wwPDB EM Validation Summary Report (i)

May 12, 2024 – 06:24 am BST

PDB ID	:	6REB
EMDB ID	:	EMD-4848
Title	:	Cryo-EM structure of Polytomella F-ATP synthase, Rotary substate 3A, composite map
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:

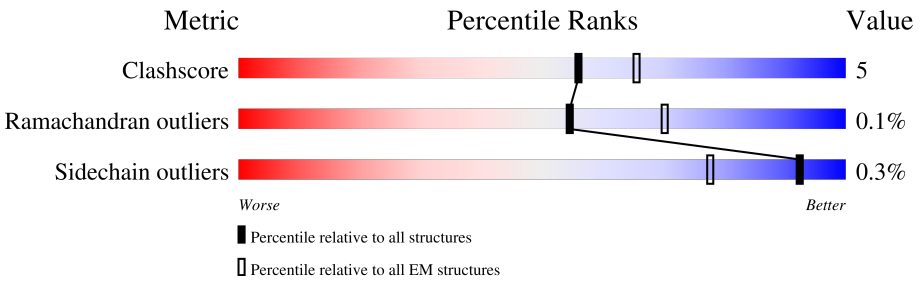
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	95%
2	1	618	85% 11%
3	2	441	85% 15%
4	3	325	67% 8% 25%
5	4	294	85% 13%
6	5	123	87% 13%
7	6	151	73% 9% 18%
8	7	190	78% 15% 7%

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Mol	Chain	Length	Quality of chain
9	8	89	89% 10% •
10	9	97	88% 12%
11	A	127	51% 7% 42%
11	B	127	50% 9% 42%
11	C	127	50% 9% 42%
11	D	127	46% 13% 42%
11	E	127	48% 10% 42%
11	F	127	50% 9% 42%
11	G	127	50% 9% 42%
11	H	127	49% 9% 42%
11	I	127	46% 12% 42%
11	J	127	48% 10% 42%
12	M	327	58% 8% 34%
13	P	229	74% 10% 16%
14	Q	74	80% 18% •
15	R	199	81% 8% • 11%
16	S	317	73% 14% 13%
17	T	562	82% 11% • 7%
17	U	562	81% 12% 7%
17	V	562	76% 17% 7%
18	X	574	79% 14% • 6%
18	Y	574	81% 10% 9%
18	Z	574	79% 16% 6%

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 53756 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	539	4095	2572	693	817	13	0	0
18	Y	521	3957	2485	670	789	13	0	0
18	Z	542	4115	2586	696	820	13	0	0

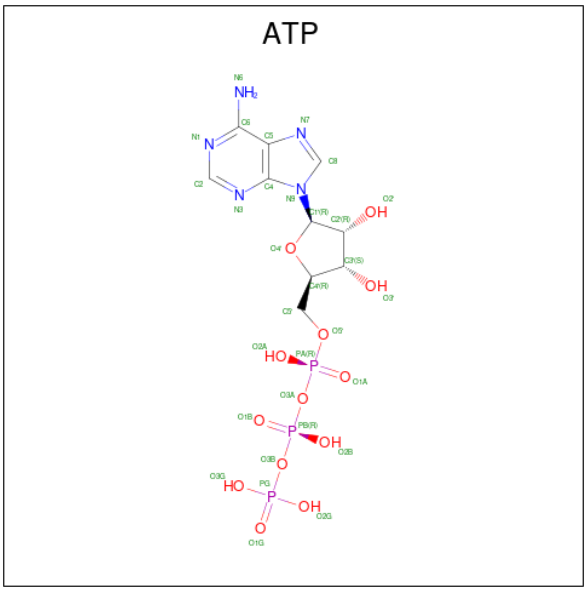
There are 6 discrepancies between the modelled and reference sequences:

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: $C_{10}H_{16}N_5O_{13}P_3$).

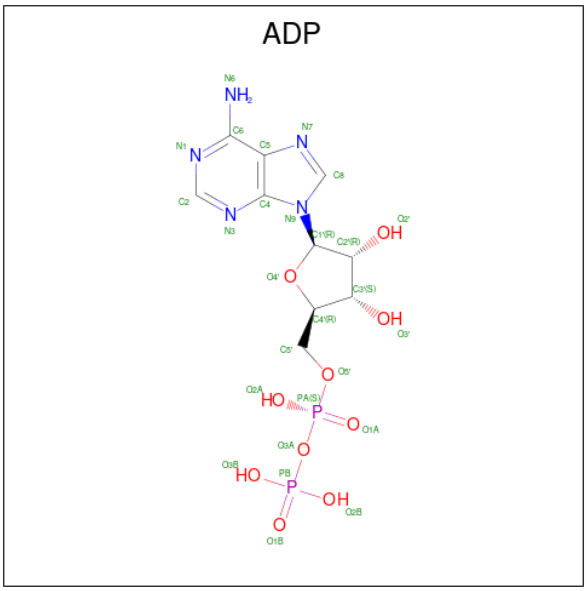


Mol	Chain	Residues	Atoms					AltConf
20	T	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	U	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	V	1	Total	C	N	O	P	0
			31	10	5	13	3	

- 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	Z	1	Total	Mg	0
			1	1	

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



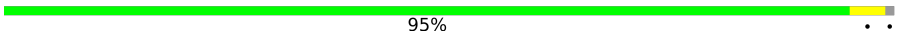
Mol	Chain	Residues	Atoms					AltConf
22	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
22	Z	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

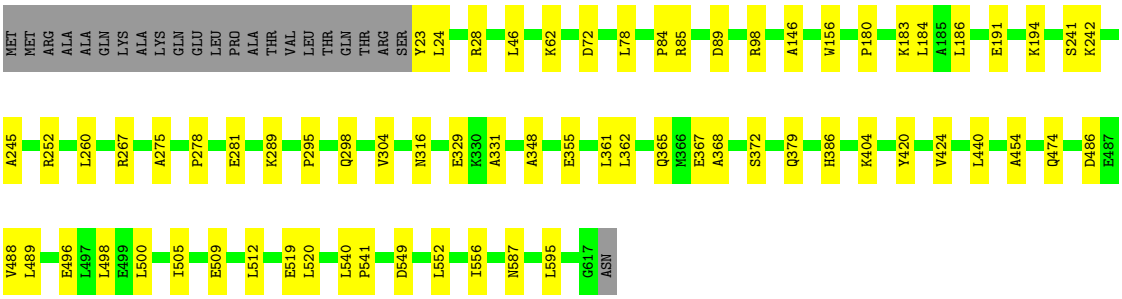
• Molecule 1: ASA-10: Polytomella F-ATP synthase associated subunit 10

Chain 0:



• Molecule 2: ATP synthase associated protein ASA1

Chain 1:

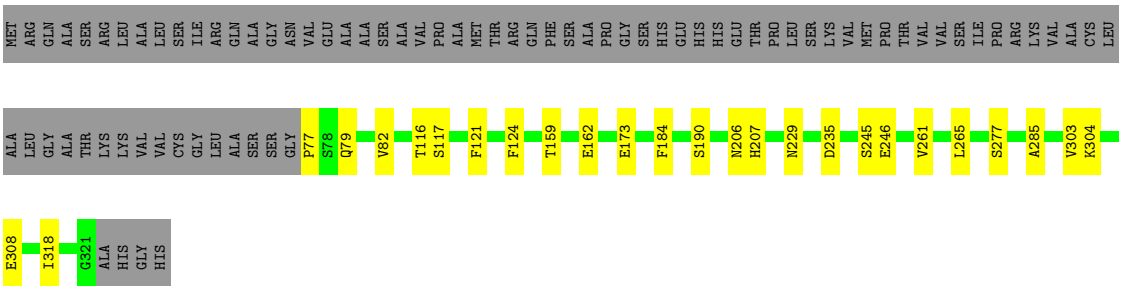


• Molecule 3: ASA-2: Polytomella F-ATP synthase associated subunit 2

Chain 2:

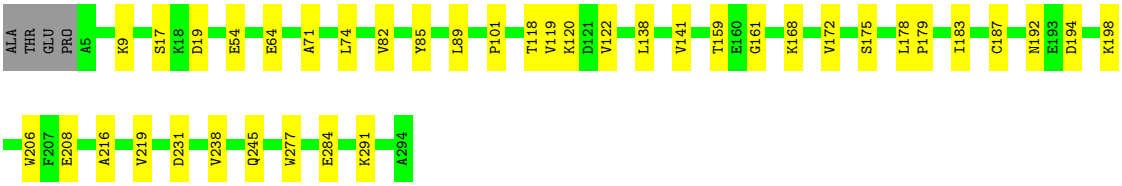
• Molecule 4: Mitochondrial F1F0 ATP synthase associated 32 kDa protein

Chain 3:



• Molecule 5: Mitochondrial ATP synthase associated protein ASA4

Chain 4:



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

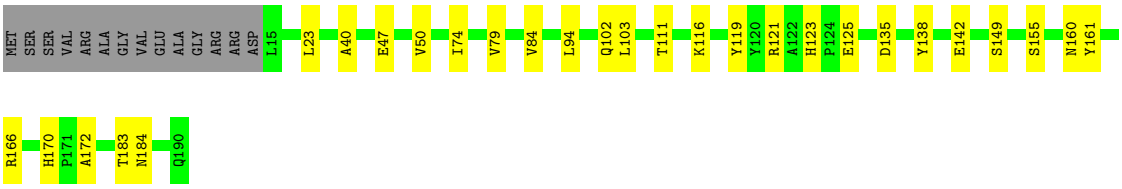
Chain 5:

• Molecule 7: Mitochondrial ATP synthase subunit ASA6

Chain 6:

• Molecule 8: Mitochondrial ATP synthase associated protein ASA7

Chain 7:

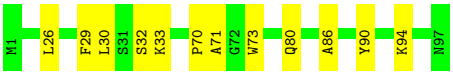


• Molecule 9: Mitochondrial ATP synthase subunit ASA8

Chain 8:

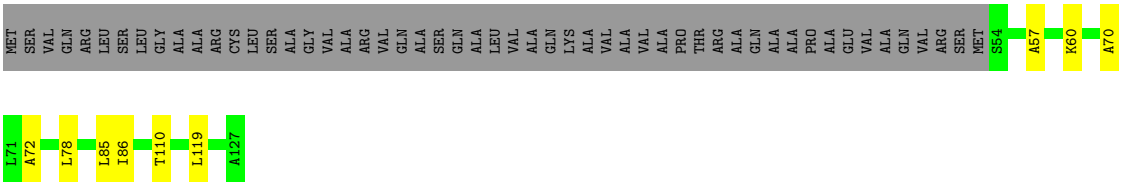
- Molecule 10: ASA-9: Polytomella F-ATP synthase associated subunit 9

Chain 9:



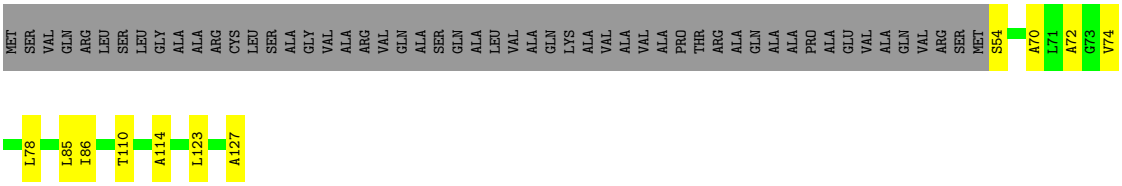
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain A:



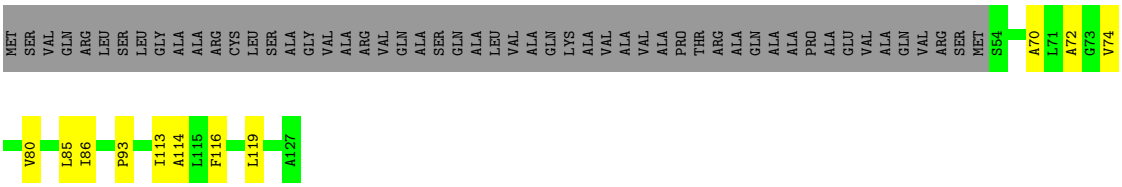
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain B:



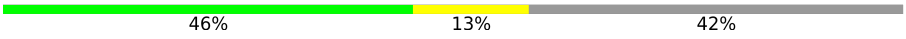
- Molecule 11: Mitochondrial ATP synthase subunit c

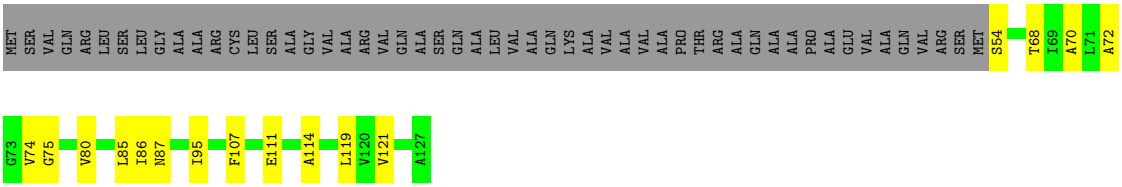
Chain C:



- Molecule 11: Mitochondrial ATP synthase subunit c

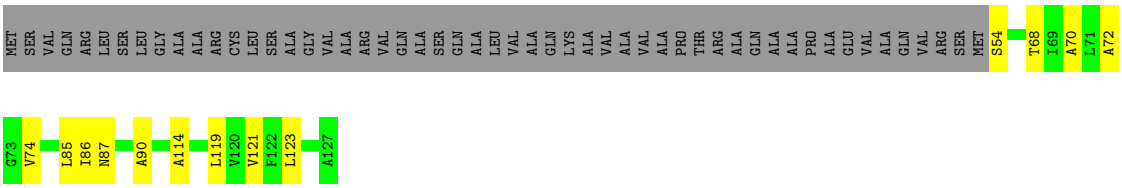
Chain D:





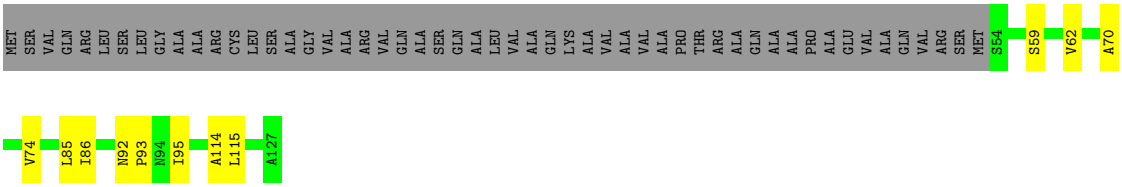
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain E: 48% 10% 42%



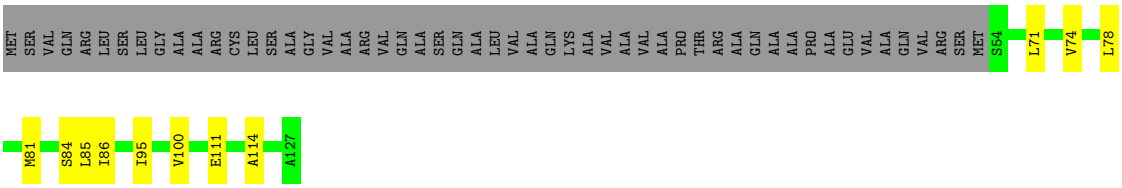
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain F: 50% 9% 42%



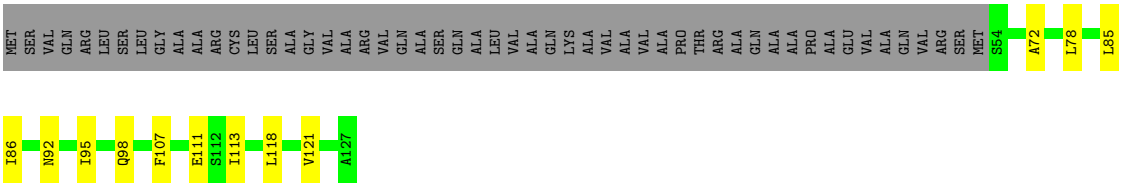
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain G: 50% 9% 42%



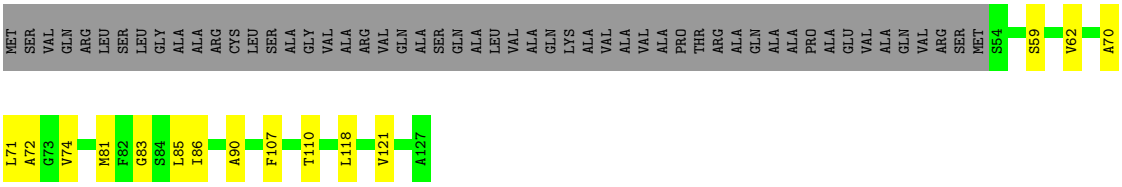
- Molecule 11: Mitochondrial ATP synthase subunit c

Chain H: 49% 9% 42%



- Molecule 11: Mitochondrial ATP synthase subunit c

Chain I: 46% 12% 42%



- Molecule 11: Mitochondrial ATP synthase subunit c

Chain J: 48% 10% 42%

MET SER VAL GLN ARG LEU SER LEU GLY ALA ALA ARG CYS LEU SER ALA GLY VAL ALA ARG VAL GLN ALA SER GLN ALA LEU VAL ALA GLN LYS ALA VAL ALA VAL ALA PRO THR ARG ALA GLN ALA ALA PRO ALA GLU VAL ALA GLN VAL ARG SER MET S54 S59 V62 A70

L71 A72 G73 V74 L78 S84 L85 I86 N92 A103 A114 A127

- Molecule 12: Mitochondrial ATP synthase subunit 6

Chain M: 58% 8% 34%

MET SER VAL LEU SER SER VAL SER MET GLY SER ARG ILE GLY SER SER LEU LEU GLY ARG SER SER ALA TYR LEU ALA GLN CYS GLY PHE SER THR ARG SER ASN LEU ASN GLY SER ILE ASP THR SER SER SER VAL PHE GLN ALA LEU SER SER ASP ASN GLU ASN LYS PRO ALA ALA

SER PRO LEU ASN VAL LYS LEU PRO GLY MET SER CYS SER SER ILE LEU LEU PRO LYS THR SER ARG ILE ALA VAL PRO PHE GLY ASN GLN THR MET ALA MET S95 Q120 N121 R133 R145 N163 T175 T200 G201 F202 K203 F204 P205 GLY HIS PHE ILE PRO GLY GLY

THR PRO TRP PRO MET ALA F219 Y229 R232 A233 V234 R239 N243 L250 L254 T255 S264 V271 F275 L280 L281 E288 V291 A292 T304 K321 K324 LYS ILE HIS

- Molecule 13: Mitochondrial ATP synthase subunit OSCP

Chain P: 74% 10% 16%

MET LEU ALA ARG VAL ALA SER VAL ALA LEU ARG ARG ALA GLU GLY LYS ILE MET PRO GLN MET VAL ARG ALA LEU SER VAL SER ALA ALA SER ALA ALA GLN ALA GLU L37 T49 Q52 E73 E79 Q83 S112 G113 A114 T118 E136 N140 K149

I157 P161 L162 D163 E166 D179 K189 I190 L195 V199 D208 M209 S210 T211 A212 I229

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

Chain Q: 80% 18%

MET CYS A3 P4 S5 G6 R10 S15 Y16 L17 I22 D25 R28 K32 K36 A39 D54 K71 N74

- Molecule 15: Mitochondrial ATP synthase subunit delta

Chain R: 81% 8% 11%

MET PHE GLY LEU LYS ARG ALA VAL THR VAL GLY ARG ARG PHE ILE SER THR SER ALA ALA ARG MET E23 A24 A25 E49 F50 N53 P71 V89 V90 T107 E117 L118 E125 V129 V136 V141 T142 V146 D153 A199

- Molecule 16: ATP synthase gamma chain, mitochondrial

Chain S: 73% 14% 13%

MET ALA LEU ARG LYS ALA VAL LEU SER LEU GLY LEU SER GLN GLY VAL ALA ALA GLU ALA VAL LEU GLY SER GLY MET PHE ASN ALA VAL GLN HIS GLU SER VAL ARG TYR ALA S39 R79 D83 V86 R87 S97 V101 V102 V105 T123 R124 L127 V137

V138 V139 V140 S141 I142 L150 I153 E154 R157 L160 V168 R169 V170 Q174 I183 K184 Q188 N195 K196 F197 T206 I210 P213 D214 L215 L216 E217 K218 Q219 L220 R239 R244 D245 L246 T247 E248 T254 E261 N262 N276 I308

M315 ASP GLU

- Molecule 17: ATP synthase subunit alpha

Chain T:

MET ARG SER PRO ALA ALA PHE VAL ALA ARG SER GLY LEU PHE LYS ALA SER LEU GLY GLN SER ASN TRP ALA GLN LYS ALA GLU GLN MET MET ALA SER VAL THR ARG THR PHE ALA A40 D41 S55 K56 Y57 P79 V90 S102 V103 Q104 E107 L108 N121 L122 Q123

I138 V151 I155 L202 F203 Q219 R220 E221 L222 I223 I224 G225 D226 K231 T232 A235 I240 H241 Q242 K243 P250 Q253 K265 R266 S267 T268 T279 G280 A281 F300 L301 Y312 F313 R314 I323 Q330 Y356 R360 R364 T378

A379 F380 D403 L408 K415 V442 L466 D467 R476 E482 K485 P493 V501 T505 H549 L559 A562

- Molecule 17: ATP synthase subunit alpha

Chain U:

MET ARG SER PRO ALA ALA PHE VAL ALA ARG SER GLY LEU PHE LYS ALA SER LEU GLY GLN SER ASN TRP ALA GLN LYS ALA GLU GLN MET MET ALA SER VAL THR ARG THR PHE ALA A40 E47 K52 L58 H61 L84 L100 V103 L108 L120 F132

L143 T147 V151 N152 L160 V180 A189 F203 R217 R220 D226 R227 Q228 K231 A235 I240 H241 Q242 K243 N246 R254 L272 T279 G280 A281 P297 F300 L301 Y304 R314 I323 V332 R335 L339

P345 L357 H358 S359 R364 A365 A366 K367 G374 G375 S376 L377 T378 A379 F380 S400 D403 R418 R429 L446 Y453 Q471 E475 R476 G477 A500 V501 R513 V514 Q515 D516 I517 I525 A562

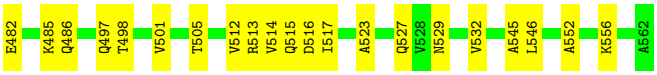
- Molecule 17: ATP synthase subunit alpha

Chain V:

MET ARG SER PRO ALA ALA PHE VAL ALA ARG SER GLY LEU PHE LYS ALA SER LEU GLY GLN SER ASN TRP ALA GLN LYS ALA GLU GLN MET MET ALA SER VAL THR ARG THR PHE ALA ALA ASP ALA K43 D46 I59 V62 L66 V90 G91 D92 Q104 E107 L108

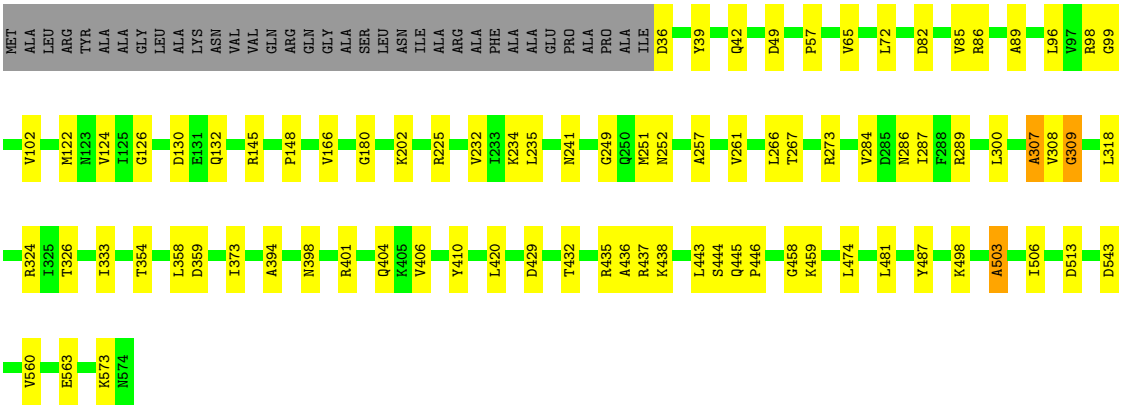
K116 L122 D125 D135 S136 V137 I138 L143 T147 I150 D172 V180 I193 Q196 P201 V206 K207 D210 R217 R220 E221 L222 D226 K231 A235 I236 K251 R254 A270 Q271 L272 R283 Y284 F300 Y304

E311 R314 I323 Y324 D325 D326 L327 Y334 L340 P344 P345 G346 R347 E348 A349 D353 L357 K370 F380 P381 V382 I406 F407 L408 E409 L412 A420 L421 N422 S428 S432 A443 L446 F459 G463 R476 R479 L480 T481



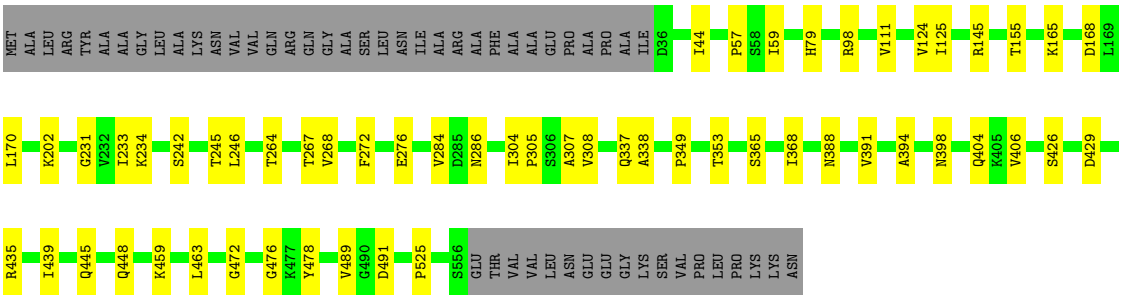
• Molecule 18: ATP synthase subunit beta

Chain X:



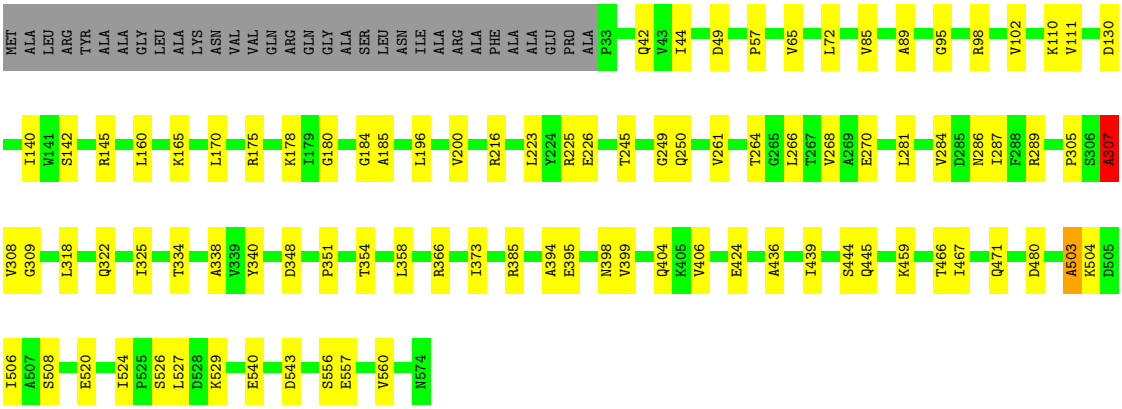
• Molecule 18: ATP synthase subunit beta

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	74956	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	35.532	Depositor
Minimum map value	-21.540	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.034	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: ZN, MG, ATP, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	0	0.50	0/628	0.52	0/856
2	1	0.49	0/4750	0.55	0/6434
3	2	0.40	0/3212	0.57	0/4371
4	3	0.45	0/1911	0.56	1/2601 (0.0%)
5	4	0.47	0/2216	0.54	0/3000
6	5	0.58	0/1011	0.67	2/1376 (0.1%)
7	6	0.51	0/946	0.60	0/1287
8	7	0.56	0/1374	0.58	1/1865 (0.1%)
9	8	0.56	0/715	0.62	0/974
10	9	0.42	0/802	0.59	0/1084
11	A	0.35	0/520	0.59	1/704 (0.1%)
11	B	0.35	0/520	0.56	0/704
11	C	0.39	0/519	0.60	1/701 (0.1%)
11	D	0.43	0/520	0.60	0/704
11	E	0.45	0/520	0.56	0/704
11	F	0.42	0/520	0.59	0/704
11	G	0.38	0/520	0.53	0/704
11	H	0.36	0/520	0.54	0/704
11	I	0.35	0/520	0.52	0/704
11	J	0.35	0/520	0.59	0/704
12	M	0.55	0/1683	0.62	0/2295
13	P	0.44	0/1553	0.58	0/2093
14	Q	0.40	0/574	0.53	0/774
15	R	0.45	0/1336	0.57	1/1827 (0.1%)
16	S	0.45	0/2153	0.59	1/2901 (0.0%)
17	T	0.59	0/4048	0.62	2/5481 (0.0%)
17	U	0.59	0/4049	0.62	1/5481 (0.0%)
17	V	0.60	0/4031	0.60	0/5456
18	X	0.56	0/4155	0.61	1/5630 (0.0%)
18	Y	0.57	0/4015	0.59	0/5440
18	Z	0.57	0/4176	0.61	0/5659
All	All	0.52	0/54537	0.59	12/73922 (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
3	2	0	1
6	5	0	1
18	X	0	2
18	Y	0	1
18	Z	0	2
All	All	0	7

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	5	106	LEU	CA-CB-CG	6.62	130.53	115.30
17	T	559	LEU	CA-CB-CG	6.41	130.04	115.30
15	R	118	LEU	CA-CB-CG	6.09	129.32	115.30
4	3	77	PRO	N-CA-CB	5.86	110.33	103.30
6	5	106	LEU	CB-CG-CD2	-5.86	101.03	111.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	222	PHE	Peptide
6	5	119	LYS	Peptide
18	X	307	ALA	Peptide
18	X	503	ALA	Mainchain
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	3	0
2	1	4661	0	4695	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	3163	0	3262	35	0
4	3	1874	0	1826	16	0
5	4	2177	0	2169	28	0
6	5	986	0	1021	16	0
7	6	926	0	941	12	0
8	7	1347	0	1345	28	0
9	8	692	0	694	8	0
10	9	776	0	757	13	0
11	A	514	0	554	7	0
11	B	514	0	554	9	0
11	C	514	0	553	8	0
11	D	514	0	554	15	0
11	E	514	0	554	11	0
11	F	514	0	554	9	0
11	G	514	0	554	12	0
11	H	514	0	554	14	0
11	I	514	0	554	11	0
11	J	514	0	554	11	0
12	M	1640	0	1665	20	0
13	P	1532	0	1602	18	0
14	Q	561	0	565	10	0
15	R	1303	0	1266	11	0
16	S	2130	0	2180	31	0
17	T	3979	0	4119	42	0
17	U	3980	0	4119	40	0
17	V	3962	0	4105	63	0
18	X	4095	0	4113	51	0
18	Y	3957	0	3967	34	0
18	Z	4115	0	4138	57	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	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	Z	1	0	0	0	0
22	X	27	0	12	0	0
22	Z	27	0	12	0	0
All	All	53756	0	54732	565	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 565 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)
10:9:90:TYR:OH	10:9:94:LYS:HE2	1.46	1.13
11:G:78:LEU:HD11	11:G:111:GLU:OE2	1.48	1.10
11:H:78:LEU:HD11	11:H:111:GLU:OE2	1.62	0.99
10:9:90:TYR:OH	10:9:94:LYS:CE	2.17	0.92
10:9:90:TYR:HH	10:9:94:LYS:HE2	1.42	0.81

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%)	75 (95%)	4 (5%)	0	100	100
2	1	593/618 (96%)	574 (97%)	19 (3%)	0	100	100
3	2	439/441 (100%)	415 (94%)	22 (5%)	2 (0%)	29	67
4	3	243/325 (75%)	235 (97%)	8 (3%)	0	100	100
5	4	288/294 (98%)	278 (96%)	10 (4%)	0	100	100
6	5	121/123 (98%)	114 (94%)	6 (5%)	1 (1%)	19	58
7	6	122/151 (81%)	110 (90%)	12 (10%)	0	100	100
8	7	174/190 (92%)	170 (98%)	4 (2%)	0	100	100
9	8	86/89 (97%)	77 (90%)	9 (10%)	0	100	100
10	9	95/97 (98%)	82 (86%)	13 (14%)	0	100	100
11	A	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	B	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
11	C	71/127 (56%)	70 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	D	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	E	72/127 (57%)	71 (99%)	1 (1%)	0	100	100
11	F	72/127 (57%)	70 (97%)	2 (3%)	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%)	72 (100%)	0	0	100	100
11	J	72/127 (57%)	70 (97%)	2 (3%)	0	100	100
12	M	213/327 (65%)	204 (96%)	9 (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%)	167 (95%)	8 (5%)	0	100	100
16	S	275/317 (87%)	260 (94%)	15 (6%)	0	100	100
17	T	521/562 (93%)	494 (95%)	26 (5%)	1 (0%)	47	79
17	U	521/562 (93%)	494 (95%)	27 (5%)	0	100	100
17	V	518/562 (92%)	492 (95%)	26 (5%)	0	100	100
18	X	537/574 (94%)	496 (92%)	39 (7%)	2 (0%)	34	69
18	Y	519/574 (90%)	496 (96%)	22 (4%)	1 (0%)	47	79
18	Z	540/574 (94%)	505 (94%)	33 (6%)	2 (0%)	34	69
All	All	7039/8234 (86%)	6691 (95%)	339 (5%)	9 (0%)	54	83

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	X	308	VAL
18	Y	308	VAL
18	Z	308	VAL
3	2	383	PRO
17	T	56	LYS

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%)	310 (99%)	2 (1%)	86	94
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%)	139 (99%)	1 (1%)	84	94
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%)	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%)	233 (99%)	2 (1%)	78	91
17	T	419/448 (94%)	416 (99%)	3 (1%)	84	94
17	U	419/448 (94%)	415 (99%)	4 (1%)	76	90
17	V	418/448 (93%)	416 (100%)	2 (0%)	88	95
18	X	447/469 (95%)	447 (100%)	0	100	100
18	Y	430/469 (92%)	430 (100%)	0	100	100
18	Z	449/469 (96%)	449 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5632/6445 (87%)	5617 (100%)	15 (0%)	92 96

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	T	243	LYS
17	V	180	VAL
17	T	300	PHE
17	V	300	PHE
17	U	378	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
17	V	244	ASN
18	Y	398	ASN
17	V	435	GLN
18	Y	83	ASN
18	Z	278	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	$\#\|Z\| > 2$
20	ATP	U	1001	21	26,33,33	0.95	0	31,52,52	1.42	5 (16%)
20	ATP	T	1001	21	26,33,33	0.93	0	31,52,52	1.43	5 (16%)
20	ATP	V	1001	21	26,33,33	0.95	0	31,52,52	1.45	4 (12%)
22	ADP	X	601	21	24,29,29	0.95	1 (4%)	29,45,45	1.44	4 (13%)
22	ADP	Z	601	21	24,29,29	0.98	1 (4%)	29,45,45	1.38	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	ATP	U	1001	21	-	0/18/38/38	0/3/3/3
20	ATP	T	1001	21	-	0/18/38/38	0/3/3/3
20	ATP	V	1001	21	-	2/18/38/38	0/3/3/3
22	ADP	X	601	21	-	0/12/32/32	0/3/3/3
22	ADP	Z	601	21	-	8/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	X	601	ADP	C5-C4	2.06	1.46	1.40
22	Z	601	ADP	C5-C4	2.01	1.46	1.40

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	X	601	ADP	C3'-C2'-C1'	3.61	106.41	100.98
22	Z	601	ADP	C3'-C2'-C1'	3.60	106.39	100.98
20	V	1001	ATP	N3-C2-N1	-3.57	123.09	128.68
20	U	1001	ATP	N3-C2-N1	-3.47	123.25	128.68
20	T	1001	ATP	N3-C2-N1	-3.38	123.40	128.68

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	Z	601	ADP	PA-O3A-PB-O2B
22	Z	601	ADP	PA-O3A-PB-O3B
22	Z	601	ADP	C5'-O5'-PA-O1A
22	Z	601	ADP	C5'-O5'-PA-O3A
20	V	1001	ATP	O4'-C4'-C5'-O5'

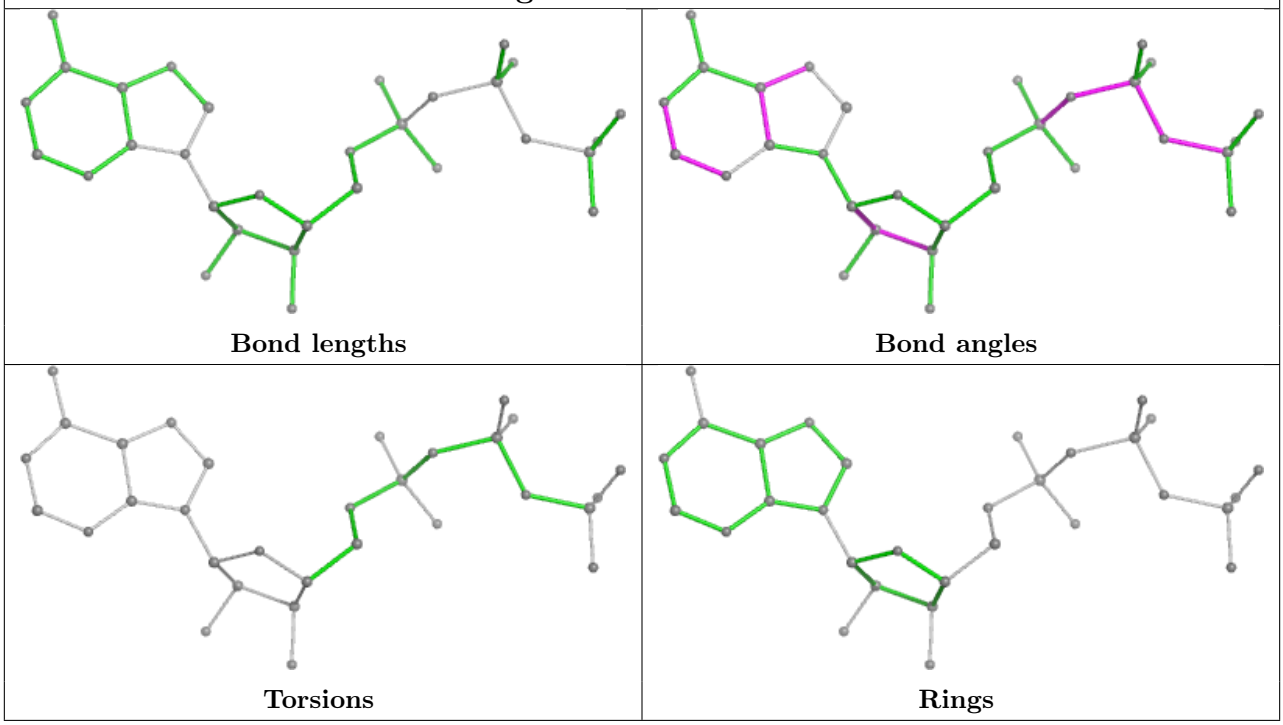
There are no ring outliers.

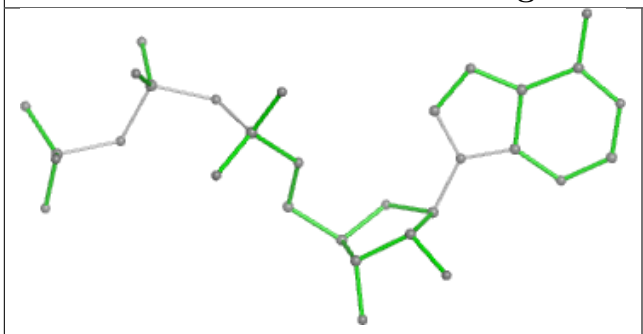
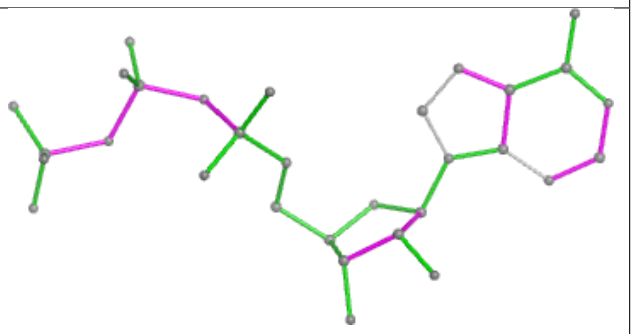
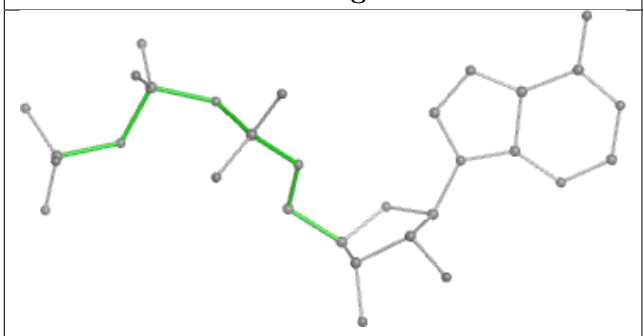
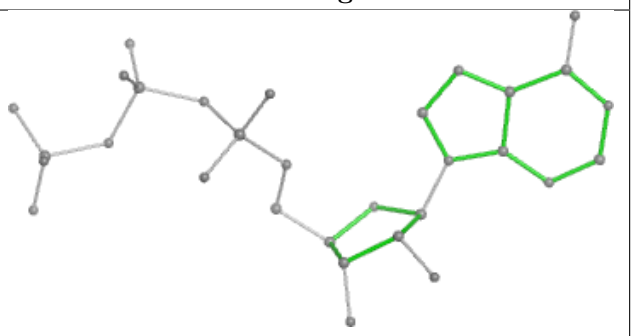
1 monomer is involved in 1 short contact:

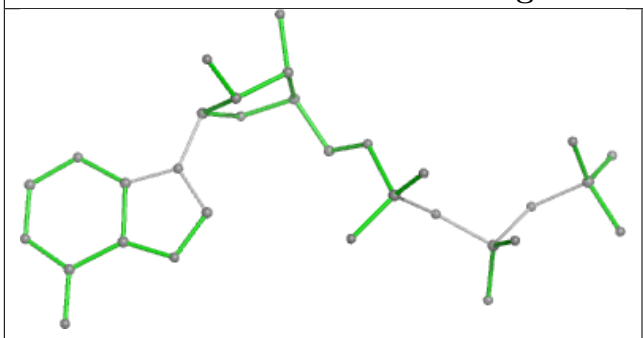
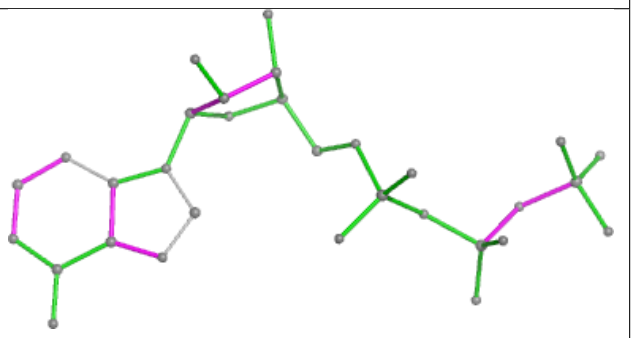
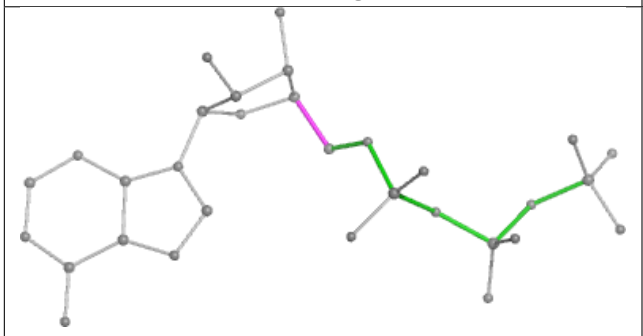
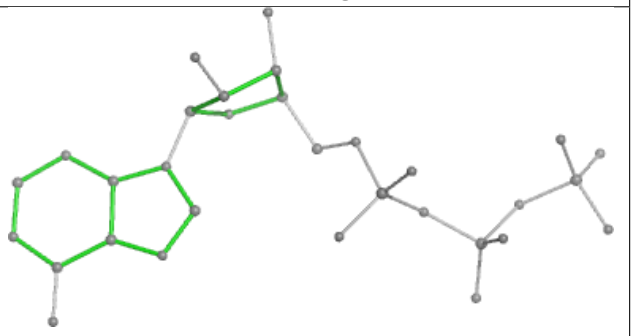
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	T	1001	ATP	1	0

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.

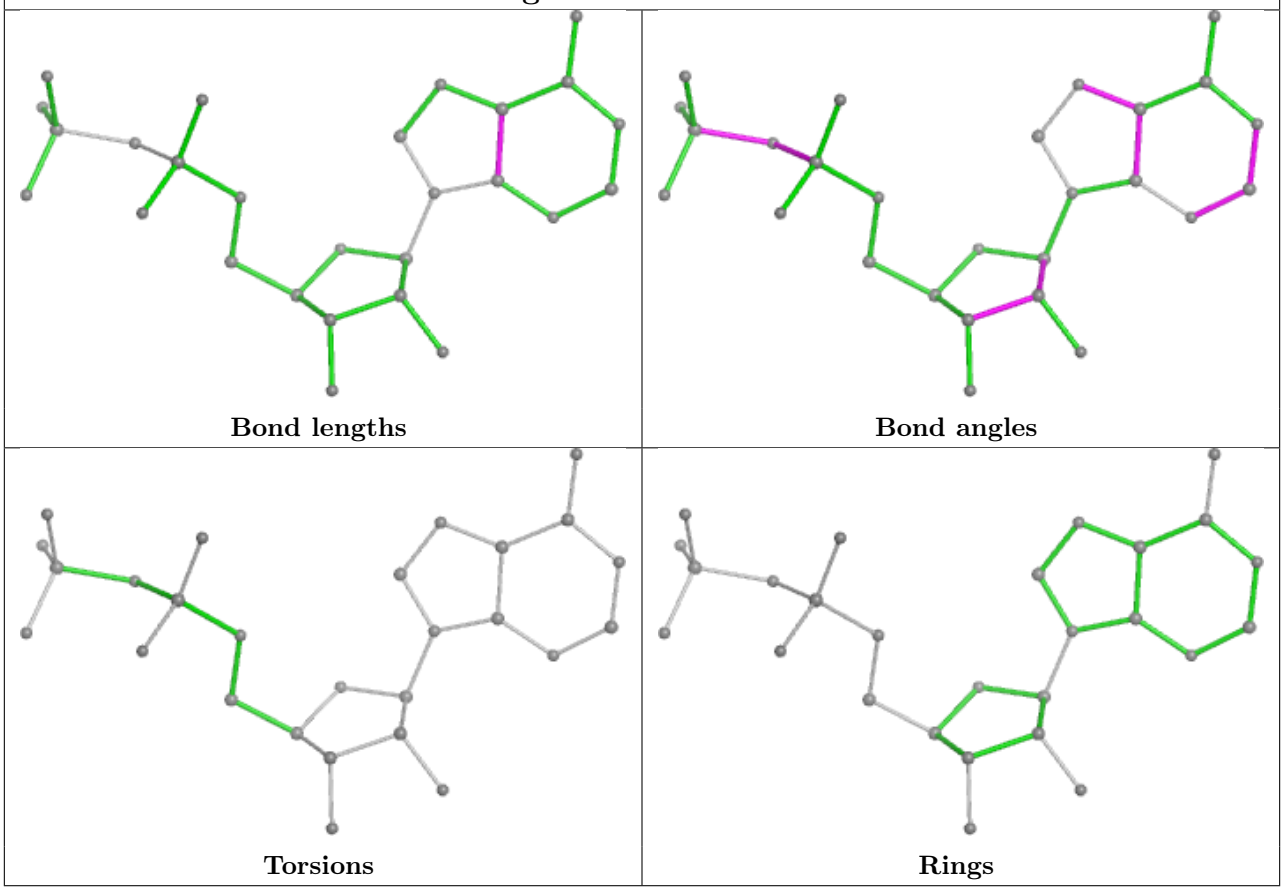
Ligand ATP U 1001



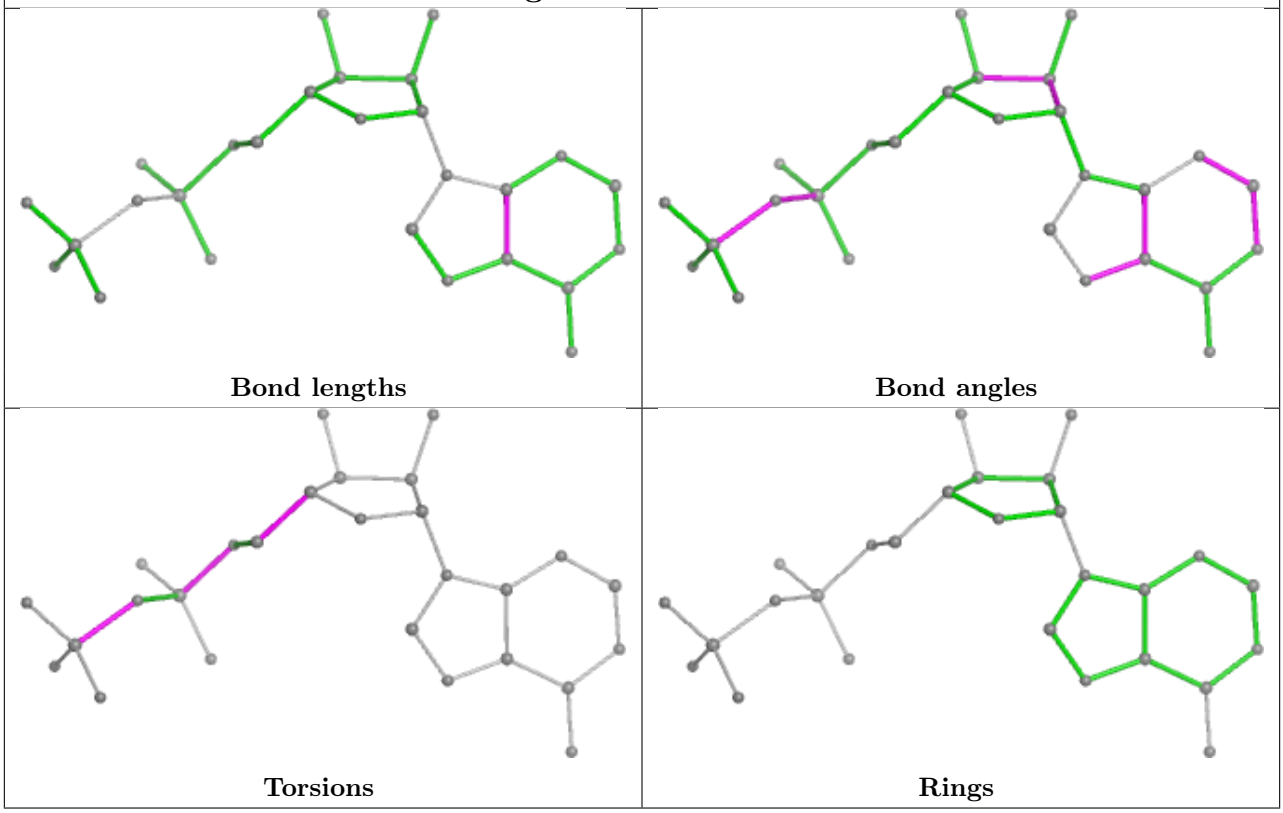
Ligand ATP T 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP V 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP X 601



Ligand ADP Z 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	4.35

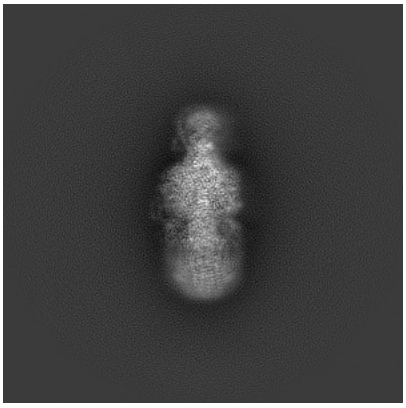
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4848. These allow visual inspection of the internal detail of the map and identification of artifacts.

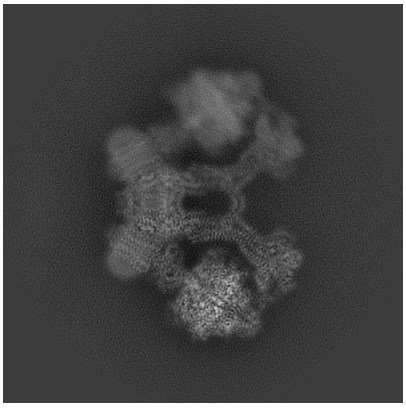
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

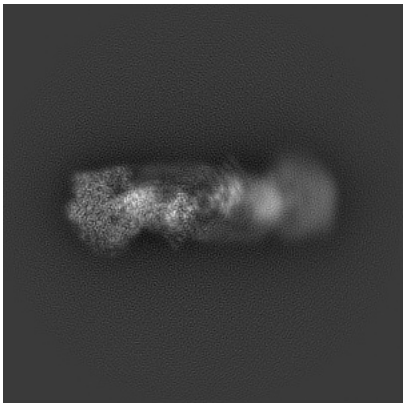
6.1.1 Primary map



X



Y

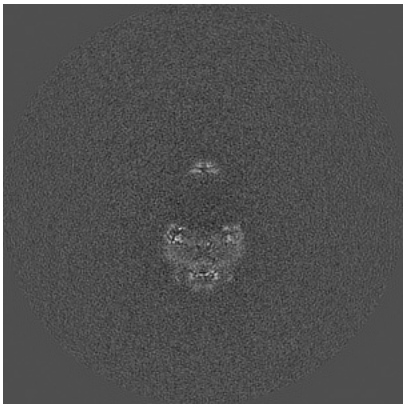


Z

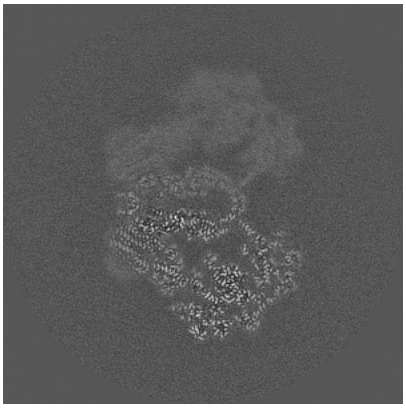
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

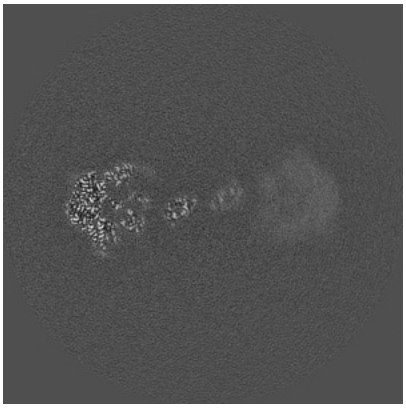
6.2.1 Primary map



X Index: 240



Y Index: 240

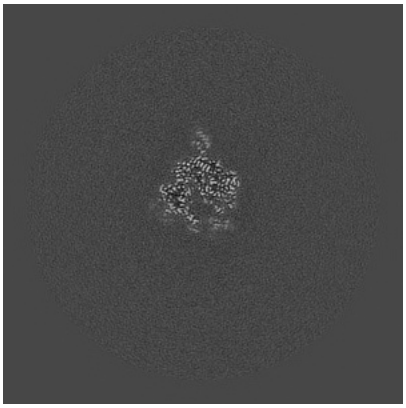


Z Index: 240

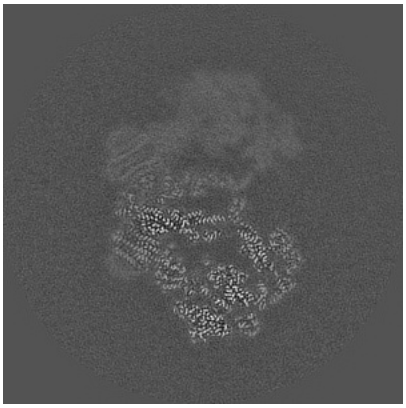
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

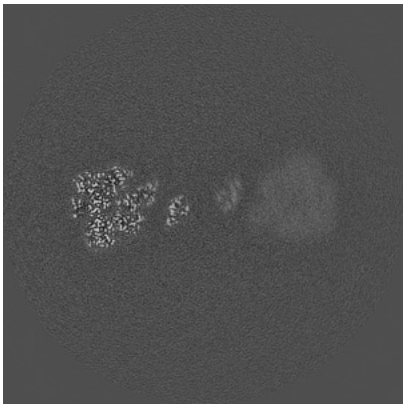
6.3.1 Primary map



X Index: 124



Y Index: 235

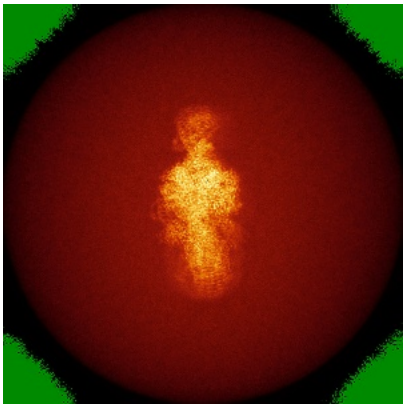


Z Index: 255

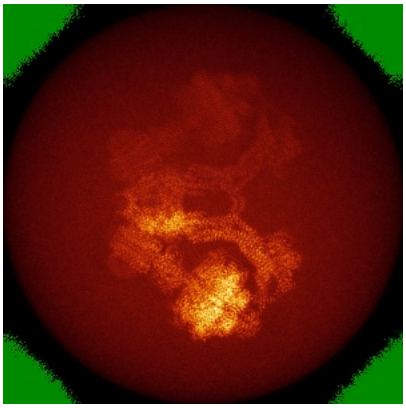
The images above show the largest variance slices of the map in three orthogonal directions.

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

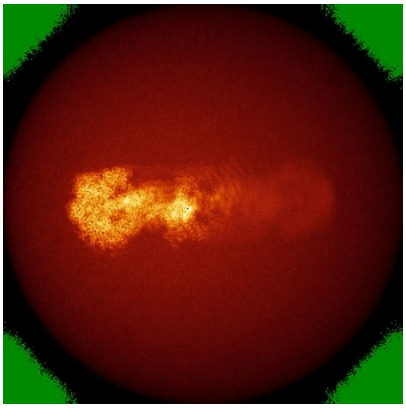
6.4.1 Primary map



X



Y

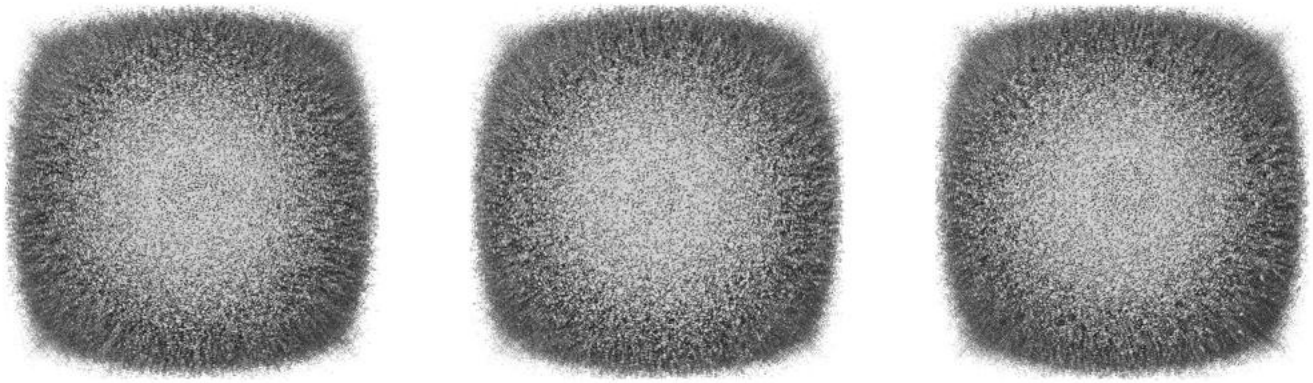


Z

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.

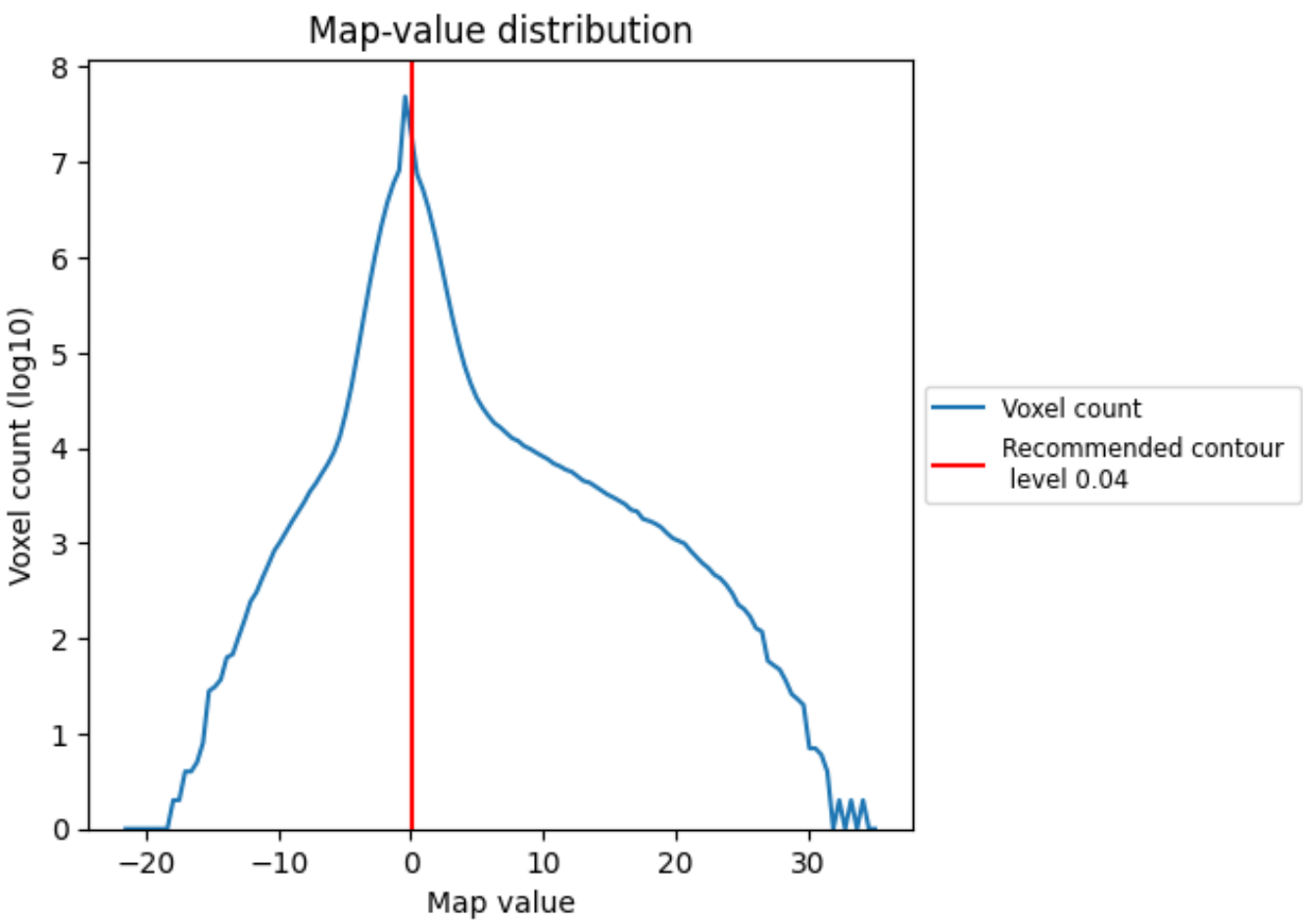
6.6 Mask visualisation (i)

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

7 Map analysis (i)

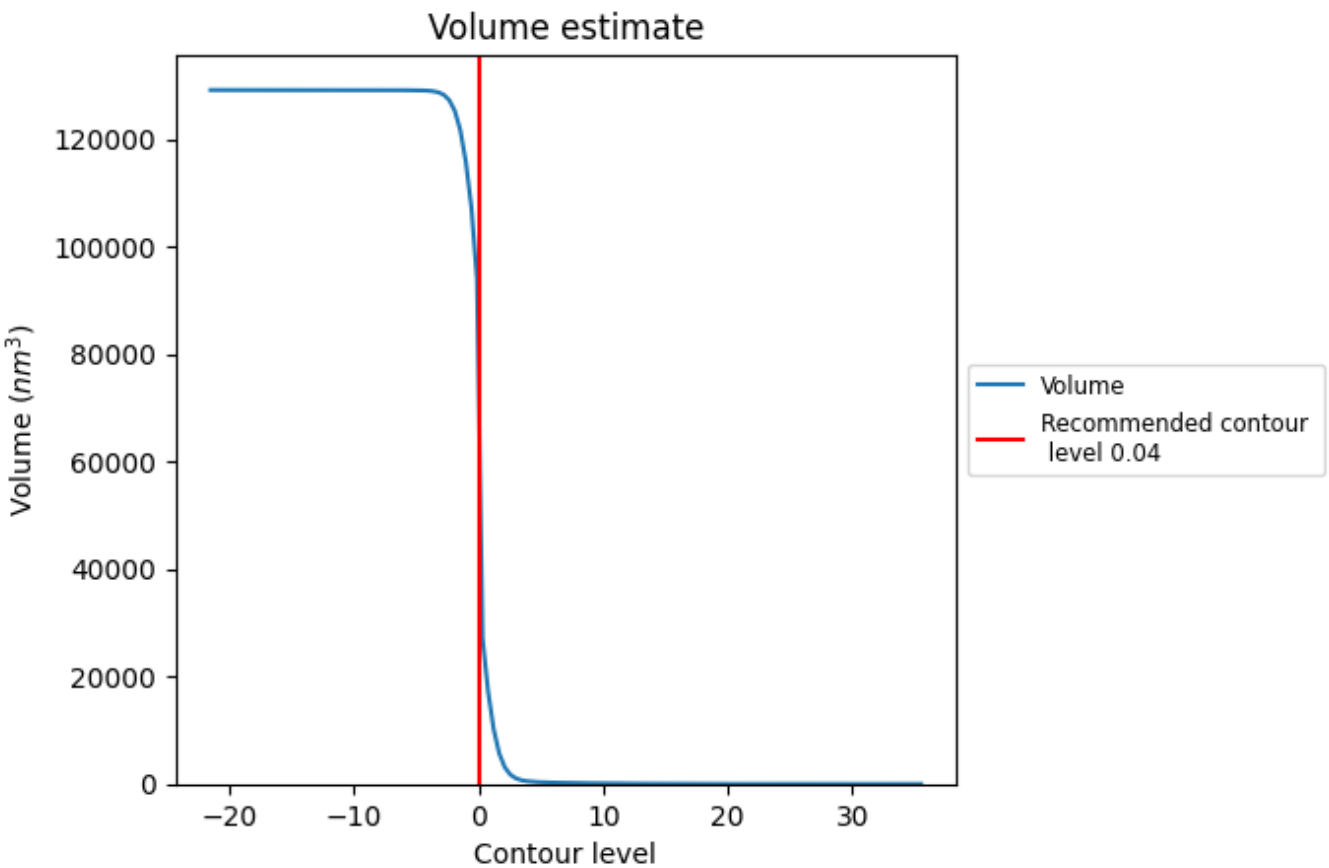
This section contains the results of statistical analysis of the map.

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.

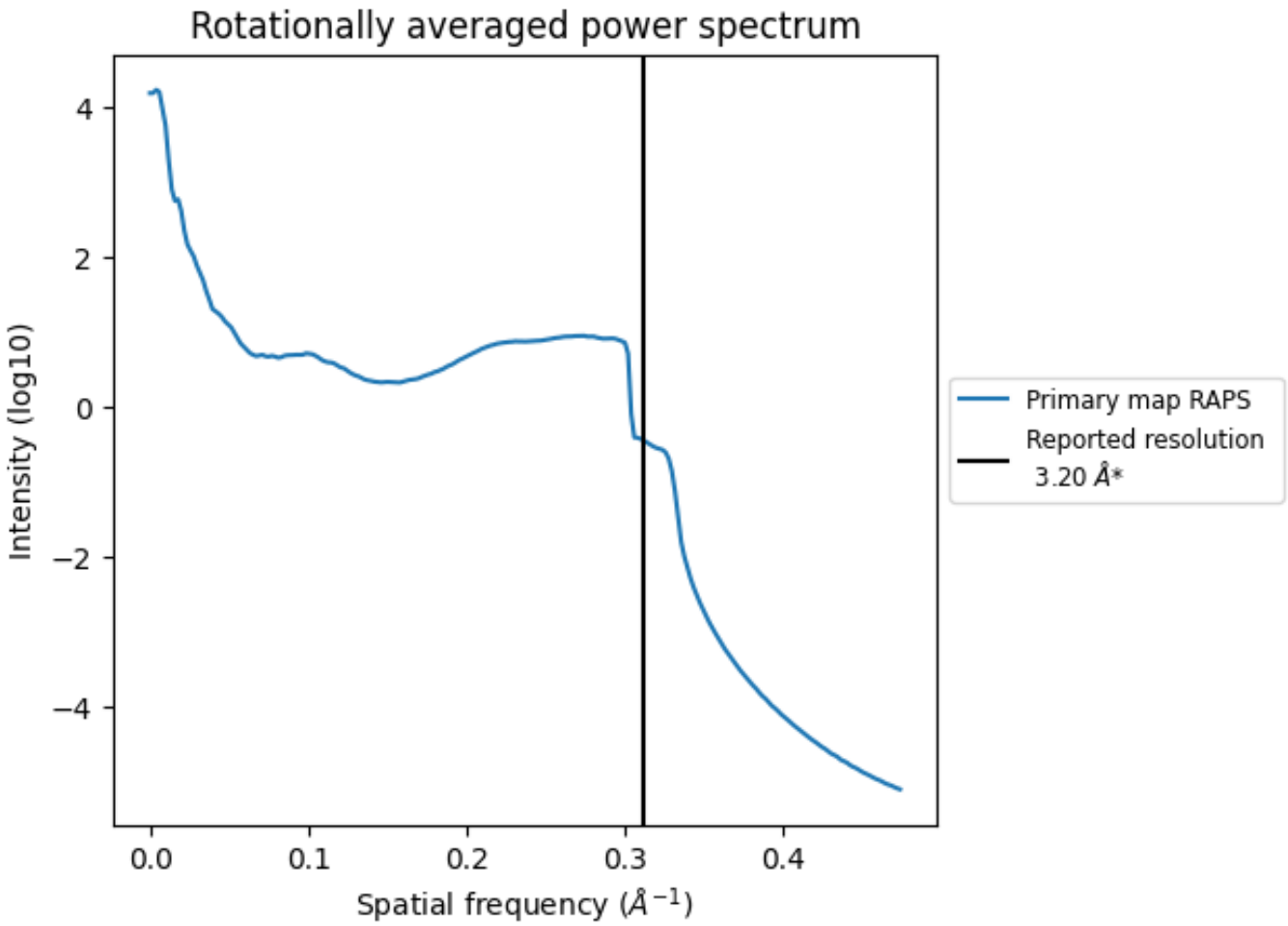
7.2 Volume estimate (i)



The volume at the recommended contour level is 67252 nm^3; this corresponds to an approximate mass of 60750 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}

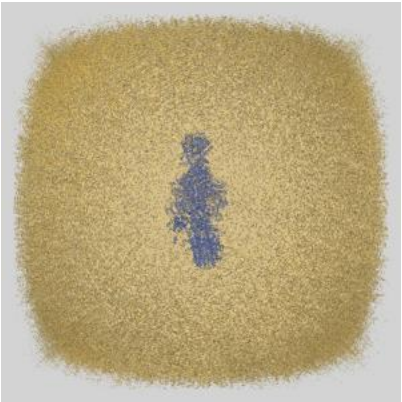
8 Fourier-Shell correlation (i)

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

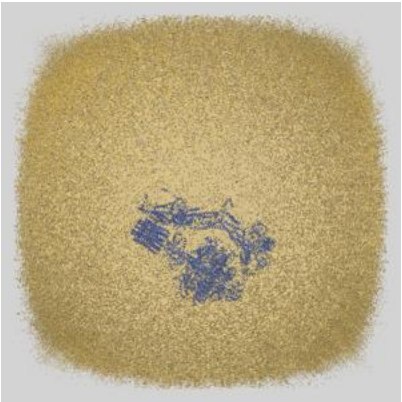
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4848 and PDB model 6REB. Per-residue inclusion information can be found in section 3 on page 10.

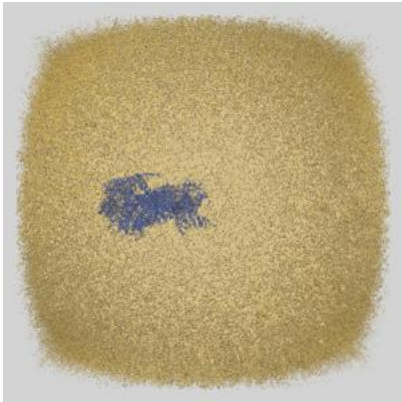
9.1 Map-model overlay (i)



X



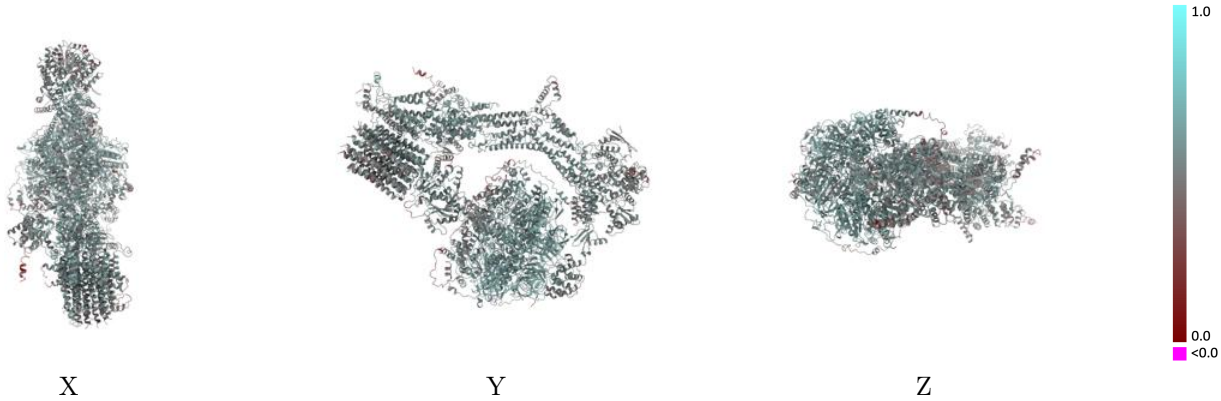
Y



Z

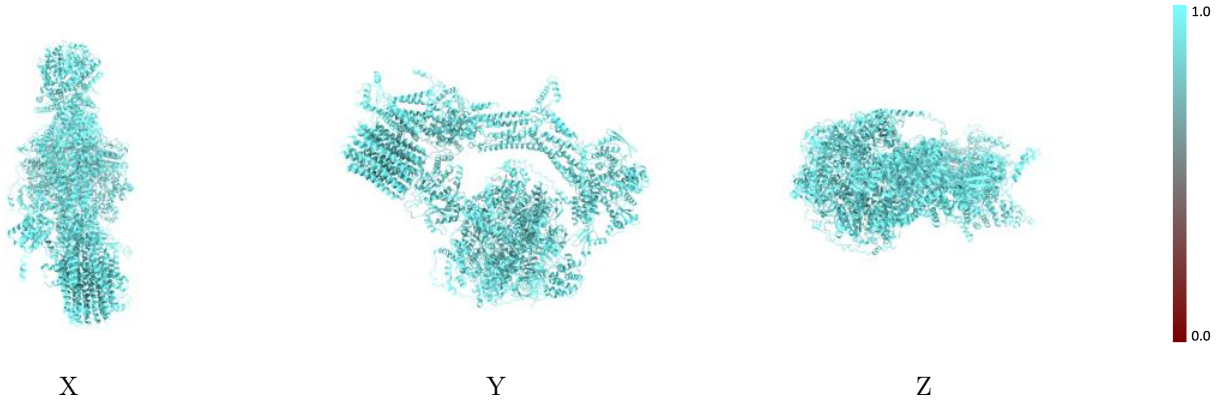
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



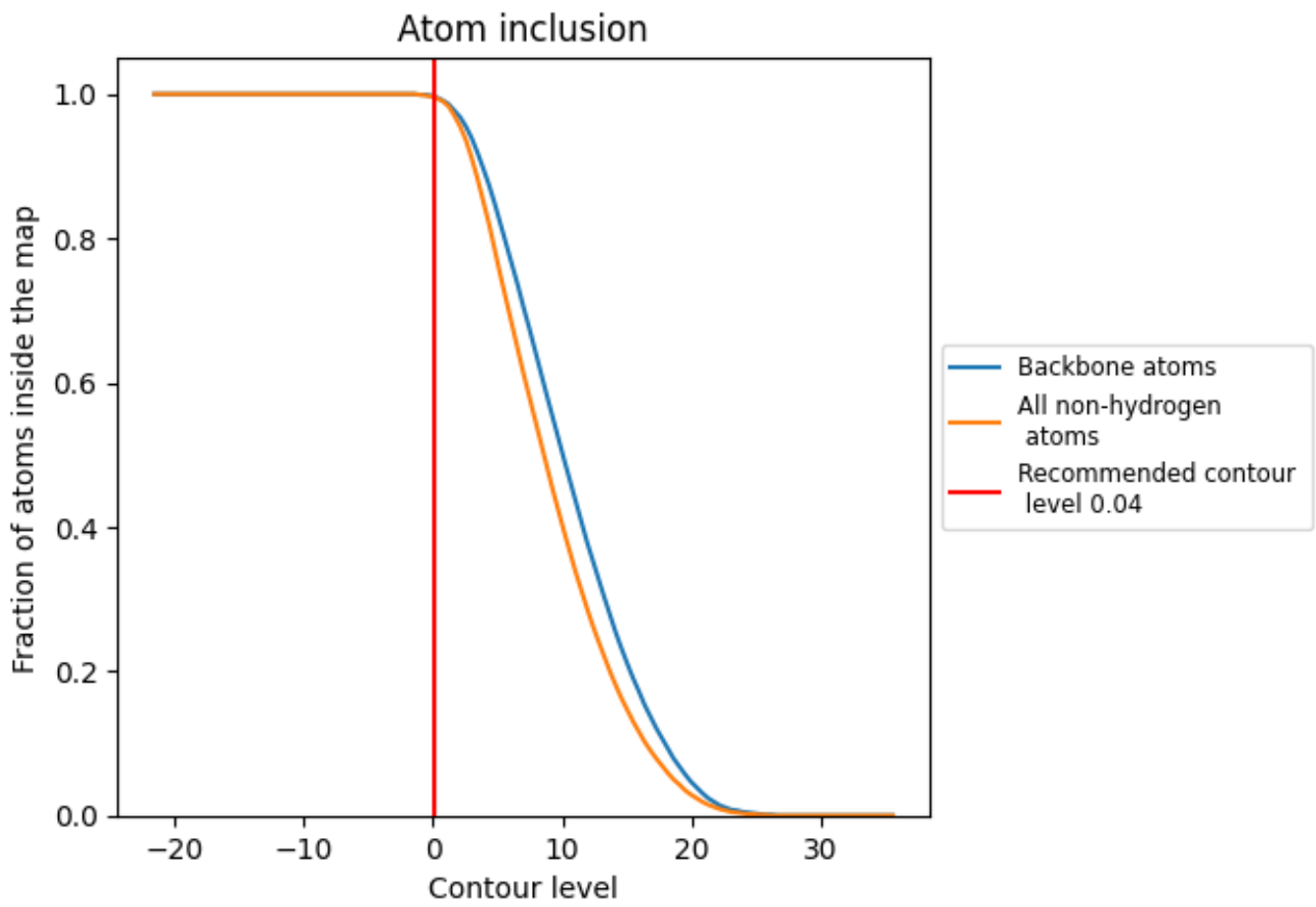
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 100% of all backbone atoms, 100% 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	0.9960	0.5410
0	0.9970	0.5340
1	0.9960	0.5400
2	0.9950	0.4940
3	0.9950	0.4990
4	0.9960	0.5130
5	0.9930	0.5630
6	0.9930	0.5470
7	0.9960	0.5390
8	0.9970	0.5580
9	0.9960	0.4800
A	0.9980	0.4840
B	0.9960	0.4920
C	0.9940	0.5200
D	0.9880	0.5360
E	0.9960	0.5430
F	0.9900	0.5320
G	0.9980	0.5010
H	0.9960	0.4950
I	1.0000	0.4770
J	0.9940	0.4750
M	0.9940	0.5400
P	0.9990	0.5220
Q	0.9960	0.5240
R	0.9920	0.5040
S	0.9970	0.5370
T	0.9940	0.5690
U	0.9980	0.5620
V	0.9990	0.5690
X	0.9980	0.5620
Y	0.9960	0.5650
Z	0.9980	0.5690