wwPDB EM Validation Summary Report (i)

May 12, 2024 – 07:20 pm BST

PDB ID	:	6RDI
EMDB ID	:	EMD-4819
Title	:	Cryo-EM structure of Polytomella F-ATP synthase, Rotary substate 1A, monomer-masked refinement
Authors	:	Murphy, B.J.; Klusch, N.; Yildiz, O.; Kuhlbrandt, W.
Deposited on	:	2019-04-12
Resolution	:	3.20 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

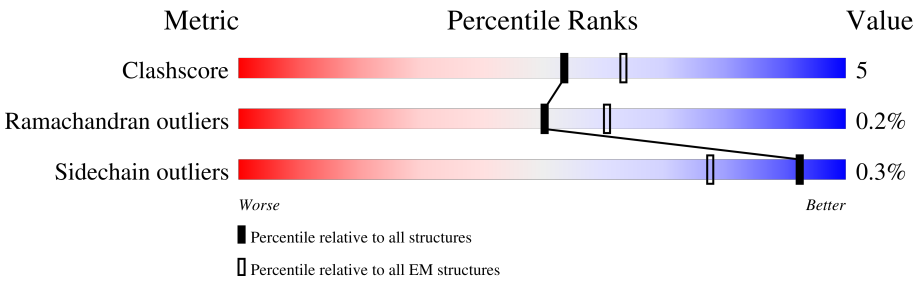
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.20 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	11% 91% 7% •
2	1	618	8% 85% 11% •
3	2	441	20% 87% 13%
4	3	325	14% 68% 8% 25%
5	4	294	15% 88% 11% •
6	5	123	• 85% 15%
7	6	151	7% 72% 10% 18%
8	7	190	13% 78% 15% 7%

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Mol	Chain	Length	Quality of chain
9	8	89	9%, 90%, 9%
10	9	97	26%, 90%, 10%
11	A	127	47%, 11%, 42%
11	B	127	50%, 9%, 42%
11	C	127	5%, 50%, 9%, 42%
11	D	127	9%, 46%, 12%, 42%
11	E	127	14%, 46%, 12%, 42%
11	F	127	12%, 43%, 16%, 42%
11	G	127	20%, 43%, 15%, 42%
11	H	127	22%, 50%, 9%, 42%
11	I	127	17%, 46%, 11%, 42%
11	J	127	6%, 50%, 8%, 42%
12	M	327	6%, 60%, 6%, 34%
13	P	229	20%, 71%, 13%, 16%
14	Q	74	38%, 77%, 20%
15	R	199	38%, 79%, 10%, 11%
16	S	317	15%, 75%, 13%, 13%
17	T	562	21%, 76%, 17%, 7%
17	U	562	24%, 77%, 15%, 7%
17	V	562	17%, 80%, 12%, 7%
18	X	574	26%, 78%, 16%, 6%
18	Y	574	25%, 75%, 16%, 9%
18	Z	574	24%, 80%, 14%, 6%

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 53748 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 ASA-2: Polytomella F-ATP synthase associated subunit 2.

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
			Total	C	N	O	S		
7	6	124	926	599	154	172	1	0	0

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

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

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

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

- Molecule 10 is a protein called ASA-9: Polytomella F-ATP synthase associated subunit 9.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

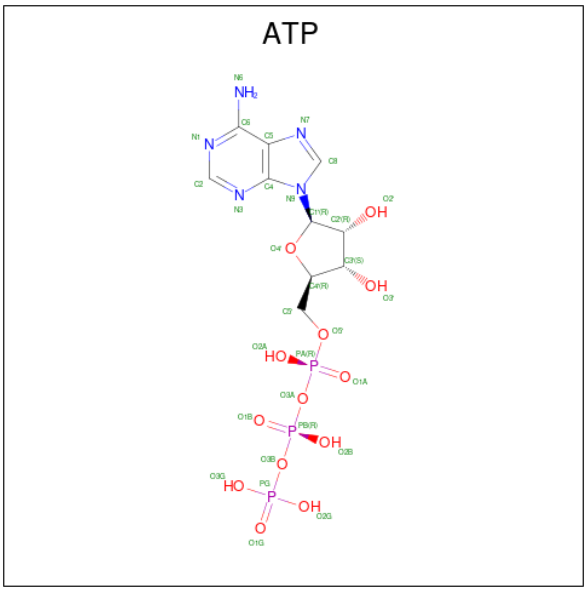
There are 6 discrepancies between the modelled and reference sequences:

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
			Total	Zn	
19	M	1	1	1	0

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

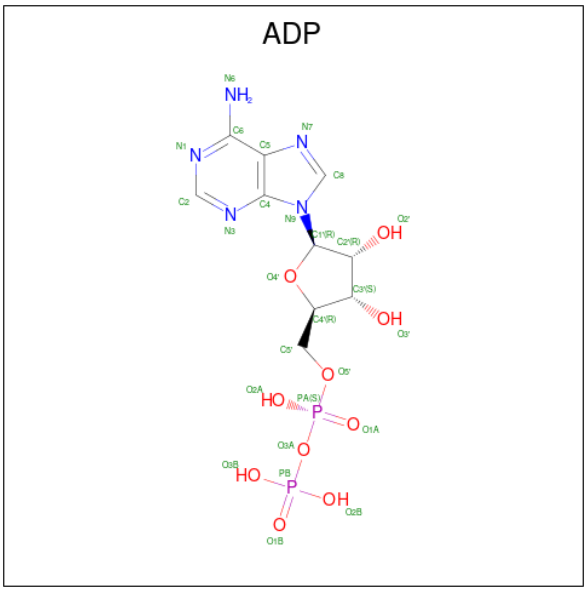


Mol	Chain	Residues	Atoms					AltConf
20	T	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	U	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	V	1	Total	C	N	O	P	0
			31	10	5	13	3	

- 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: $C_{10}H_{15}N_5O_{10}P_2$).



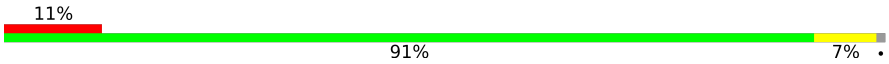
Mol	Chain	Residues	Atoms					AltConf
22	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
22	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	

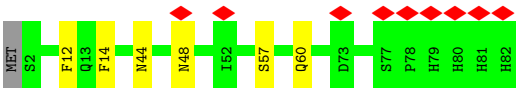
3 Residue-property plots (i)

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

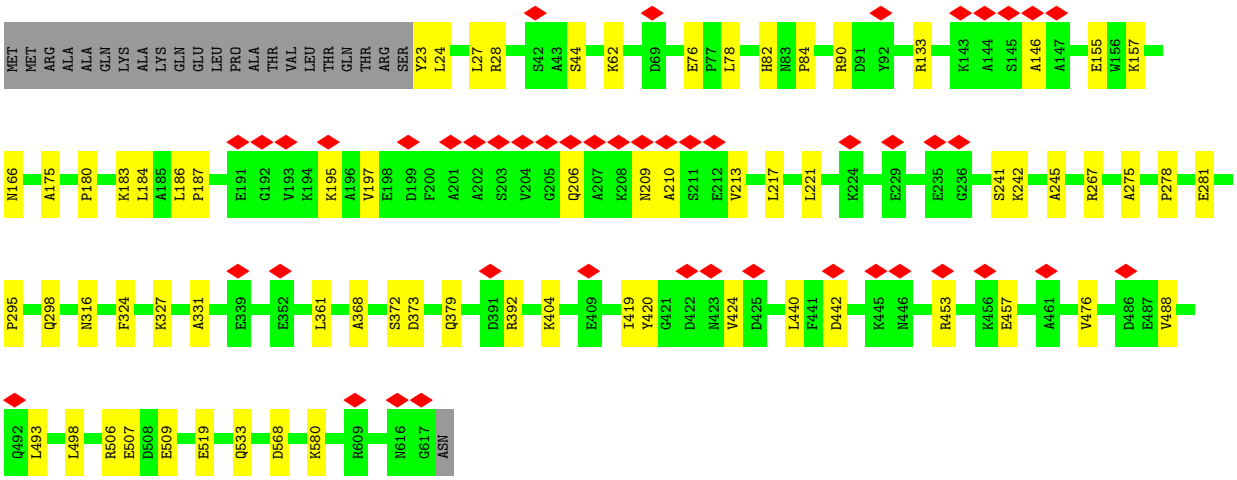
Chain 0:





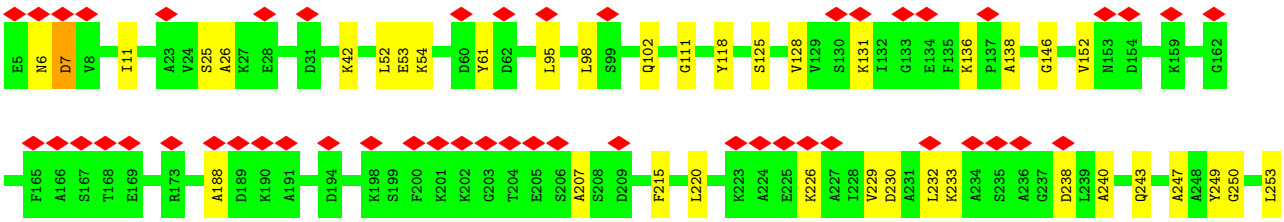
• Molecule 2: ATP synthase associated protein ASA1

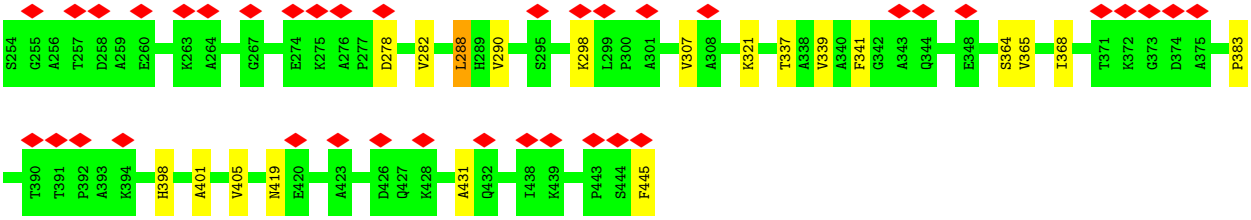
Chain 1:



• Molecule 3: ASA-2: Polytomella F-ATP synthase associated subunit 2

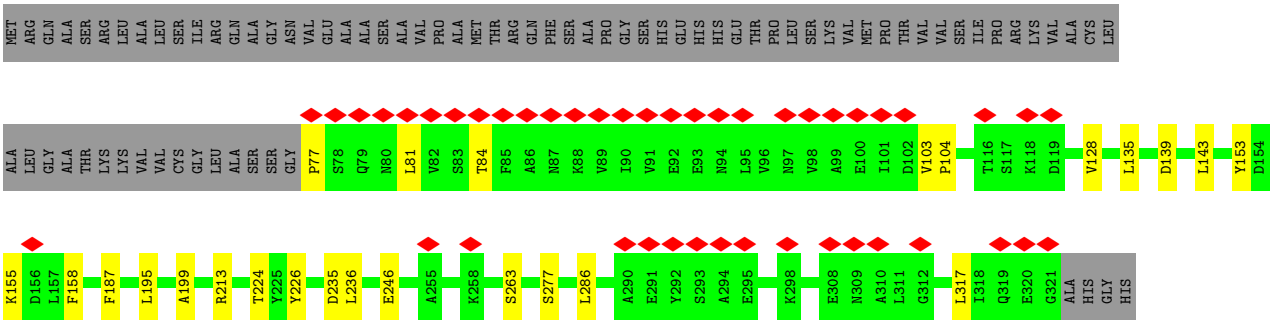
Chain 2:





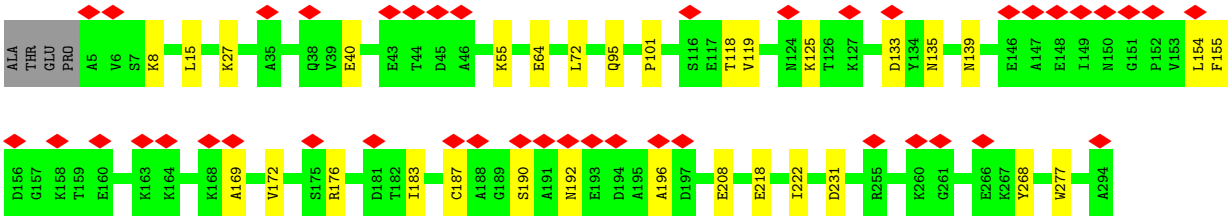
- Molecule 4: Mitochondrial F1F0 ATP synthase associated 32 kDa protein

Chain 3:



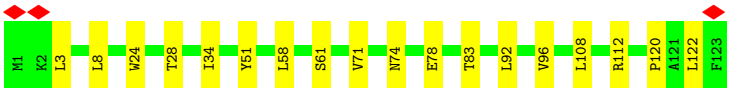
- Molecule 5: Mitochondrial ATP synthase associated protein ASA4

Chain 4:



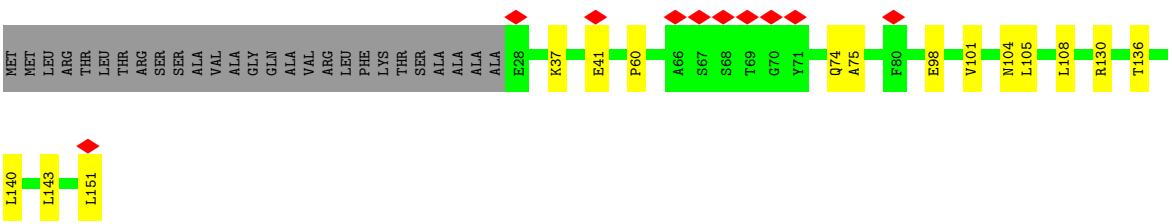
- Molecule 6: Mitochondrial F1F0 ATP synthase associated 14 kDa protein

Chain 5:



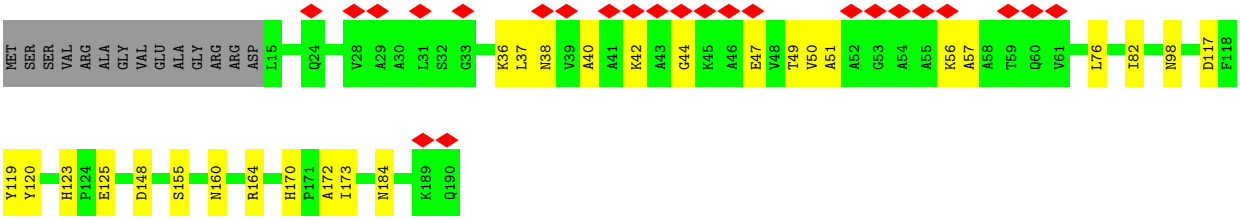
- Molecule 7: Mitochondrial ATP synthase subunit ASA6

Chain 6:



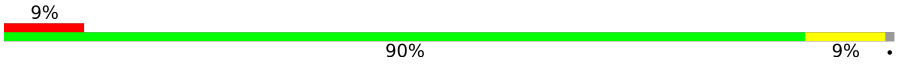
• Molecule 8: Mitochondrial ATP synthase associated protein ASA7

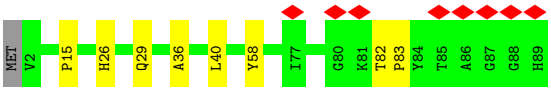
Chain 7:



• Molecule 9: Mitochondrial ATP synthase subunit ASA8

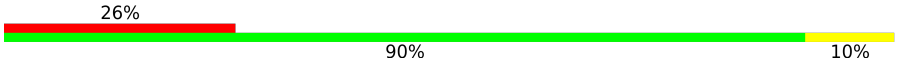
Chain 8:

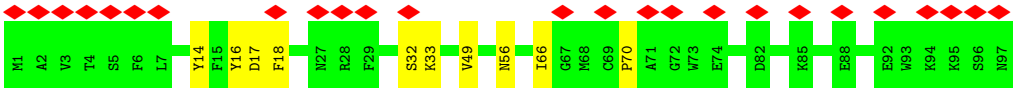




• Molecule 10: ASA-9: Polytomella F-ATP synthase associated subunit 9

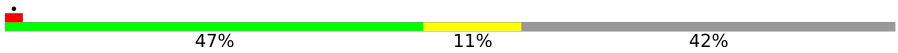
Chain 9:

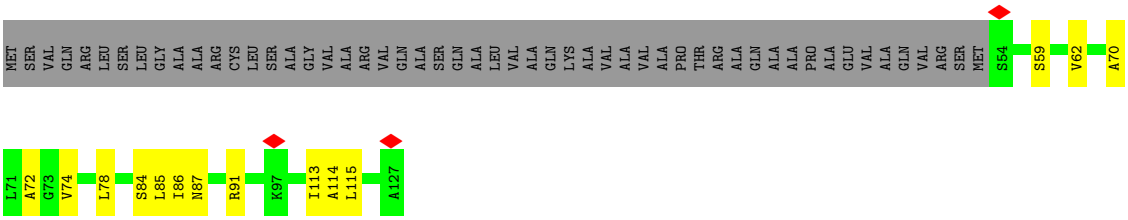




• Molecule 11: Mitochondrial ATP synthase subunit c

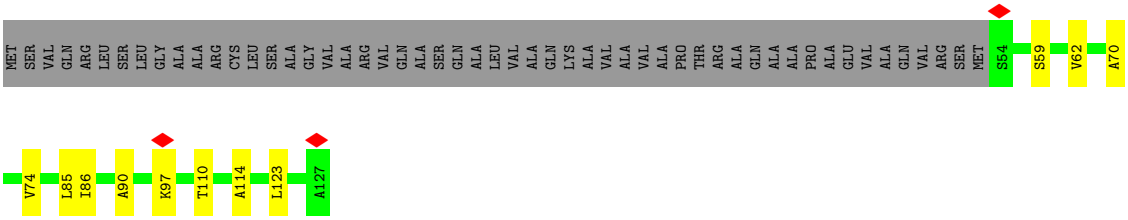
Chain A:





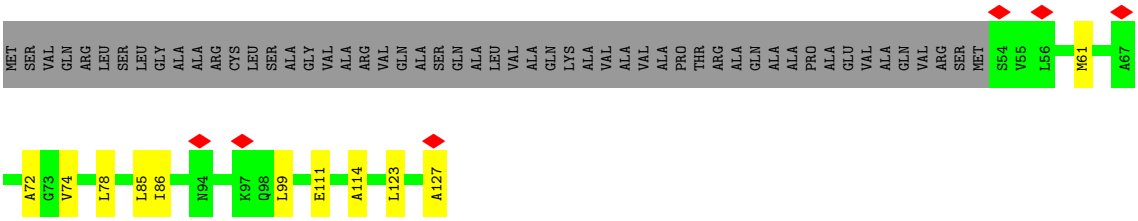
• Molecule 11: Mitochondrial ATP synthase subunit c

Chain B:



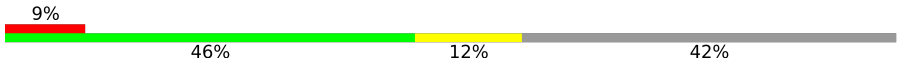
• Molecule 11: Mitochondrial ATP synthase subunit c

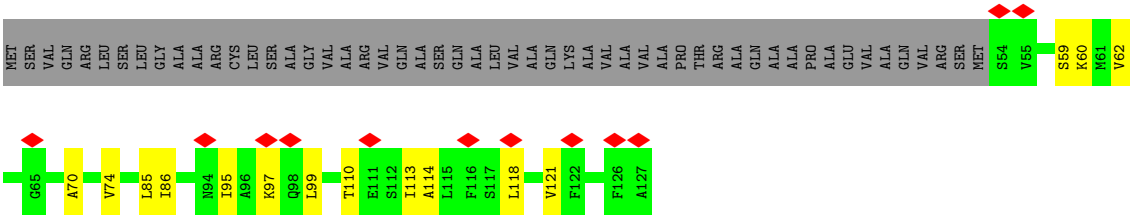
Chain C:



• Molecule 11: Mitochondrial ATP synthase subunit c

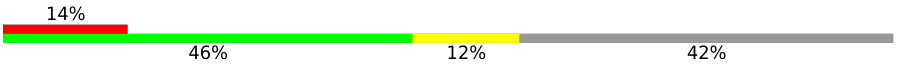
Chain D:

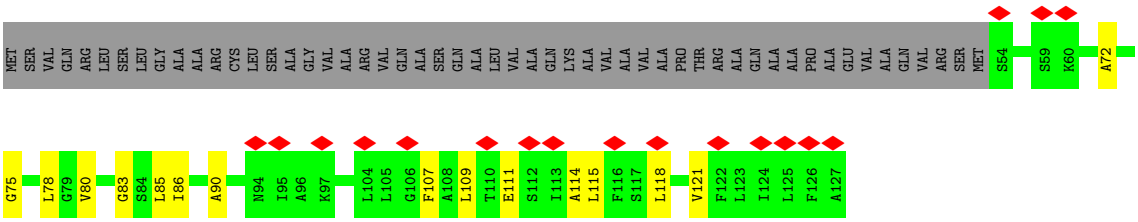




• Molecule 11: Mitochondrial ATP synthase subunit c

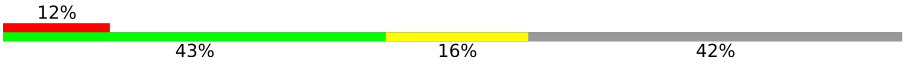
Chain E:

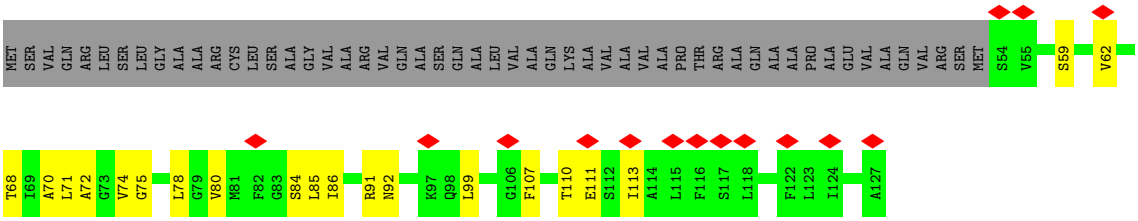




• Molecule 11: Mitochondrial ATP synthase subunit c

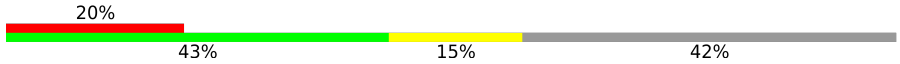
Chain F:

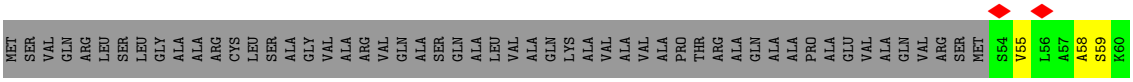


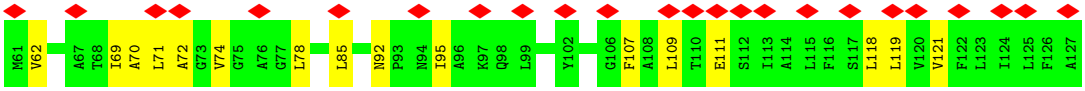


• Molecule 11: Mitochondrial ATP synthase subunit c

Chain G:

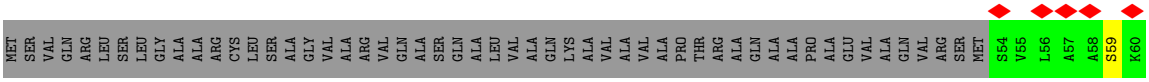


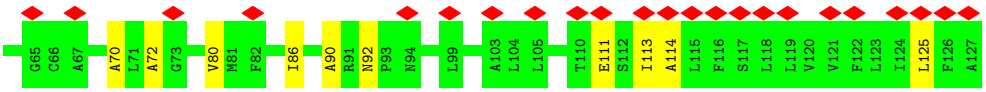




• Molecule 11: Mitochondrial ATP synthase subunit c

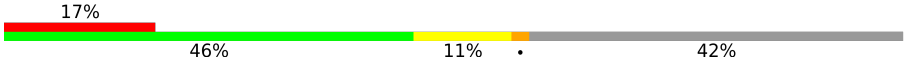
Chain H:

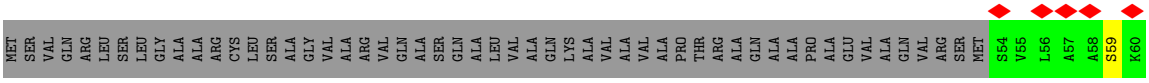


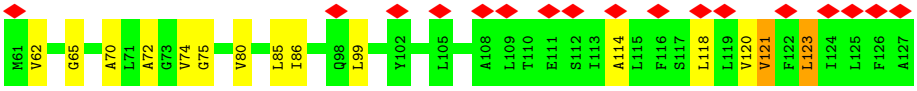


• Molecule 11: Mitochondrial ATP synthase subunit c

Chain I:

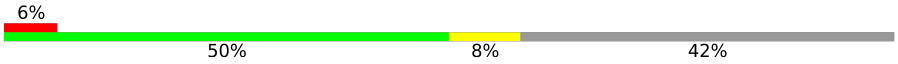


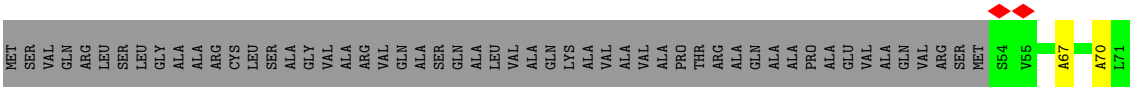


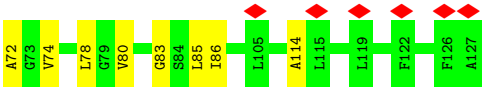


• Molecule 11: Mitochondrial ATP synthase subunit c

Chain J:

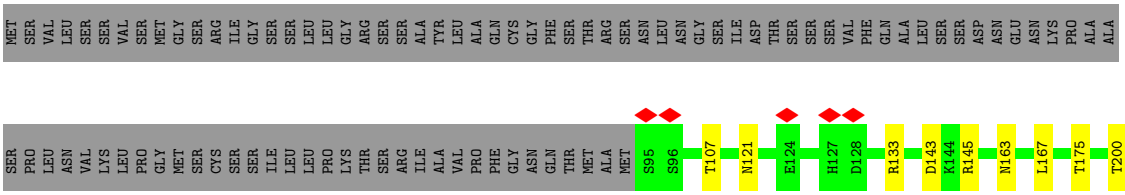


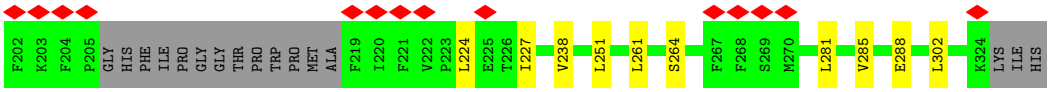




• Molecule 12: Mitochondrial ATP synthase subunit 6

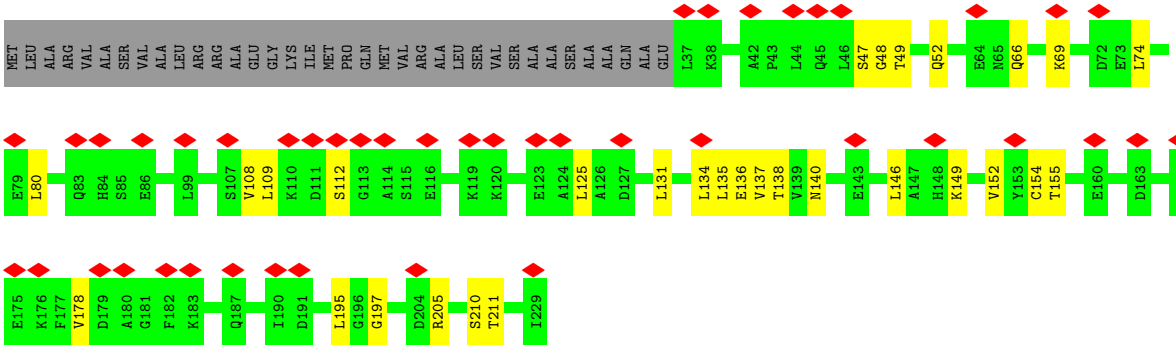
Chain M:





- Molecule 13: Mitochondrial ATP synthase subunit OSCP

Chain P:

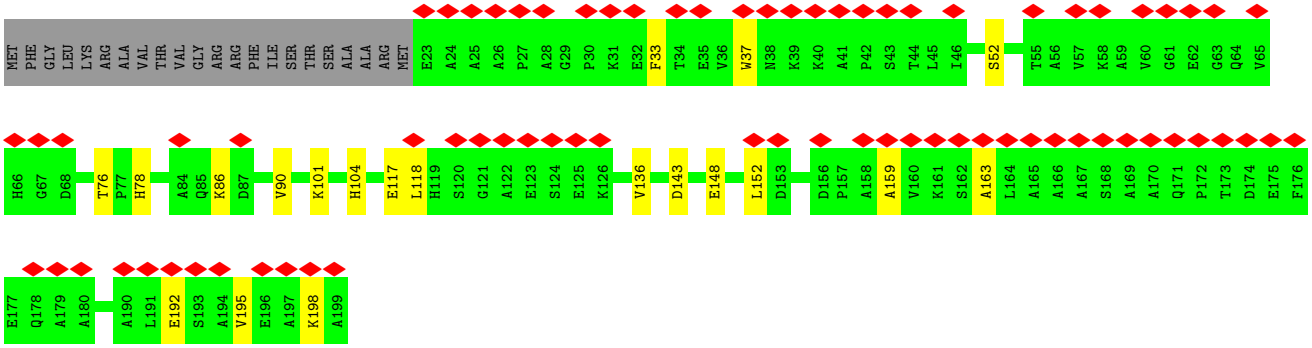


- Molecule 14: epsilon: Polytomella F-ATP synthase epsilon subunit

Chain Q:

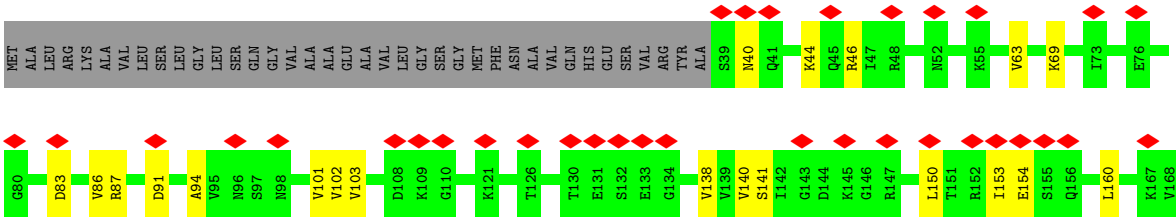
- Molecule 15: Mitochondrial ATP synthase subunit delta

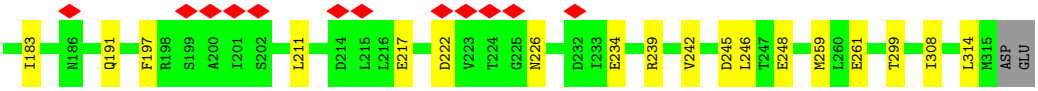
Chain R:



- Molecule 16: ATP synthase gamma chain, mitochondrial

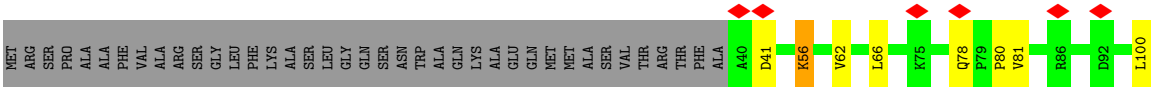
Chain S:

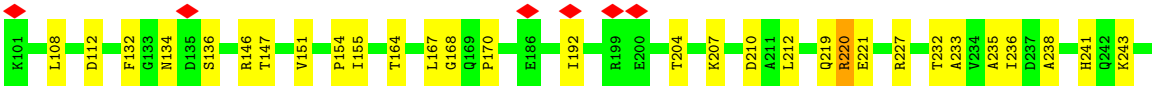


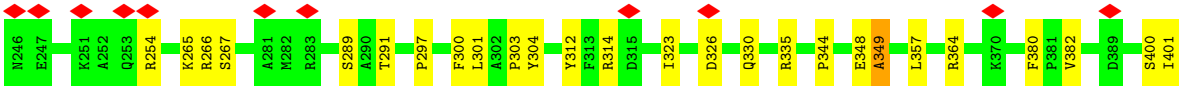


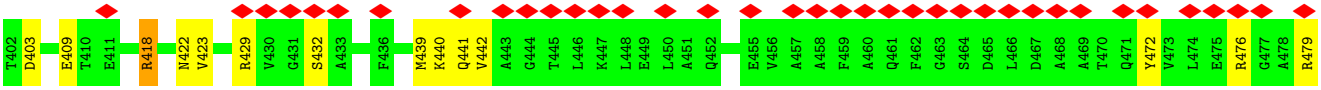
• Molecule 17: ATP synthase subunit alpha

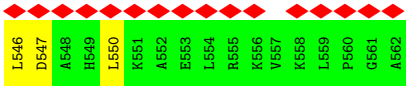
Chain T:





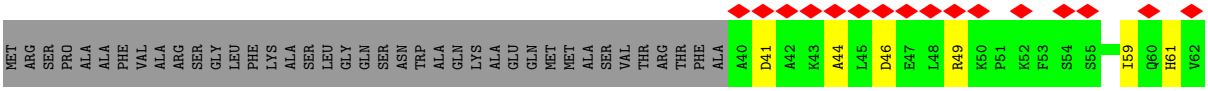


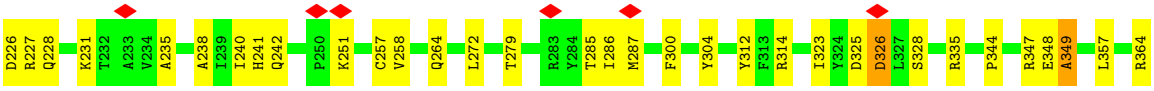


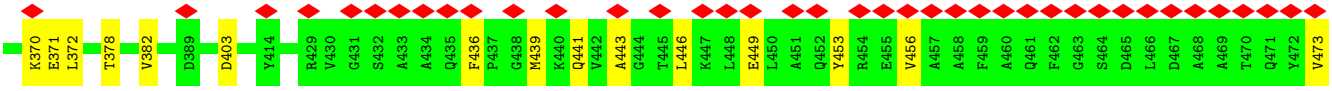


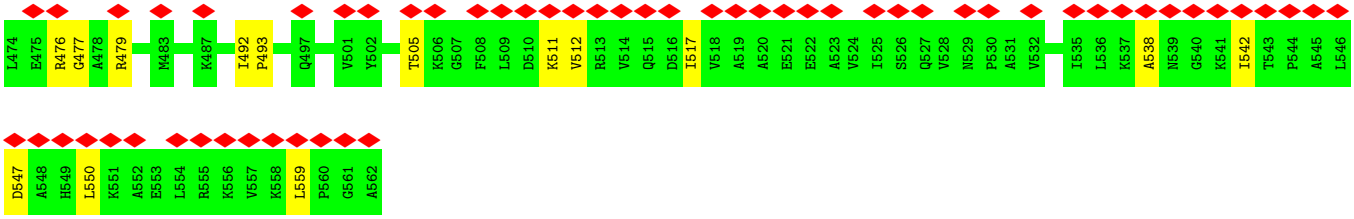
• Molecule 17: ATP synthase subunit alpha

Chain U:



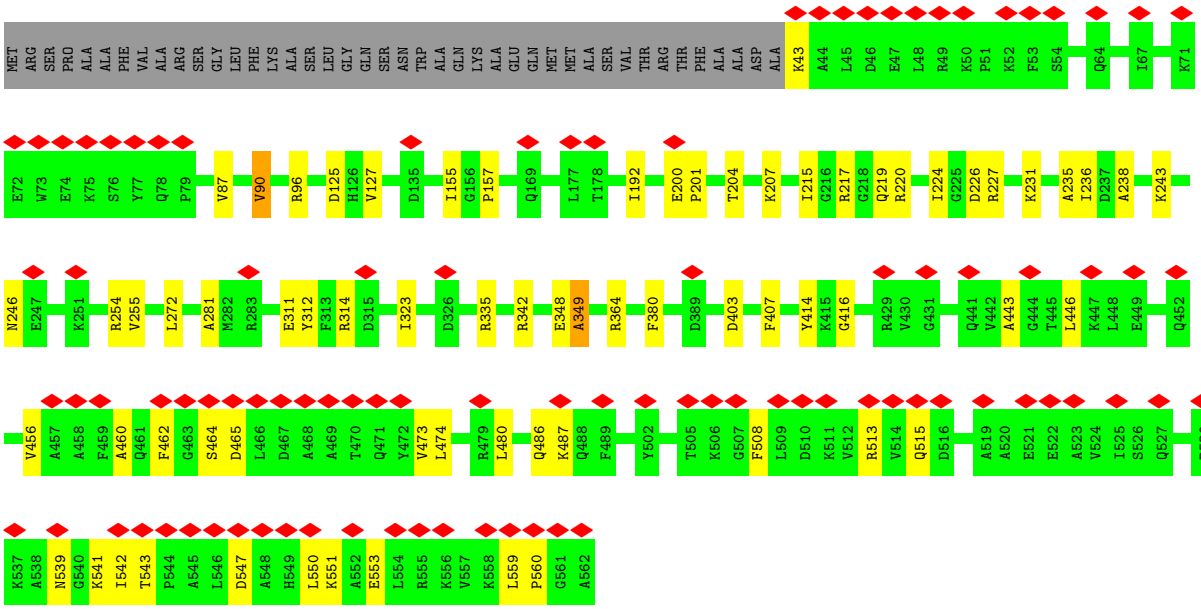






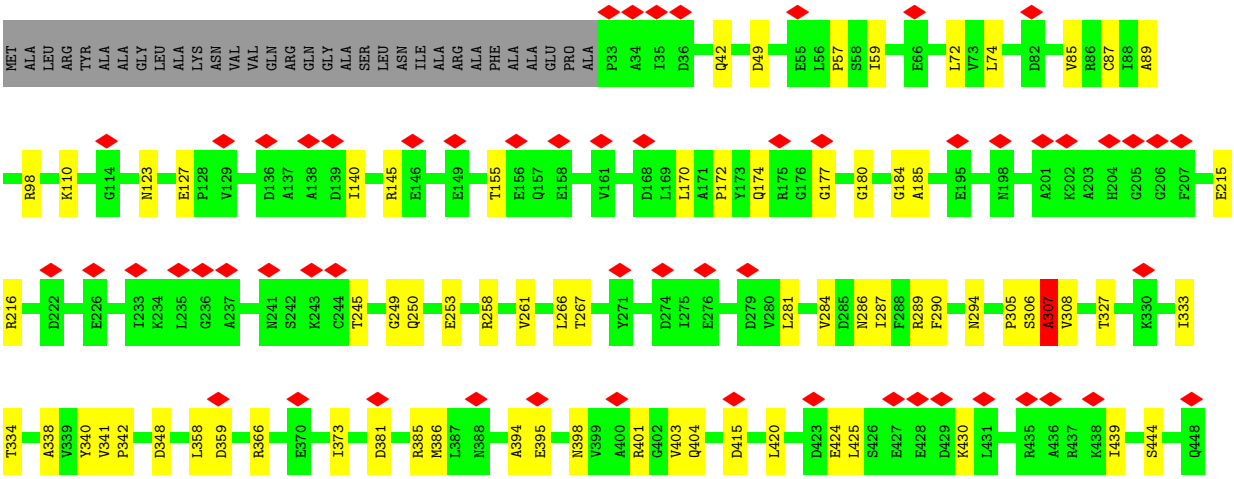
• Molecule 17: ATP synthase subunit alpha

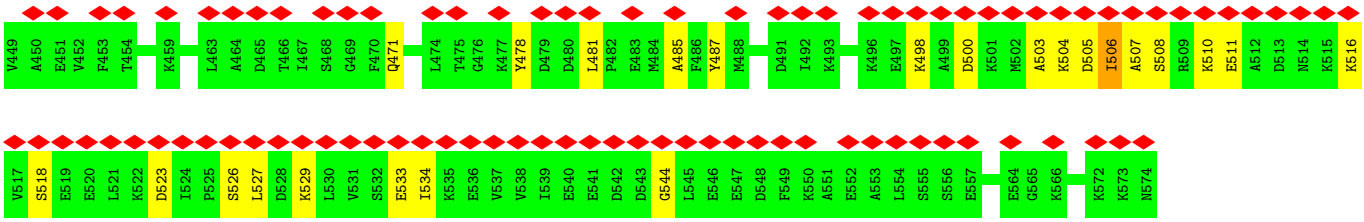
Chain V:



• Molecule 18: ATP synthase subunit beta

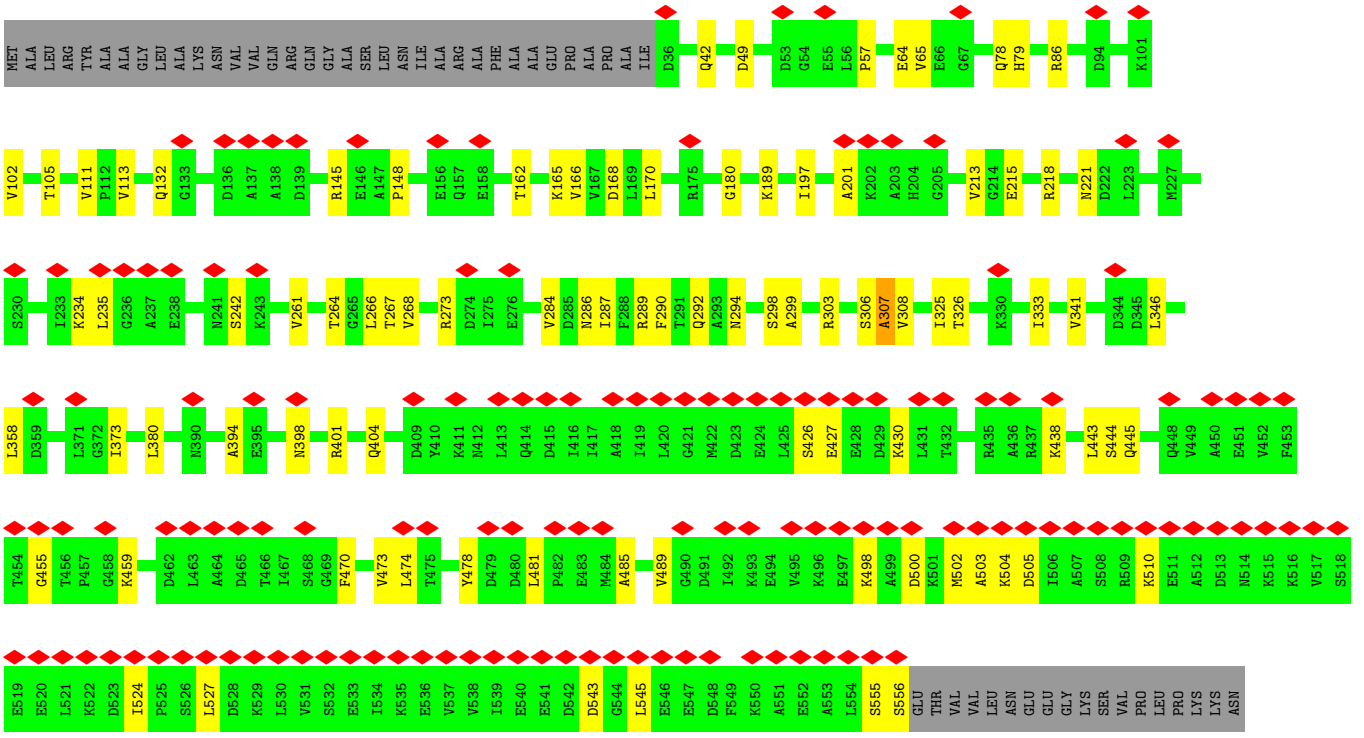
Chain X:





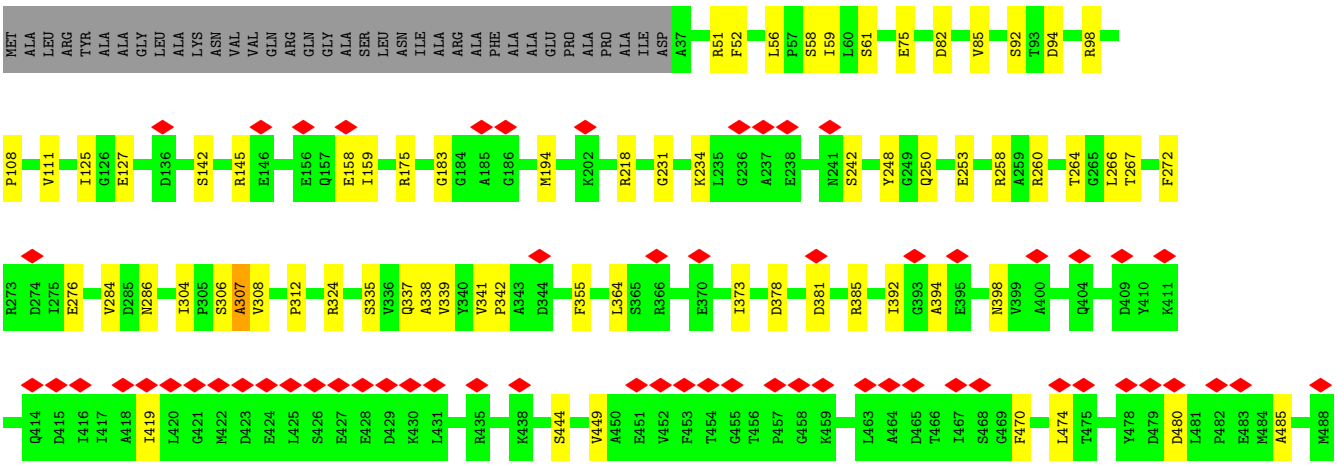
• Molecule 18: ATP synthase subunit beta

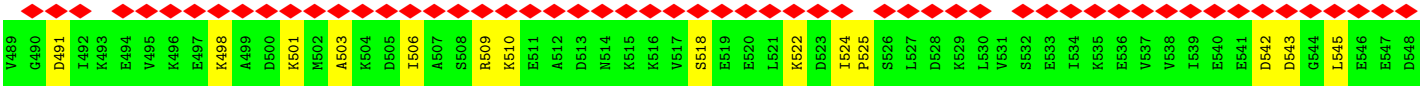
Chain Y:



• Molecule 18: ATP synthase subunit beta

Chain Z:




V489
G490
D491
I492
K493
E494
V495
K496
E497
K498
A499
D500
K501
M502
A503
K504
D505
I506
A507
S508
R509
K510
E511
A512
D513
N514
K515
K516
V517
S518
E519
E520
L521
K522
D523
I524
P525
S526
L527
D528
K529
L530
V531
S532
E533
I534
K535
E536
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V538
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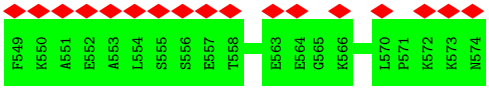
E541
D542
D543
G544
L545
E546
E547
D548


F549
K550
A551
E552
A553
L554
S555
S556
E557
T558
E563
E564
G565
K566
L570
P571
K572
K573
N574

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124537	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	0.227	Depositor
Minimum map value	-0.141	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	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 (i)

5.1 Standard geometry (i)

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	0.46	0/628	0.54	0/856
2	1	0.45	0/4750	0.53	0/6434
3	2	0.38	0/3212	0.57	1/4371 (0.0%)
4	3	0.41	0/1911	0.56	1/2601 (0.0%)
5	4	0.43	0/2216	0.53	0/3000
6	5	0.55	0/1011	0.63	2/1376 (0.1%)
7	6	0.47	0/946	0.57	0/1287
8	7	0.51	0/1374	0.57	0/1865
9	8	0.52	0/715	0.61	0/974
10	9	0.39	0/802	0.57	1/1084 (0.1%)
11	A	0.42	0/520	0.55	0/704
11	B	0.43	0/520	0.54	0/704
11	C	0.35	0/519	0.53	0/701
11	D	0.34	0/520	0.55	0/704
11	E	0.35	0/520	0.55	1/704 (0.1%)
11	F	0.36	0/520	0.60	0/704
11	G	0.35	0/520	0.60	1/704 (0.1%)
11	H	0.34	0/520	0.54	0/704
11	I	0.35	0/520	0.59	1/704 (0.1%)
11	J	0.35	0/520	0.56	0/704
12	M	0.50	0/1683	0.62	1/2295 (0.0%)
13	P	0.38	0/1553	0.59	0/2093
14	Q	0.39	0/574	0.55	0/774
15	R	0.43	0/1336	0.55	0/1827
16	S	0.44	0/2153	0.57	0/2901
17	T	0.53	0/4048	0.61	1/5481 (0.0%)
17	U	0.55	0/4049	0.61	0/5481
17	V	0.52	0/4031	0.61	1/5456 (0.0%)
18	X	0.53	0/4176	0.58	1/5659 (0.0%)
18	Y	0.50	0/4015	0.60	1/5440 (0.0%)
18	Z	0.50	0/4147	0.57	0/5619
All	All	0.47	0/54529	0.58	13/73911 (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
17	T	0	2
17	U	0	1
17	V	0	2
18	X	0	2
18	Y	0	1
18	Z	0	2
All	All	0	10

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	167	LEU	CA-CB-CG	7.43	132.40	115.30
12	M	261	LEU	CA-CB-CG	6.47	130.18	115.30
4	3	77	PRO	N-CA-CB	5.78	110.23	103.30
18	Y	505	ASP	CB-CG-OD1	5.77	123.49	118.30
18	X	266	LEU	CA-CB-CG	5.63	128.24	115.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	T	348	GLU	Peptide
17	T	487	LYS	Peptide
17	U	348	GLU	Peptide
17	V	348	GLU	Peptide
17	V	487	LYS	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	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1	4661	0	4695	44	0
3	2	3163	0	3262	36	0
4	3	1874	0	1826	15	0
5	4	2177	0	2169	23	0
6	5	986	0	1021	13	0
7	6	926	0	941	13	0
8	7	1347	0	1345	24	0
9	8	692	0	694	5	0
10	9	776	0	757	7	0
11	A	514	0	554	12	0
11	B	514	0	554	10	0
11	C	514	0	553	14	0
11	D	514	0	554	14	0
11	E	514	0	554	14	0
11	F	514	0	554	18	0
11	G	514	0	554	19	0
11	H	514	0	554	14	0
11	I	514	0	554	14	0
11	J	514	0	554	11	0
12	M	1640	0	1665	13	0
13	P	1532	0	1603	17	0
14	Q	561	0	565	10	0
15	R	1303	0	1266	14	0
16	S	2130	0	2180	27	0
17	T	3979	0	4120	59	0
17	U	3980	0	4119	60	0
17	V	3962	0	4105	44	0
18	X	4115	0	4137	56	0
18	Y	3957	0	3966	53	0
18	Z	4087	0	4110	54	0
19	M	1	0	0	0	0
20	T	31	0	12	0	0
20	U	31	0	12	0	0
20	V	31	0	12	0	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
22	Y	27	0	12	0	0
All	All	53748	0	54729	592	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 5.

The worst 5 of 592 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:C:78:LEU:HD11	11:C:111:GLU:OE2	1.46	1.16
17:T:78:GLN:O	17:T:80:PRO:HD3	1.50	1.12
11:E:107:PHE:O	11:E:111:GLU:HG2	1.62	0.99
17:U:228:GLN:NE2	18:Z:385:ARG:HH21	1.64	0.96
11:G:78:LEU:HD11	11:G:111:GLU:OE2	1.69	0.92

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	79
4	3	243/325 (75%)	235 (97%)	8 (3%)	0	100	100
5	4	288/294 (98%)	277 (96%)	11 (4%)	0	100	100
6	5	121/123 (98%)	112 (93%)	8 (7%)	1 (1%)	19	58
7	6	122/151 (81%)	111 (91%)	11 (9%)	0	100	100
8	7	174/190 (92%)	169 (97%)	5 (3%)	0	100	100
9	8	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
10	9	95/97 (98%)	85 (90%)	10 (10%)	0	100	100
11	A	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	B	72/127 (57%)	72 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	C	71/127 (56%)	71 (100%)	0	0	100	100
11	D	72/127 (57%)	72 (100%)	0	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%)	71 (99%)	1 (1%)	0	100	100
11	I	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	J	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
12	M	213/327 (65%)	205 (96%)	8 (4%)	0	100	100
13	P	191/229 (83%)	178 (93%)	13 (7%)	0	100	100
14	Q	70/74 (95%)	68 (97%)	2 (3%)	0	100	100
15	R	175/199 (88%)	161 (92%)	14 (8%)	0	100	100
16	S	275/317 (87%)	258 (94%)	17 (6%)	0	100	100
17	T	521/562 (93%)	494 (95%)	23 (4%)	4 (1%)	19	58
17	U	521/562 (93%)	490 (94%)	30 (6%)	1 (0%)	47	79
17	V	518/562 (92%)	495 (96%)	22 (4%)	1 (0%)	47	79
18	X	540/574 (94%)	498 (92%)	39 (7%)	3 (1%)	25	64
18	Y	519/574 (90%)	480 (92%)	36 (7%)	3 (1%)	25	64
18	Z	536/574 (93%)	505 (94%)	29 (5%)	2 (0%)	34	69
All	All	7038/8234 (86%)	6670 (95%)	352 (5%)	16 (0%)	50	79

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	Z	308	VAL
3	2	383	PRO
17	T	493	PRO
17	U	349	ALA
18	X	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%)	63 (100%)	0	100	100
2	1	493/512 (96%)	492 (100%)	1 (0%)	93	98
3	2	312/312 (100%)	309 (99%)	3 (1%)	76	90
4	3	195/258 (76%)	195 (100%)	0	100	100
5	4	220/223 (99%)	220 (100%)	0	100	100
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%)	49 (98%)	1 (2%)	55	80
11	J	50/86 (58%)	50 (100%)	0	100	100
12	M	178/272 (65%)	178 (100%)	0	100	100
13	P	171/196 (87%)	171 (100%)	0	100	100
14	Q	56/58 (97%)	56 (100%)	0	100	100
15	R	134/151 (89%)	134 (100%)	0	100	100
16	S	235/265 (89%)	235 (100%)	0	100	100
17	T	419/448 (94%)	415 (99%)	4 (1%)	76	90
17	U	419/448 (94%)	417 (100%)	2 (0%)	88	95
17	V	418/448 (93%)	414 (99%)	4 (1%)	76	90
18	X	449/469 (96%)	447 (100%)	2 (0%)	91	95
18	Y	430/469 (92%)	430 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	Z	446/469 (95%)	445 (100%)	1 (0%)	93	98
All	All	5631/6445 (87%)	5613 (100%)	18 (0%)	92	96

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	V	227	ARG
18	Z	501	LYS
18	X	245	THR
17	T	418	ARG
17	V	220	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
17	V	244	ASN
18	Z	250	GLN
17	V	271	GLN
18	X	337	GLN
11	I	98	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	$\#\|Z\| > 2$
22	ADP	Y	601	21	24,29,29	0.95	1 (4%)	29,45,45	1.32	4 (13%)
20	ATP	U	1001	21	26,33,33	0.97	1 (3%)	31,52,52	1.57	6 (19%)
20	ATP	T	1001	21	26,33,33	0.95	1 (3%)	31,52,52	1.48	5 (16%)
22	ADP	X	601	21	24,29,29	1.02	1 (4%)	29,45,45	1.28	3 (10%)
20	ATP	V	1001	21	26,33,33	0.96	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
22	ADP	Y	601	21	-	2/12/32/32	0/3/3/3
20	ATP	U	1001	21	-	2/18/38/38	0/3/3/3
20	ATP	T	1001	21	-	4/18/38/38	0/3/3/3
22	ADP	X	601	21	-	4/12/32/32	0/3/3/3
20	ATP	V	1001	21	-	1/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	601	ADP	C5-C4	2.19	1.46	1.40
20	U	1001	ATP	C5-C4	2.09	1.46	1.40
22	Y	601	ADP	C5-C4	2.06	1.46	1.40
20	T	1001	ATP	C5-C4	2.02	1.46	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	U	1001	ATP	PB-O3B-PG	-3.88	119.51	132.83
20	T	1001	ATP	N3-C2-N1	-3.28	123.54	128.68
20	V	1001	ATP	PB-O3B-PG	-3.28	121.58	132.83
22	Y	601	ADP	N3-C2-N1	-3.20	123.67	128.68
20	U	1001	ATP	N3-C2-N1	-3.12	123.80	128.68

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

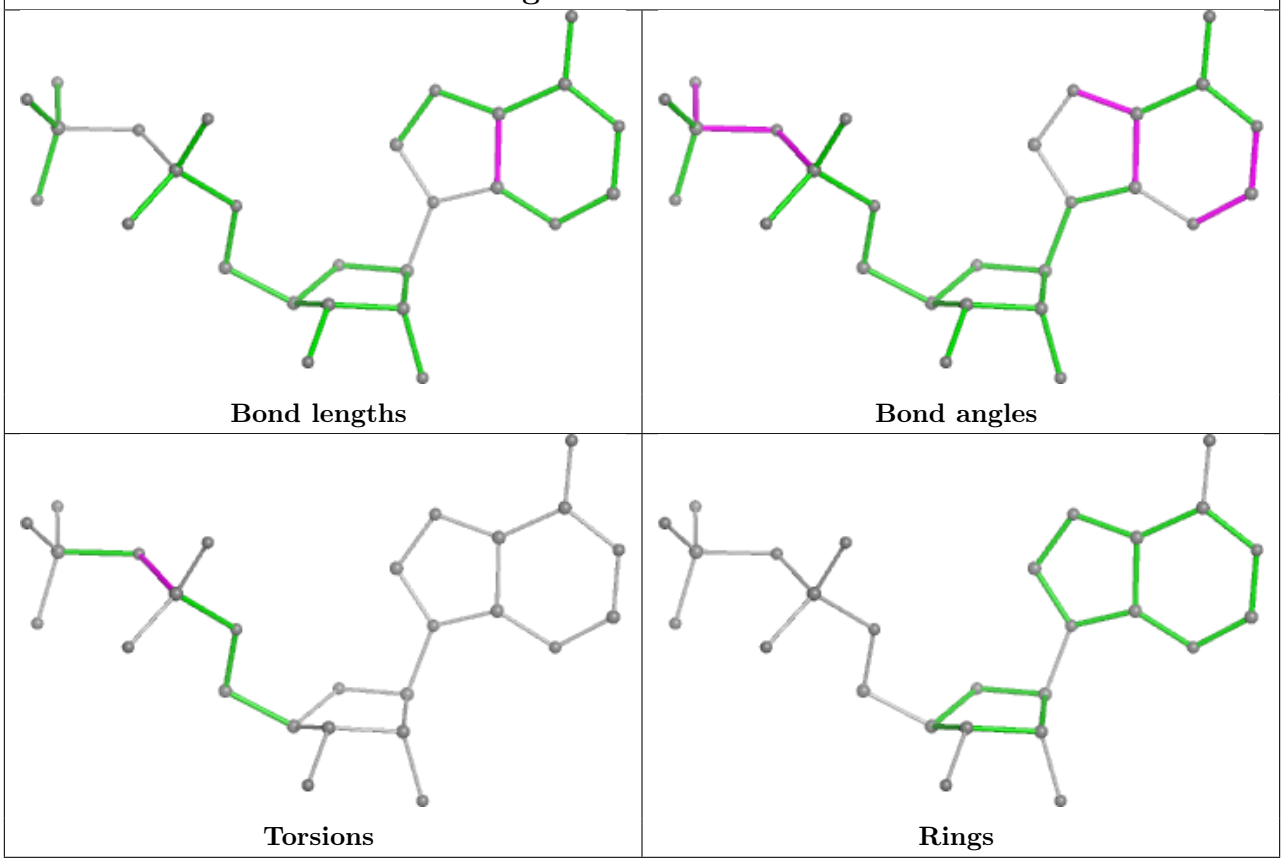
Mol	Chain	Res	Type	Atoms
20	T	1001	ATP	C5'-O5'-PA-O3A
22	X	601	ADP	PA-O3A-PB-O2B
22	X	601	ADP	PA-O3A-PB-O3B
20	T	1001	ATP	C5'-O5'-PA-O1A
20	T	1001	ATP	PG-O3B-PB-O2B

There are no ring outliers.

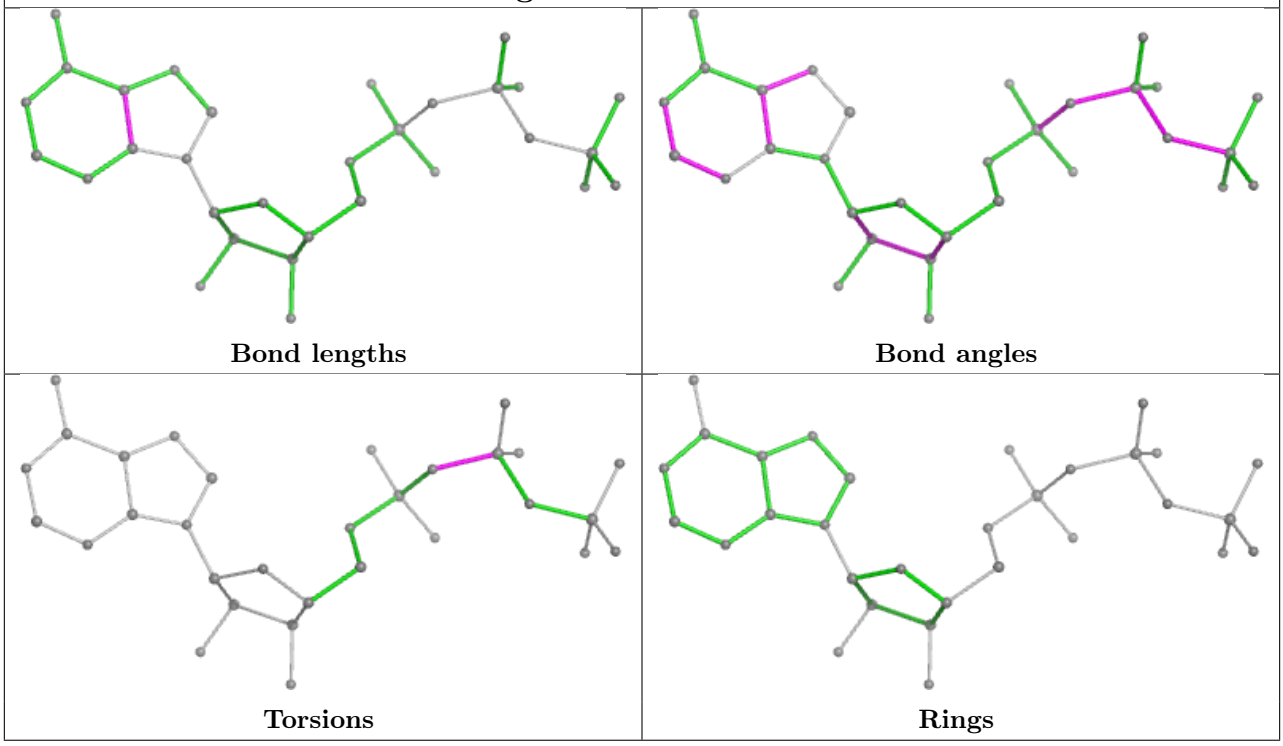
No monomer is involved in short contacts.

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.

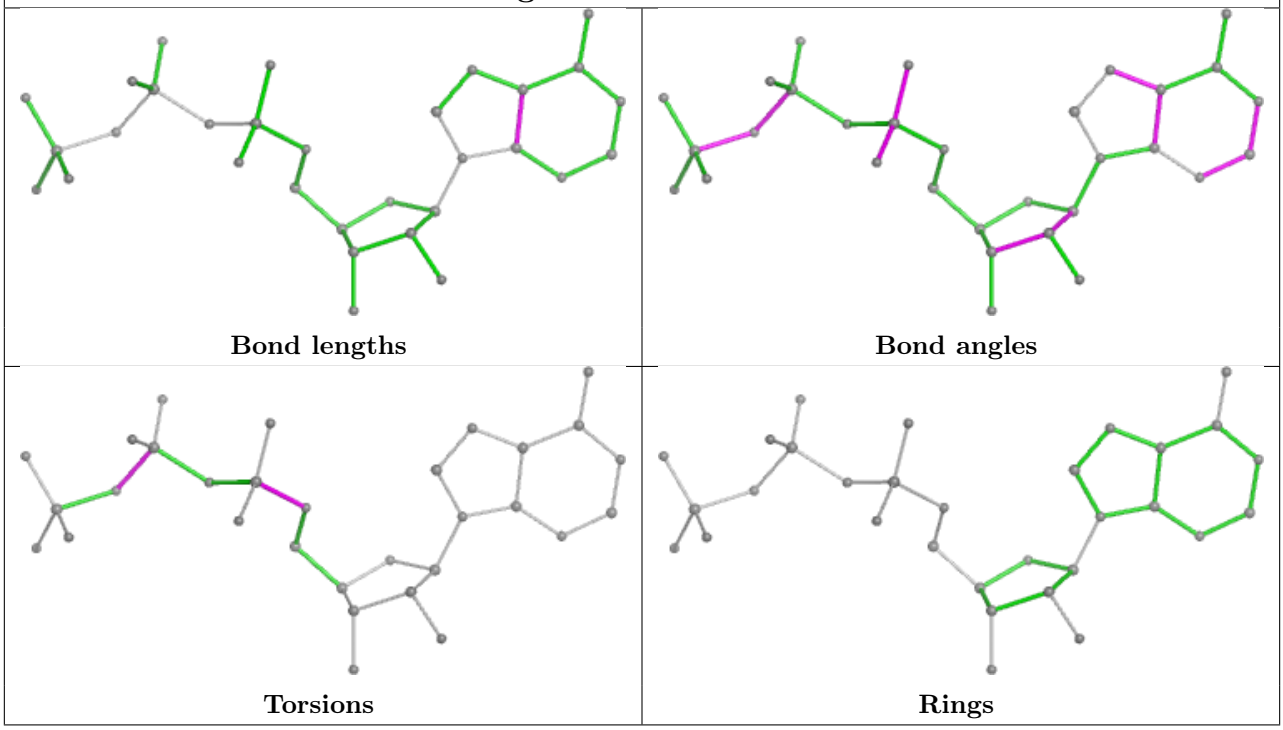
Ligand ADP Y 601



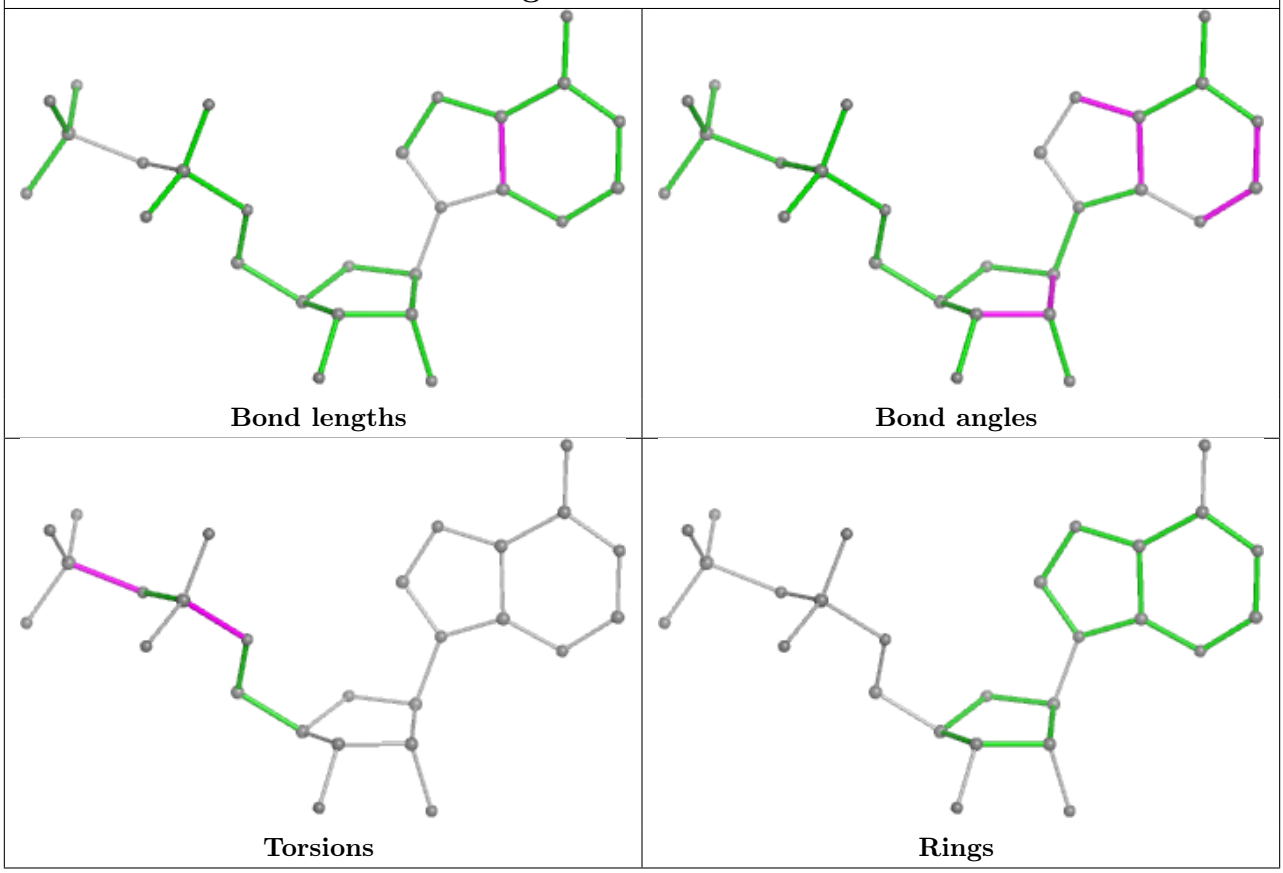
Ligand ATP U 1001

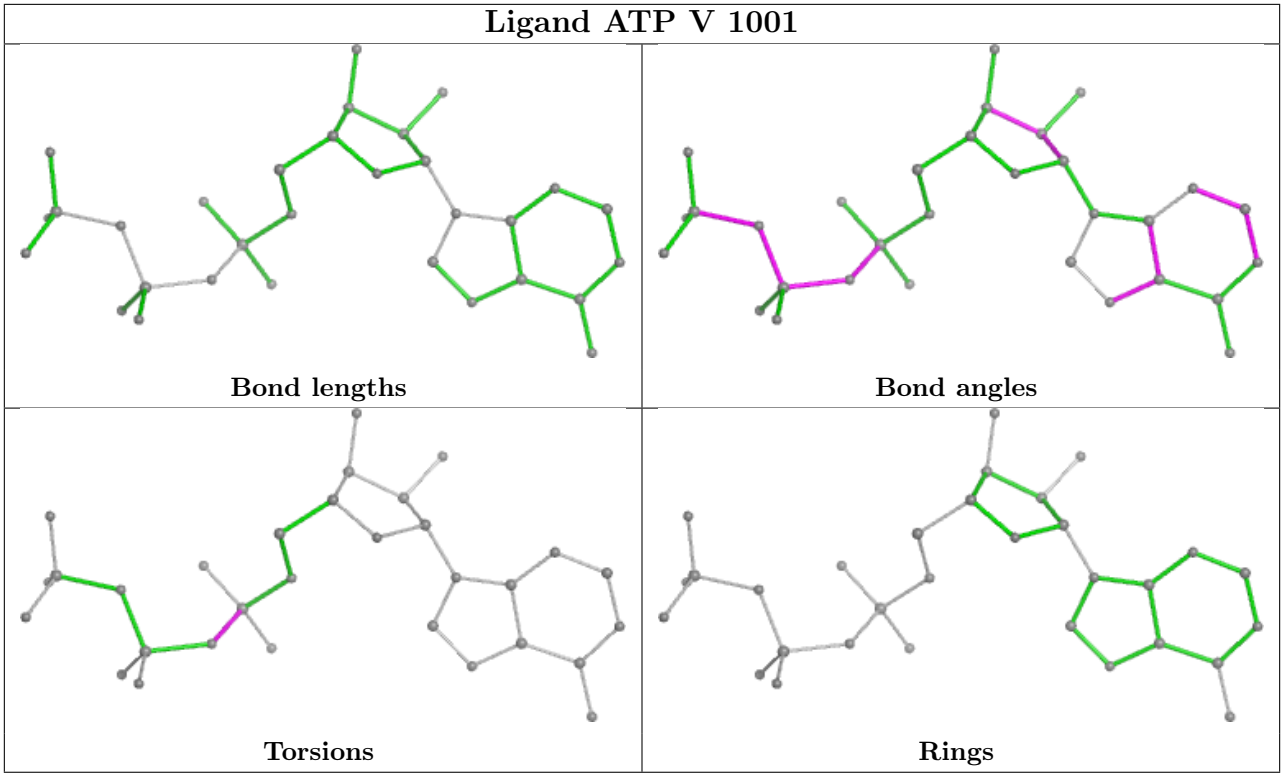


Ligand ATP T 1001



Ligand ADP X 601





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	3.27

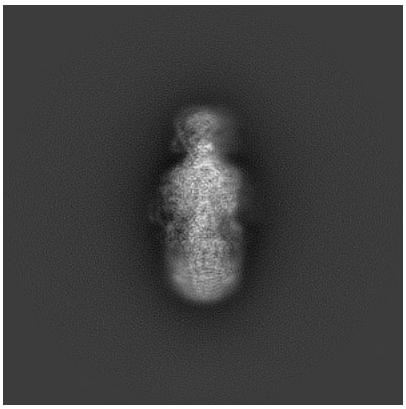
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4819. These allow visual inspection of the internal detail of the map and identification of artifacts.

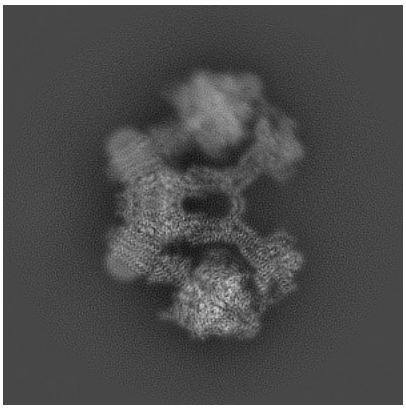
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

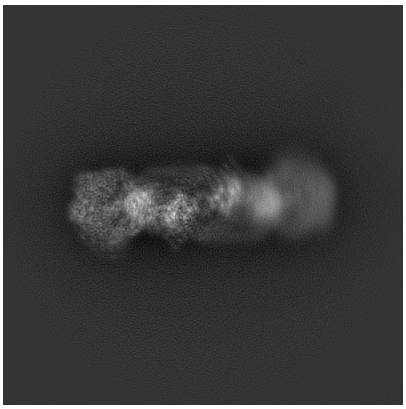
6.1.1 Primary map



X

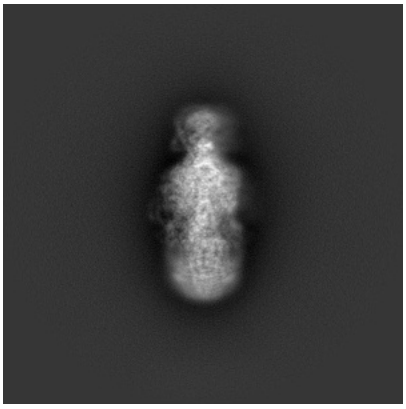


Y

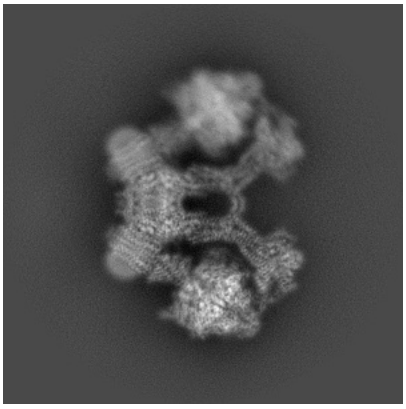


Z

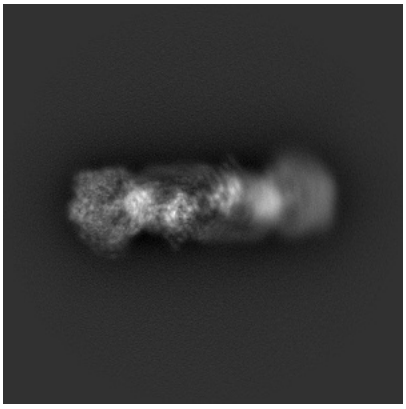
6.1.2 Raw map



X



Y

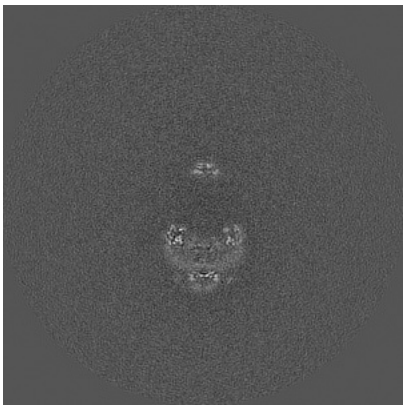


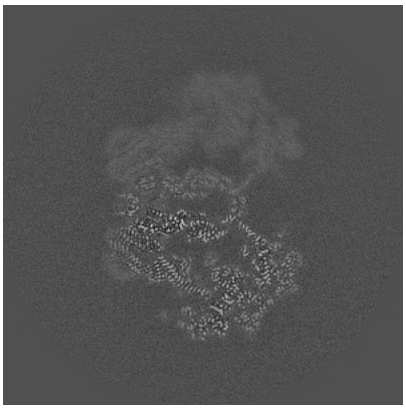
Z

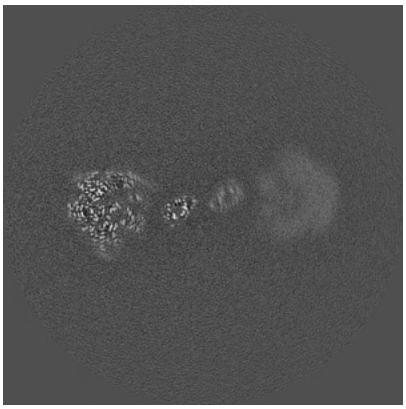
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

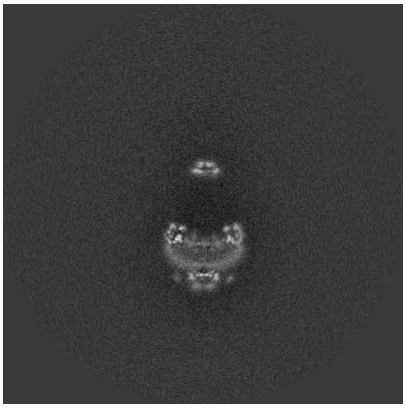
6.2.1 Primary map

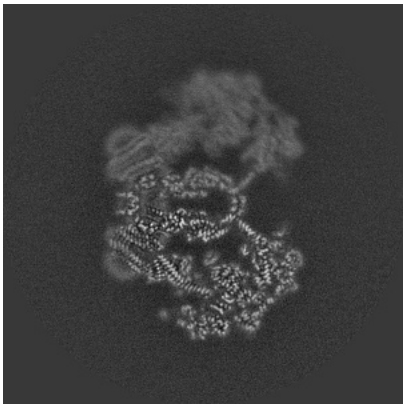

X Index: 240

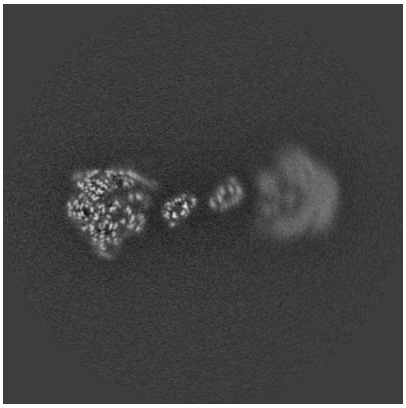

Y Index: 240


Z Index: 240

6.2.2 Raw map


X Index: 240

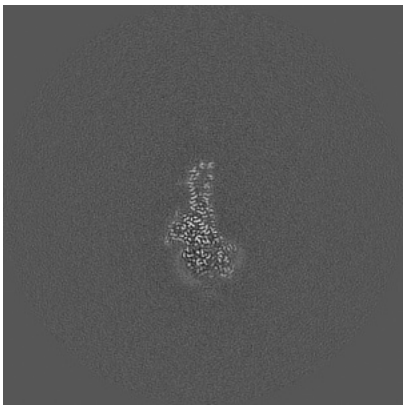

Y Index: 240

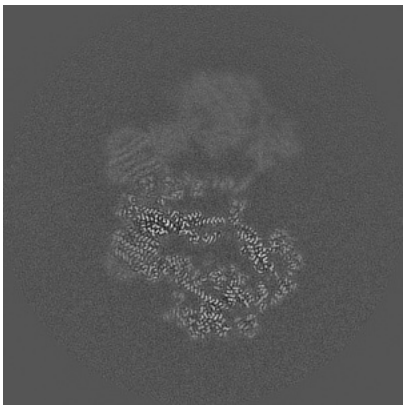

Z Index: 240

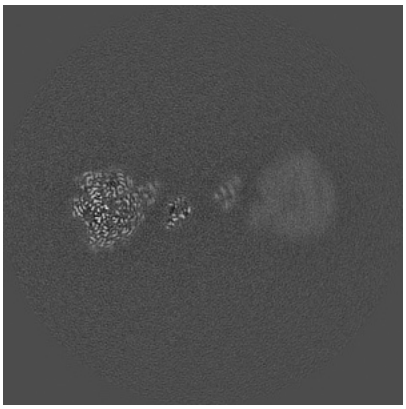
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

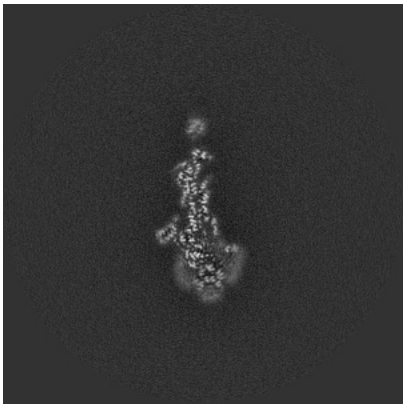
6.3.1 Primary map

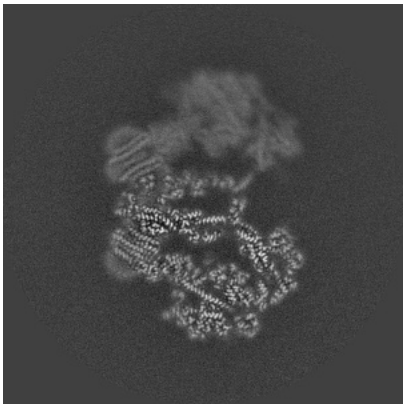

X Index: 216

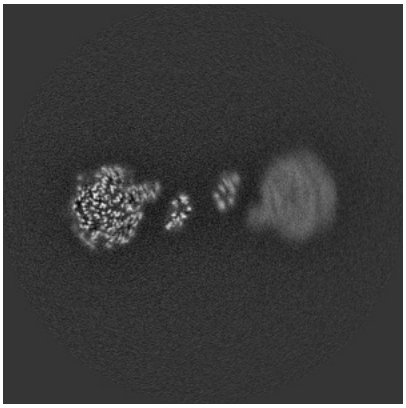

Y Index: 235


Z Index: 257

6.3.2 Raw map


X Index: 205

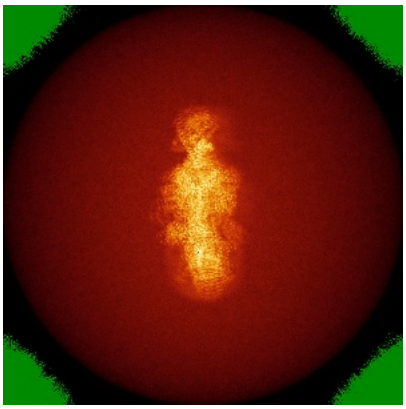

Y Index: 235


Z Index: 262

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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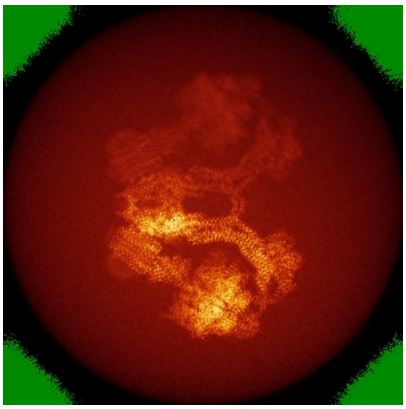
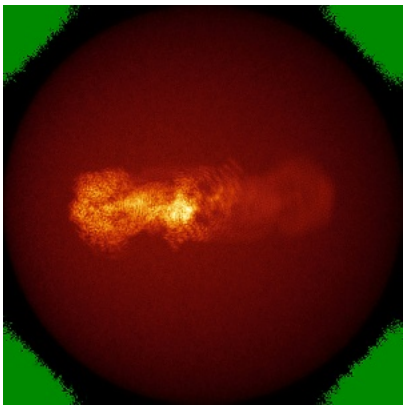
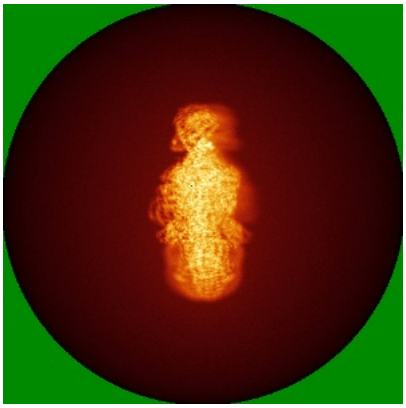
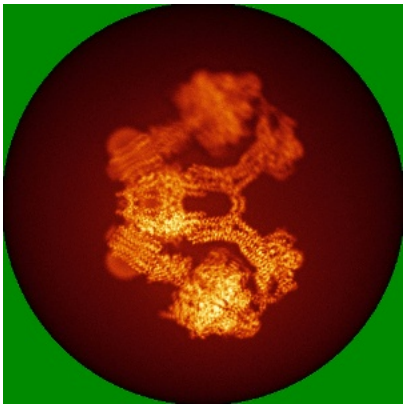
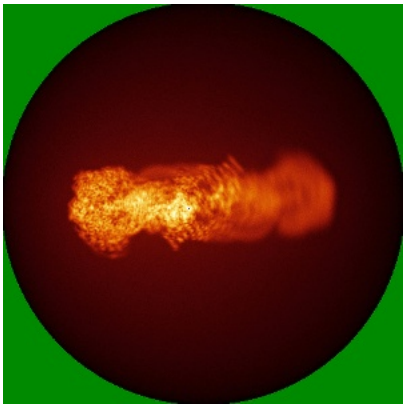

Y


Z

6.4.2 Raw 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.

6.5.2 Raw map

X

Y

Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

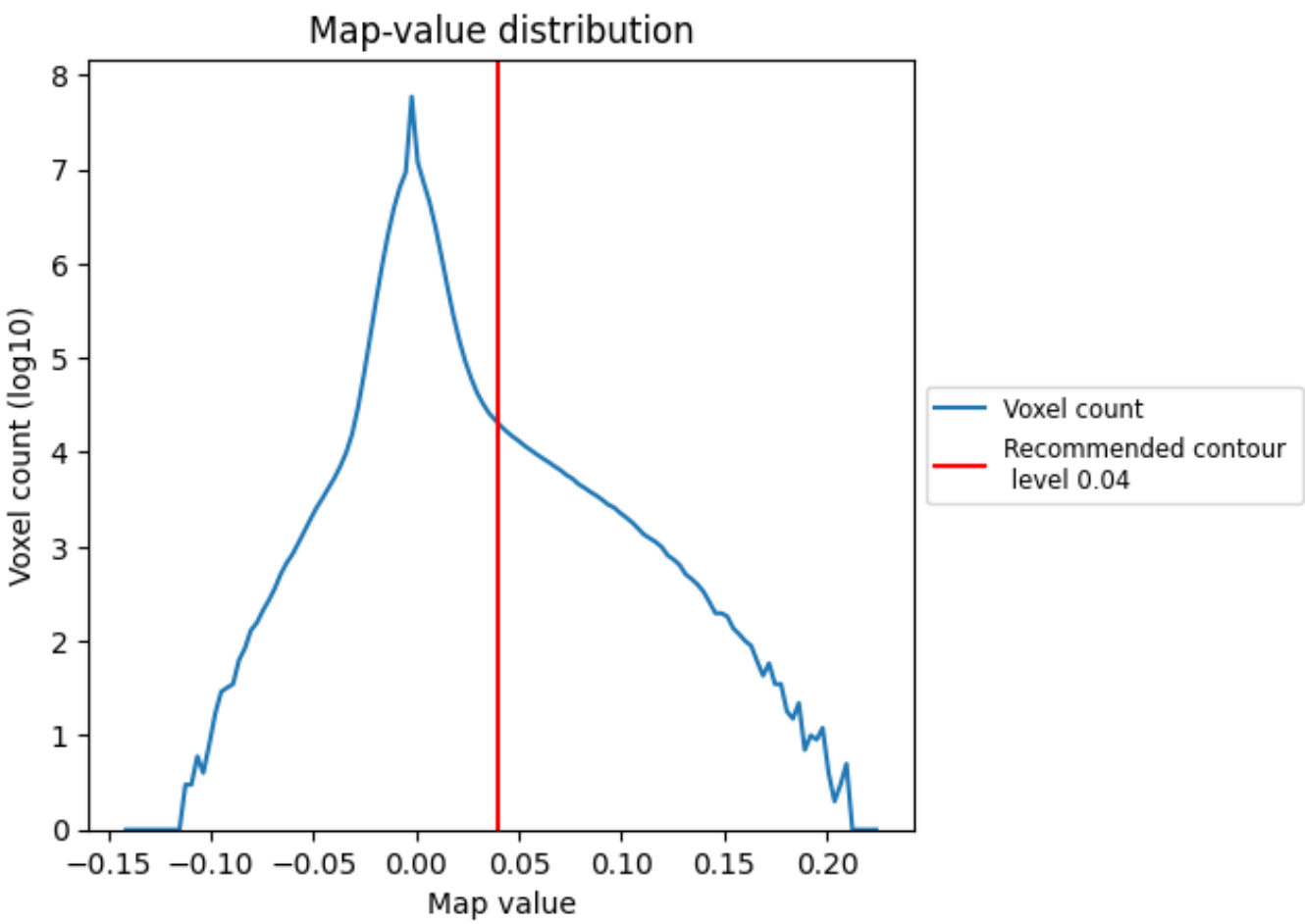
6.6 Mask visualisation (i)

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

7 Map analysis (i)

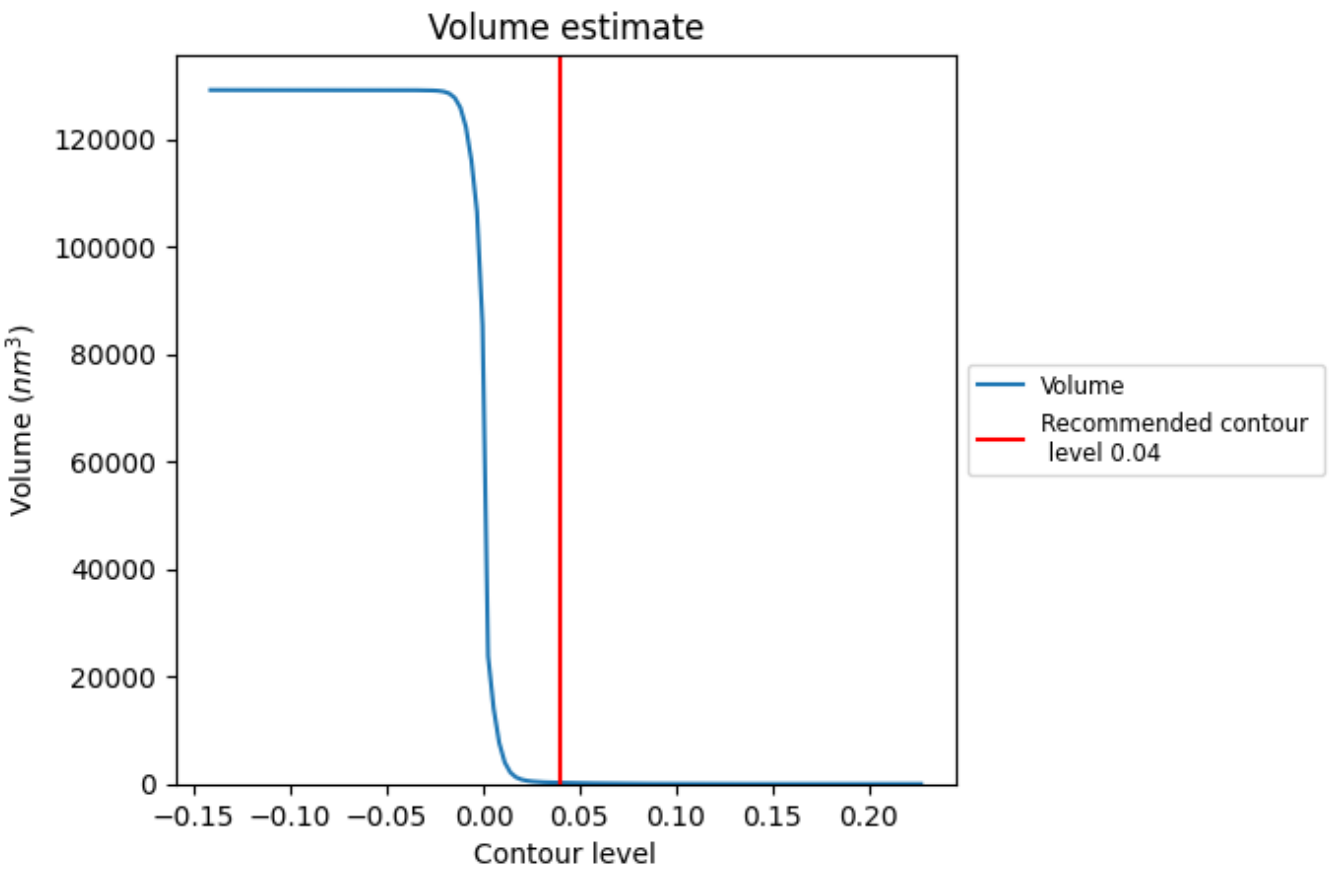
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

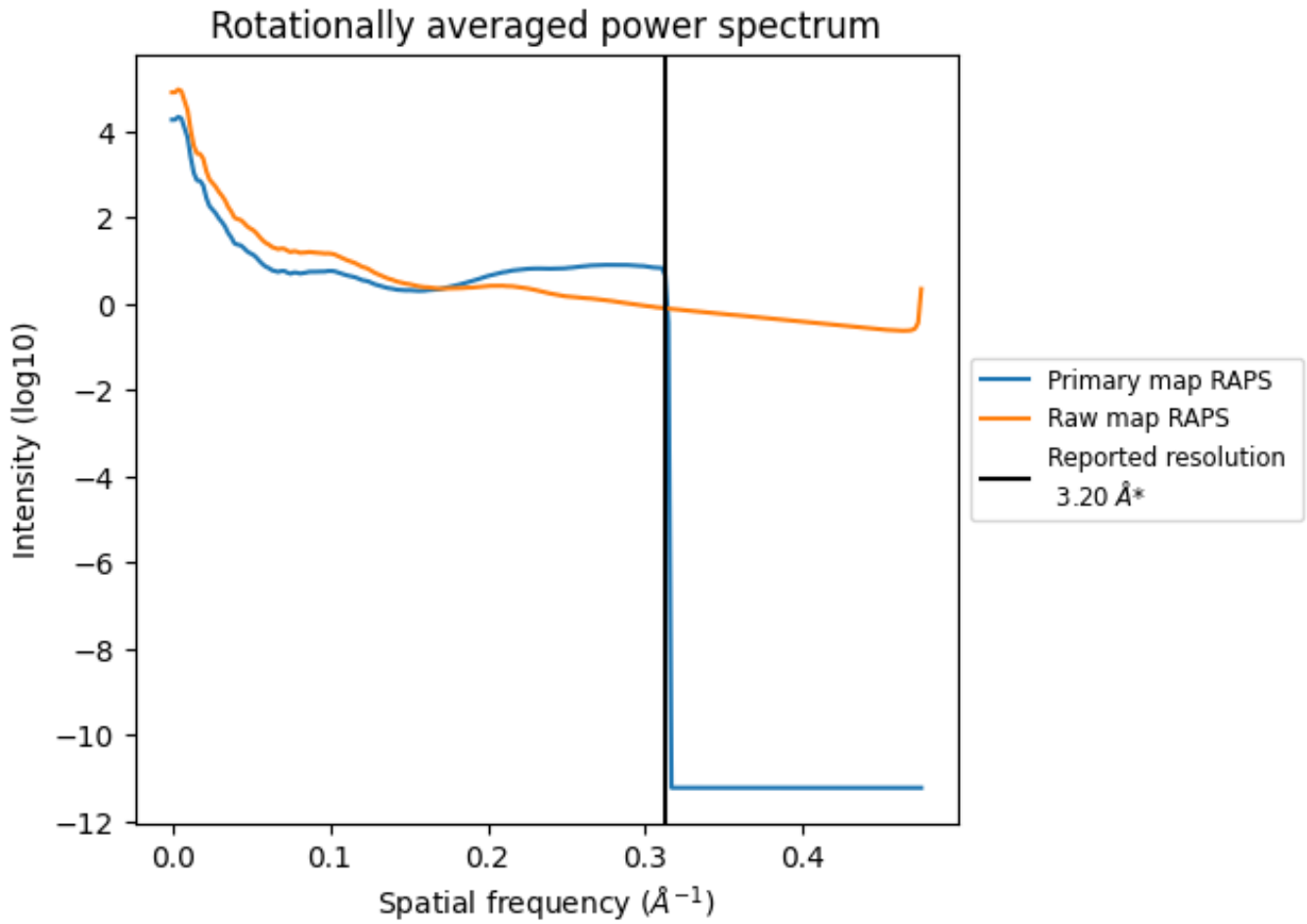
7.2 Volume estimate (i)



The volume at the recommended contour level is 220 nm^3; this corresponds to an approximate mass of 198 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)

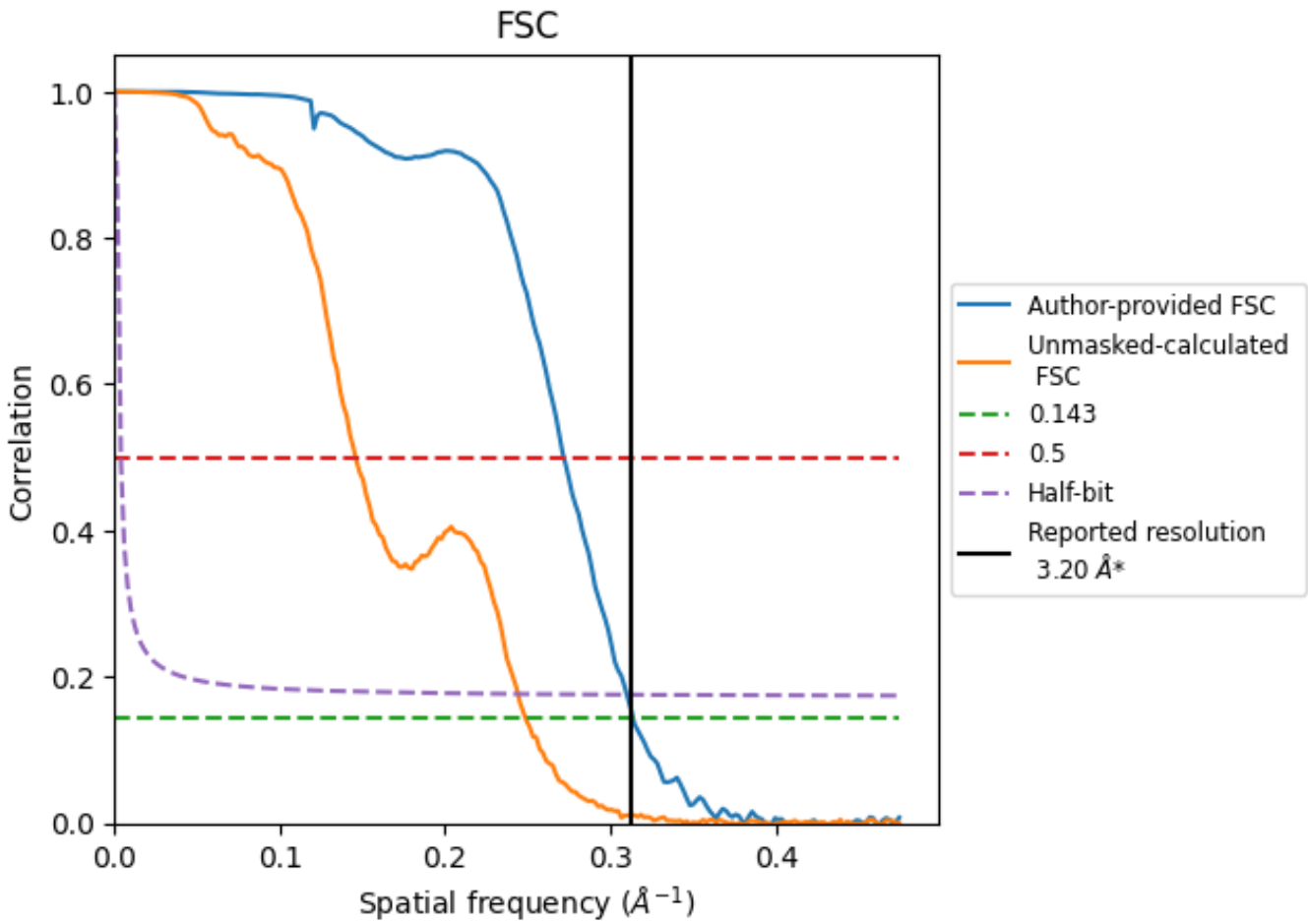


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

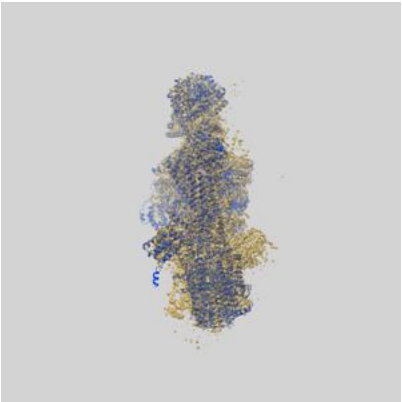
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.68	3.23
Unmasked-calculated*	4.02	6.85	4.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.02 differs from the reported value 3.2 by more than 10 %

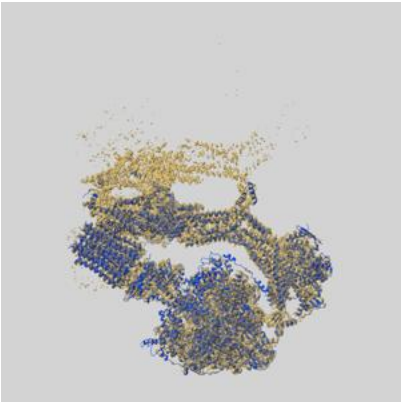
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4819 and PDB model 6RDI. Per-residue inclusion information can be found in section 3 on page 10.

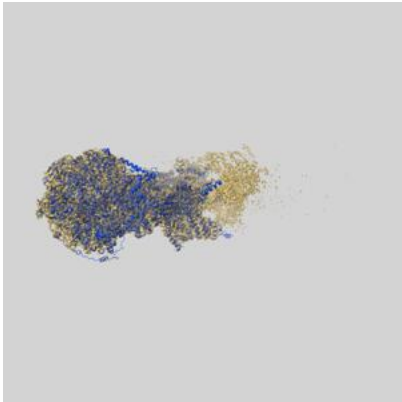
9.1 Map-model overlay (i)



X



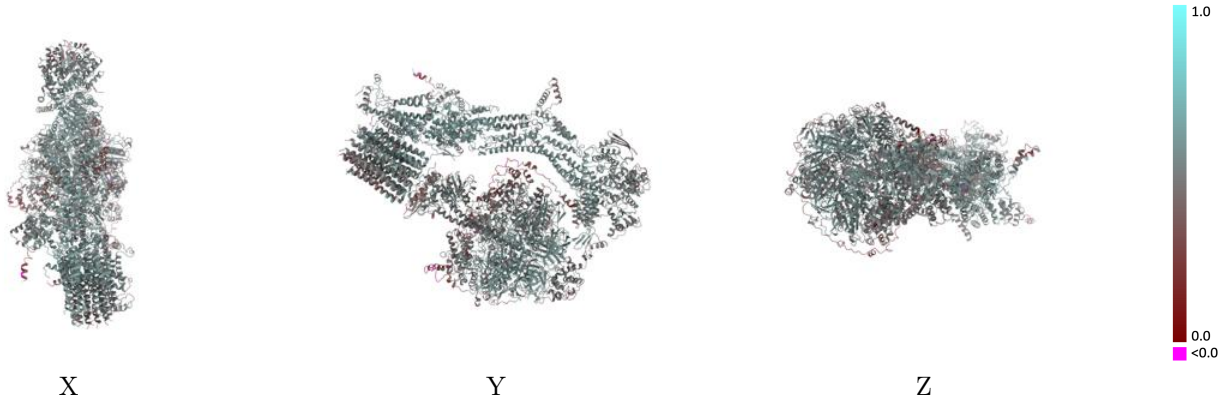
Y



Z

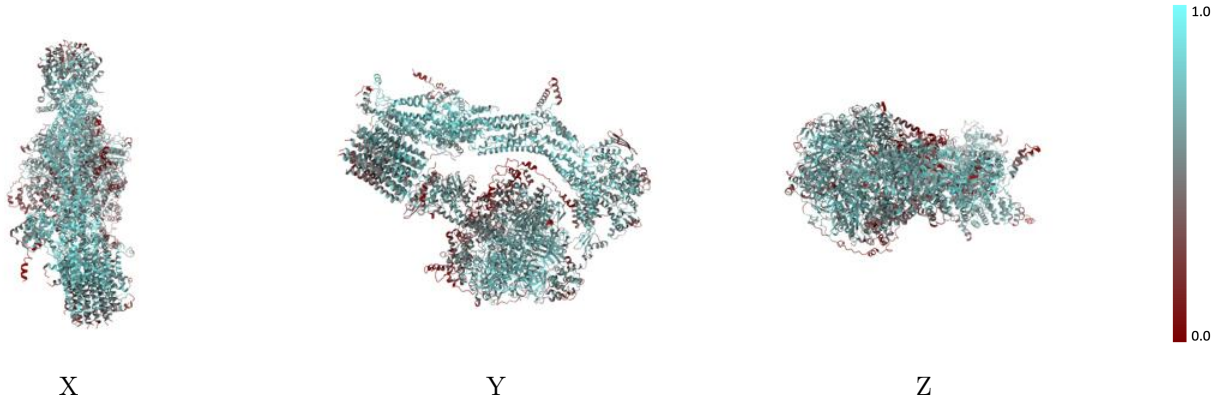
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



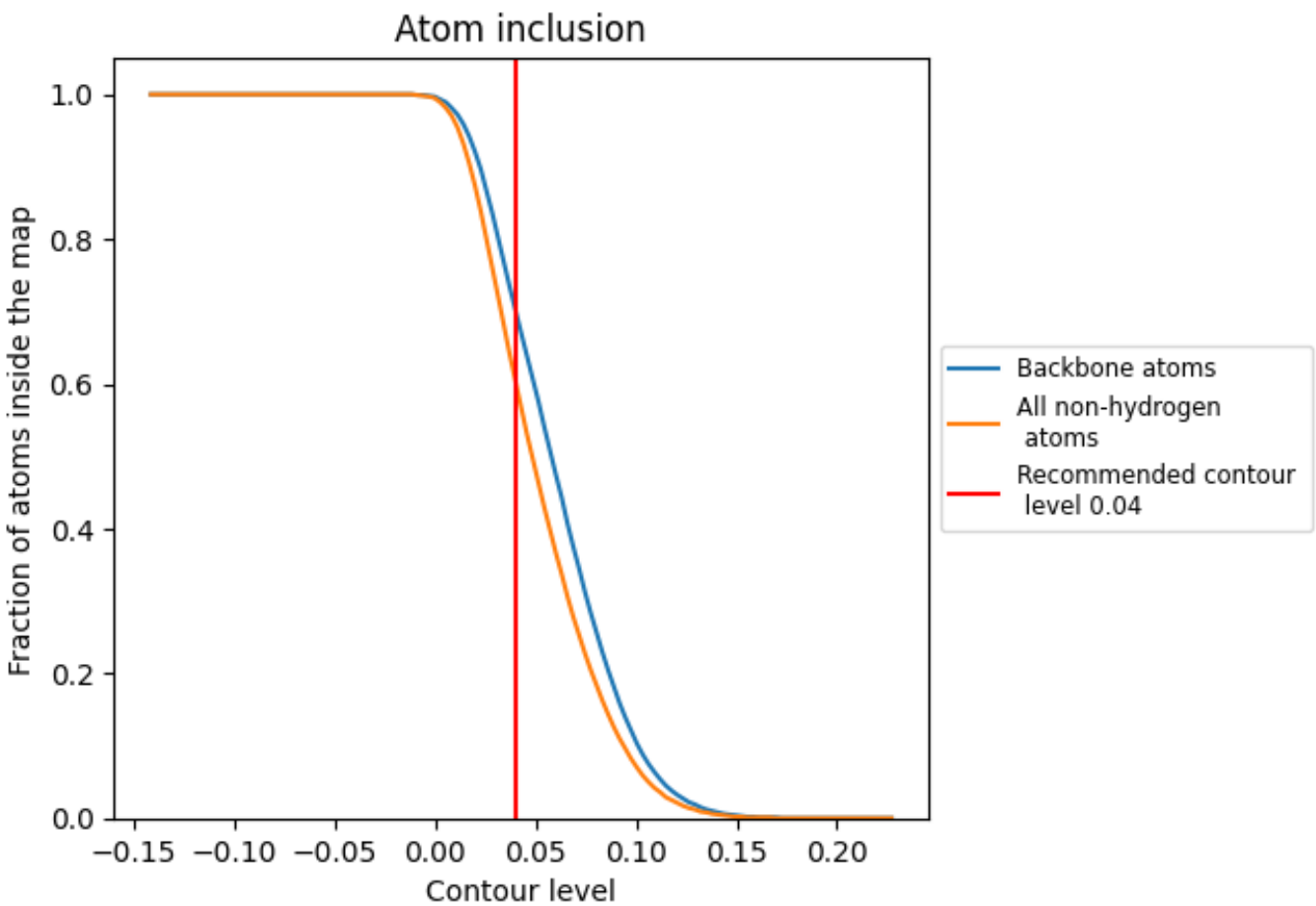
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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, 70% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.6030	0.5090
0	0.7020	0.5490
1	0.7080	0.5530
2	0.5780	0.5000
3	0.6030	0.5060
4	0.6380	0.5210
5	0.7920	0.5790
6	0.7220	0.5560
7	0.7000	0.5440
8	0.7400	0.5670
9	0.5640	0.4870
A	0.7070	0.5500
B	0.7100	0.5510
C	0.6280	0.5340
D	0.5620	0.5120
E	0.5360	0.4800
F	0.5480	0.4700
G	0.4950	0.4430
H	0.4950	0.4580
I	0.5050	0.5060
J	0.6180	0.5330
M	0.7140	0.5610
P	0.5510	0.4820
Q	0.4930	0.4850
R	0.4890	0.4660
S	0.5940	0.5020
T	0.5850	0.5000
U	0.5670	0.4900
V	0.6270	0.5230
X	0.5390	0.4780
Y	0.5360	0.4900
Z	0.5650	0.4940