wwPDB EM Validation Summary Report

May 11, 2024 – 09:28 pm BST

PDB ID	:	6RD4
EMDB ID	:	EMD-4805
Title	:	CryoEM structure of Polytomella F-ATP synthase, Full dimer, composite map
Authors	:	Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.
Deposited on	:	2019-04-12
Resolution	:	2.90 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:

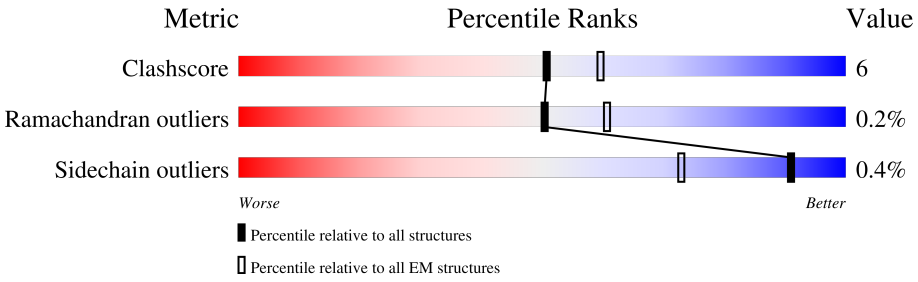
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	158937	4297
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	0	82	95% . .
2	1	618	86% 10% .
3	2	441	87% 13%
4	3	325	65% 11% 25%
5	4	294	90% 8% .
6	5	123	86% 14%
7	6	151	75% 7% 18%
8	7	190	78% 14% 7%

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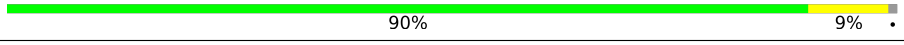
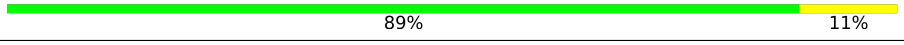
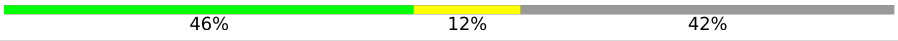
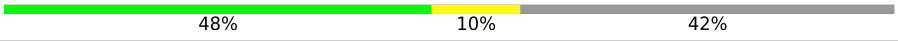
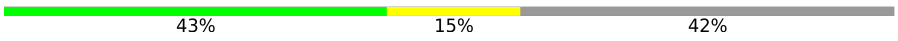
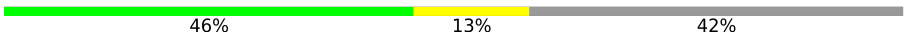
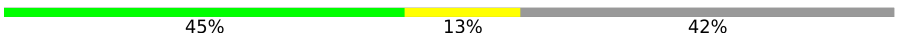
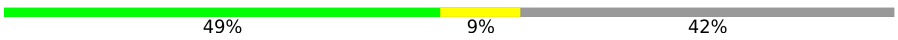
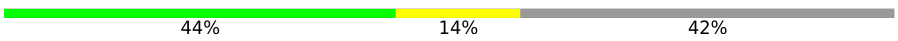
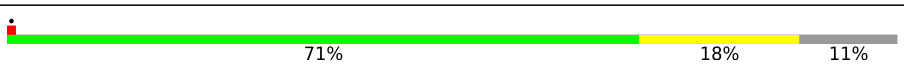
Mol	Chain	Length	Quality of chain
9	8	89	
10	9	97	
11	A	127	
11	B	127	
11	C	127	
11	D	127	
11	E	127	
11	F	127	
11	G	127	
11	H	127	
11	I	127	
11	J	127	
12	M	327	
13	P	229	
14	Q	74	
15	R	199	
16	S	317	
17	T	562	
17	U	562	
17	V	562	
18	X	574	
18	Y	574	
18	Z	574	

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 53776 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 ASA-10: Polytomella F-ATP synthase associated subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	81	607	388	107	110	2	0	0

- Molecule 2 is a protein called ATP synthase associated protein ASA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	595	4661	2958	798	900	5	0	0

- Molecule 3 is a protein called Mitochondrial ATP synthase subunit ASA2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	2	441	3163	2020	532	611	0	0

- Molecule 4 is a protein called Mitochondrial F1F0 ATP synthase associated 32 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	245	1874	1204	299	370	1	0	0

- Molecule 5 is a protein called Mitochondrial ATP synthase associated protein ASA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	290	2177	1385	356	434	2	0	0

- Molecule 6 is a protein called Mitochondrial F1F0 ATP synthase associated 14 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	123	986	640	172	170	4	0	0

- Molecule 7 is a protein called Mitochondrial ATP synthase subunit ASA6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	124	Total	C	N	O	S	0	0
			926	599	154	172	1		

- Molecule 8 is a protein called Mitochondrial ATP synthase associated protein ASA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	176	Total	C	N	O	S	0	0
			1347	860	227	259	1		

- Molecule 9 is a protein called Mitochondrial ATP synthase subunit ASA8.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	8	88	Total	C	N	O	0	0
			692	456	115	121		

- Molecule 10 is a protein called Mitochondrial ATP synthase subunit ASA9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	97	Total	C	N	O	S	0	0
			776	514	124	132	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	B	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	C	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	D	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	E	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	F	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	G	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	H	74	Total	C	N	O	S	0	0
			514	340	83	88	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	74	Total	C	N	O	S	0	0
			514	340	83	88	3		
11	J	74	Total	C	N	O	S	0	0
			514	340	83	88	3		

- Molecule 12 is a protein called Mitochondrial ATP synthase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	217	Total	C	N	O	S	0	0
			1640	1077	267	288	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	193	Total	C	N	O	S	0	0
			1532	988	250	290	4		

- Molecule 14 is a protein called epsilon: Polytomella F-ATP synthase epsilon subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	72	Total	C	N	O	S	0	0
			561	358	102	99	2		

- Molecule 15 is a protein called Mitochondrial ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	177	Total	C	N	O	S	0	0
			1303	833	213	256	1		

- Molecule 16 is a protein called ATP synthase gamma chain, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	277	Total	C	N	O	S	0	0
			2130	1327	377	416	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	523	Total	C	N	O	S	0	0
			3979	2537	703	728	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	523	Total	C	N	O	S	0	0
			3980	2537	703	729	11		
17	V	520	Total	C	N	O	S	0	0
			3962	2527	700	724	11		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	266	ARG	LYS	conflict	UNP A0ZW40
U	266	ARG	LYS	conflict	UNP A0ZW40
V	266	ARG	LYS	conflict	UNP A0ZW40

- Molecule 18 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	542	Total	C	N	O	S	0	0
			4115	2586	696	820	13		
18	Y	521	Total	C	N	O	S	0	0
			3957	2485	670	789	13		
18	Z	538	Total	C	N	O	S	0	0
			4087	2568	692	814	13		

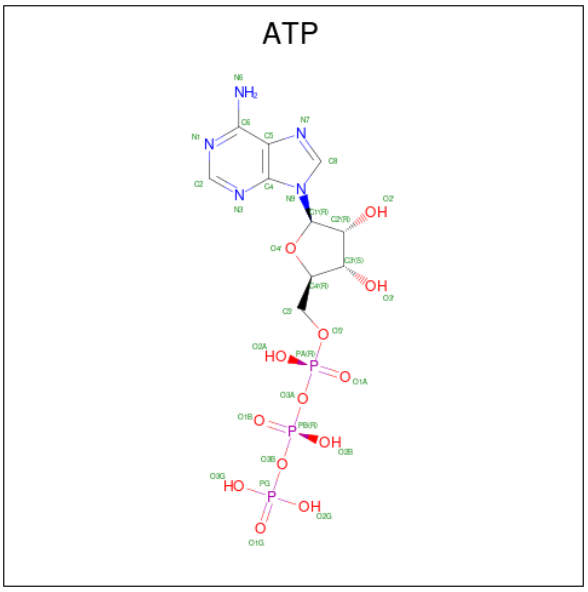
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	350	ALA	GLY	conflict	UNP A0ZW41
X	387	LEU	ARG	conflict	UNP A0ZW41
Y	350	ALA	GLY	conflict	UNP A0ZW41
Y	387	LEU	ARG	conflict	UNP A0ZW41
Z	350	ALA	GLY	conflict	UNP A0ZW41
Z	387	LEU	ARG	conflict	UNP A0ZW41

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	M	1	Total	Zn	0
			1	1	

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

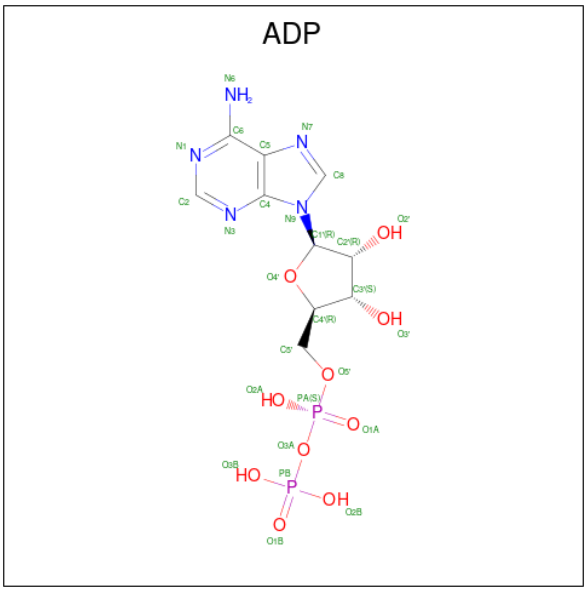


Mol	Chain	Residues	Atoms					AltConf
20	T	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	U	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	V	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
21	T	1	Total	Mg	0
			1	1	
21	U	1	Total	Mg	0
			1	1	
21	V	1	Total	Mg	0
			1	1	
21	X	1	Total	Mg	0
			1	1	
21	Y	1	Total	Mg	0
			1	1	

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 23 is water.

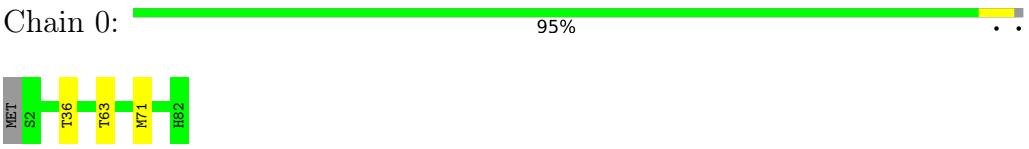
Mol	Chain	Residues	Atoms		AltConf
23	1	2	Total	O	0
			2	2	
23	6	5	Total	O	0
			5	5	
23	A	1	Total	O	0
			1	1	
23	M	20	Total	O	0
			20	20	

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.

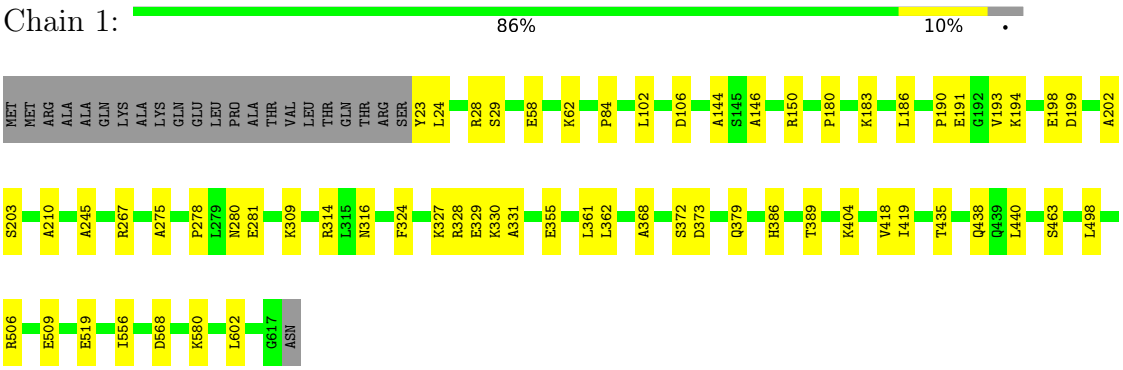
• Molecule 1: ASA-10: Polytomella F-ATP synthase associated subunit 10

Chain 0:



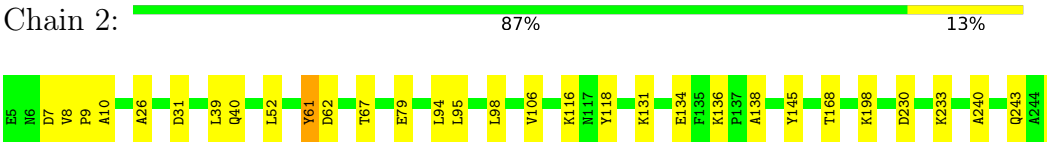
• Molecule 2: ATP synthase associated protein ASA1

Chain 1:



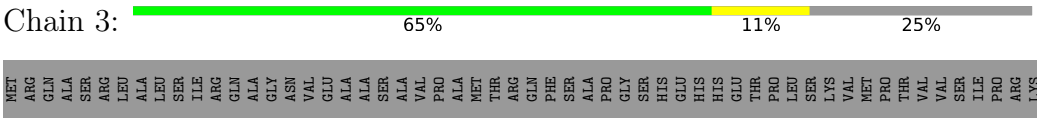
• Molecule 3: Mitochondrial ATP synthase subunit ASA2

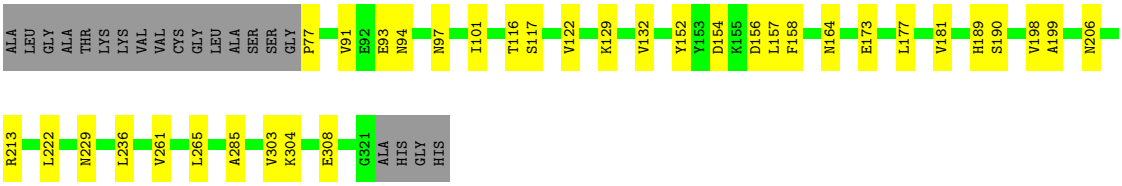
Chain 2:



• Molecule 4: Mitochondrial F1F0 ATP synthase associated 32 kDa protein

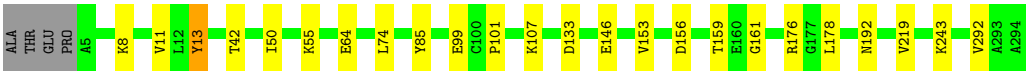
Chain 3:





• Molecule 5: Mitochondrial ATP synthase associated protein ASA4

Chain 4:

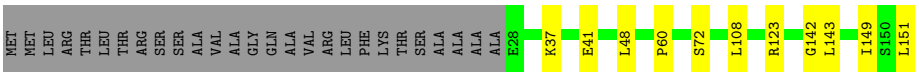


• Molecule 6: Mitochondrial F1F0 ATP synthase associated 14 kDa protein

Chain 5:

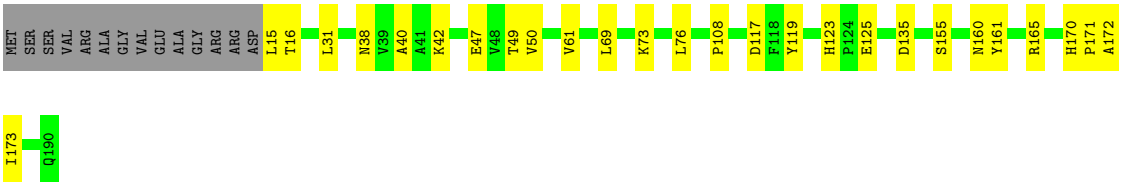
• Molecule 7: Mitochondrial ATP synthase subunit ASA6

Chain 6:



• Molecule 8: Mitochondrial ATP synthase associated protein ASA7

Chain 7:

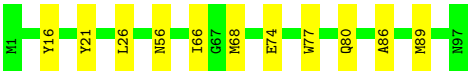


• Molecule 9: Mitochondrial ATP synthase subunit ASA8

Chain 8:

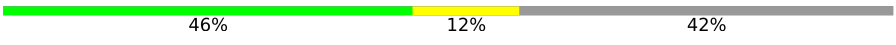
• Molecule 10: Mitochondrial ATP synthase subunit ASA9

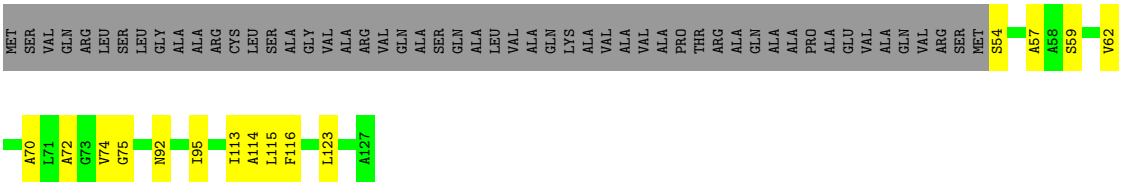
Chain 9:



• Molecule 11: Mitochondrial ATP synthase subunit c

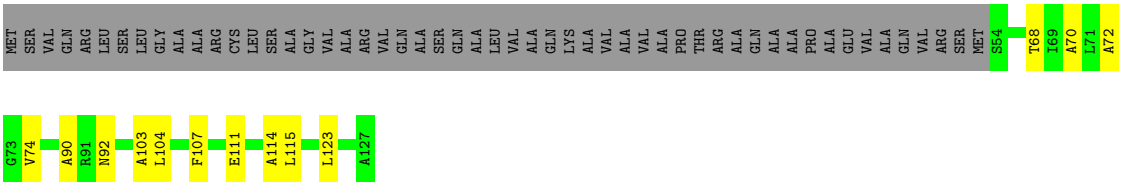
Chain A:





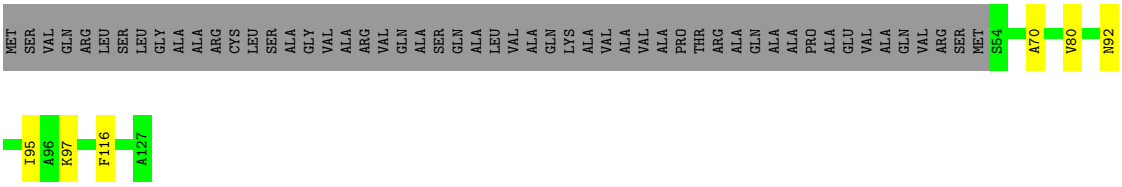
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain B:



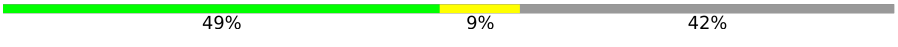
• Molecule 11: Mitochondrial ATP synthase subunit c

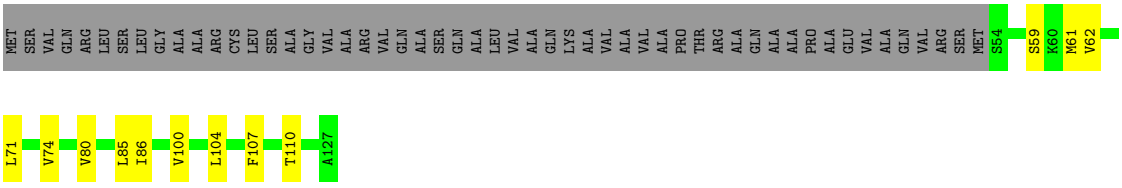
Chain C:



• Molecule 11: Mitochondrial ATP synthase subunit c

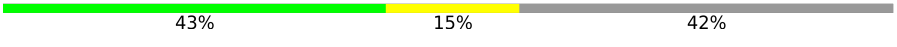
Chain D:

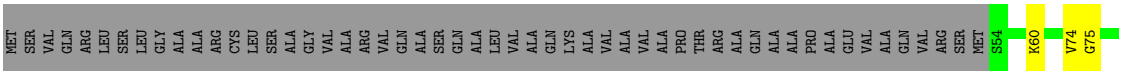




• Molecule 11: Mitochondrial ATP synthase subunit c

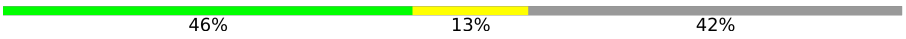
Chain E:





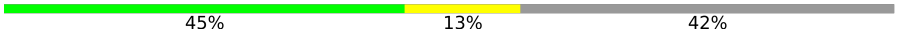
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain F:



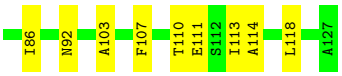
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain G:



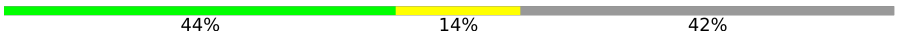
• Molecule 11: Mitochondrial ATP synthase subunit c

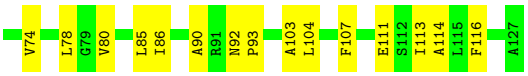
Chain H:



• Molecule 11: Mitochondrial ATP synthase subunit c

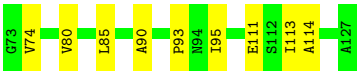
Chain I:





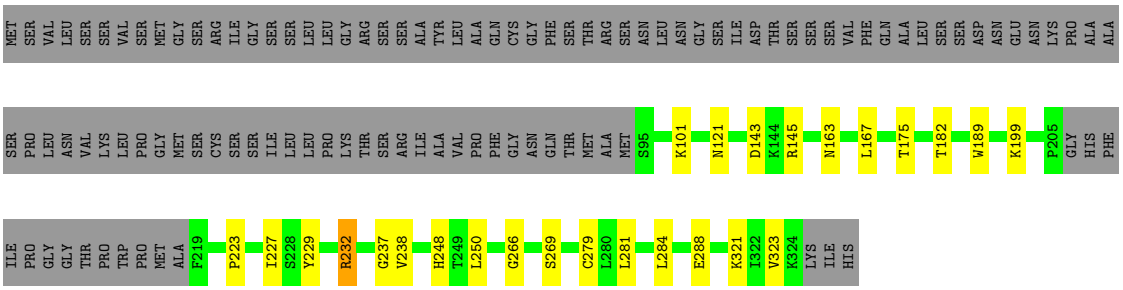
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain J:



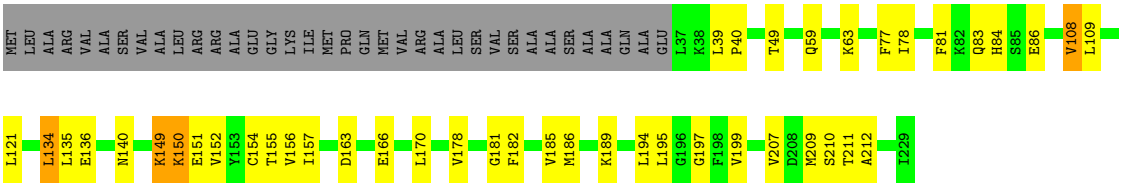
• Molecule 12: Mitochondrial ATP synthase subunit 6

Chain M:



• Molecule 13: Mitochondrial ATP synthase subunit OSCP

Chain P:

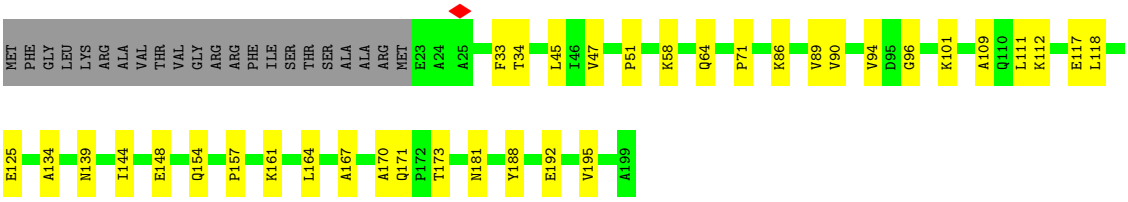


• Molecule 14: epsilon: Polytomella F-ATP synthase epsilon subunit

Chain Q:

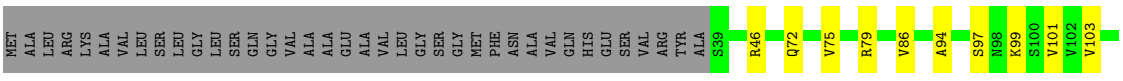
• Molecule 15: Mitochondrial ATP synthase subunit delta

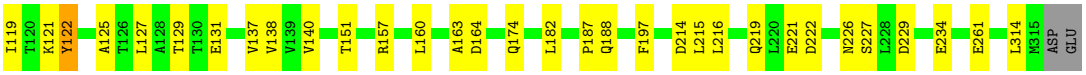
Chain R:



• Molecule 16: ATP synthase gamma chain, mitochondrial

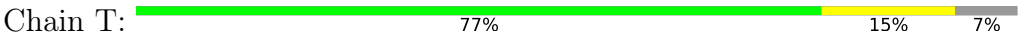
Chain S:

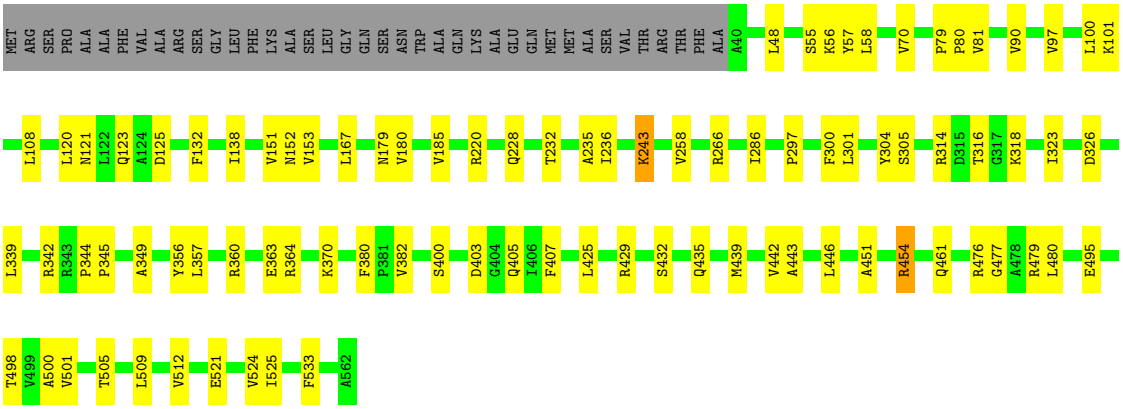




• Molecule 17: ATP synthase subunit alpha

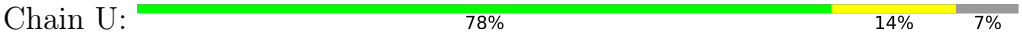
Chain T:

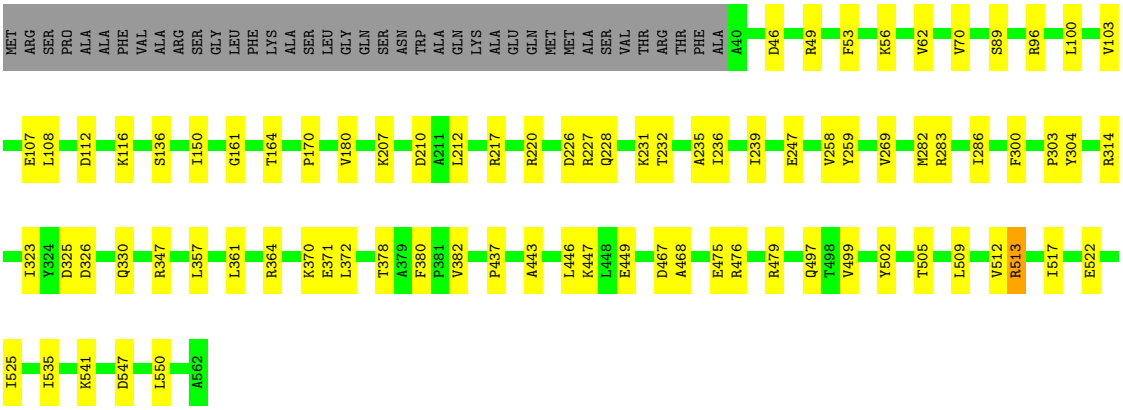




• Molecule 17: ATP synthase subunit alpha

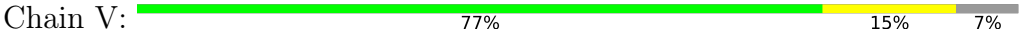
Chain U:

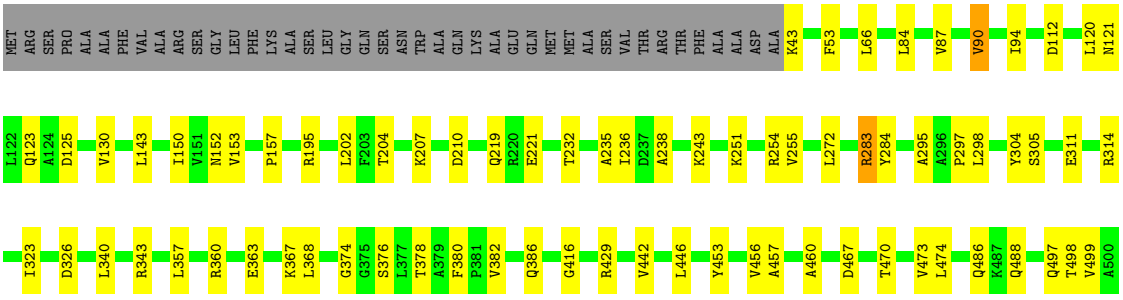


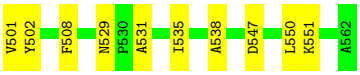


• Molecule 17: ATP synthase subunit alpha

Chain V:

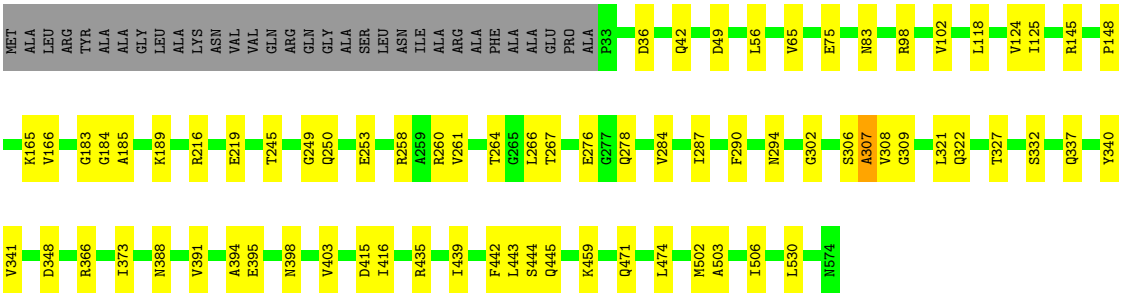






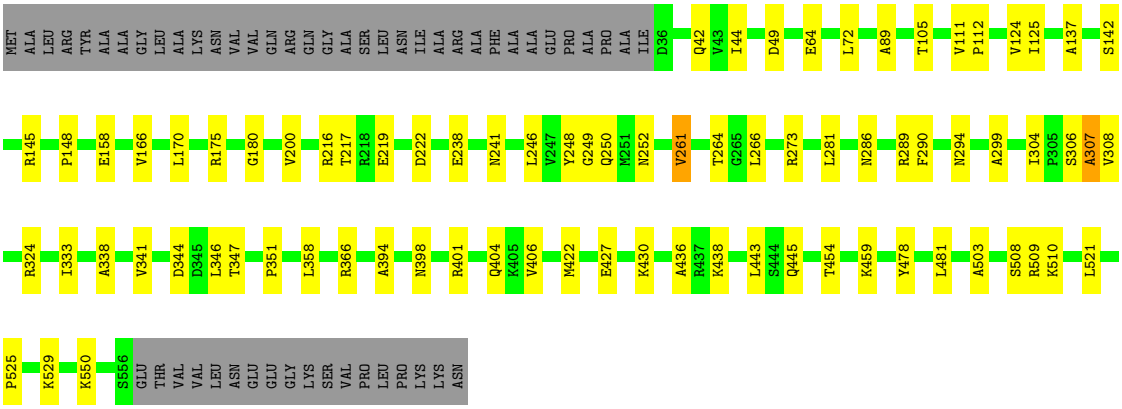
• Molecule 18: ATP synthase subunit beta

Chain X:



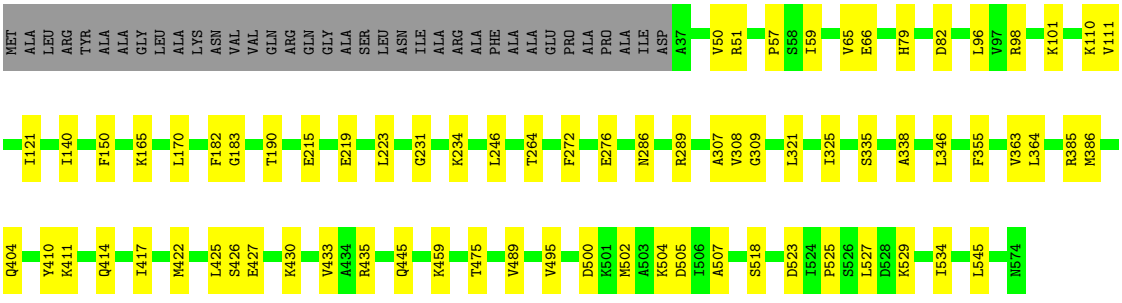
• Molecule 18: ATP synthase subunit beta

Chain Y:



• Molecule 18: ATP synthase subunit beta

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	388670	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	-400	Depositor
Maximum defocus (nm)	-5000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	62.159	Depositor
Minimum map value	-30.456	Depositor
Average map value	0.003	Depositor
Map value standard deviation	1.264	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	505.44, 505.44, 505.44	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.053, 1.053, 1.053	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, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.70	0/628	0.55	0/856
2	1	0.69	0/4750	0.59	0/6434
3	2	0.53	0/3212	0.58	0/4371
4	3	0.63	0/1911	0.59	1/2601 (0.0%)
5	4	0.61	0/2216	0.59	1/3000 (0.0%)
6	5	0.90	1/1011 (0.1%)	0.68	0/1376
7	6	0.72	0/946	0.63	0/1287
8	7	0.79	0/1374	0.63	0/1865
9	8	0.83	0/715	0.66	0/974
10	9	0.52	0/802	0.59	0/1084
11	A	0.48	0/520	0.59	1/704 (0.1%)
11	B	0.49	0/520	0.66	1/704 (0.1%)
11	C	0.40	0/519	0.61	1/701 (0.1%)
11	D	0.35	0/520	0.59	0/704
11	E	0.36	0/520	0.63	0/704
11	F	0.39	0/520	0.63	1/704 (0.1%)
11	G	0.41	0/520	0.65	0/704
11	H	0.39	0/520	0.61	0/704
11	I	0.37	0/520	0.55	0/704
11	J	0.40	0/520	0.59	0/704
12	M	0.77	0/1683	0.66	0/2295
13	P	0.49	0/1553	0.65	1/2093 (0.0%)
14	Q	0.45	0/574	0.64	0/774
15	R	0.46	0/1336	0.57	0/1827
16	S	0.53	0/2153	0.63	0/2901
17	T	0.70	0/4048	0.65	0/5481
17	U	0.71	0/4049	0.64	0/5481
17	V	0.68	0/4031	0.64	0/5456
18	X	0.69	0/4176	0.66	2/5659 (0.0%)
18	Y	0.61	1/4015 (0.0%)	0.64	2/5440 (0.0%)
18	Z	0.63	1/4147 (0.0%)	0.62	1/5619 (0.0%)
All	All	0.64	3/54529 (0.0%)	0.62	12/73911 (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
13	P	0	2
17	T	0	1
18	X	0	1
18	Y	0	2
18	Z	0	2
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Y	261	VAL	CB-CG2	-6.08	1.40	1.52
18	Z	50	VAL	CB-CG2	-5.39	1.41	1.52
6	5	113	VAL	CB-CG2	-5.28	1.41	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	X	36	ASP	CB-CG-OD1	8.78	126.20	118.30
13	P	134	LEU	CB-CG-CD1	-7.58	98.11	111.00
11	B	123	LEU	CA-CB-CG	6.76	130.86	115.30
18	X	266	LEU	CA-CB-CG	6.45	130.13	115.30
11	C	95	ILE	CG1-CB-CG2	-6.25	97.66	111.40

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	P	149	LYS	Peptide
13	P	185	VAL	Peptide
17	T	509	LEU	Peptide
18	X	307	ALA	Peptide
18	Y	307	ALA	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	607	0	584	1	0
2	1	4661	0	4695	45	0
3	2	3163	0	3262	37	0
4	3	1874	0	1826	18	0
5	4	2177	0	2169	16	0
6	5	986	0	1021	13	0
7	6	926	0	941	8	0
8	7	1347	0	1345	24	0
9	8	692	0	694	6	0
10	9	776	0	757	10	0
11	A	514	0	554	15	0
11	B	514	0	554	13	0
11	C	514	0	553	6	0
11	D	514	0	554	9	0
11	E	514	0	554	16	0
11	F	514	0	554	17	0
11	G	514	0	554	27	0
11	H	514	0	554	18	0
11	I	514	0	554	21	0
11	J	514	0	554	19	0
12	M	1640	0	1665	24	0
13	P	1532	0	1603	36	0
14	Q	561	0	565	19	0
15	R	1303	0	1266	23	0
16	S	2130	0	2180	30	0
17	T	3979	0	4119	61	0
17	U	3980	0	4119	55	0
17	V	3962	0	4105	54	0
18	X	4115	0	4137	41	0
18	Y	3957	0	3966	46	0
18	Z	4087	0	4110	39	0
19	M	1	0	0	0	0
20	T	31	0	12	1	0
20	U	31	0	12	0	0
20	V	31	0	12	1	0
21	T	1	0	0	0	0
21	U	1	0	0	0	0
21	V	1	0	0	0	0
21	X	1	0	0	0	0
21	Y	1	0	0	0	0
22	X	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	Y	27	0	12	2	0
23	1	2	0	0	0	0
23	6	5	0	0	0	0
23	A	1	0	0	0	0
23	M	20	0	0	3	0
All	All	53776	0	54728	635	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 6.

The worst 5 of 635 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)
11:I:111:GLU:OE2	11:J:113:ILE:HD11	1.22	1.37
11:H:111:GLU:OE2	11:I:113:ILE:HD11	1.36	1.22
12:M:229:TYR:O	12:M:232:ARG:HG2	1.49	1.11
14:Q:51:PRO:HD2	14:Q:59:ALA:O	1.54	1.07
13:P:149:LYS:O	13:P:151:GLU:N	1.88	1.06

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	0	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
2	1	593/618 (96%)	572 (96%)	21 (4%)	0	100	100
3	2	439/441 (100%)	415 (94%)	23 (5%)	1 (0%)	47	78
4	3	243/325 (75%)	234 (96%)	8 (3%)	1 (0%)	34	66
5	4	288/294 (98%)	275 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	5	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
7	6	122/151 (81%)	113 (93%)	8 (7%)	1 (1%)	19	51
8	7	174/190 (92%)	165 (95%)	9 (5%)	0	100	100
9	8	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
10	9	95/97 (98%)	79 (83%)	15 (16%)	1 (1%)	14	42
11	A	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	B	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	C	71/127 (56%)	69 (97%)	2 (3%)	0	100	100
11	D	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	E	72/127 (57%)	72 (100%)	0	0	100	100
11	F	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	G	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	H	72/127 (57%)	72 (100%)	0	0	100	100
11	I	72/127 (57%)	72 (100%)	0	0	100	100
11	J	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
12	M	213/327 (65%)	206 (97%)	7 (3%)	0	100	100
13	P	191/229 (83%)	178 (93%)	11 (6%)	2 (1%)	15	45
14	Q	70/74 (95%)	64 (91%)	3 (4%)	3 (4%)	2	10
15	R	175/199 (88%)	165 (94%)	10 (6%)	0	100	100
16	S	275/317 (87%)	268 (98%)	7 (2%)	0	100	100
17	T	521/562 (93%)	499 (96%)	21 (4%)	1 (0%)	47	78
17	U	521/562 (93%)	494 (95%)	26 (5%)	1 (0%)	47	78
17	V	518/562 (92%)	504 (97%)	14 (3%)	0	100	100
18	X	540/574 (94%)	498 (92%)	40 (7%)	2 (0%)	34	66
18	Y	519/574 (90%)	480 (92%)	37 (7%)	2 (0%)	34	66
18	Z	536/574 (93%)	502 (94%)	32 (6%)	2 (0%)	34	66
All	All	7038/8234 (86%)	6688 (95%)	333 (5%)	17 (0%)	50	78

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	383	PRO
13	P	150	LYS

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Mol	Chain	Res	Type
14	Q	57	ALA
18	X	308	VAL
18	Y	308	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	63/64 (98%)	62 (98%)	1 (2%)	62 86
2	1	493/512 (96%)	492 (100%)	1 (0%)	93 98
3	2	312/312 (100%)	310 (99%)	2 (1%)	86 96
4	3	195/258 (76%)	195 (100%)	0	100 100
5	4	220/223 (99%)	219 (100%)	1 (0%)	88 96
6	5	107/107 (100%)	107 (100%)	0	100 100
7	6	96/115 (84%)	96 (100%)	0	100 100
8	7	140/150 (93%)	140 (100%)	0	100 100
9	8	71/72 (99%)	71 (100%)	0	100 100
10	9	79/79 (100%)	79 (100%)	0	100 100
11	A	50/86 (58%)	50 (100%)	0	100 100
11	B	50/86 (58%)	50 (100%)	0	100 100
11	C	50/86 (58%)	50 (100%)	0	100 100
11	D	50/86 (58%)	50 (100%)	0	100 100
11	E	50/86 (58%)	50 (100%)	0	100 100
11	F	50/86 (58%)	50 (100%)	0	100 100
11	G	50/86 (58%)	50 (100%)	0	100 100
11	H	50/86 (58%)	50 (100%)	0	100 100
11	I	50/86 (58%)	50 (100%)	0	100 100
11	J	50/86 (58%)	50 (100%)	0	100 100
12	M	178/272 (65%)	176 (99%)	2 (1%)	73 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	P	171/196 (87%)	170 (99%)	1 (1%)	86 96
14	Q	56/58 (97%)	56 (100%)	0	100 100
15	R	134/151 (89%)	133 (99%)	1 (1%)	84 95
16	S	235/265 (89%)	233 (99%)	2 (1%)	78 93
17	T	419/448 (94%)	415 (99%)	4 (1%)	76 92
17	U	419/448 (94%)	415 (99%)	4 (1%)	76 92
17	V	418/448 (93%)	415 (99%)	3 (1%)	84 95
18	X	449/469 (96%)	449 (100%)	0	100 100
18	Y	430/469 (92%)	430 (100%)	0	100 100
18	Z	446/469 (95%)	445 (100%)	1 (0%)	93 98
All	All	5631/6445 (87%)	5608 (100%)	23 (0%)	91 97

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	T	454	ARG
17	U	378	THR
17	U	300	PHE
17	U	513	ARG
12	M	279	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
17	T	539	ASN
17	V	278	GLN
17	U	246	ASN
17	V	121	ASN
17	V	539	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 11 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
20	ATP	V	1000	21	26,33,33	1.05	1 (3%)	31,52,52	1.46	5 (16%)
22	ADP	Y	601	21	24,29,29	1.02	2 (8%)	29,45,45	1.25	4 (13%)
22	ADP	X	601	21	24,29,29	1.08	1 (4%)	29,45,45	1.31	4 (13%)
20	ATP	U	1001	21	26,33,33	1.04	0	31,52,52	1.38	5 (16%)
20	ATP	T	1001	21	26,33,33	1.03	0	31,52,52	1.41	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
20	ATP	V	1000	21	-	3/18/38/38	0/3/3/3
22	ADP	Y	601	21	-	4/12/32/32	0/3/3/3
22	ADP	X	601	21	-	4/12/32/32	0/3/3/3
20	ATP	U	1001	21	-	3/18/38/38	0/3/3/3
20	ATP	T	1001	21	-	5/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	V	1000	ATP	C2'-C1'	-2.18	1.50	1.53
22	Y	601	ADP	C2'-C1'	-2.13	1.50	1.53
22	Y	601	ADP	C5-C4	2.12	1.46	1.40
22	X	601	ADP	C2'-C1'	-2.04	1.50	1.53

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	T	1001	ATP	N3-C2-N1	-3.33	123.47	128.68
22	X	601	ADP	N3-C2-N1	-3.23	123.62	128.68
20	V	1000	ATP	N3-C2-N1	-3.13	123.79	128.68
20	U	1001	ATP	C3'-C2'-C1'	2.77	105.15	100.98
20	V	1000	ATP	PB-O3B-PG	-2.77	123.33	132.83

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	X	601	ADP	PA-O3A-PB-O2B
22	X	601	ADP	O4'-C4'-C5'-O5'
22	Y	601	ADP	C5'-O5'-PA-O2A
20	U	1001	ATP	O4'-C4'-C5'-O5'
20	U	1001	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

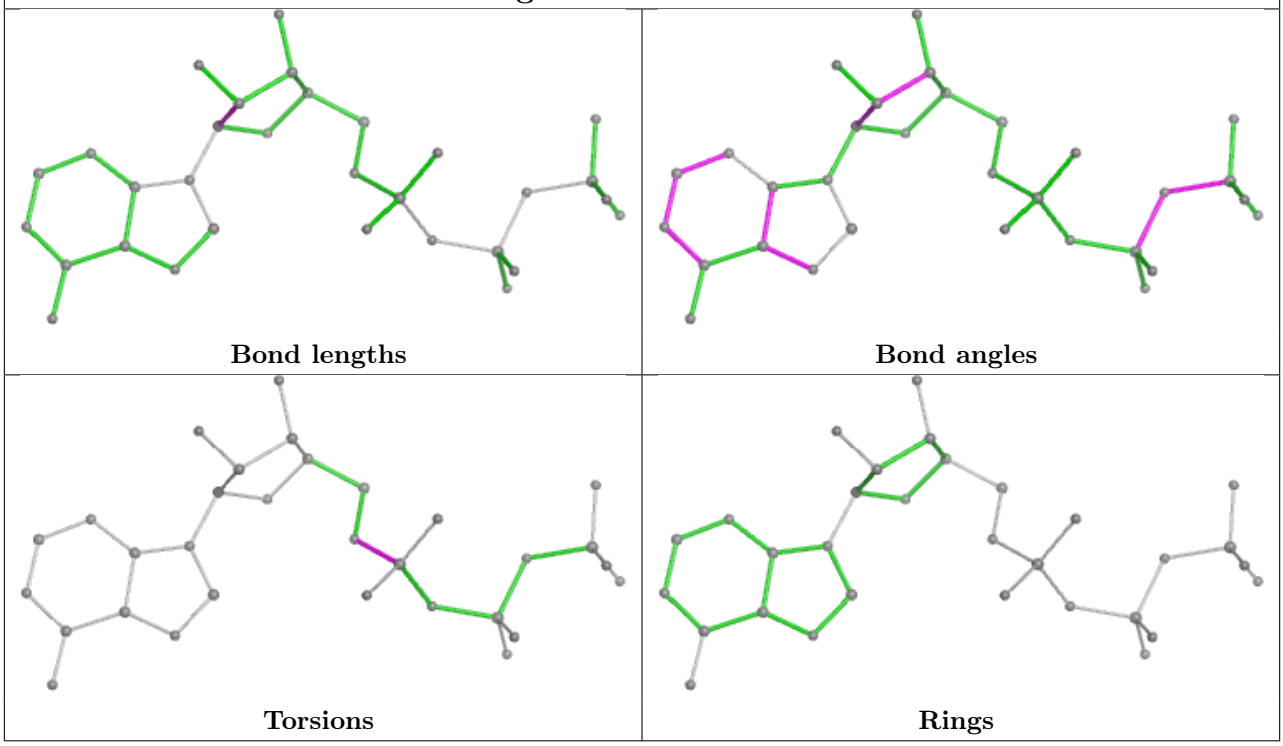
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	V	1000	ATP	1	0
22	Y	601	ADP	2	0
20	T	1001	ATP	1	0

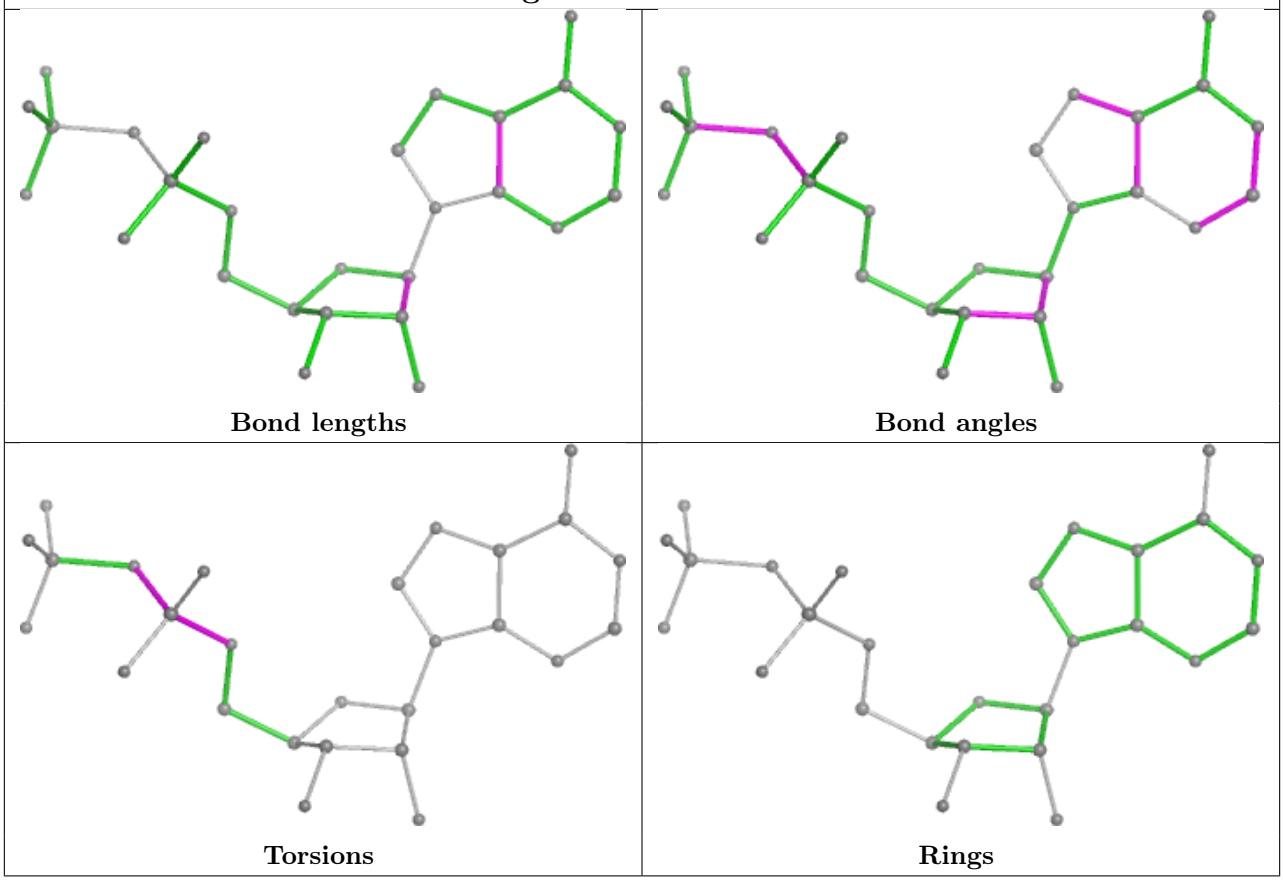
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

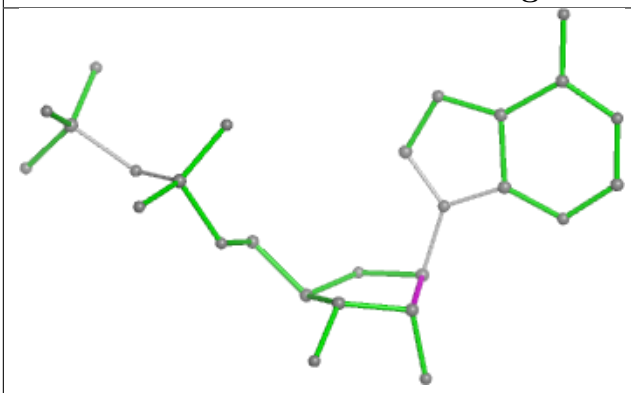
Ligand ATP V 1000



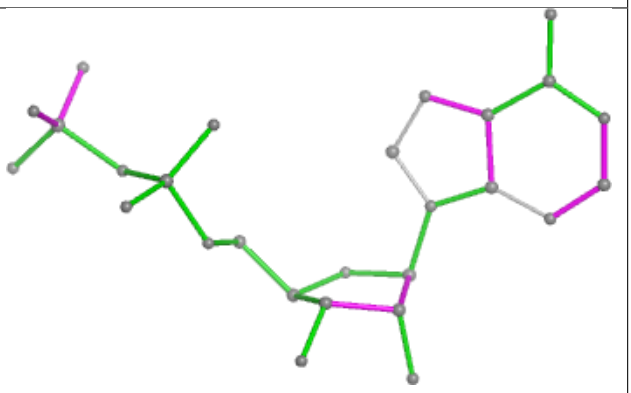
Ligand ADP Y 601



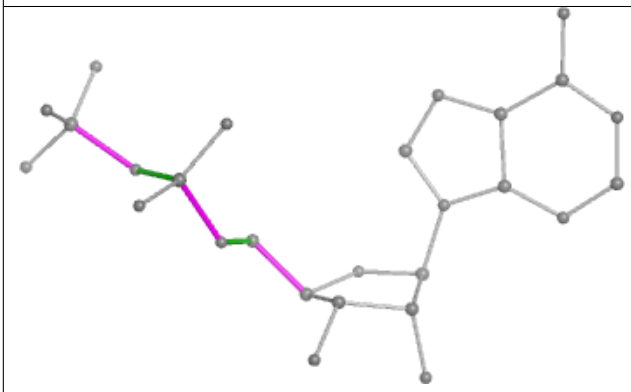
Ligand ADP X 601



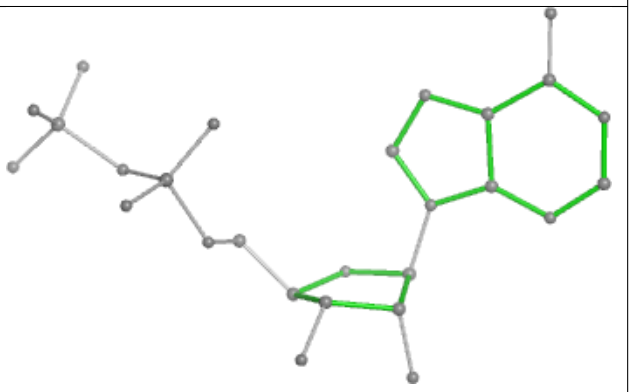
Bond lengths



Bond angles

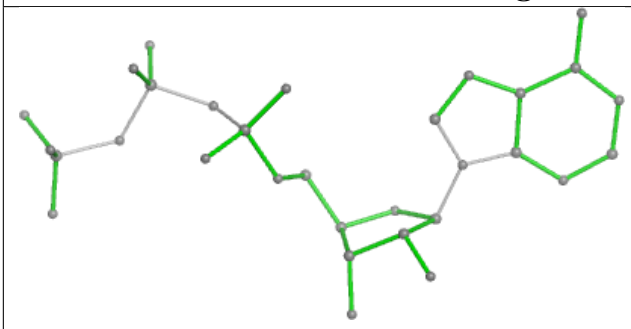


Torsions

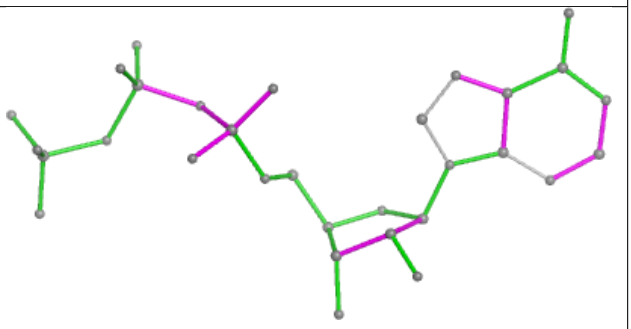


Rings

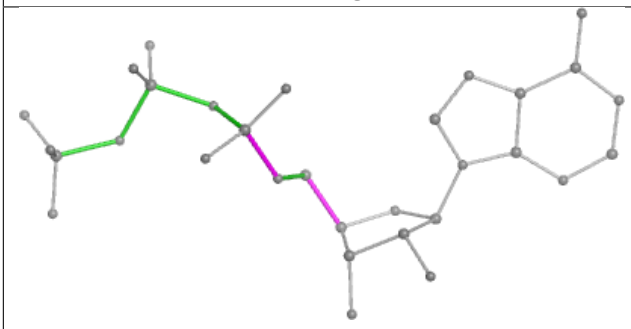
Ligand ATP U 1001



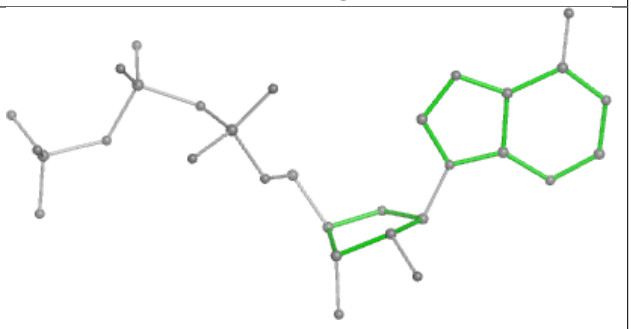
Bond lengths



Bond angles

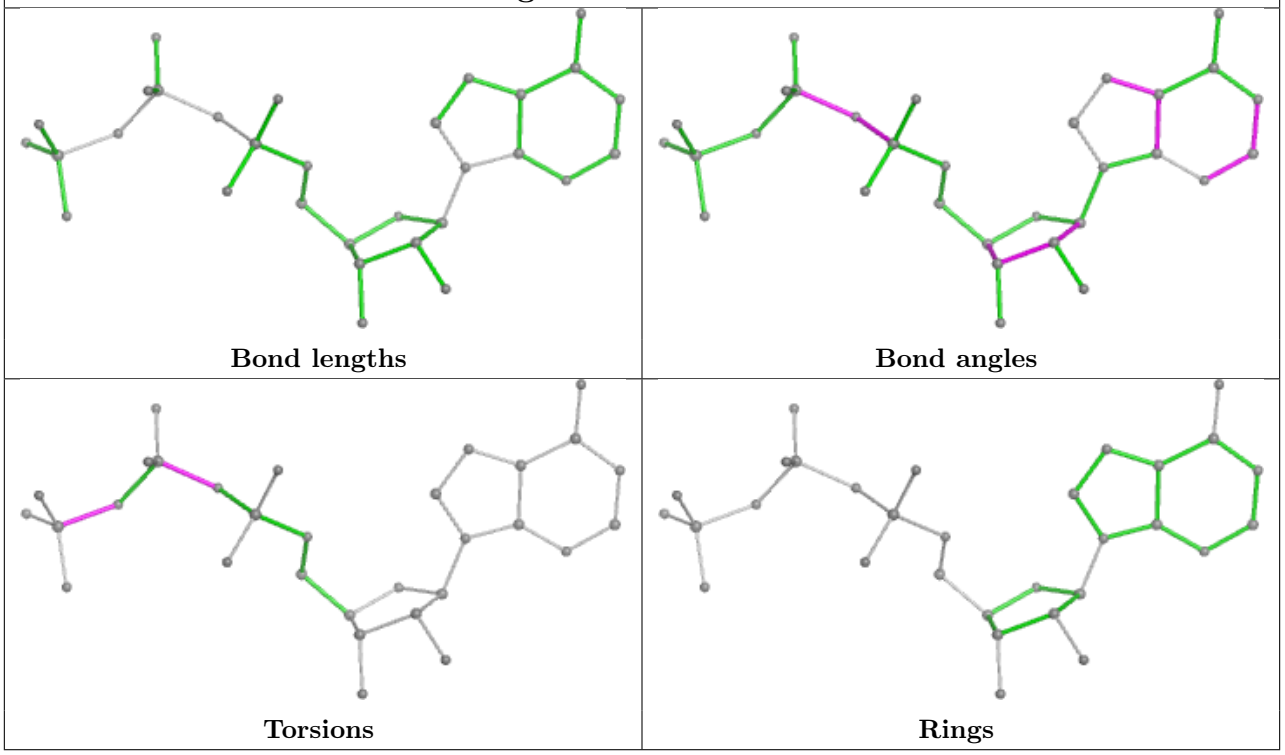


Torsions



Rings

Ligand ATP T 1001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	126:PHE	C	127:ALA	N	3.48

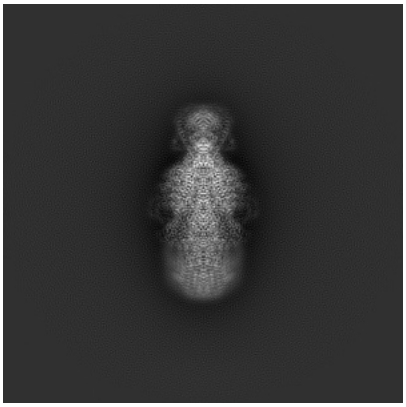
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4805. These allow visual inspection of the internal detail of the map and identification of artifacts.

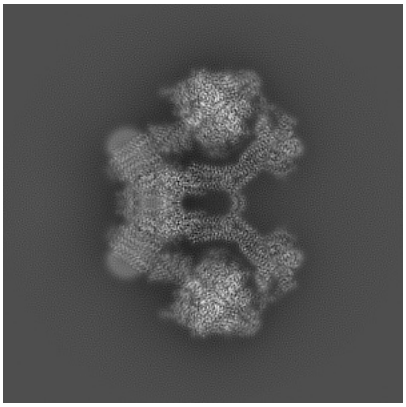
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

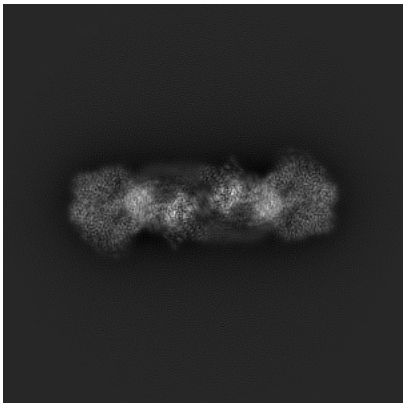
6.1.1 Primary map



X



Y

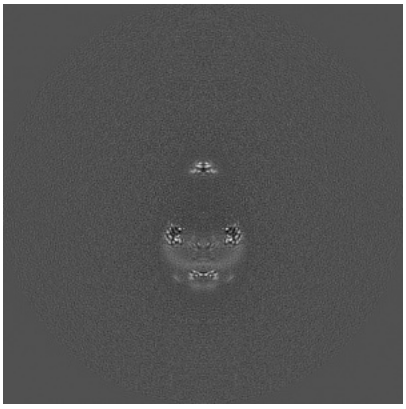


Z

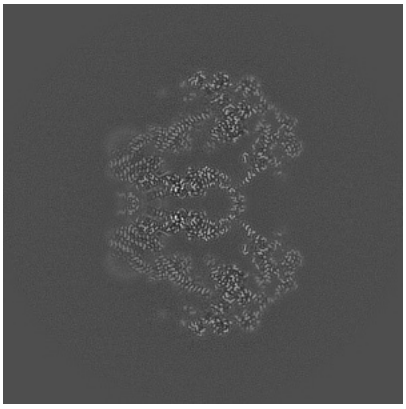
The images above show the map projected in three orthogonal directions.

6.2 Central slices

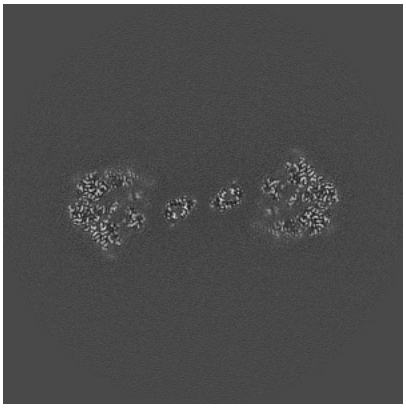
6.2.1 Primary map



X Index: 240



Y Index: 240

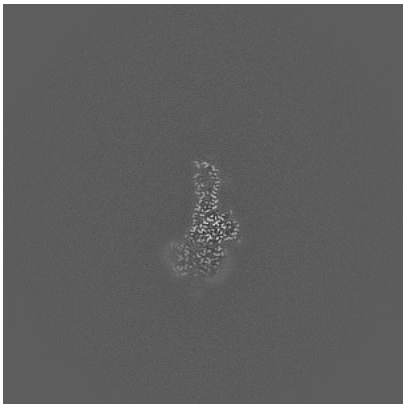


Z Index: 240

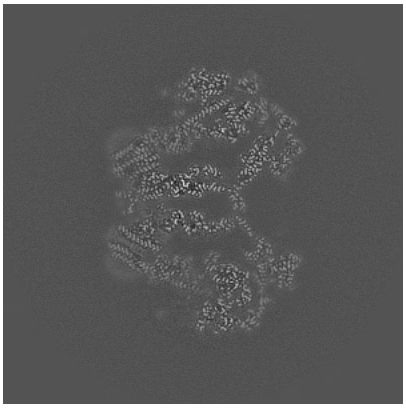
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

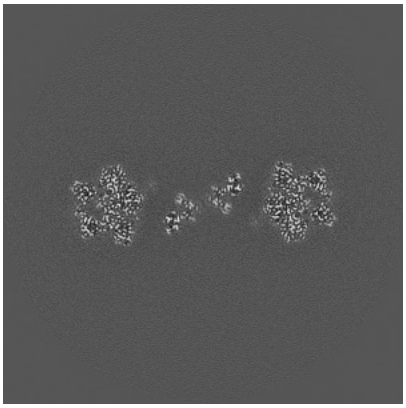
6.3.1 Primary map



X Index: 264



Y Index: 245

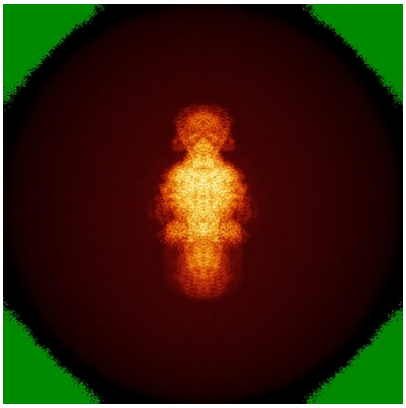


Z Index: 272

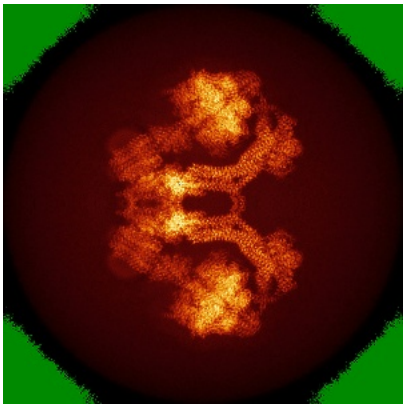
The images above show the largest variance slices of the map in three orthogonal directions.

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

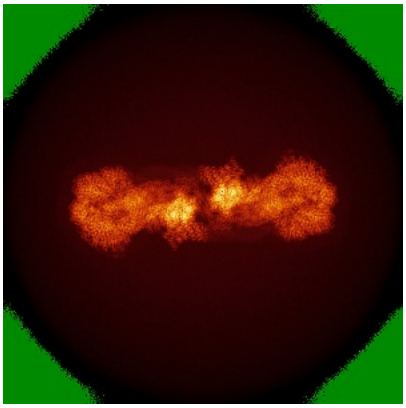
6.4.1 Primary map



X



Y

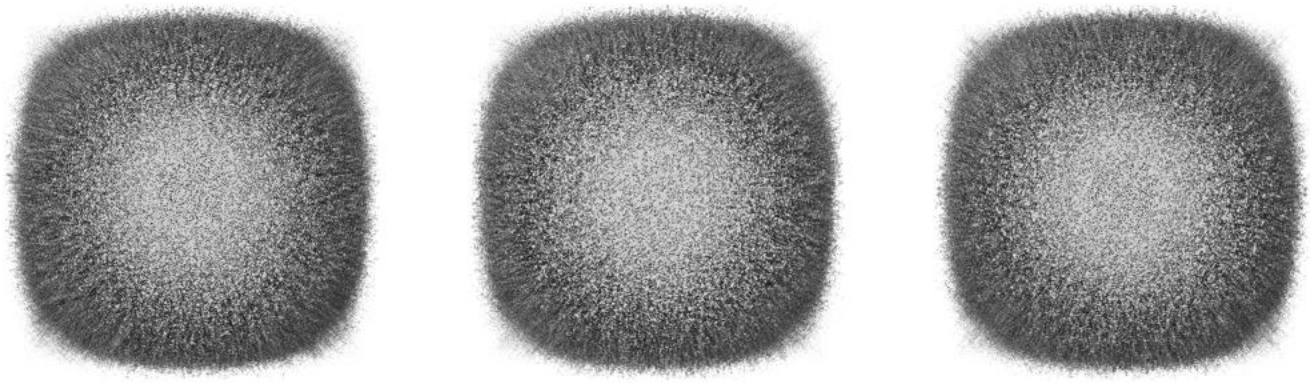


Z

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

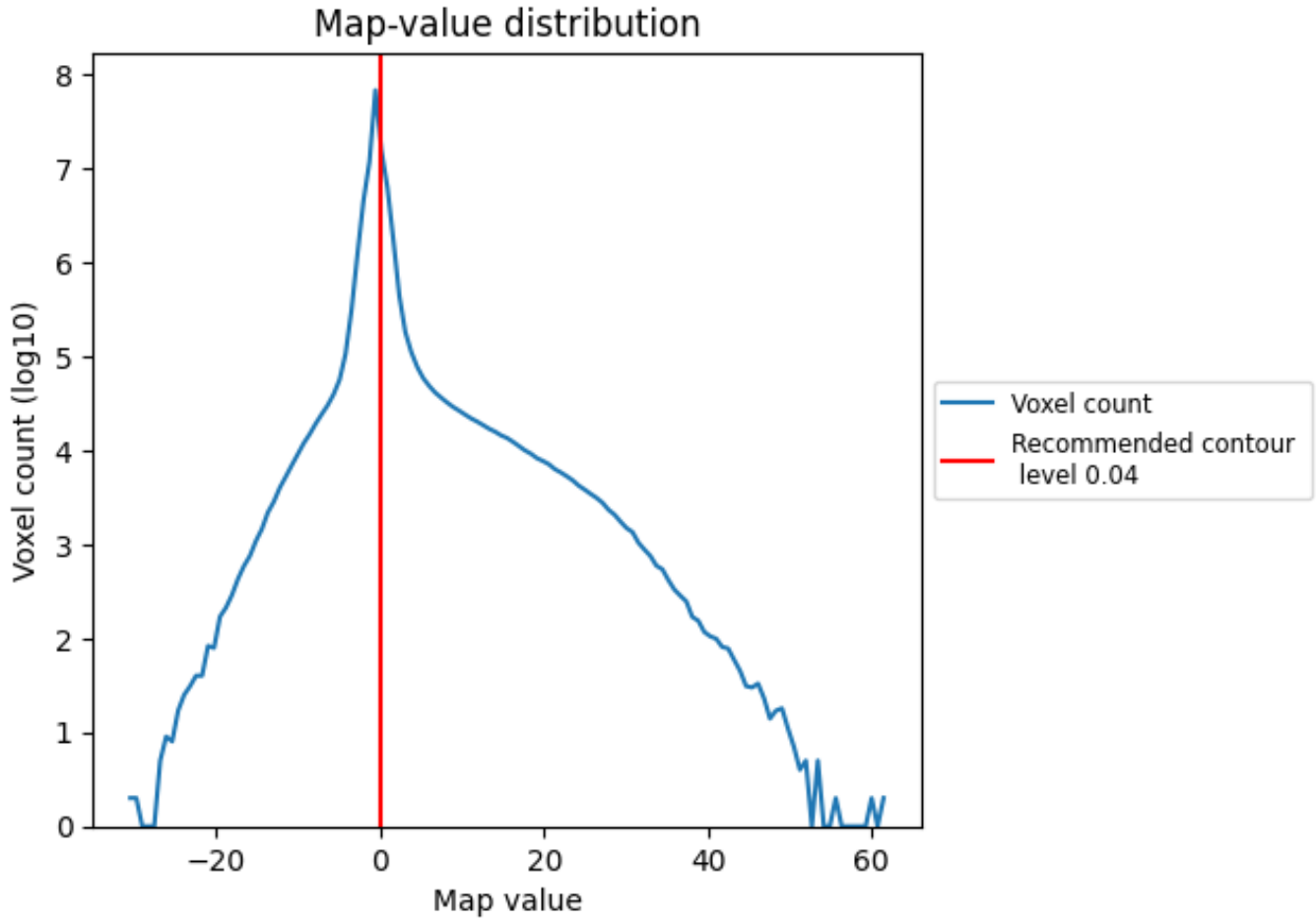
6.6 Mask visualisation (i)

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

7 Map analysis

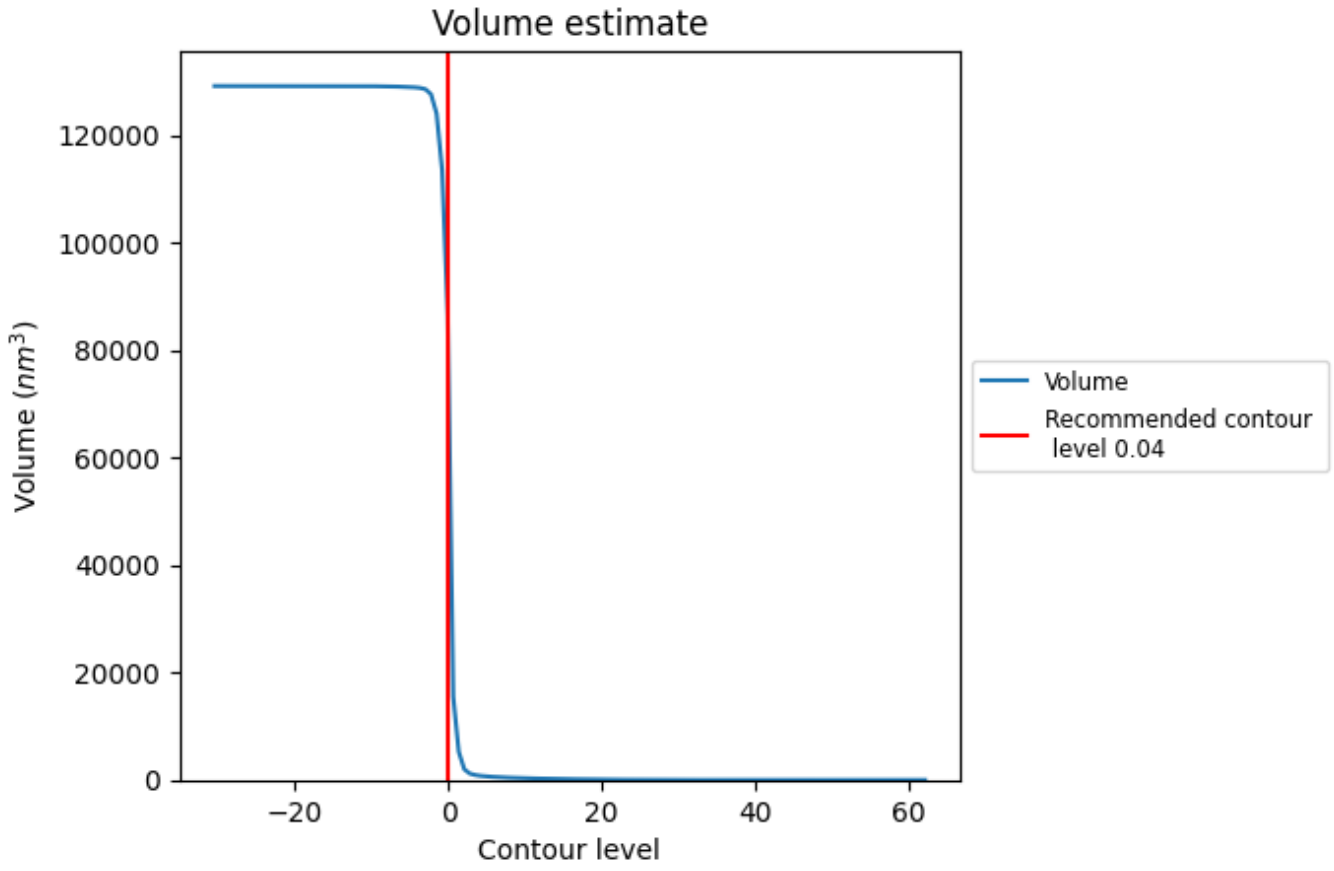
This section contains the results of statistical analysis of the map.

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.

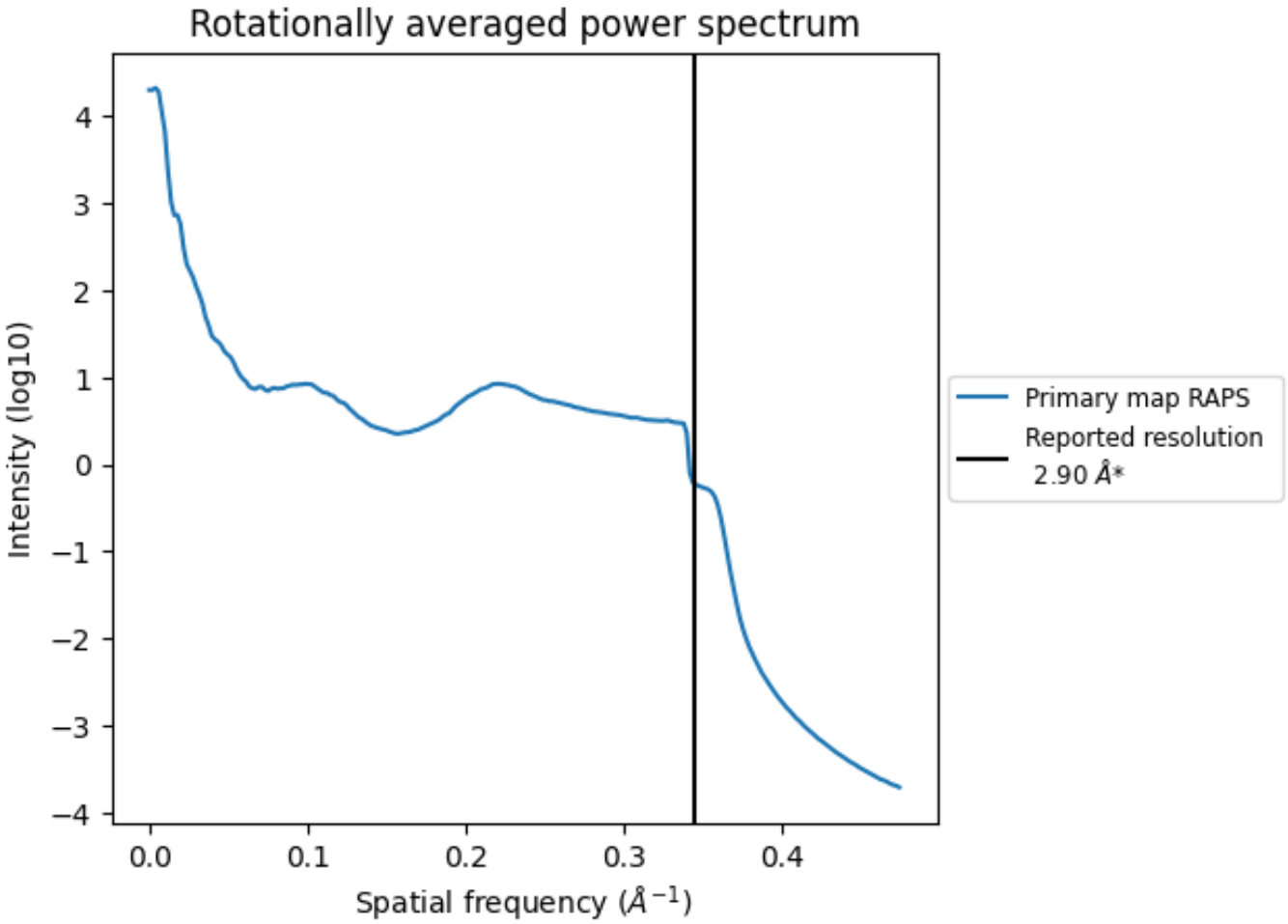
7.2 Volume estimate (i)



The volume at the recommended contour level is 76065 nm^3; this corresponds to an approximate mass of 68712 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 0.345 Å^{-1}

8 Fourier-Shell correlation (i)

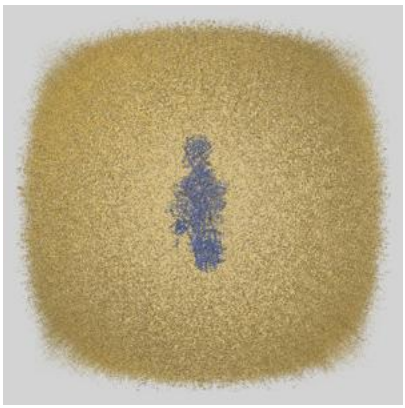
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

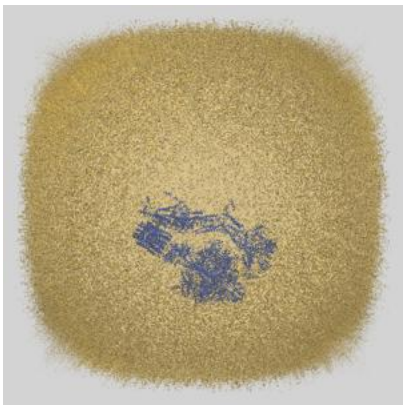
This section contains information regarding the fit between EMDB map EMD-4805 and PDB model 6RD4. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlays

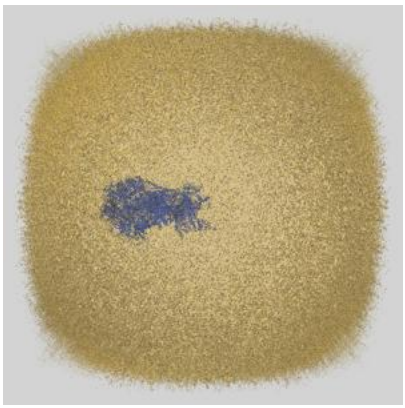
9.1.1 Map-model overlay



X

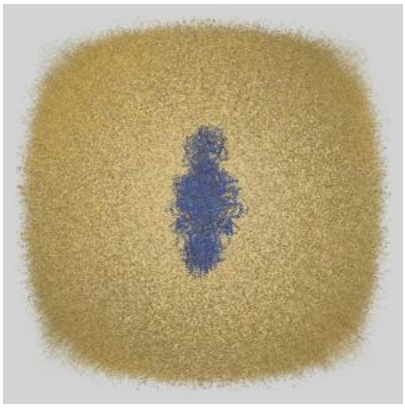


Y

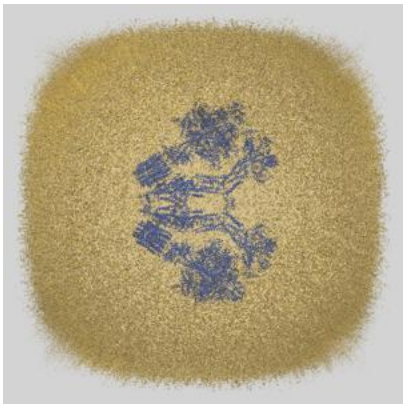


Z

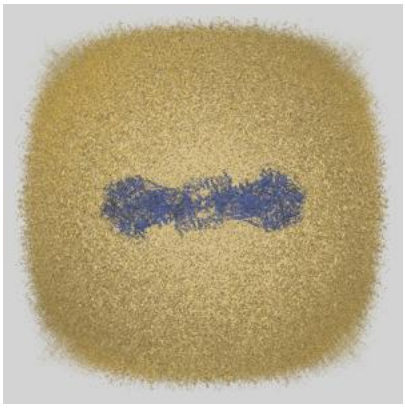
9.1.2 Map-model assembly overlay



X



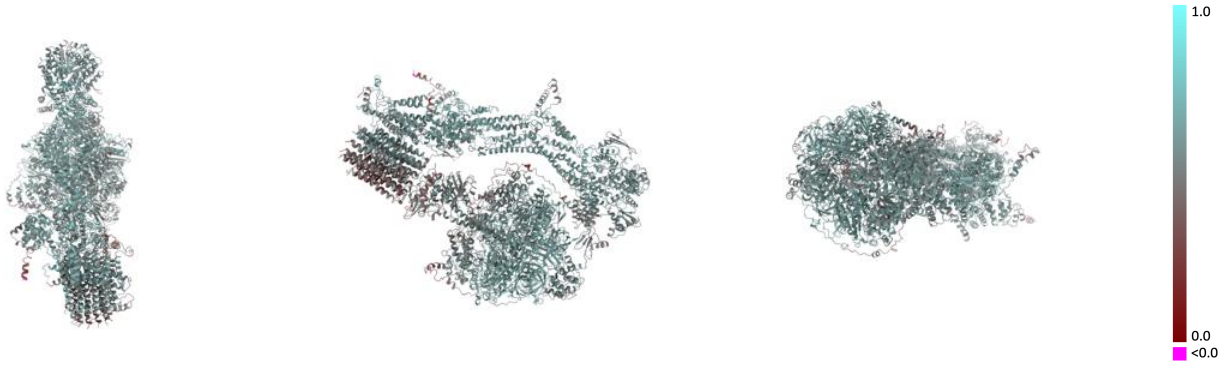
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

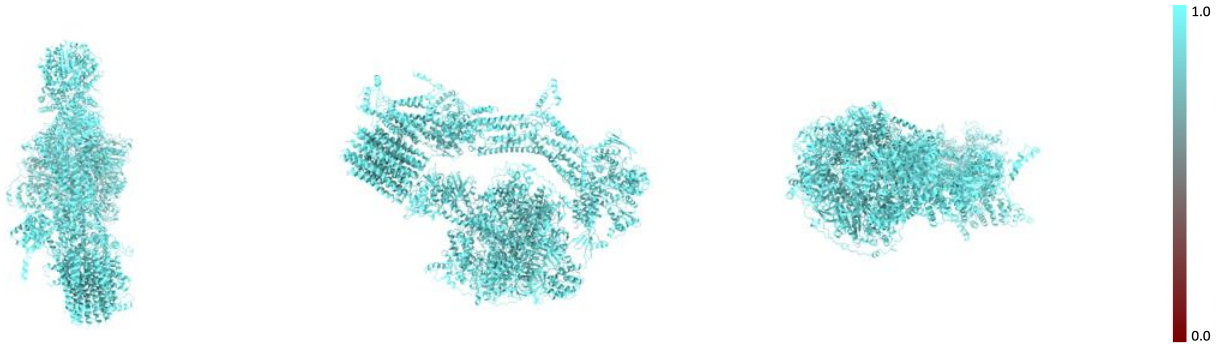
9.2 Q-score mapped to coordinate model (i)



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.

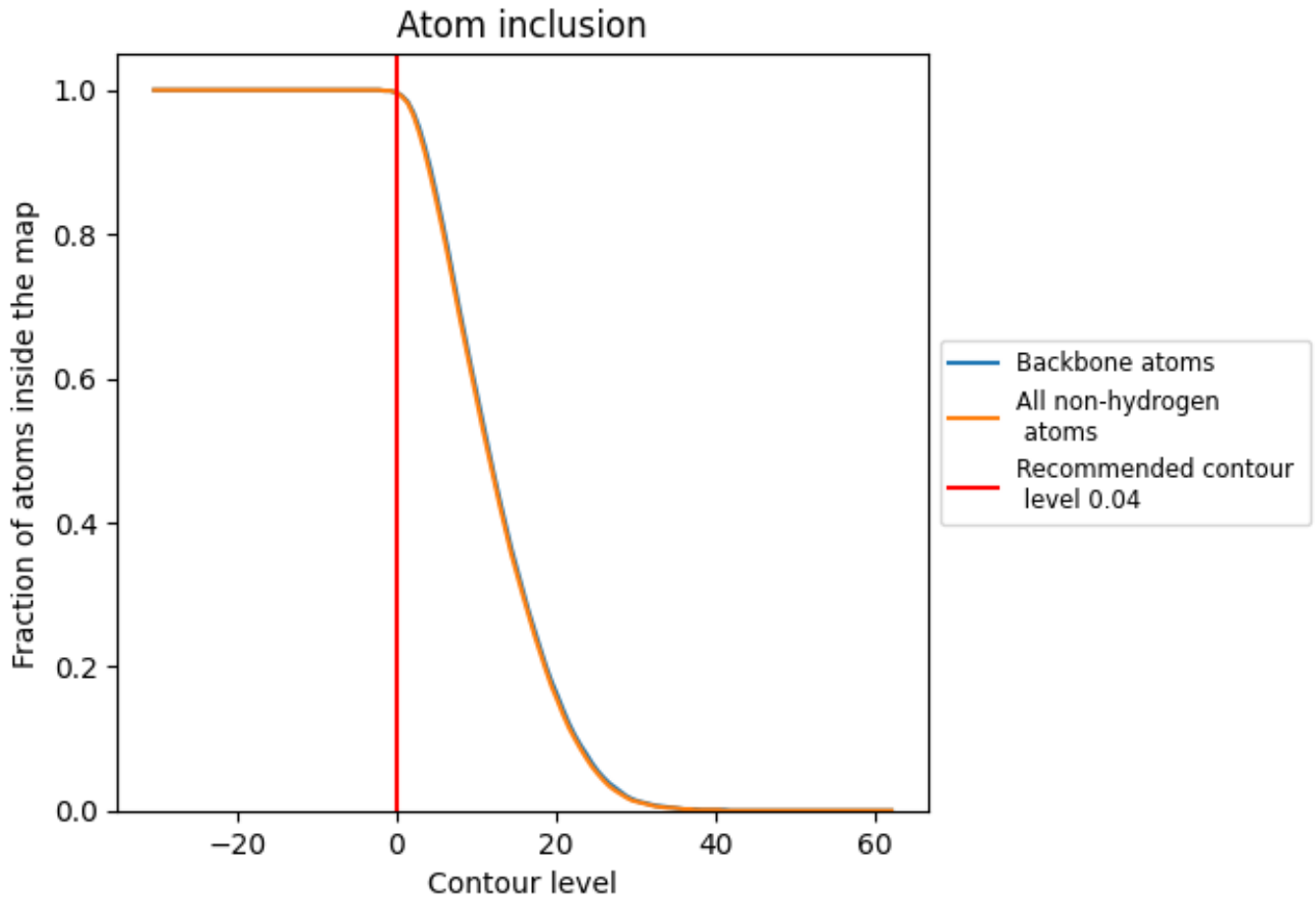
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9960	0.5570
0	1.0000	0.5830
1	0.9980	0.5900
2	1.0000	0.5610
3	0.9970	0.5560
4	0.9980	0.5640
5	0.9990	0.6190
6	0.9970	0.5840
7	0.9990	0.5980
8	1.0000	0.5990
9	0.9950	0.4780
A	0.9980	0.5550
B	0.9960	0.5640
C	0.9920	0.5270
D	0.9860	0.4680
E	0.9880	0.4180
F	0.9730	0.3790
G	0.9670	0.3620
H	0.9670	0.3700
I	0.9770	0.4210
J	0.9840	0.4860
M	0.9970	0.5850
P	0.9980	0.5090
Q	0.9980	0.4690
R	0.9900	0.4470
S	0.9950	0.5150
T	0.9990	0.5820
U	1.0000	0.5840
V	0.9990	0.5860
X	0.9960	0.5840
Y	0.9970	0.5770
Z	0.9960	0.5600