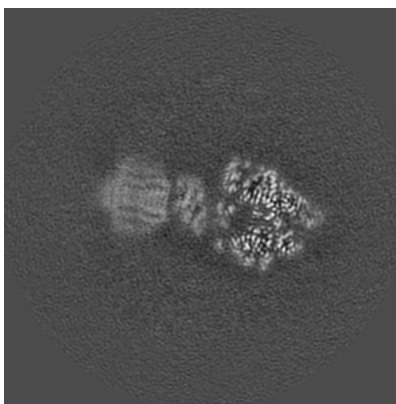
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

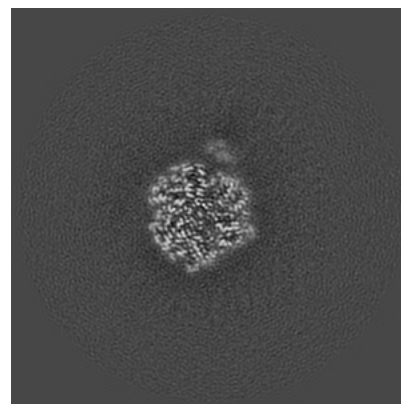
6.3.1 Primary map



X Index: 151



Y Index: 145

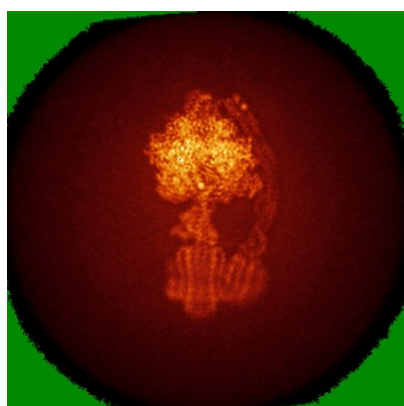


Z Index: 207

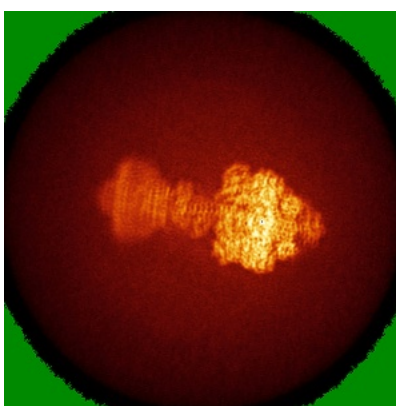
The images above show the largest variance slices of the map in three orthogonal directions.

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

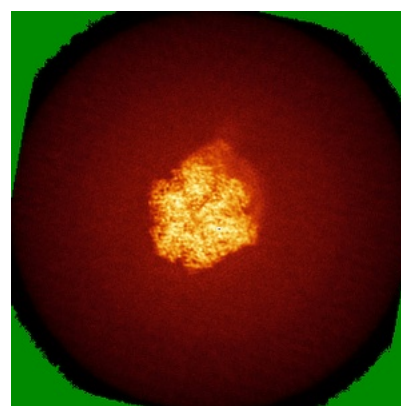
6.4.1 Primary map



X



Y

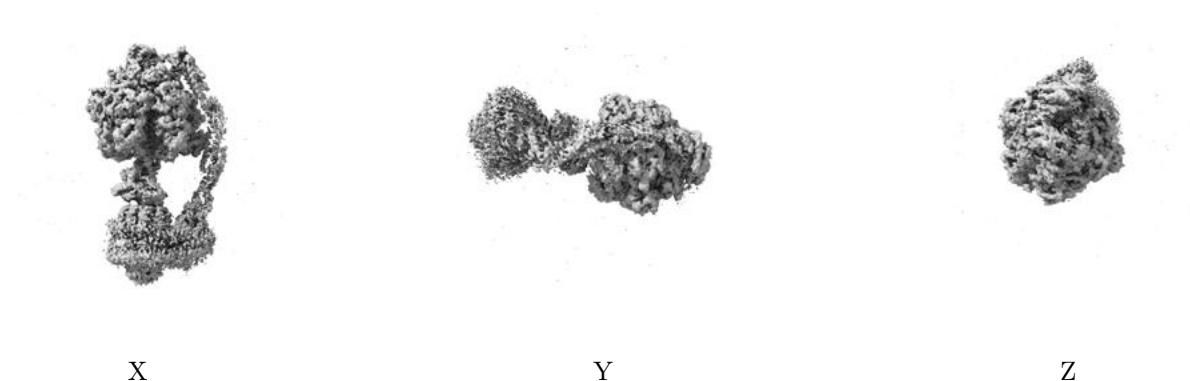


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0218. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

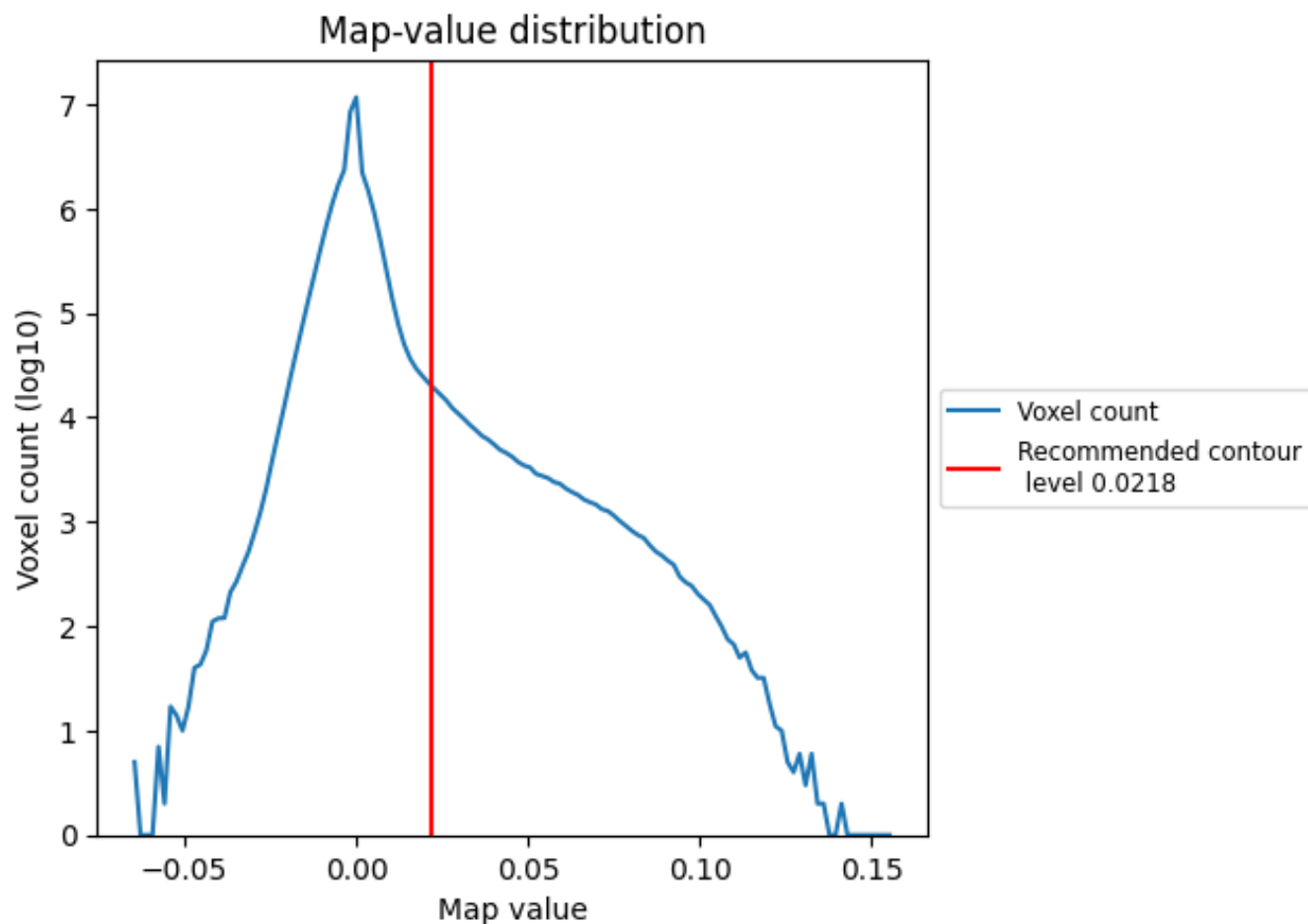
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

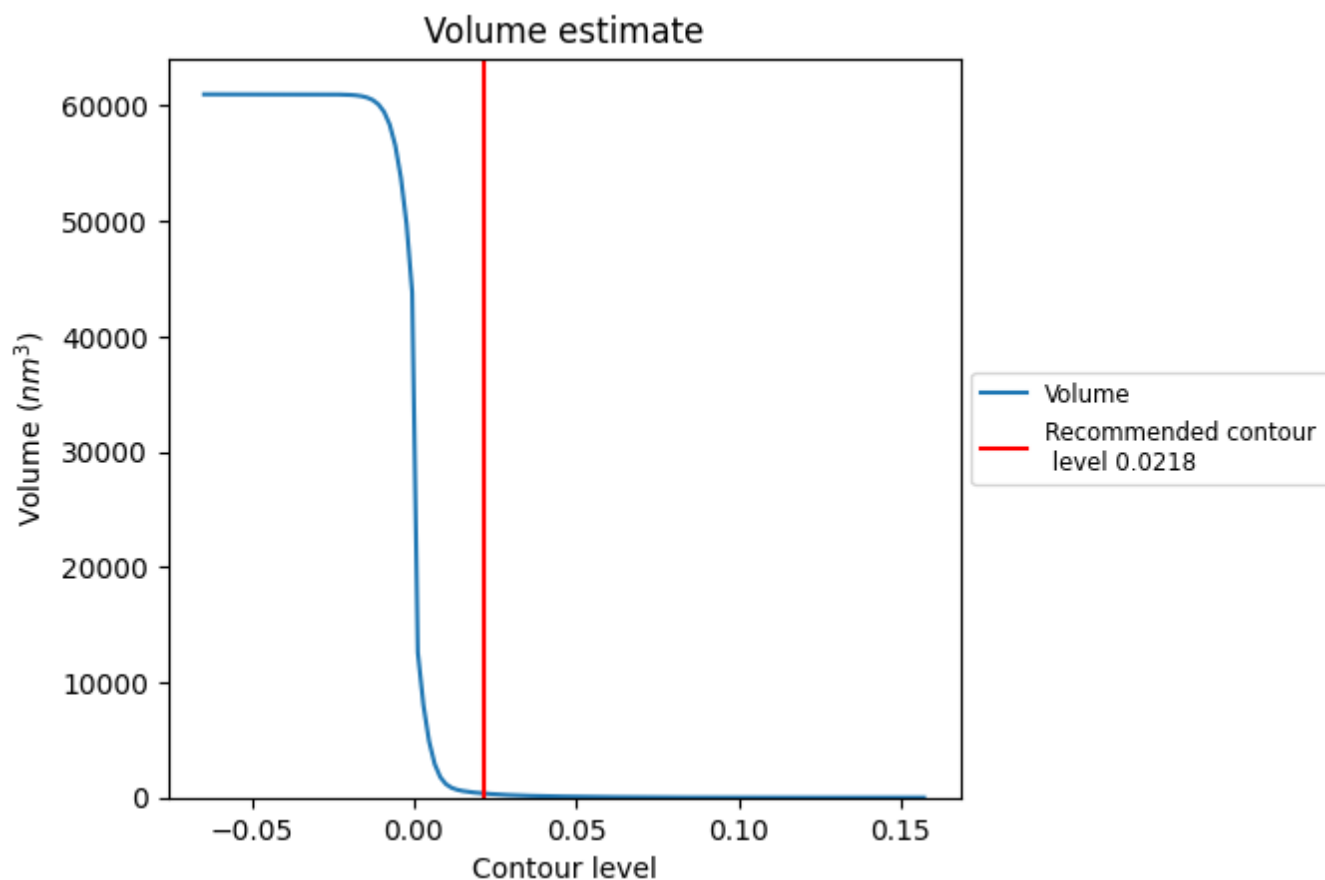
This section contains the results of statistical analysis of the map.

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.

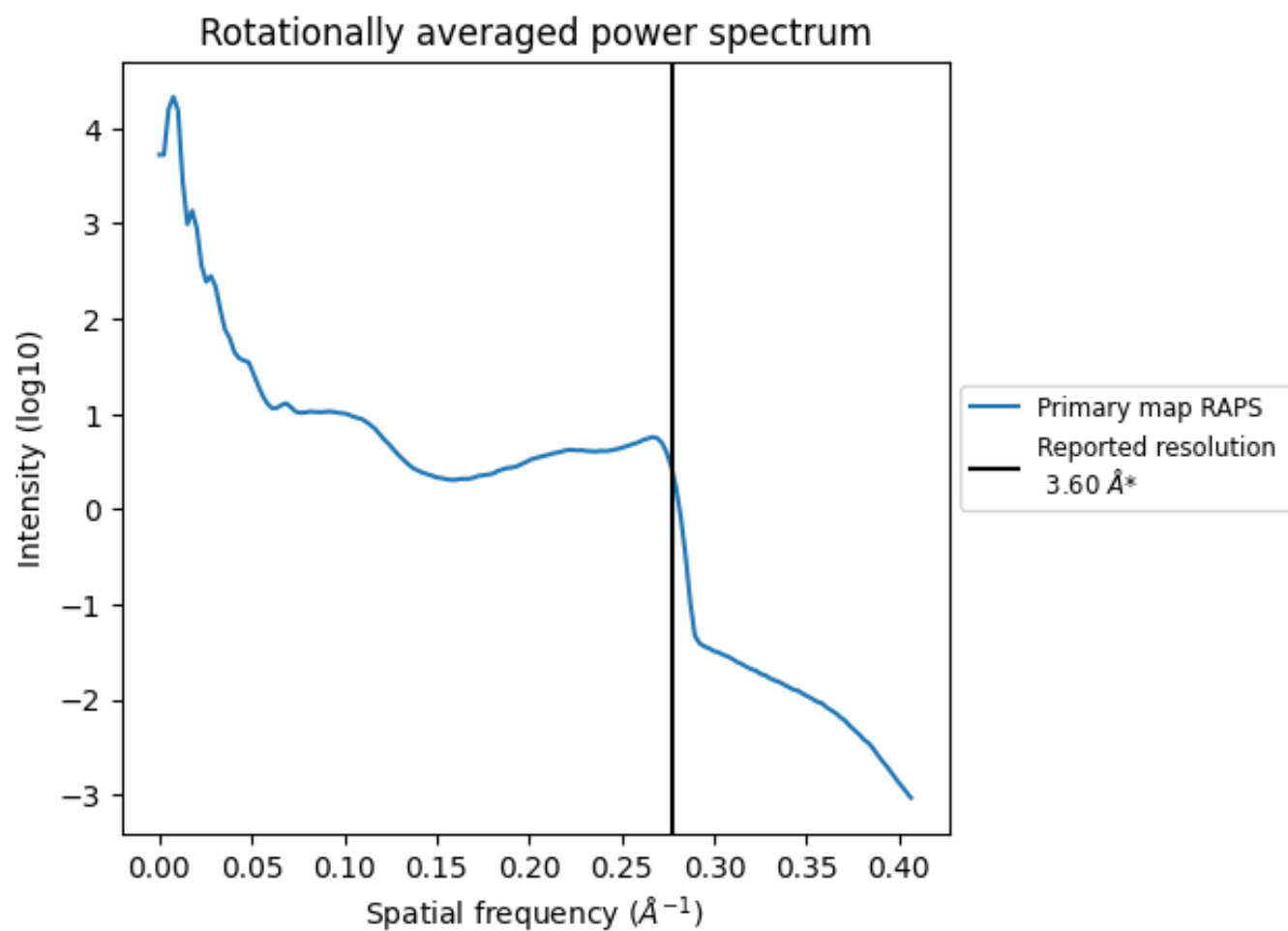
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 350 nm³; this corresponds to an approximate mass of 316 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

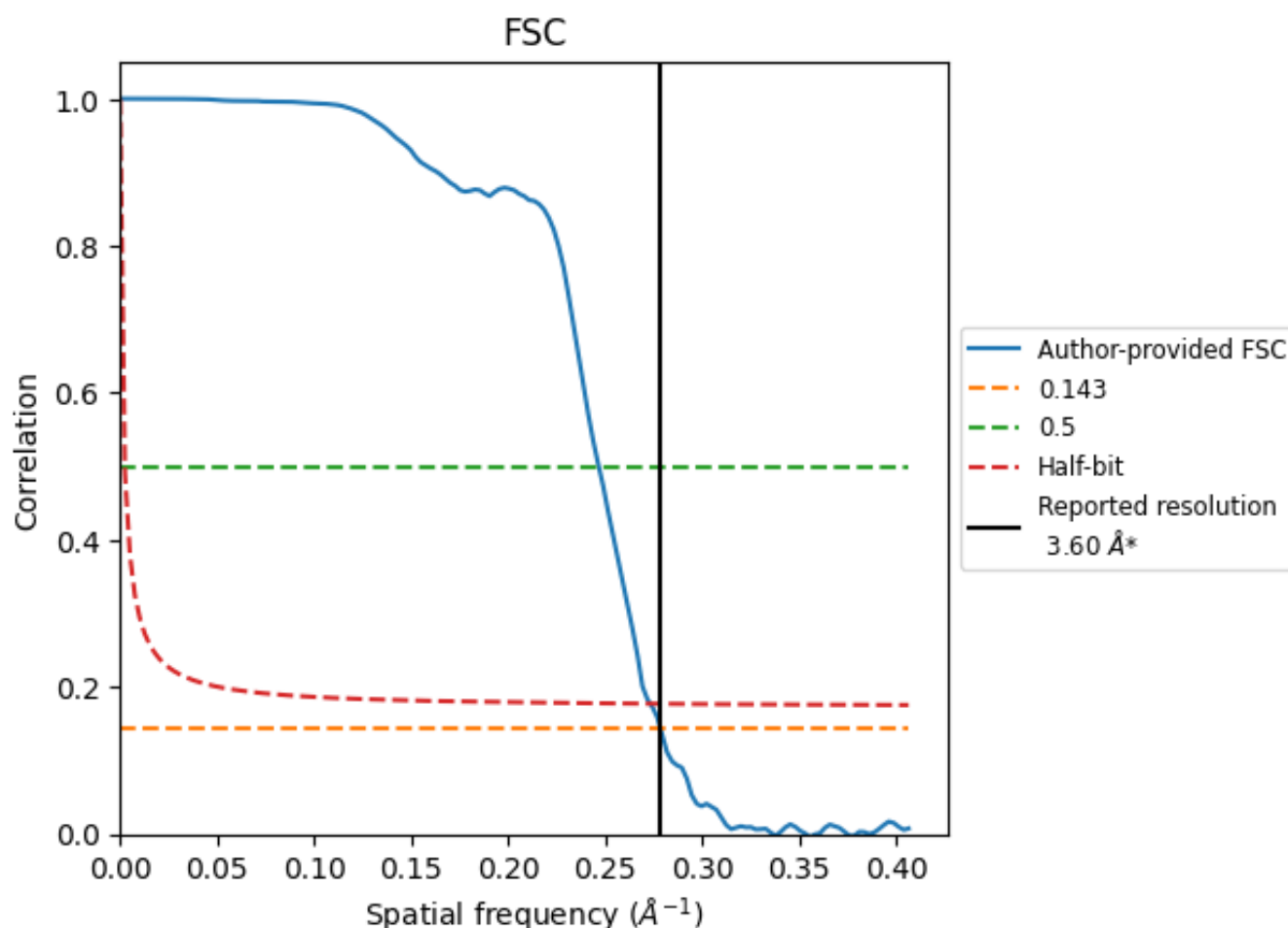


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

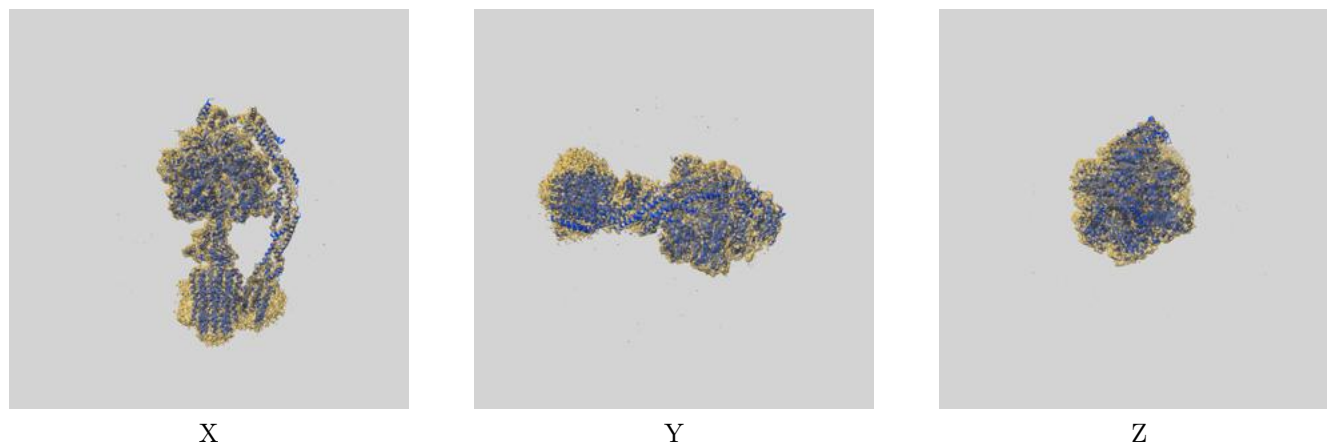
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	4.05	3.66
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

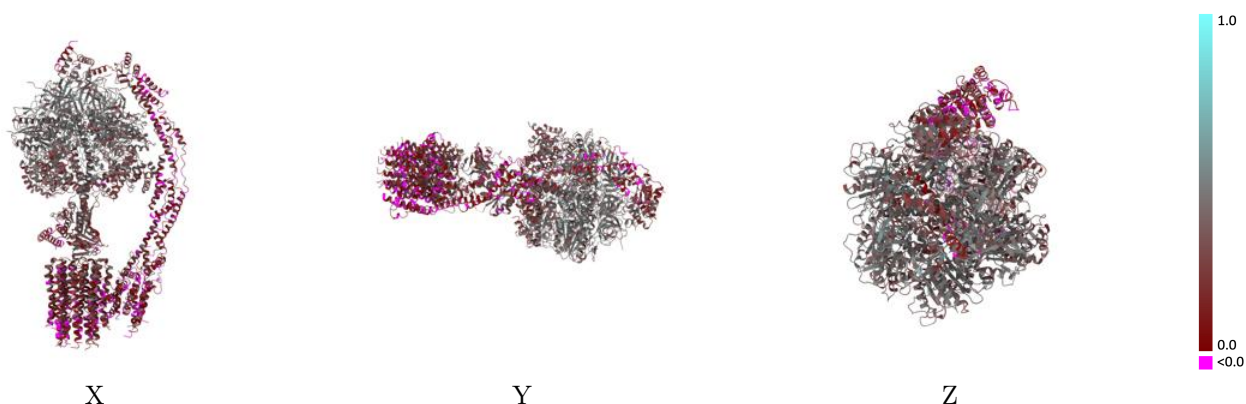
This section contains information regarding the fit between EMDB map EMD-7548 and PDB model 6CP6. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



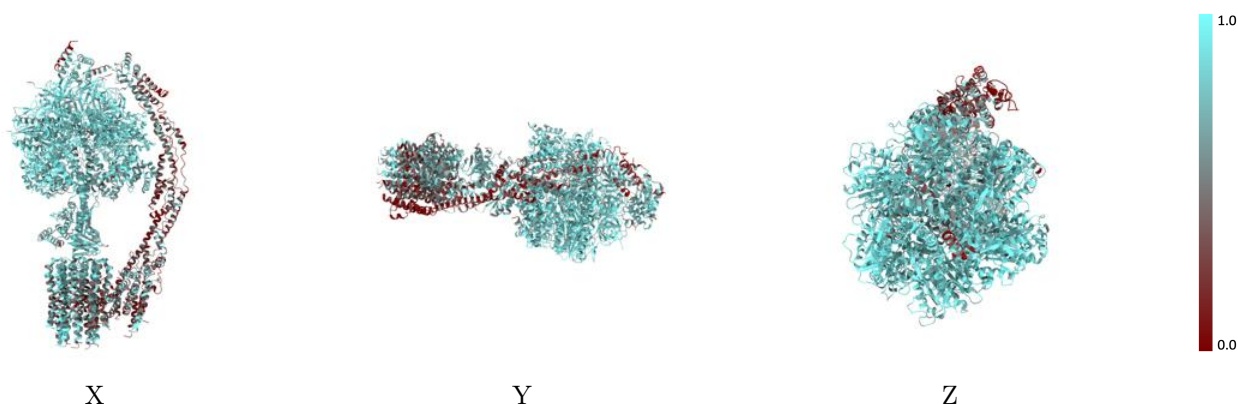
The images above show the 3D surface view of the map at the recommended contour level 0.0218 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



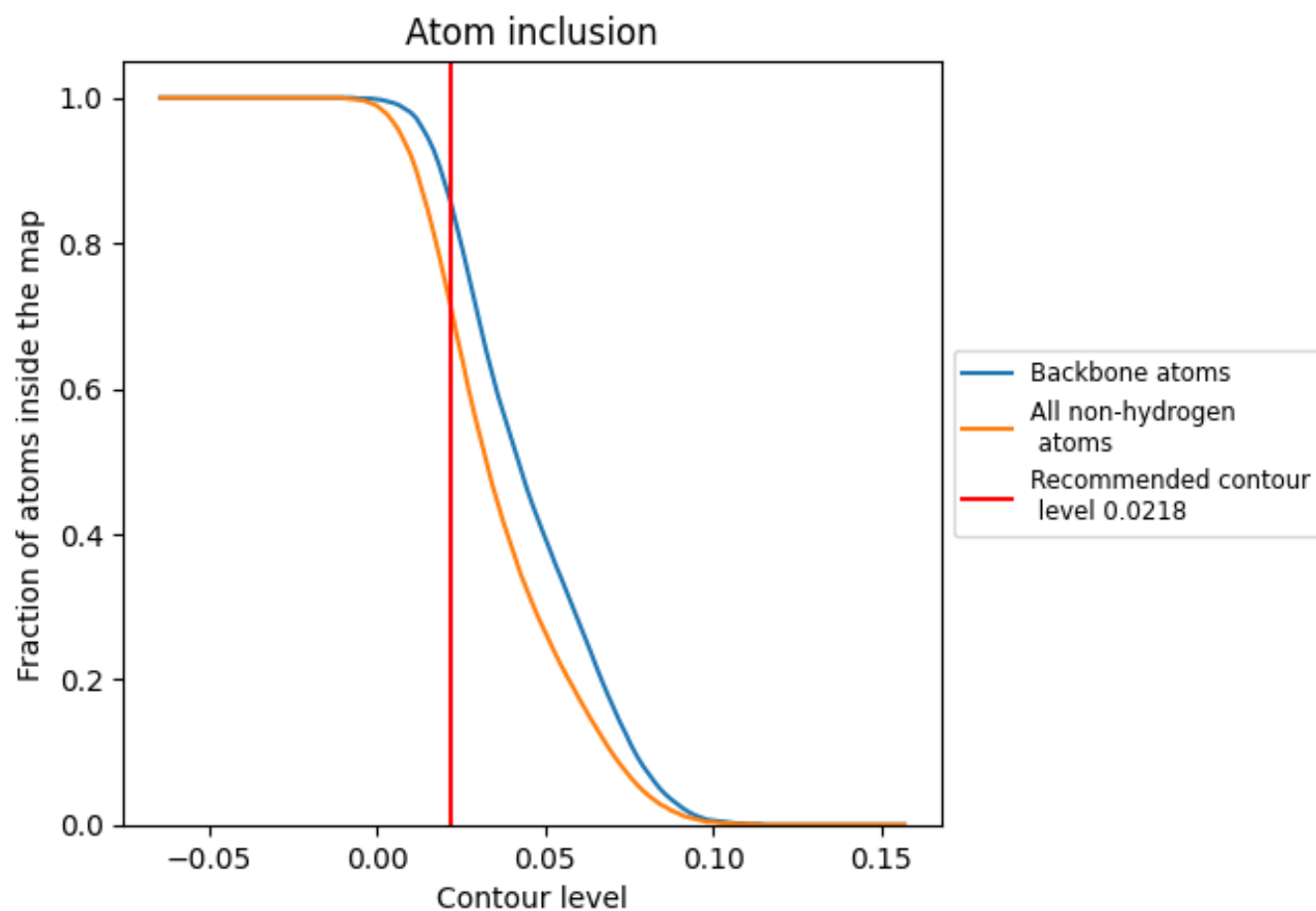
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0218).

























































9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 72% 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 (0.0218) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7150	 0.3140
6	 0.1820	 0.0570
7	 0.2900	 0.1500
8	 0.5150	 0.1460
A	 0.8570	 0.4060
B	 0.8130	 0.3900
C	 0.8510	 0.4090
D	 0.8540	 0.4140
E	 0.8280	 0.3930
F	 0.8610	 0.4250
G	 0.7590	 0.3240
H	 0.6990	 0.2440
I	 0.7940	 0.2560
J	 0.5310	 0.1420
K	 0.5450	 0.1890
L	 0.6030	 0.1790
M	 0.6800	 0.1590
N	 0.6730	 0.1720
O	 0.6360	 0.1170
P	 0.6820	 0.1820
Q	 0.5580	 0.1700
R	 0.4230	 0.1750
S	 0.6460	 0.2230
T	 0.6530	 0.2340
U	 0.1930	 0.0870
X	 0.4040	 0.1130
Y	 0.6940	 0.2820
Z	 0.3500	 0.1460

