Full wwPDB EM Validation Report ⓘ

Mar 18, 2024 – 01:39 PM JST

PDB ID	:	6J5J
EMDB ID	:	EMD-0669
Title	:	Cryo-EM structure of the mammalian E-state ATP synthase
Authors	:	Gu, J.; Zhang, L.; Yi, J.; Yang, M.
Deposited on	:	2019-01-11
Resolution	:	3.45 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:

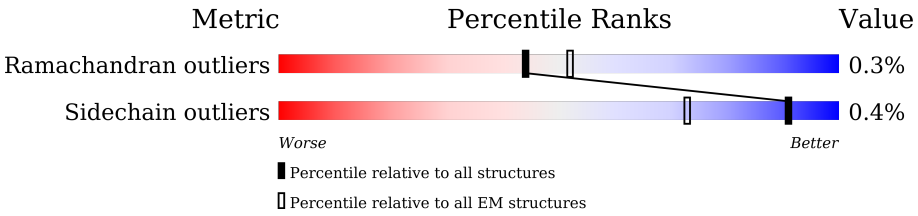
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.45 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 <=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	509	99%
1	B	509	98%
1	C	509	96%
2	D	469	99%
2	E	469	98%
2	F	469	99%
3	J	83	7% 66% 34%
4	G	272	100%
5	H	132	7% 95%

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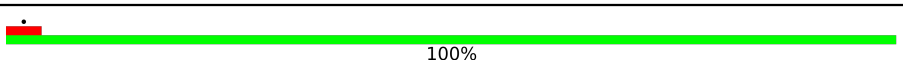
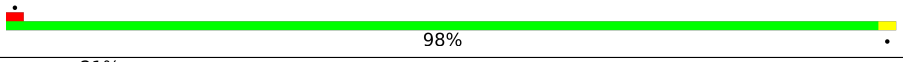
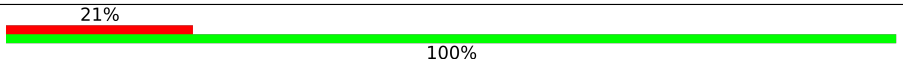
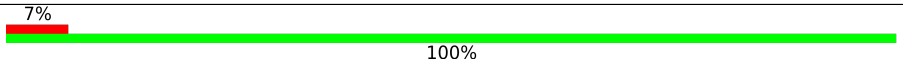
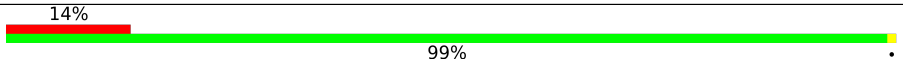
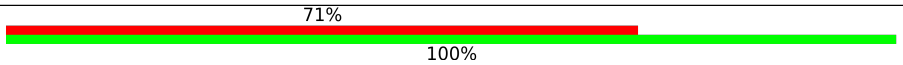
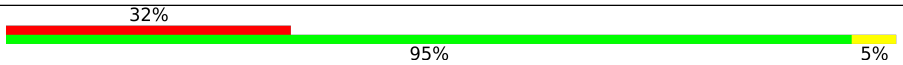
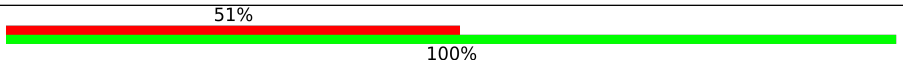
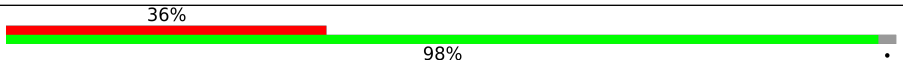
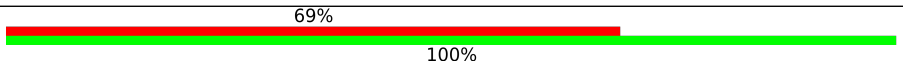
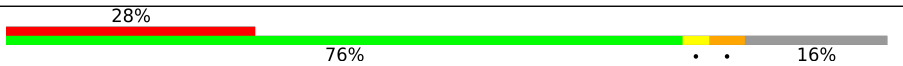
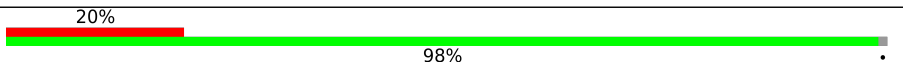
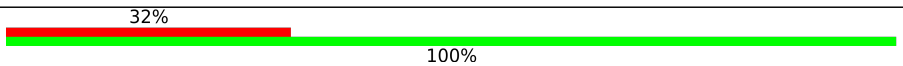
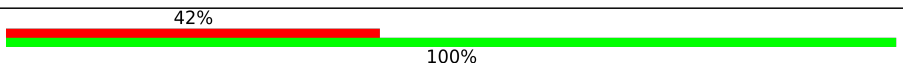
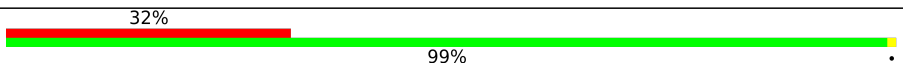
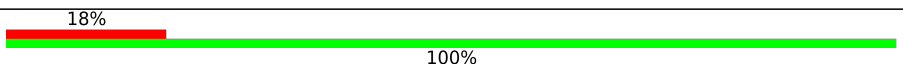
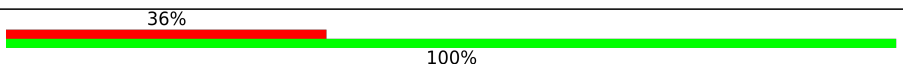
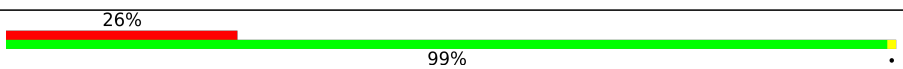
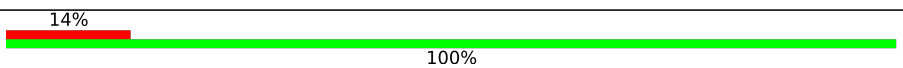
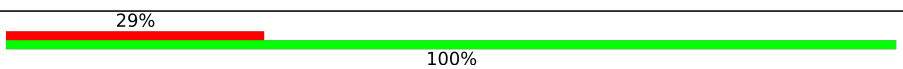
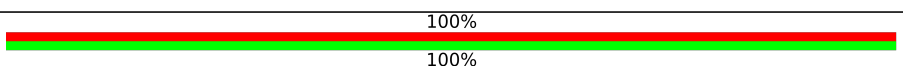
Mol	Chain	Length	Quality of chain
6	I	48	
7	S	187	
8	b	209	
9	c	70	
10	d	147	
11	e	63	
12	f	87	
13	g	84	
14	i	42	
15	k	29	
16	8	67	
17	a	226	
18	K	72	
18	L	72	
18	M	72	
18	N	72	
18	O	72	
18	P	72	
18	Q	72	
18	R	72	
19	u	42	

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 38168 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 alpha, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	504	Total	C	N	O	S	0	0
			3837	2417	676	732	12		
1	B	501	Total	C	N	O	S	0	0
			3814	2400	673	729	12		
1	C	488	Total	C	N	O	S	0	0
			3722	2347	657	706	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	469	Total	C	N	O	S	0	0
			3555	2253	603	687	12		
2	E	465	Total	C	N	O	S	0	0
			3522	2234	597	679	12		
2	F	466	Total	C	N	O	S	0	0
			3527	2237	598	680	12		

- Molecule 3 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	55	Total	C	N	O	0	0
			406	242	80	84		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	272	Total	C	N	O	S	0	0
			2112	1332	366	407	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	132	Total	C	N	O	S	0	0
			970	607	165	196	2		

- Molecule 6 is a protein called ATP synthase F1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	48	Total	C	N	O	S	0	0
			377	241	69	66	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	187	Total	C	N	O	S	0	0
			1429	910	244	266	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	b	209	Total	C	N	O	S	0	0
			1478	916	277	280	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	c	70	Total	C	N	O	0	0
			428	263	84	81		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	d	147	Total	C	N	O	0	0
			741	446	148	147		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	e	63	Total	C	N	O	0	0
			315	189	63	63		

- Molecule 12 is a protein called ATP synthase subunit f, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	87	Total	C	N	O	S	0	0
			530	327	103	98	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	g	84	Total	C	N	O	0	0
			420	252	84	84		

- Molecule 14 is a protein called ATP synthase membrane subunit DAPIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	i	41	Total	C	N	O	S	0	0
			301	199	48	52	2		

- Molecule 15 is a protein called subunit k analog.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	k	29	Total	C	N	O	0	0
			145	87	29	29		

- Molecule 16 is a protein called ATP synthase protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	8	56	Total	C	N	O	S	0	0
			374	242	60	70	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	223	Total	C	N	O	S	0	0
			1702	1131	269	290	12		

- Molecule 18 is a protein called Mitochondrial H+ transporting ATP synthase subunit c isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	72	Total	C	N	O	S	0	0
			513	340	80	89	4		
18	L	72	Total	C	N	O	S	0	0
			513	340	80	89	4		

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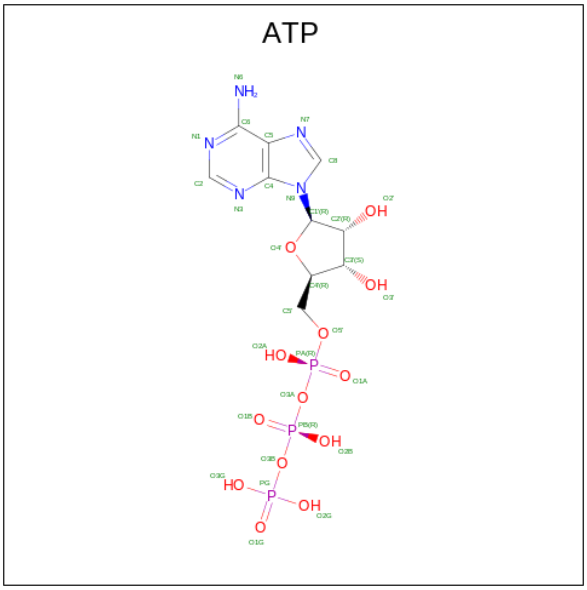
Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	72	Total	C	N	O	S	0	0
			513	340	80	89	4		
18	N	72	Total	C	N	O	S	0	0
			510	338	80	89	3		
18	O	72	Total	C	N	O	S	0	0
			513	340	80	89	4		
18	P	72	Total	C	N	O	S	0	0
			513	340	80	89	4		
18	Q	72	Total	C	N	O	S	0	0
			513	340	80	89	4		
18	R	72	Total	C	N	O	S	0	0
			513	340	80	89	4		

- Molecule 19 is a protein called ATP synthase membrane subunit 6.8PL.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	u	42	Total	C	N	O	0	0
			210	126	42	42		

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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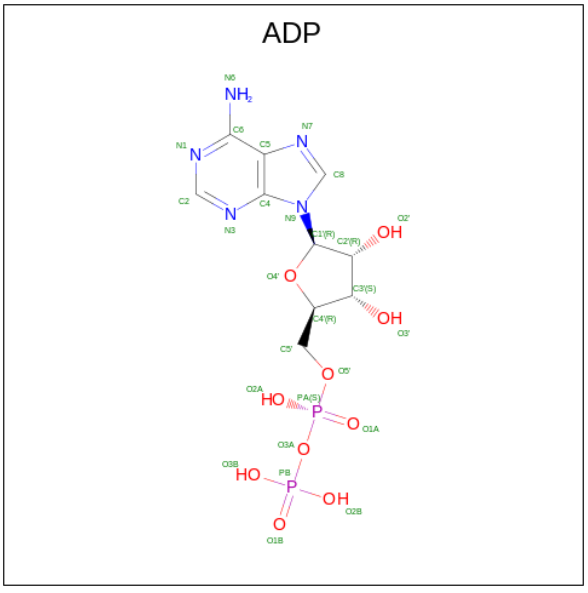
Mol	Chain	Residues	Atoms					AltConf
20	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



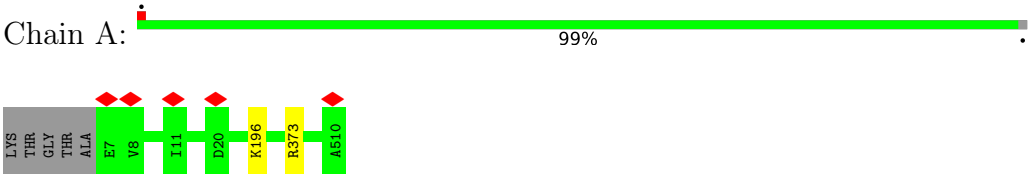
Mol	Chain	Residues	Atoms					AltConf
22	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
22	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

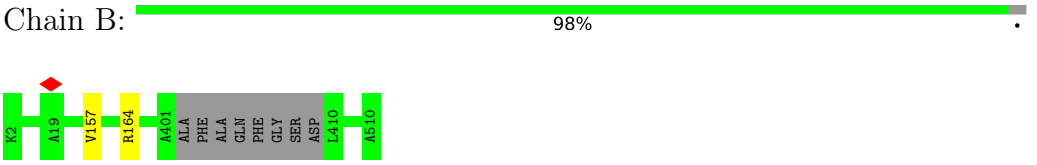
• Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain A:



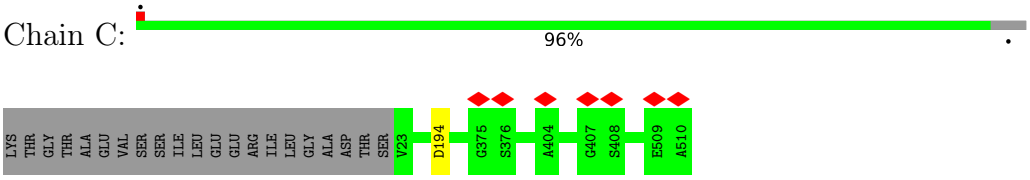
• Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain B:



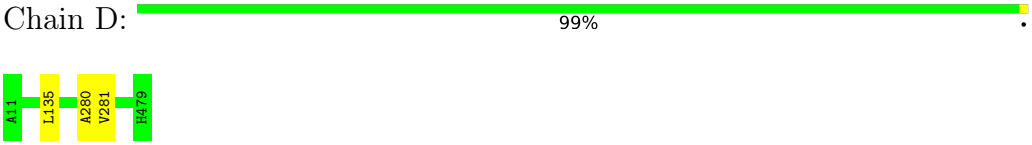
• Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain C:



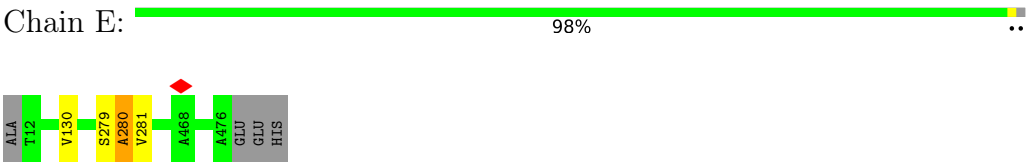
• Molecule 2: ATP synthase subunit beta

Chain D:



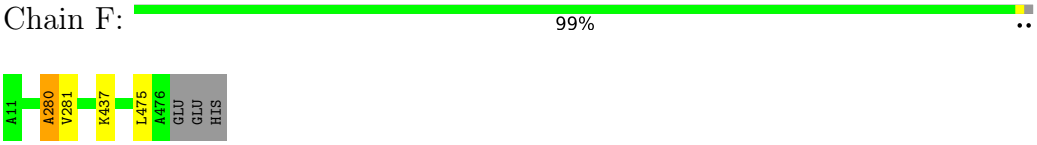
• Molecule 2: ATP synthase subunit beta

Chain E:



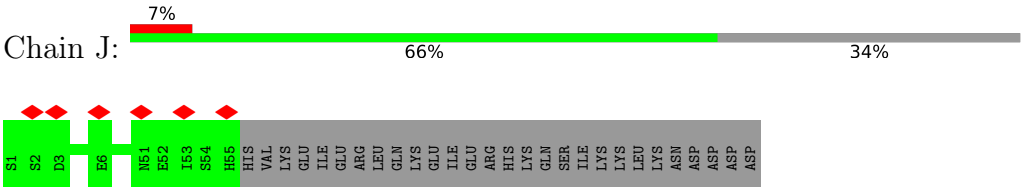
• Molecule 2: ATP synthase subunit beta

Chain F:



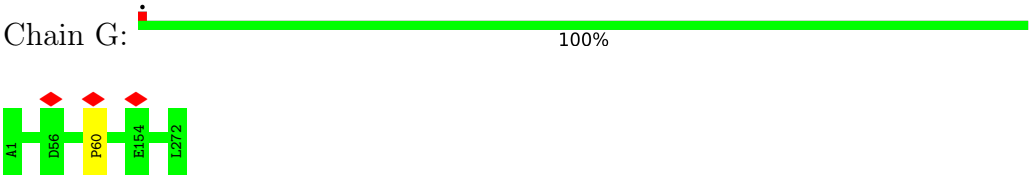
• Molecule 3: ATPase inhibitor, mitochondrial

Chain J:



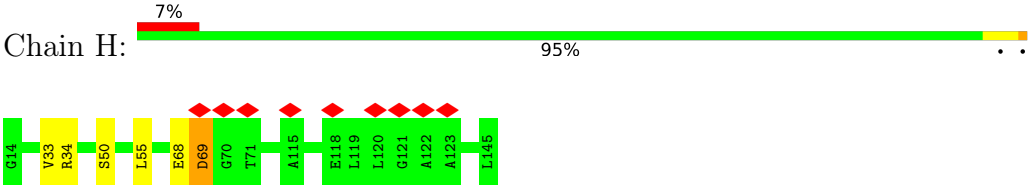
• Molecule 4: ATP synthase subunit gamma

Chain G:



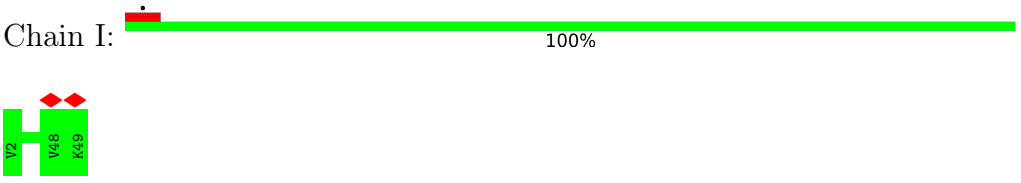
• Molecule 5: ATP synthase subunit delta, mitochondrial

Chain H:



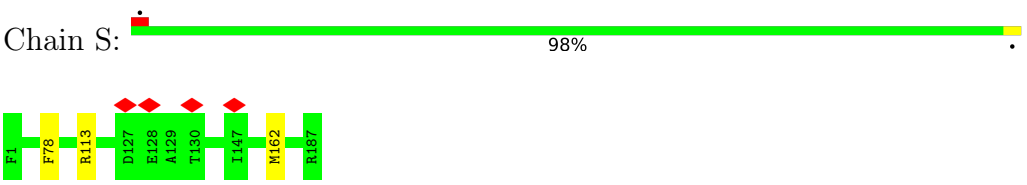
• Molecule 6: ATP synthase F1 subunit epsilon

Chain I:



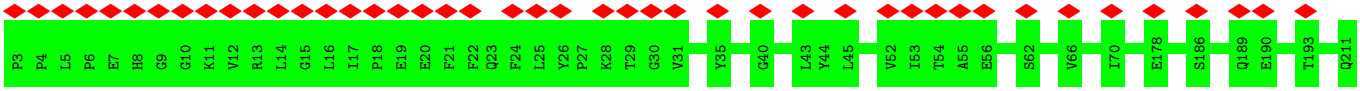
• Molecule 7: ATP synthase subunit O, mitochondrial

Chain S:



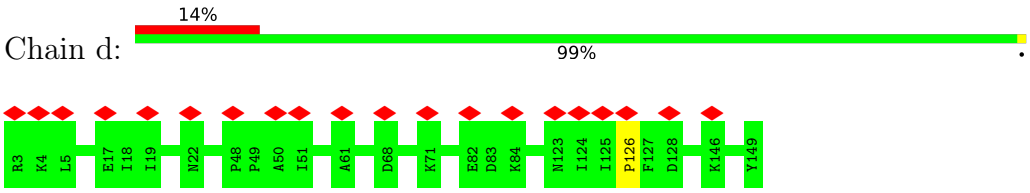
• Molecule 8: ATP synthase peripheral stalk-membrane subunit b

Chain b:

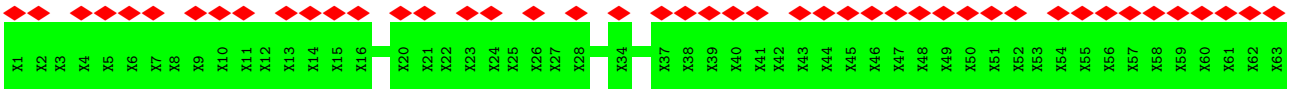


• Molecule 9: ATP synthase-coupling factor 6, mitochondrial

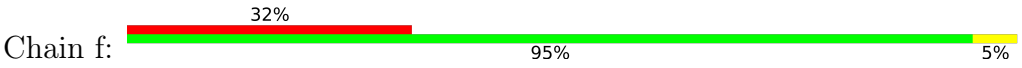
• Molecule 10: ATP synthase subunit d, mitochondrial

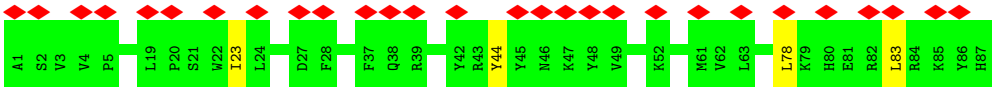


• Molecule 11: ATP synthase subunit e

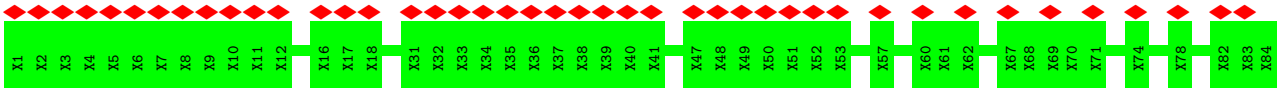


• Molecule 12: ATP synthase subunit f, mitochondrial

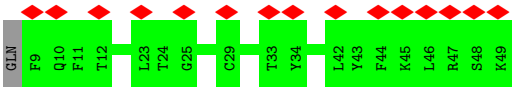




• Molecule 13: ATP synthase subunit g

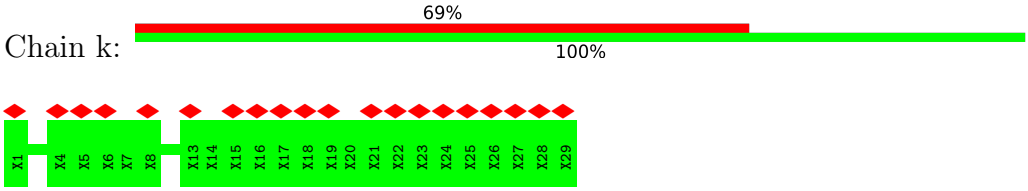


• Molecule 14: ATP synthase membrane subunit DAPIT



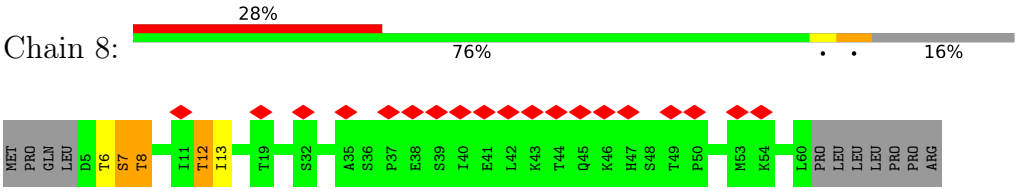
• Molecule 15: subunit k analog

Chain k:



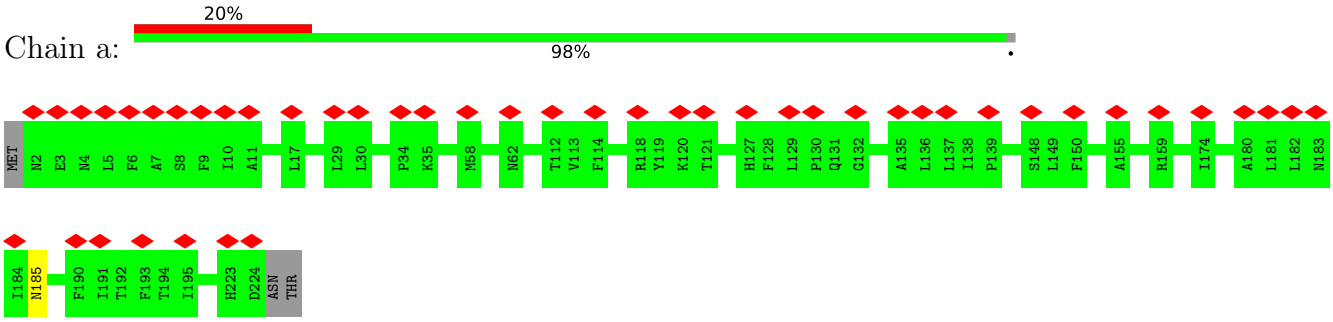
• Molecule 16: ATP synthase protein 8

Chain 8:



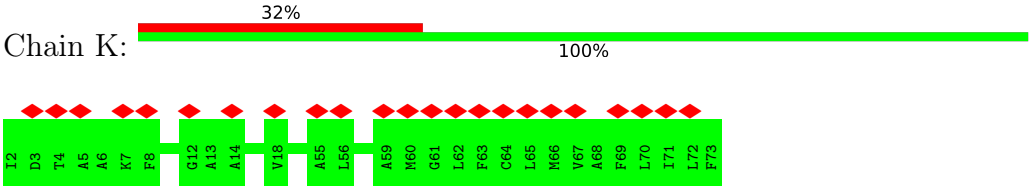
• Molecule 17: ATP synthase subunit a

Chain a:



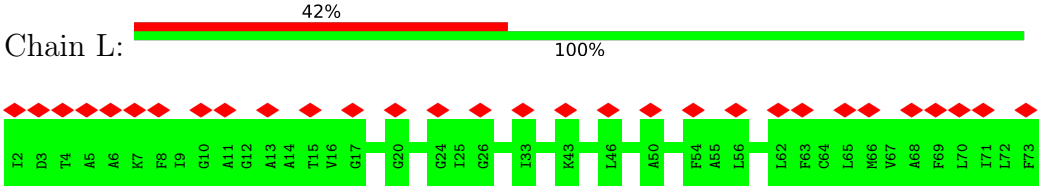
• Molecule 18: Mitochondrial H+ transporting ATP synthase subunit c isoform 1

Chain K:



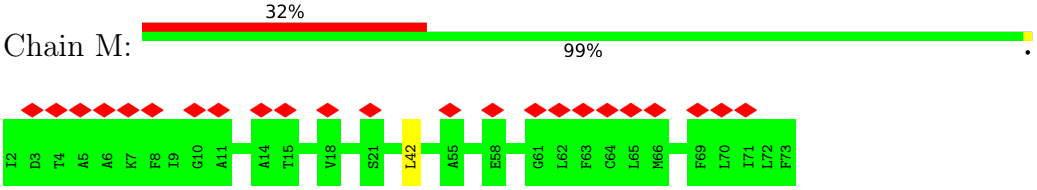
• Molecule 18: Mitochondrial H+ transporting ATP synthase subunit c isoform 1

Chain L:



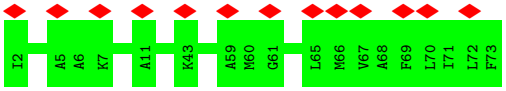
• Molecule 18: Mitochondrial H+ transporting ATP synthase subunit c isoform 1

Chain M:



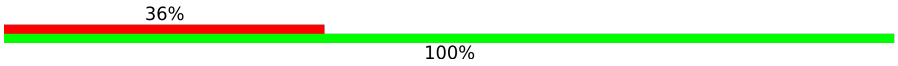
• Molecule 18: Mitochondrial H+ transporting ATP synthase subunit c isoform 1

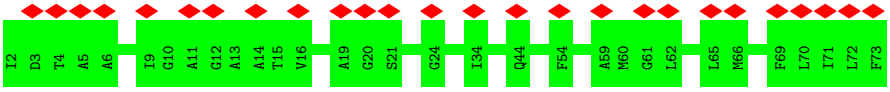
Chain N:



• Molecule 18: Mitochondrial H+ transporting ATP synthase subunit c isoform 1

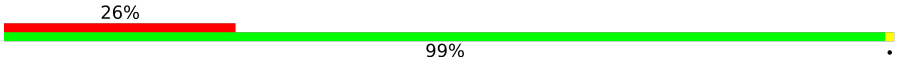
Chain O:

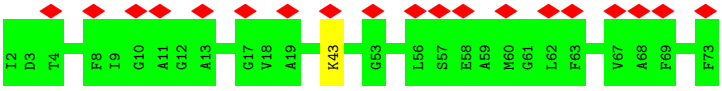




• Molecule 18: Mitochondrial H+ transporting ATP synthase subunit c isoform 1

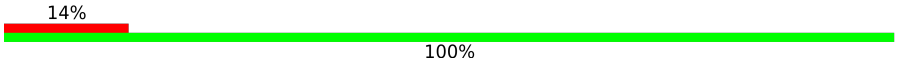
Chain P:

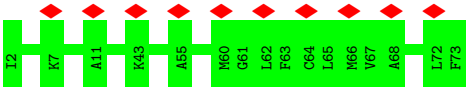




• Molecule 18: Mitochondrial H+ transporting ATP synthase subunit c isoform 1

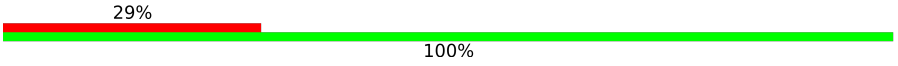
Chain Q:

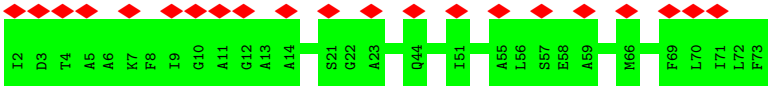




• Molecule 18: Mitochondrial H+ transporting ATP synthase subunit c isoform 1

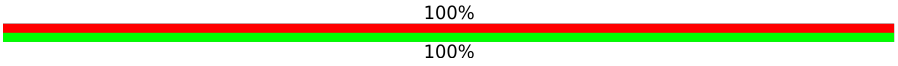
Chain R:

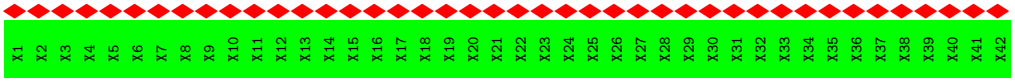




• Molecule 19: ATP synthase membrane subunit 6.8PL

Chain u:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	312331	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.185	Depositor
Minimum map value	-0.119	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	331.2, 331.2, 331.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	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, MG, ADP

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	0.32	0/3888	0.52	0/5247
1	B	0.29	0/3862	0.52	0/5210
1	C	0.30	0/3773	0.53	0/5091
2	D	0.32	0/3613	0.52	0/4900
2	E	0.29	0/3579	0.51	0/4854
2	F	0.30	0/3584	0.51	1/4861 (0.0%)
3	J	0.28	0/410	0.41	0/548
4	G	0.28	0/2138	0.49	0/2874
5	H	0.30	0/983	0.63	1/1338 (0.1%)
6	I	0.28	0/382	0.50	0/511
7	S	0.27	0/1447	0.57	0/1947
8	b	0.25	0/1489	0.48	0/2010
9	c	0.26	0/431	0.43	0/587
10	d	0.24	0/742	0.42	0/1036
12	f	0.34	0/535	0.66	2/730 (0.3%)
14	i	0.34	0/306	0.50	0/414
16	8	0.44	0/380	0.76	0/522
17	a	0.43	0/1739	0.68	0/2379
18	K	0.41	0/522	0.54	0/703
18	L	0.38	0/522	0.56	0/703
18	M	0.43	0/522	0.59	0/703
18	N	0.44	0/519	0.50	0/700
18	O	0.40	0/522	0.59	0/703
18	P	0.34	0/522	0.53	0/703
18	Q	0.34	0/522	0.48	0/703
18	R	0.40	0/522	0.57	0/703
All	All	0.32	0/37454	0.53	4/50680 (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	D	0	1
2	E	0	1
2	F	0	1
5	H	0	2
7	S	0	1
12	f	0	2
16	8	0	4
All	All	0	12

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	475	LEU	CA-CB-CG	5.34	127.58	115.30
5	H	55	LEU	CA-CB-CG	5.20	127.25	115.30
12	f	83	LEU	CA-CB-CG	5.12	127.08	115.30
12	f	78	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	8	12	THR	Peptide
16	8	6	THR	Peptide
16	8	7	SER	Peptide
16	8	8	THR	Peptide
2	D	280	ALA	Peptide
2	E	280	ALA	Peptide
2	F	280	ALA	Peptide
5	H	33	VAL	Peptide
5	H	68	GLU	Peptide
7	S	78	PHE	Peptide
12	f	23	ILE	Peptide
12	f	44	TYR	Peptide

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	502/509 (99%)	479 (95%)	23 (5%)	0	100	100
1	B	497/509 (98%)	476 (96%)	21 (4%)	0	100	100
1	C	486/509 (96%)	459 (94%)	27 (6%)	0	100	100
2	D	467/469 (100%)	434 (93%)	32 (7%)	1 (0%)	47	80
2	E	463/469 (99%)	442 (96%)	18 (4%)	3 (1%)	25	62
2	F	464/469 (99%)	432 (93%)	30 (6%)	2 (0%)	34	70
3	J	53/83 (64%)	51 (96%)	2 (4%)	0	100	100
4	G	270/272 (99%)	258 (96%)	11 (4%)	1 (0%)	34	70
5	H	130/132 (98%)	118 (91%)	9 (7%)	3 (2%)	6	34
6	I	46/48 (96%)	38 (83%)	8 (17%)	0	100	100
7	S	185/187 (99%)	162 (88%)	23 (12%)	0	100	100
8	b	207/209 (99%)	195 (94%)	12 (6%)	0	100	100
9	c	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
10	d	145/147 (99%)	132 (91%)	12 (8%)	1 (1%)	22	60
12	f	85/87 (98%)	63 (74%)	22 (26%)	0	100	100
14	i	39/42 (93%)	38 (97%)	1 (3%)	0	100	100
16	8	54/67 (81%)	46 (85%)	4 (7%)	4 (7%)	1	10
17	a	221/226 (98%)	195 (88%)	26 (12%)	0	100	100
18	K	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
18	L	70/72 (97%)	66 (94%)	4 (6%)	0	100	100
18	M	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
18	N	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
18	O	70/72 (97%)	66 (94%)	4 (6%)	0	100	100
18	P	70/72 (97%)	66 (94%)	4 (6%)	0	100	100
18	Q	70/72 (97%)	65 (93%)	5 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	R	70/72 (97%)	65 (93%)	5 (7%)	0	100 100
All	All	4942/5080 (97%)	4612 (93%)	315 (6%)	15 (0%)	44 75

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	281	VAL
2	E	281	VAL
2	F	281	VAL
5	H	50	SER
5	H	69	ASP
10	d	126	PRO
16	8	13	ILE
16	8	7	SER
16	8	8	THR
16	8	12	THR
2	F	280	ALA
5	H	34	ARG
2	E	280	ALA
2	E	279	SER
4	G	60	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
1	A	406/410 (99%)	404 (100%)	2 (0%)	88 95
1	B	405/410 (99%)	403 (100%)	2 (0%)	88 95
1	C	393/410 (96%)	392 (100%)	1 (0%)	92 98
2	D	378/378 (100%)	377 (100%)	1 (0%)	92 98
2	E	375/378 (99%)	374 (100%)	1 (0%)	92 98
2	F	375/378 (99%)	374 (100%)	1 (0%)	92 98
3	J	36/68 (53%)	36 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	G	230/230 (100%)	230 (100%)	0	100 100
5	H	104/105 (99%)	103 (99%)	1 (1%)	76 89
6	I	38/38 (100%)	38 (100%)	0	100 100
7	S	162/163 (99%)	160 (99%)	2 (1%)	71 87
8	b	124/182 (68%)	124 (100%)	0	100 100
9	c	22/63 (35%)	22 (100%)	0	100 100
10	d	1/127 (1%)	1 (100%)	0	100 100
12	f	27/75 (36%)	27 (100%)	0	100 100
14	i	29/36 (81%)	29 (100%)	0	100 100
16	8	29/66 (44%)	29 (100%)	0	100 100
17	a	188/199 (94%)	187 (100%)	1 (0%)	88 95
18	K	49/49 (100%)	49 (100%)	0	100 100
18	L	49/49 (100%)	49 (100%)	0	100 100
18	M	49/49 (100%)	48 (98%)	1 (2%)	55 79
18	N	48/49 (98%)	48 (100%)	0	100 100
18	O	49/49 (100%)	49 (100%)	0	100 100
18	P	49/49 (100%)	48 (98%)	1 (2%)	55 79
18	Q	49/49 (100%)	49 (100%)	0	100 100
18	R	49/49 (100%)	49 (100%)	0	100 100
All	All	3713/4108 (90%)	3699 (100%)	14 (0%)	91 97

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	LYS
1	A	373	ARG
1	B	157	VAL
1	B	164	ARG
1	C	194	ASP
2	D	135	LEU
2	E	130	VAL
2	F	437	LYS
5	H	69	ASP
7	S	113	ARG
7	S	162	MET

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Mol	Chain	Res	Type
17	a	185	ASN
18	M	42	LEU
18	P	43	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	415	GLN
1	A	477	GLN
1	B	471	HIS
1	C	330	GLN
1	C	441	GLN
1	C	475	GLN
1	C	503	ASN
2	D	54	HIS
2	E	53	GLN
2	E	114	GLN
2	E	387	GLN
2	F	174	ASN
2	F	225	ASN
2	F	363	ASN
2	F	369	HIS
2	F	421	GLN
2	F	457	GLN
4	G	225	GLN
5	H	51	HIS
5	H	138	ASN
6	I	17	GLN
8	b	158	HIS
8	b	162	GLN
16	8	25	GLN
17	a	39	ASN
17	a	47	GLN
17	a	63	GLN
17	a	83	ASN
18	L	44	GLN
18	R	39	ASN

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	$\#\|Z\| > 2$
22	ADP	D	501	21	24,29,29	0.99	1 (4%)	29,45,45	1.82	4 (13%)
20	ATP	A	601	21	26,33,33	0.91	1 (3%)	31,52,52	1.48	5 (16%)
22	ADP	F	501	21	24,29,29	0.98	1 (4%)	29,45,45	1.39	4 (13%)
20	ATP	C	601	21	26,33,33	0.91	1 (3%)	31,52,52	1.62	5 (16%)
20	ATP	B	601	21	26,33,33	0.94	1 (3%)	31,52,52	1.58	5 (16%)

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
22	ADP	D	501	21	-	4/12/32/32	0/3/3/3
20	ATP	A	601	21	-	1/18/38/38	0/3/3/3
22	ADP	F	501	21	-	6/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	ATP	C	601	21	-	2/18/38/38	0/3/3/3
20	ATP	B	601	21	-	4/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	501	ADP	C5-C4	2.36	1.47	1.40
20	C	601	ATP	C5-C4	2.36	1.47	1.40
20	B	601	ATP	C5-C4	2.29	1.47	1.40
20	A	601	ATP	C5-C4	2.21	1.46	1.40
22	D	501	ADP	C5-C4	2.01	1.46	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	501	ADP	N3-C2-N1	-6.67	118.25	128.68
20	C	601	ATP	PA-O3A-PB	-4.01	119.05	132.83
20	B	601	ATP	PB-O3B-PG	-3.81	119.74	132.83
22	D	501	ADP	C2-N1-C6	3.74	125.14	118.75
20	C	601	ATP	C3'-C2'-C1'	3.61	106.41	100.98
22	F	501	ADP	C3'-C2'-C1'	3.57	106.35	100.98
20	B	601	ATP	PA-O3A-PB	-3.49	120.85	132.83
20	A	601	ATP	PB-O3B-PG	-3.45	120.98	132.83
20	B	601	ATP	C3'-C2'-C1'	3.29	105.94	100.98
20	A	601	ATP	N3-C2-N1	-3.29	123.53	128.68
20	C	601	ATP	PB-O3B-PG	-3.27	121.61	132.83
20	C	601	ATP	N3-C2-N1	-3.19	123.69	128.68
20	B	601	ATP	N3-C2-N1	-3.13	123.78	128.68
22	F	501	ADP	N3-C2-N1	-3.07	123.88	128.68
22	D	501	ADP	C4-C5-N7	-3.06	106.20	109.40
20	A	601	ATP	C4-C5-N7	-2.77	106.51	109.40
20	A	601	ATP	C3'-C2'-C1'	2.64	104.96	100.98
20	B	601	ATP	C4-C5-N7	-2.61	106.68	109.40
22	D	501	ADP	C3'-C2'-C1'	2.49	104.73	100.98
22	F	501	ADP	C4-C5-N7	-2.46	106.83	109.40
20	A	601	ATP	PA-O3A-PB	-2.37	124.69	132.83
20	C	601	ATP	C4-C5-N7	-2.23	107.08	109.40
22	F	501	ADP	PA-O3A-PB	-2.04	125.83	132.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

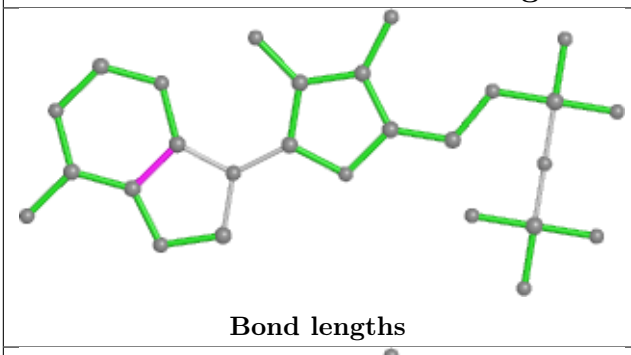
Mol	Chain	Res	Type	Atoms
20	B	601	ATP	PB-O3B-PG-O3G
20	C	601	ATP	C5'-O5'-PA-O3A
22	D	501	ADP	C5'-O5'-PA-O1A
22	D	501	ADP	C5'-O5'-PA-O2A
22	D	501	ADP	C5'-O5'-PA-O3A
22	F	501	ADP	PA-O3A-PB-O3B
22	F	501	ADP	C5'-O5'-PA-O1A
20	B	601	ATP	PB-O3B-PG-O1G
22	F	501	ADP	C5'-O5'-PA-O3A
20	B	601	ATP	PA-O3A-PB-O2B
20	C	601	ATP	C5'-O5'-PA-O2A
22	F	501	ADP	C5'-O5'-PA-O2A
22	D	501	ADP	PB-O3A-PA-O2A
20	A	601	ATP	O4'-C4'-C5'-O5'
20	B	601	ATP	PA-O3A-PB-O1B
22	F	501	ADP	O4'-C4'-C5'-O5'
22	F	501	ADP	PA-O3A-PB-O1B

There are no ring outliers.

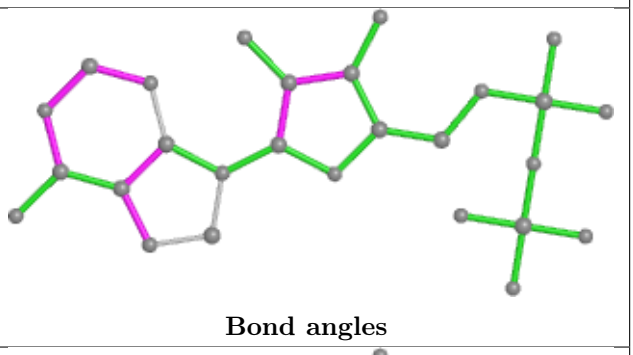
No monomer is involved in short contacts.

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 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.

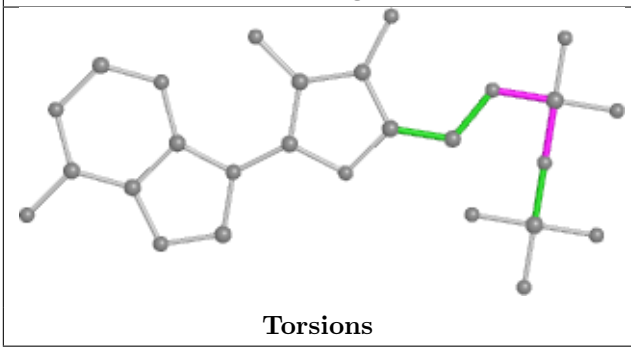
Ligand ADP D 501



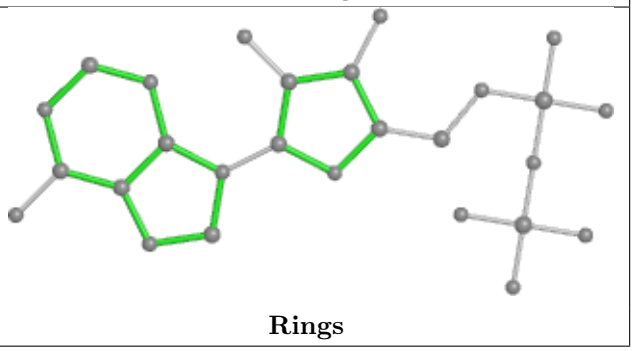
Bond lengths



Bond angles

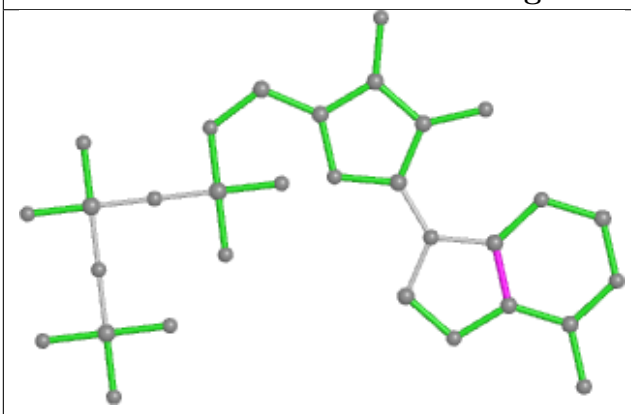


Torsions

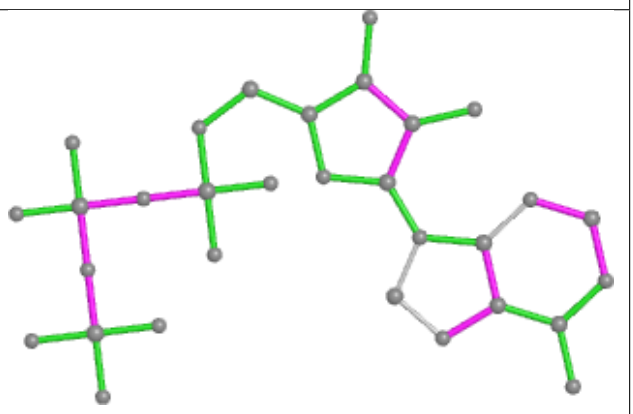


Rings

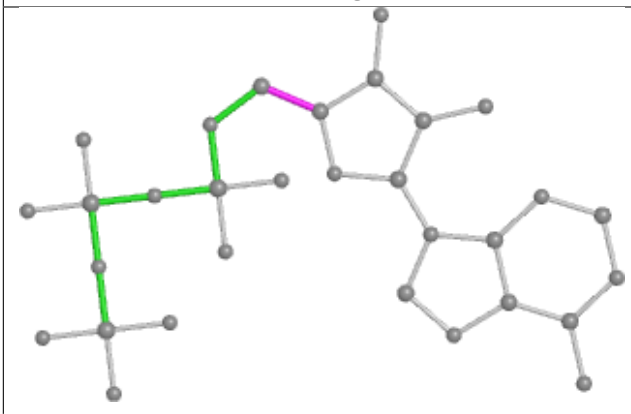
Ligand ATP A 601



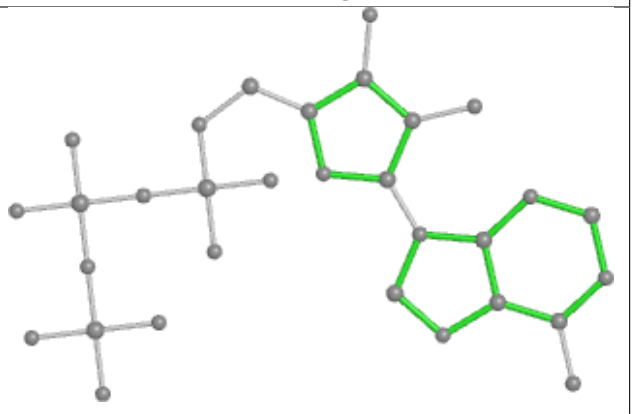
Bond lengths



Bond angles

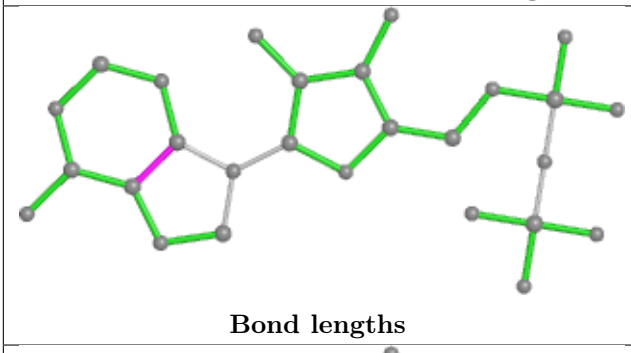


Torsions

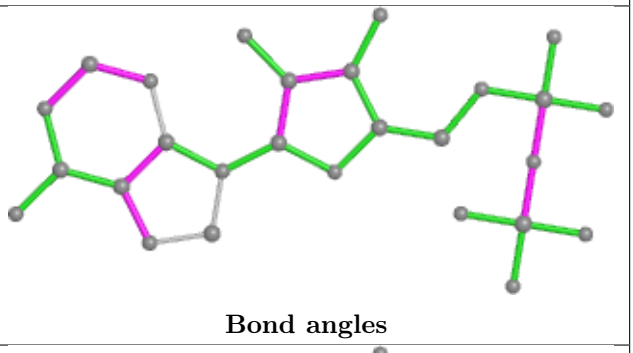


Rings

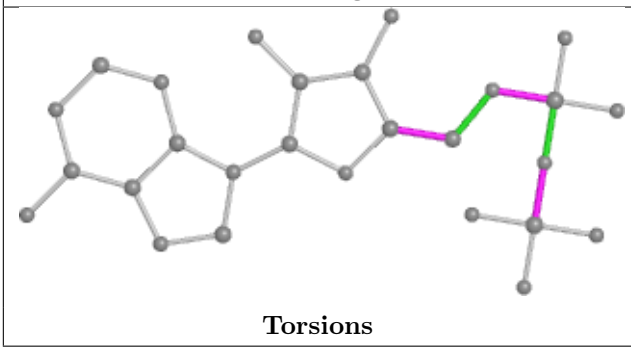
Ligand ADP F 501



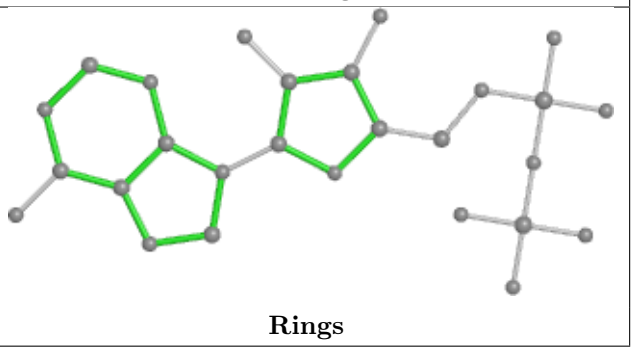
Bond lengths



Bond angles

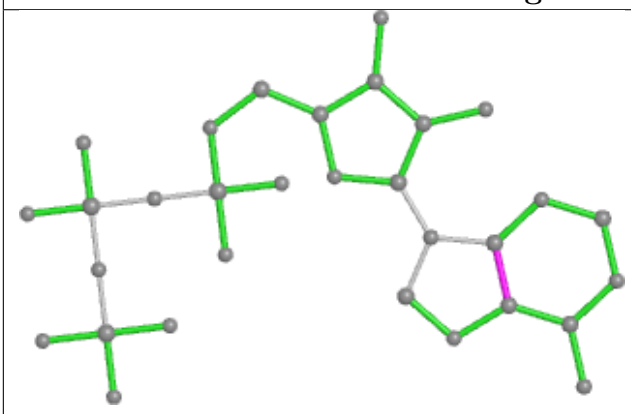


Torsions

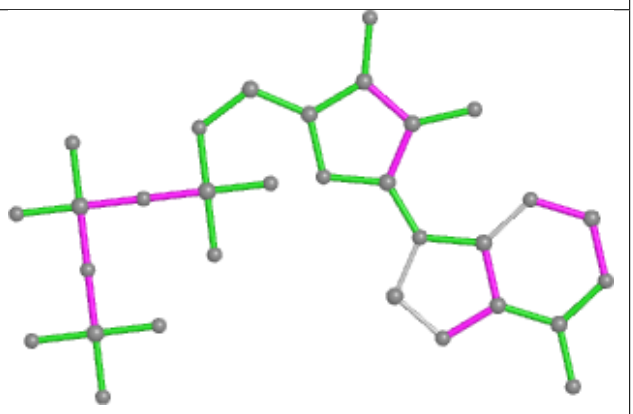


Rings

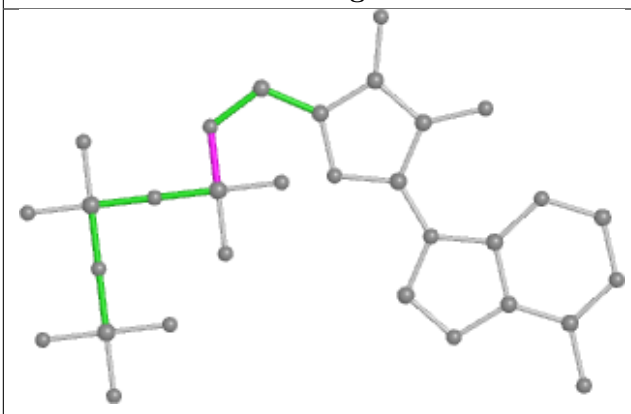
Ligand ATP C 601



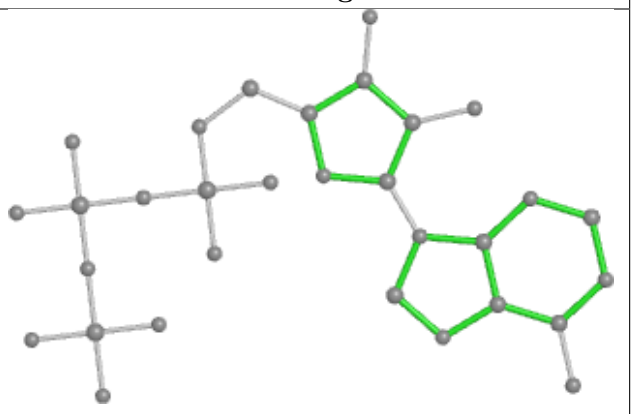
Bond lengths



Bond angles

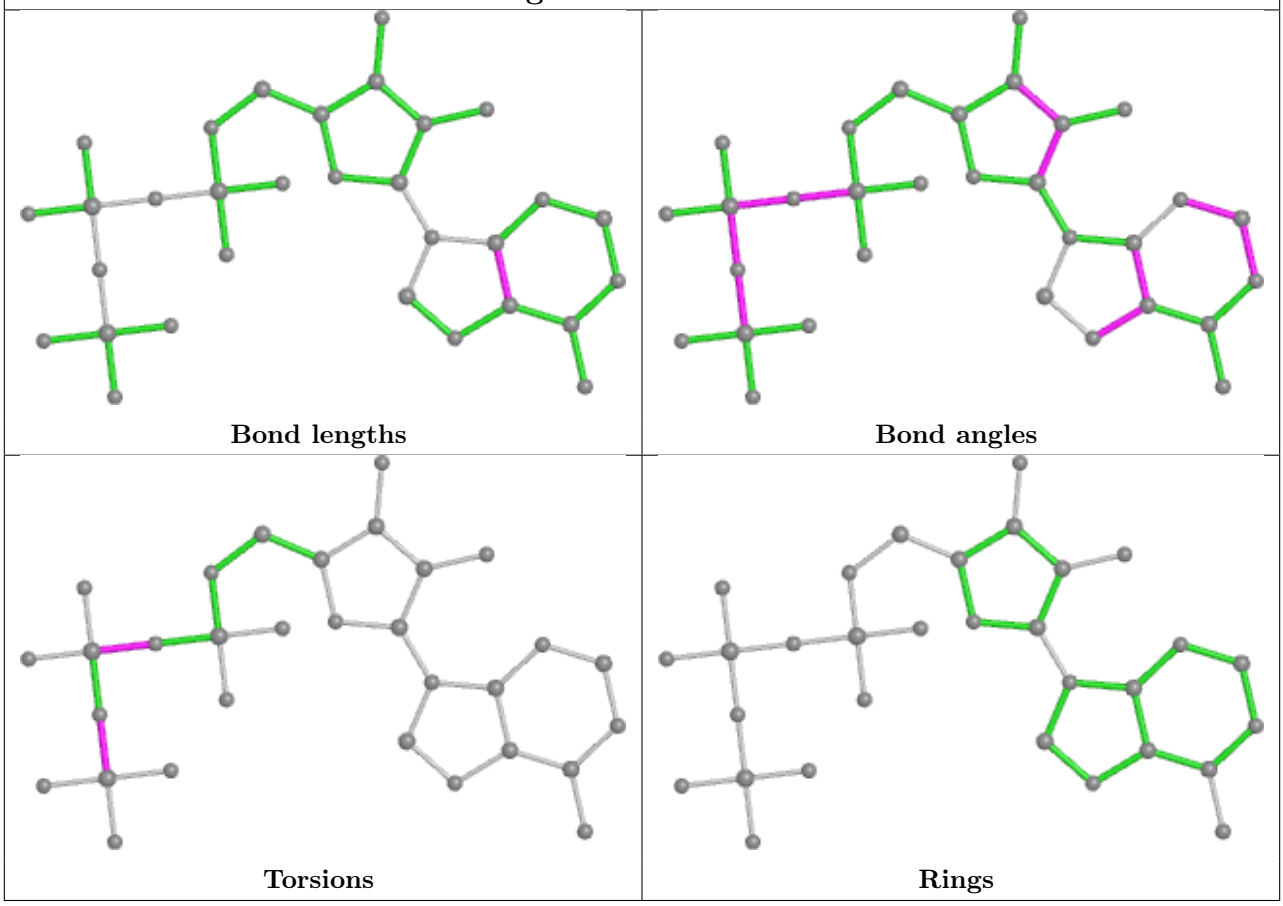


Torsions



Rings

Ligand ATP B 601



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.

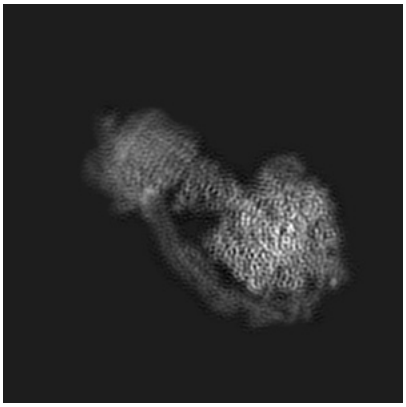
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0669. These allow visual inspection of the internal detail of the map and identification of artifacts.

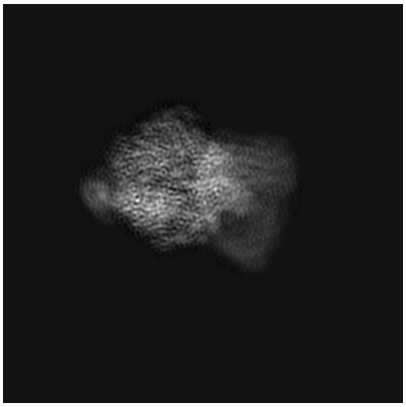
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

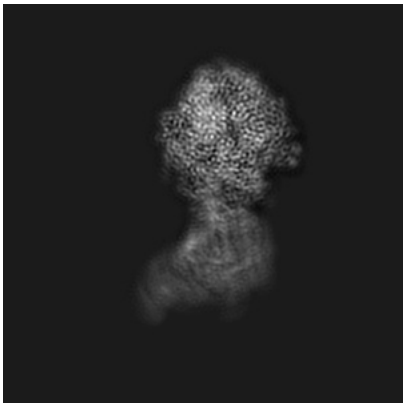
6.1.1 Primary map



X



Y

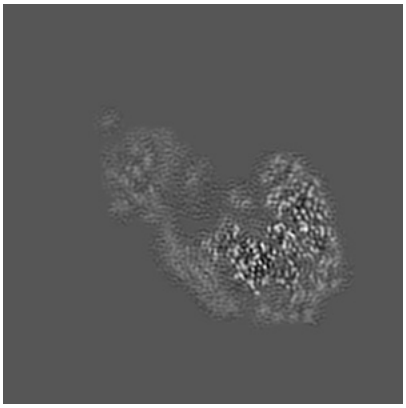


Z

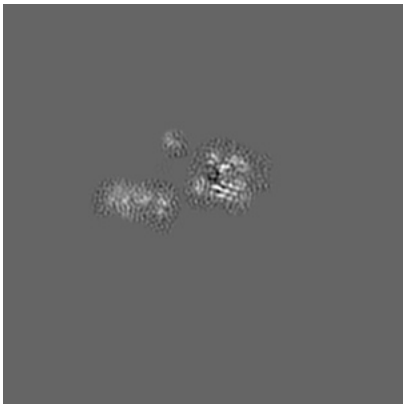
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 120



Y Index: 120

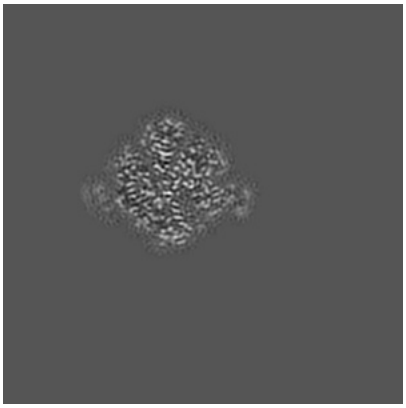
Z Index: 120

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

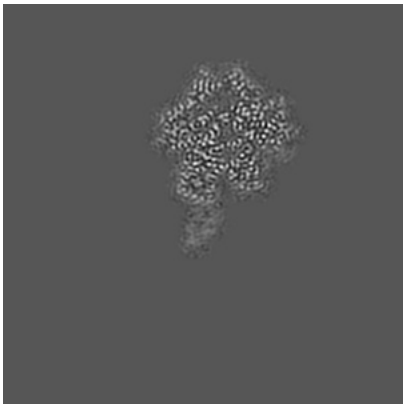
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 142



Y Index: 171

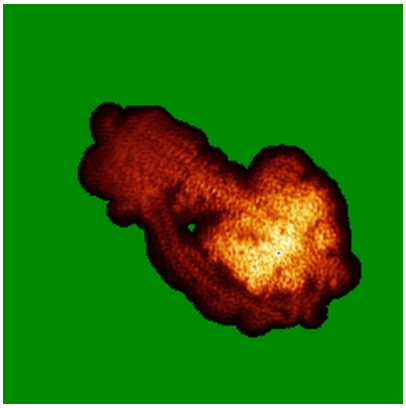


Z Index: 94

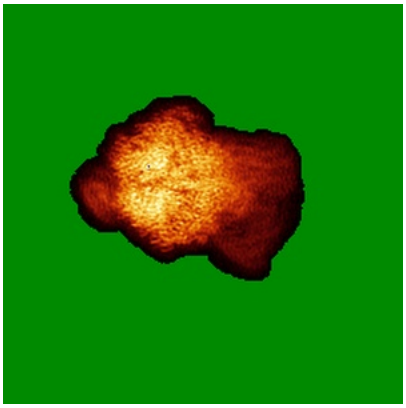
The images above show the largest variance slices of the map in three orthogonal directions.

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

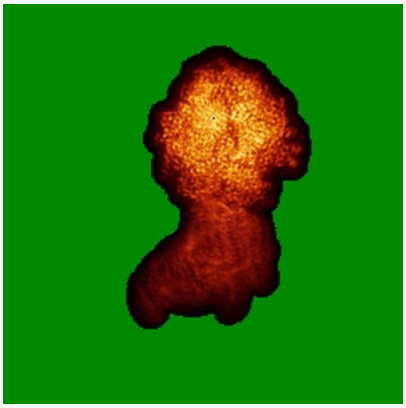
6.4.1 Primary map



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 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

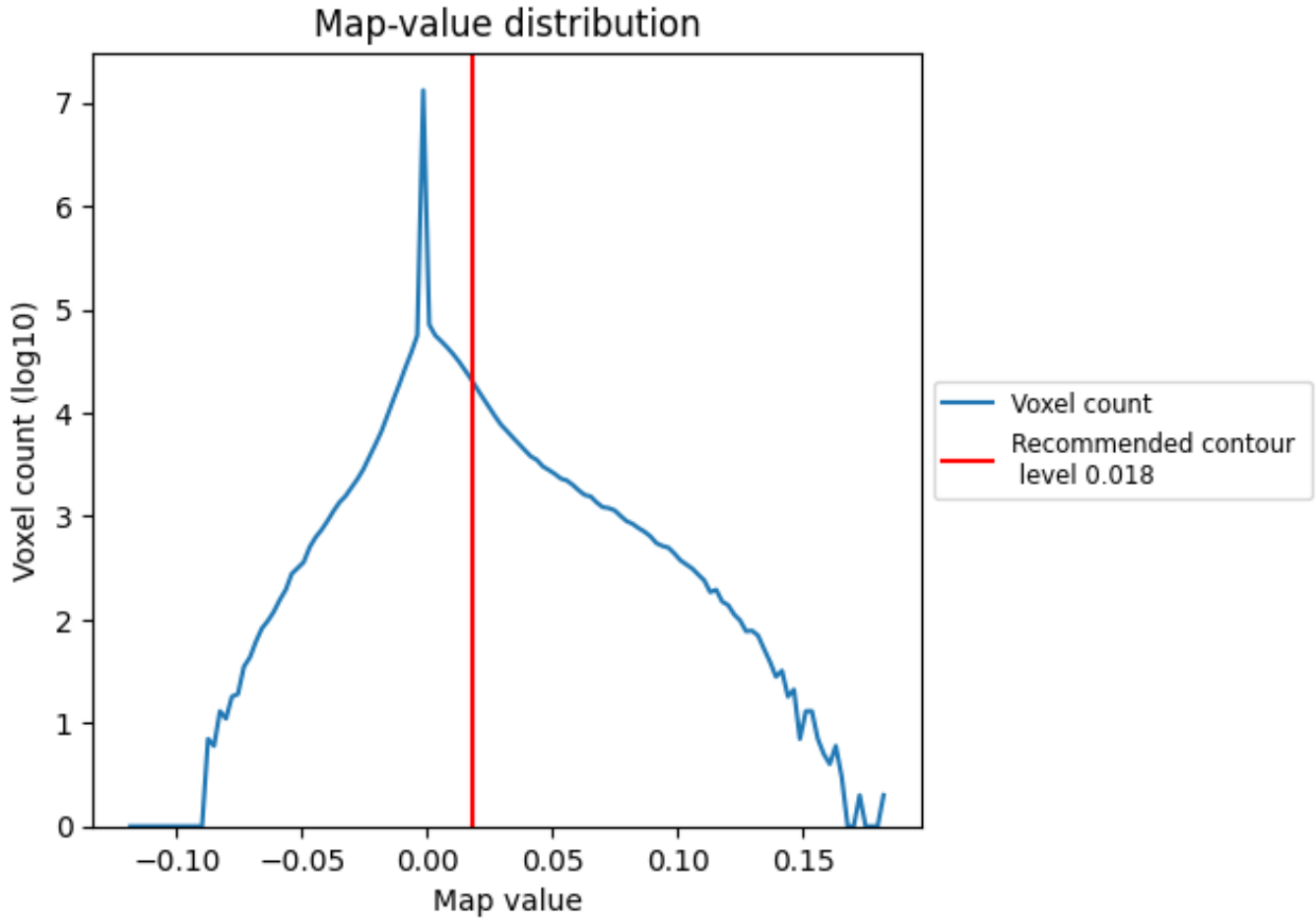
6.6 Mask visualisation (i)

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

7 Map analysis

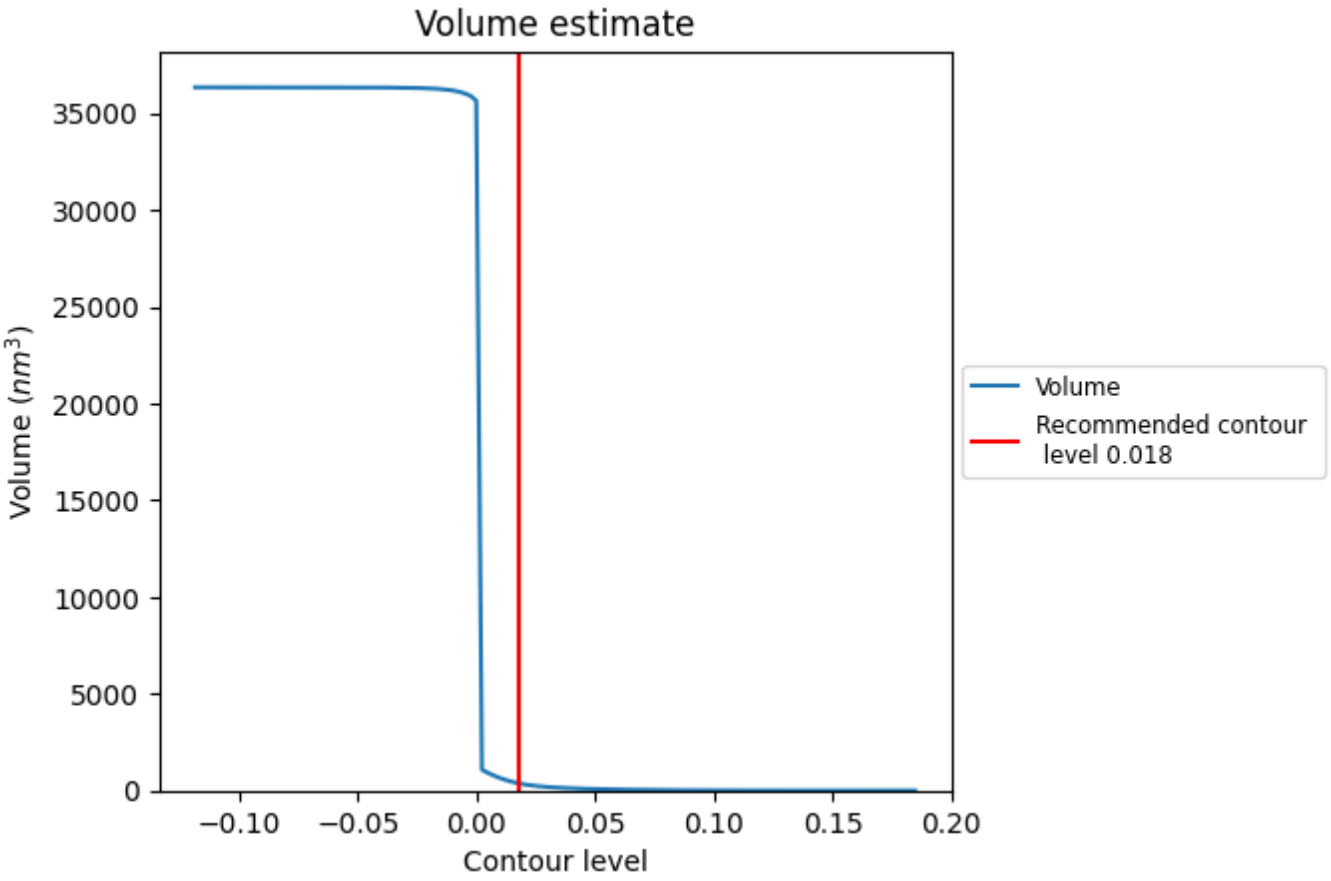
This section contains the results of statistical analysis of the map.

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.

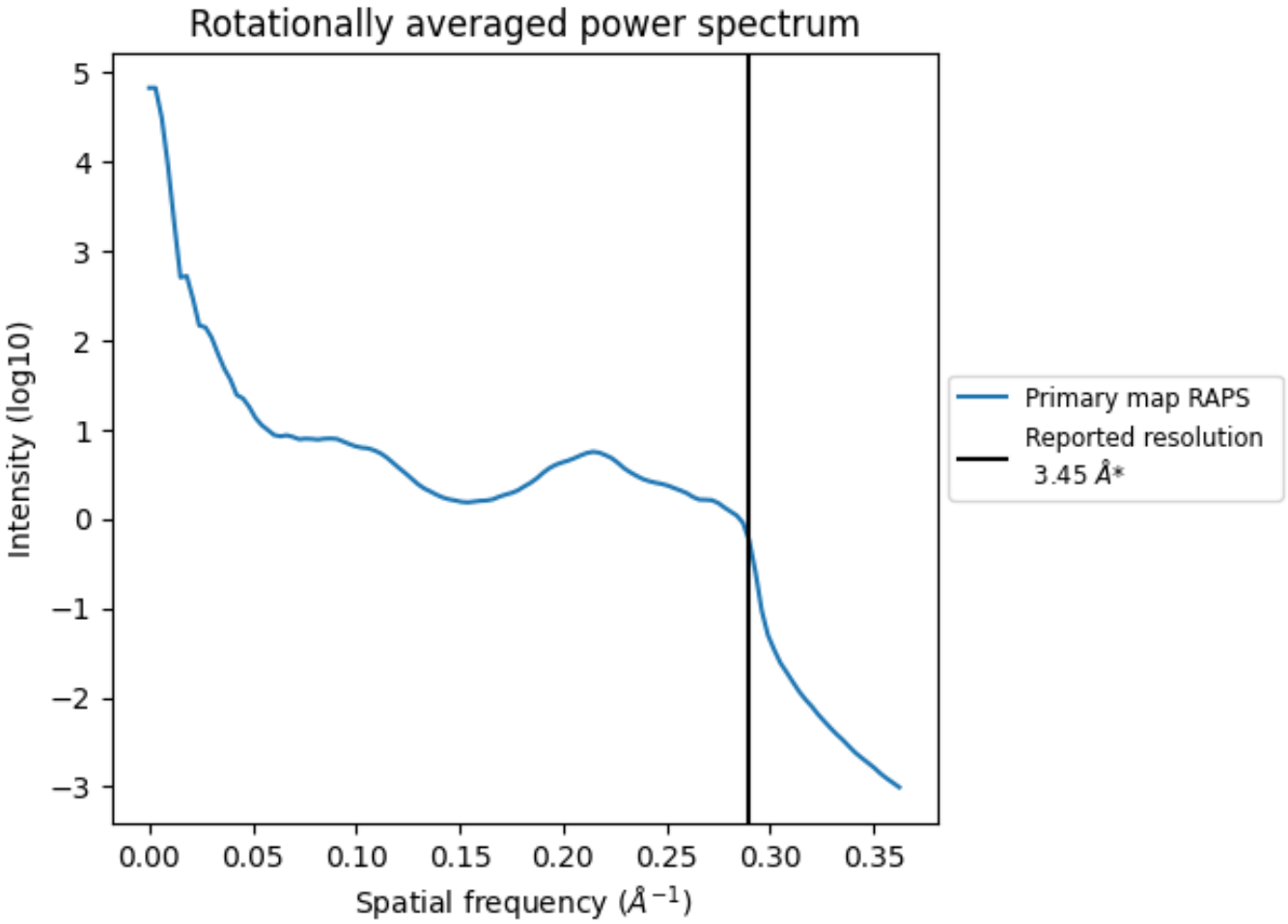
7.2 Volume estimate (i)



The volume at the recommended contour level is 370 nm^3; this corresponds to an approximate mass of 334 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 0.290 Å^{-1}

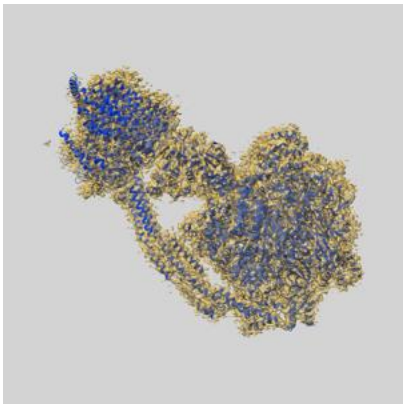
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

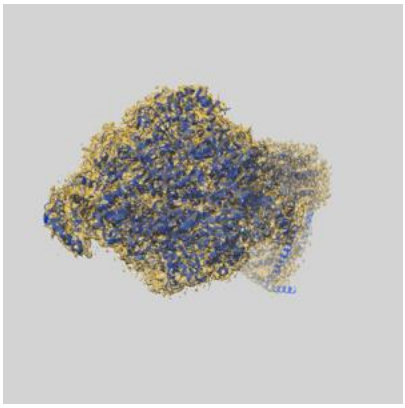
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0669 and PDB model 6J5J. Per-residue inclusion information can be found in section 3 on page 9.

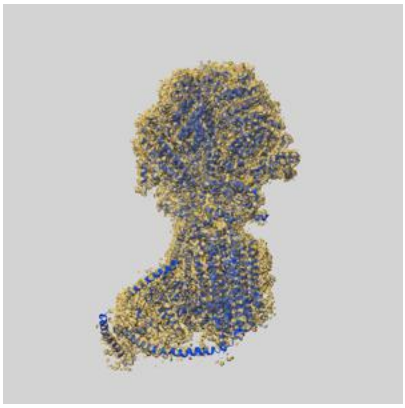
9.1 Map-model overlay



X



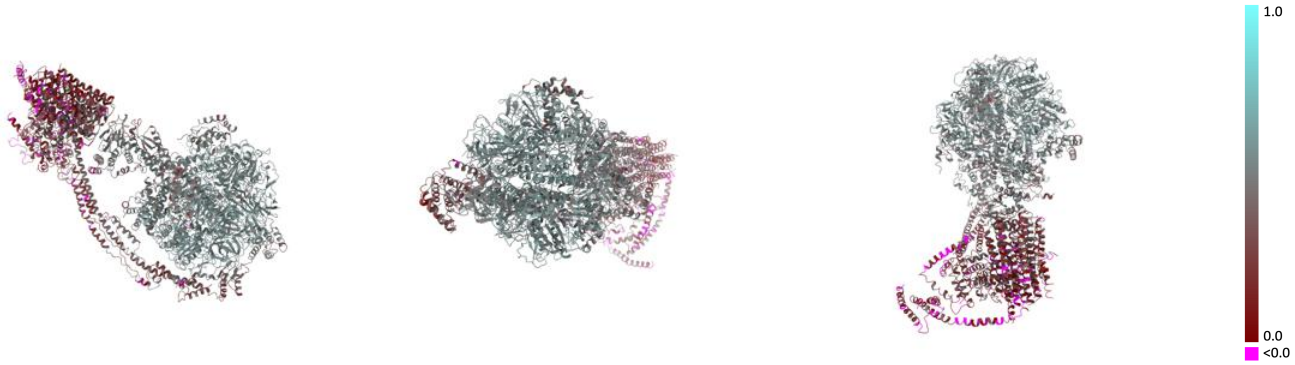
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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.

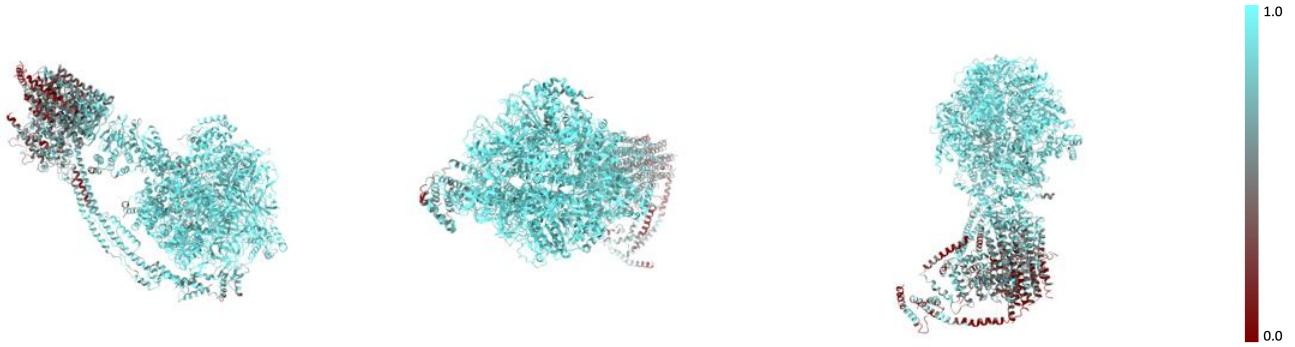
9.2 Q-score mapped to coordinate model (i)



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.

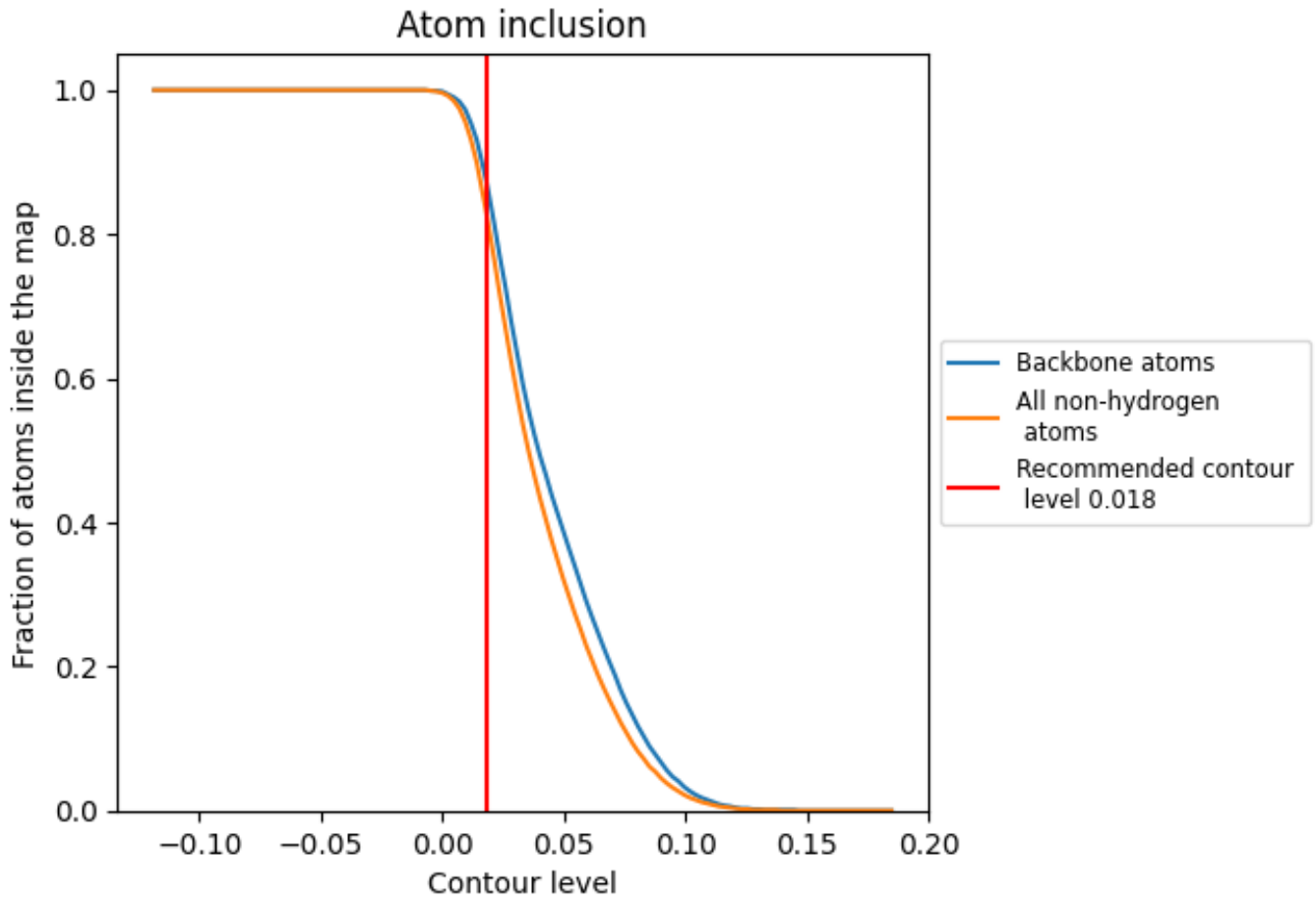
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 83% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8320	0.4400
8	0.5620	0.2440
A	0.9390	0.5300
B	0.9500	0.5220
C	0.9250	0.5210
D	0.9520	0.5410
E	0.9450	0.5250
F	0.9540	0.5400
G	0.8910	0.4800
H	0.8110	0.4260
I	0.8690	0.4400
J	0.7860	0.4620
K	0.5150	0.2450
L	0.4930	0.2480
M	0.5250	0.2420
N	0.6640	0.3080
O	0.5230	0.2320
P	0.5720	0.2030
Q	0.6380	0.2410
R	0.6050	0.2600
S	0.8670	0.4370
a	0.6140	0.2860
b	0.7130	0.2990
c	0.7710	0.3030
d	0.7770	0.2800
e	0.3430	0.1510
f	0.5550	0.1960
g	0.4710	0.1190
i	0.4650	0.1660
k	0.2970	0.1700
u	0.0670	0.0720