wwPDB EM Validation Summary Report (i)

Mar 10, 2024 – 06:15 PM EDT

PDB ID	:	6OQS
EMDB ID	:	EMD-20168
Title	:	E. coli ATP synthase State 1b
Authors	:	Stewart, A.G.; Sobti, M.; Walshe, J.L.
Deposited on	:	2019-04-29
Resolution	:	3.30 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:

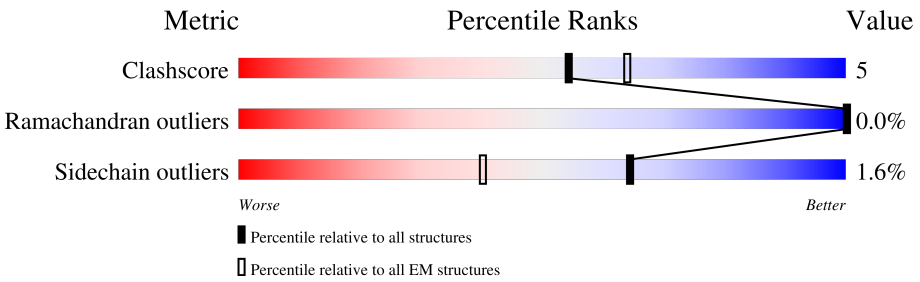
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	W	177	86% 11% •
2	A	513	87% 12% •
2	B	513	7% 85% 14%
2	C	513	89% 10%
3	X	156	31% 84% 15% •
3	Y	156	39% 79% 19% •
4	H	139	15% 86% 12% •
5	G	287	9% 91% 8% •

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Mol	Chain	Length	Quality of chain
6	D	471	86% 11%
6	E	471	86% 11%
6	F	471	88% 9%
7	I	79	62% 84% 14%
7	J	79	15% 84% 14%
7	L	79	25% 77% 20%
7	M	79	30% 86% 11%
7	N	79	52% 78% 19%
7	O	79	57% 84% 14%
7	P	79	65% 78% 19%
7	Q	79	44% 84% 14%
7	R	79	37% 84% 13%
7	S	79	48% 71% 27%
8	a	271	47% 96%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 36971 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	W	173	1320	827	233	254	6	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	64	ALA	CYS	conflict	UNP V0ZA15
W	140	ALA	CYS	conflict	UNP V0ZA15

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	512	3869	2433	682	745	9	0	0
2	B	513	3871	2432	683	746	10	0	0
2	A	508	3832	2408	676	739	9	0	0

- Molecule 3 is a protein called ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	X	156	1210	757	218	232	3	0	0
3	Y	156	1210	757	218	232	3	0	0

- Molecule 4 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	136	1034	649	180	201	4	0	0

- Molecule 5 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	284	2186	1373	382	419	12	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	87	ALA	CYS	conflict	UNP J7RYJ3
G	112	ALA	CYS	conflict	UNP J7RYJ3

- Molecule 6 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	458	3520	2219	602	685	14	0	0
6	E	460	3533	2227	604	687	15	0	0
6	D	460	3533	2227	604	687	15	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	MET	-	initiating methionine	UNP A0A0F6CB56
F	-10	ARG	-	expression tag	UNP A0A0F6CB56
F	-9	GLY	-	expression tag	UNP A0A0F6CB56
F	-8	SER	-	expression tag	UNP A0A0F6CB56
F	-7	HIS	-	expression tag	UNP A0A0F6CB56
F	-6	HIS	-	expression tag	UNP A0A0F6CB56
F	-5	HIS	-	expression tag	UNP A0A0F6CB56
F	-4	HIS	-	expression tag	UNP A0A0F6CB56
F	-3	HIS	-	expression tag	UNP A0A0F6CB56
F	-2	HIS	-	expression tag	UNP A0A0F6CB56
F	-1	GLY	-	expression tag	UNP A0A0F6CB56
F	137	ALA	CYS	conflict	UNP A0A0F6CB56
E	-11	MET	-	initiating methionine	UNP A0A0F6CB56
E	-10	ARG	-	expression tag	UNP A0A0F6CB56
E	-9	GLY	-	expression tag	UNP A0A0F6CB56
E	-8	SER	-	expression tag	UNP A0A0F6CB56
E	-7	HIS	-	expression tag	UNP A0A0F6CB56
E	-6	HIS	-	expression tag	UNP A0A0F6CB56
E	-5	HIS	-	expression tag	UNP A0A0F6CB56

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP A0A0F6CB56
E	-3	HIS	-	expression tag	UNP A0A0F6CB56
E	-2	HIS	-	expression tag	UNP A0A0F6CB56
E	-1	GLY	-	expression tag	UNP A0A0F6CB56
E	137	ALA	CYS	conflict	UNP A0A0F6CB56
D	-11	MET	-	initiating methionine	UNP A0A0F6CB56
D	-10	ARG	-	expression tag	UNP A0A0F6CB56
D	-9	GLY	-	expression tag	UNP A0A0F6CB56
D	-8	SER	-	expression tag	UNP A0A0F6CB56
D	-7	HIS	-	expression tag	UNP A0A0F6CB56
D	-6	HIS	-	expression tag	UNP A0A0F6CB56
D	-5	HIS	-	expression tag	UNP A0A0F6CB56
D	-4	HIS	-	expression tag	UNP A0A0F6CB56
D	-3	HIS	-	expression tag	UNP A0A0F6CB56
D	-2	HIS	-	expression tag	UNP A0A0F6CB56
D	-1	GLY	-	expression tag	UNP A0A0F6CB56
D	137	ALA	CYS	conflict	UNP A0A0F6CB56

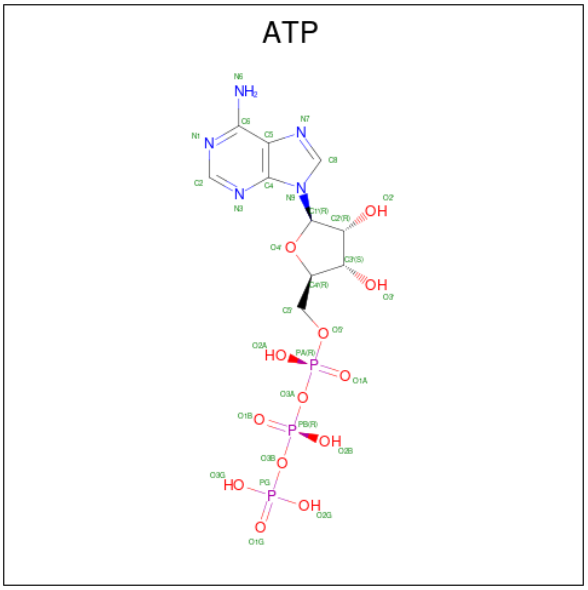
- Molecule 7 is a protein called ATP synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	77	557	370	88	92	7	0	0
7	J	77	557	370	88	92	7	0	0
7	L	77	557	370	88	92	7	0	0
7	M	77	557	370	88	92	7	0	0
7	N	77	557	370	88	92	7	0	0
7	O	77	557	370	88	92	7	0	0
7	P	77	557	370	88	92	7	0	0
7	Q	77	557	370	88	92	7	0	0
7	R	76	552	367	87	91	7	0	0
7	S	77	557	370	88	92	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	a	266	2104	1419	326	349	10	0	0

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

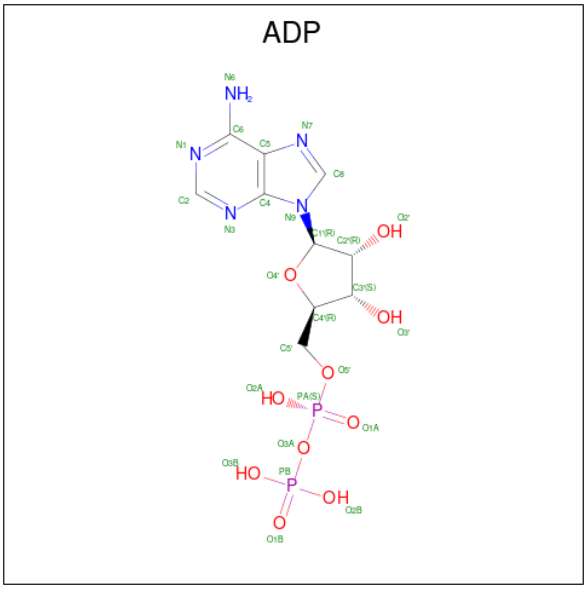


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	C	1	31	10	5	13	3	0
			Total	C	N	O	P	
9	B	1	31	10	5	13	3	0
			Total	C	N	O	P	
9	A	1	31	10	5	13	3	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

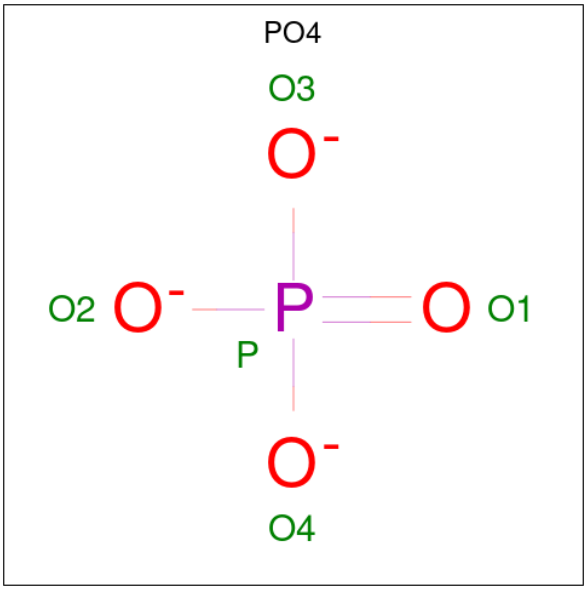
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
10	C	1	1	1	0
			Total	Mg	
10	B	1	1	1	0
			Total	Mg	
10	A	1	1	1	0
			Total	Mg	
10	F	1	1	1	0
			Total	Mg	
10	D	1	1	1	0

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 12 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



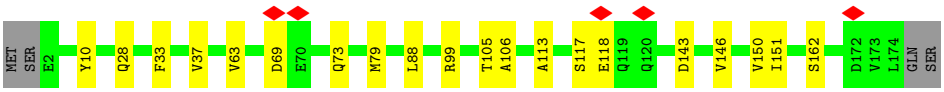
Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
12	D	1	5	4	1	0

3 Residue-property plots (i)

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

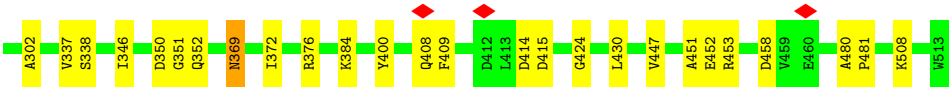
• Molecule 1: ATP synthase subunit delta

Chain W:



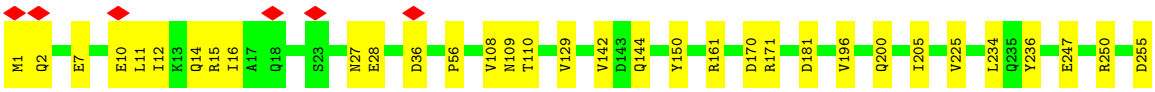
• Molecule 2: ATP synthase subunit alpha

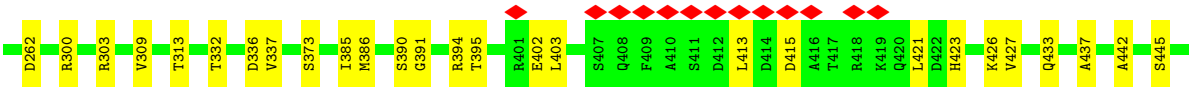
Chain C:

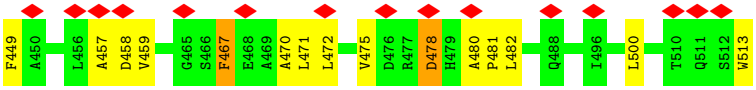


• Molecule 2: ATP synthase subunit alpha

Chain B:

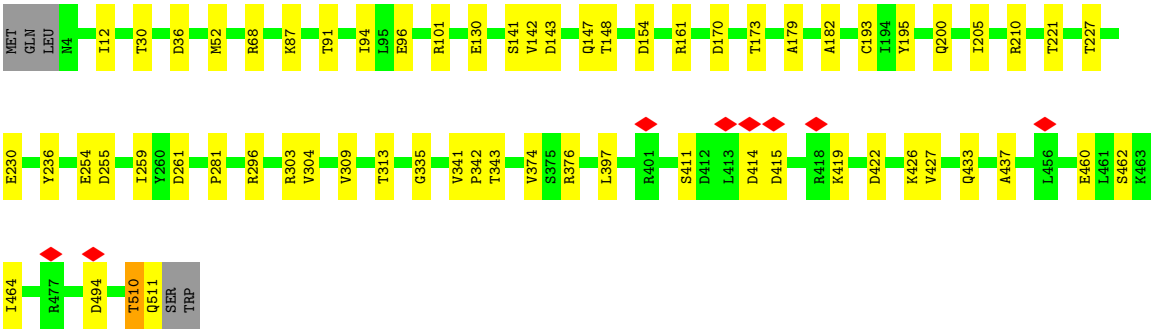






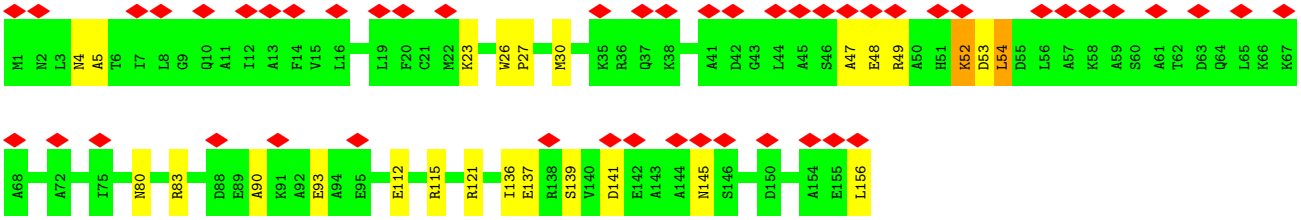
• Molecule 2: ATP synthase subunit alpha

Chain A:



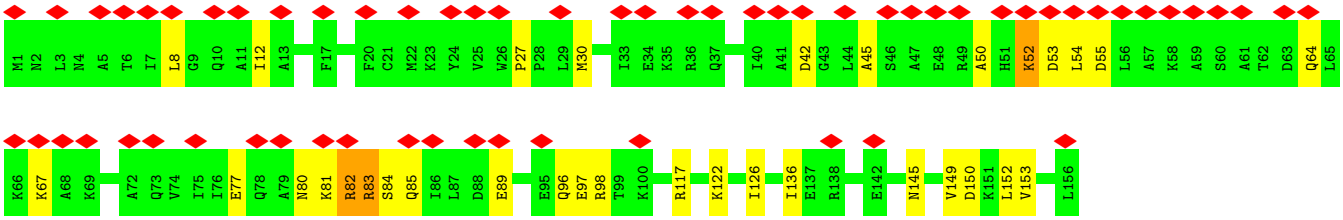
- Molecule 3: ATP synthase subunit b

Chain X:



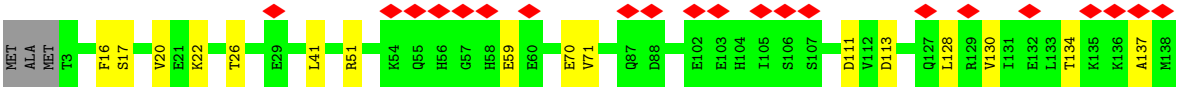
- Molecule 3: ATP synthase subunit b

Chain Y:



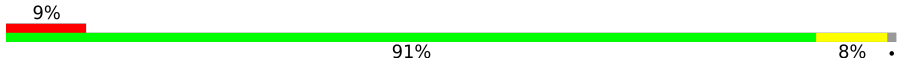
- Molecule 4: ATP synthase epsilon chain

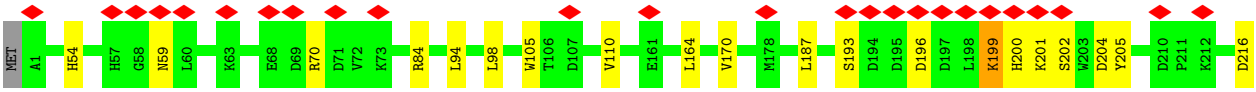
Chain H:

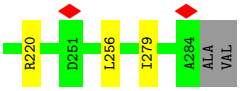


- Molecule 5: ATP synthase gamma chain

Chain G:

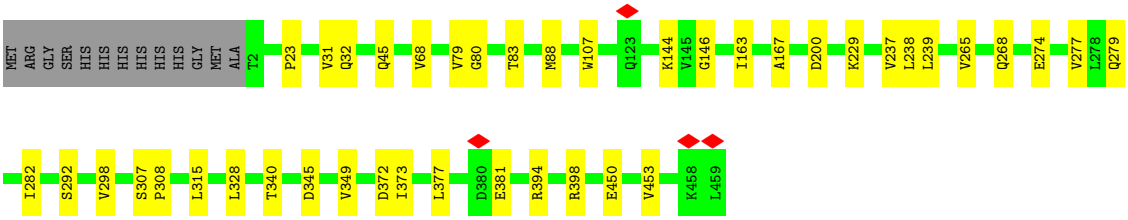






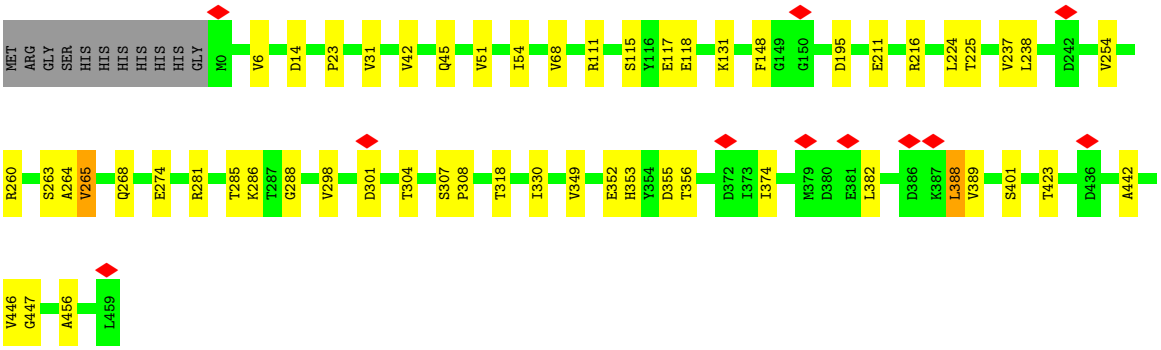
• Molecule 6: ATP synthase subunit beta

Chain F:



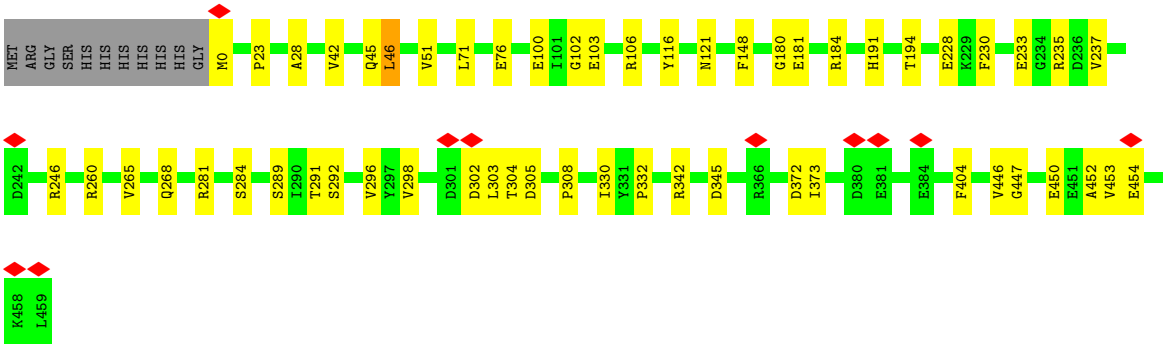
• Molecule 6: ATP synthase subunit beta

Chain E:



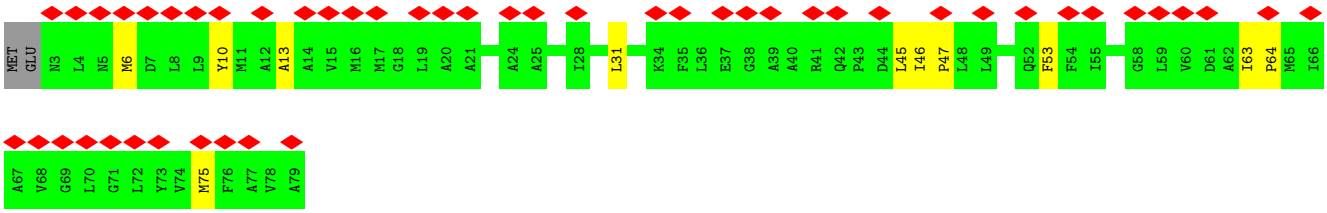
• Molecule 6: ATP synthase subunit beta

Chain D:



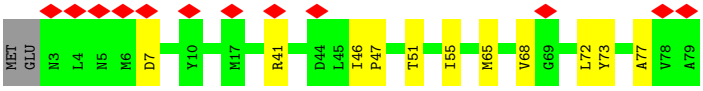
• Molecule 7: ATP synthase subunit c

Chain I:



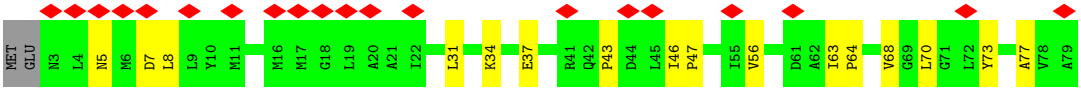
- Molecule 7: ATP synthase subunit c

Chain J:



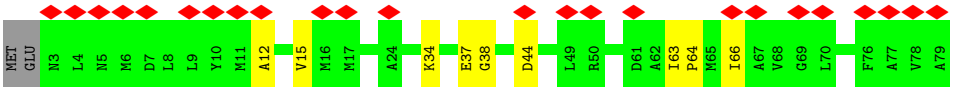
- Molecule 7: ATP synthase subunit c

Chain L:



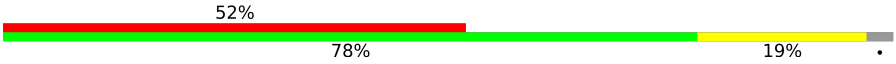
- Molecule 7: ATP synthase subunit c

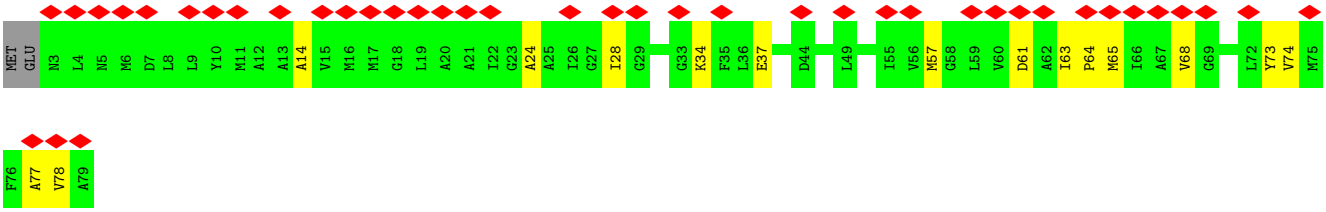
Chain M:



- Molecule 7: ATP synthase subunit c

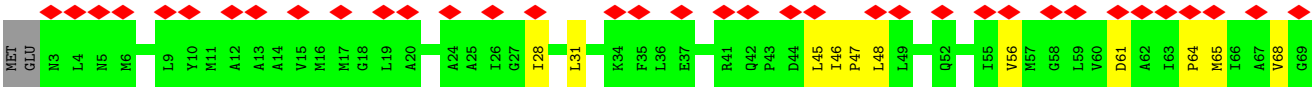
Chain N:

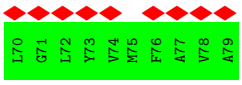




- Molecule 7: ATP synthase subunit c

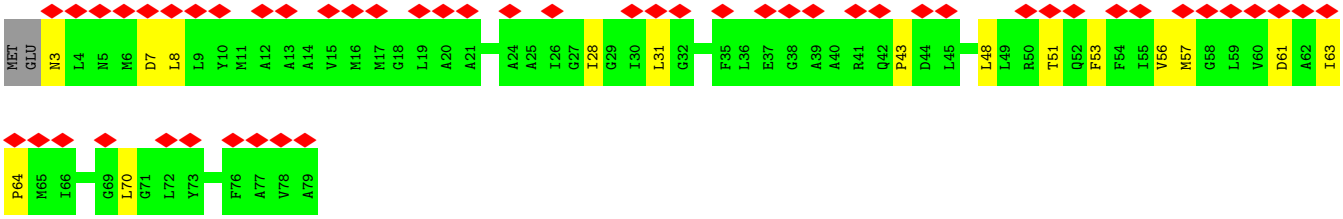
Chain O:





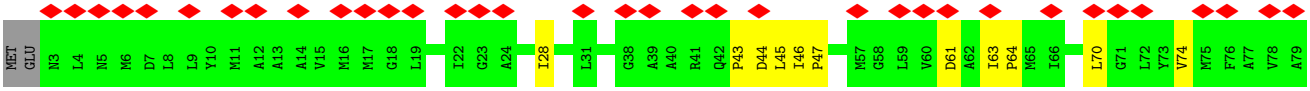
• Molecule 7: ATP synthase subunit c

Chain P:



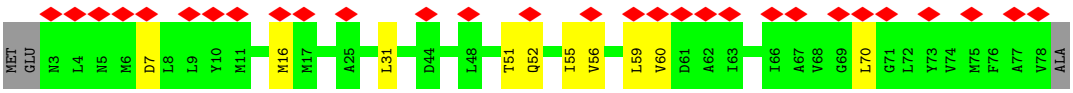
• Molecule 7: ATP synthase subunit c

Chain Q:



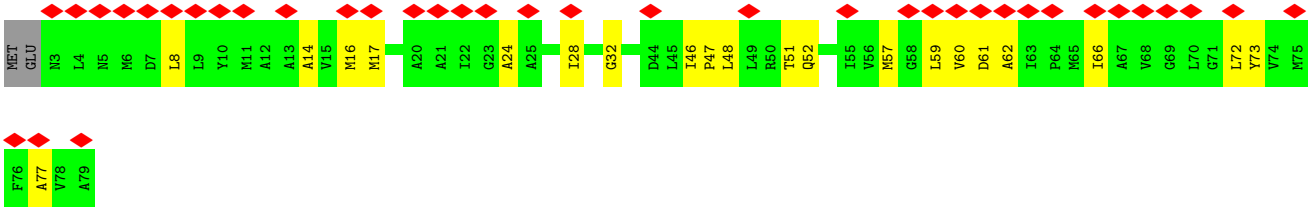
• Molecule 7: ATP synthase subunit c

Chain R:



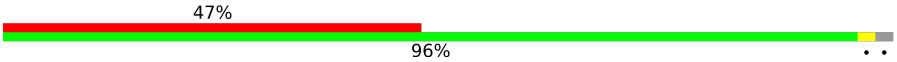
• Molecule 7: ATP synthase subunit c

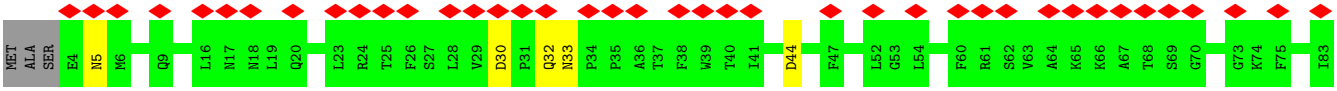
Chain S:

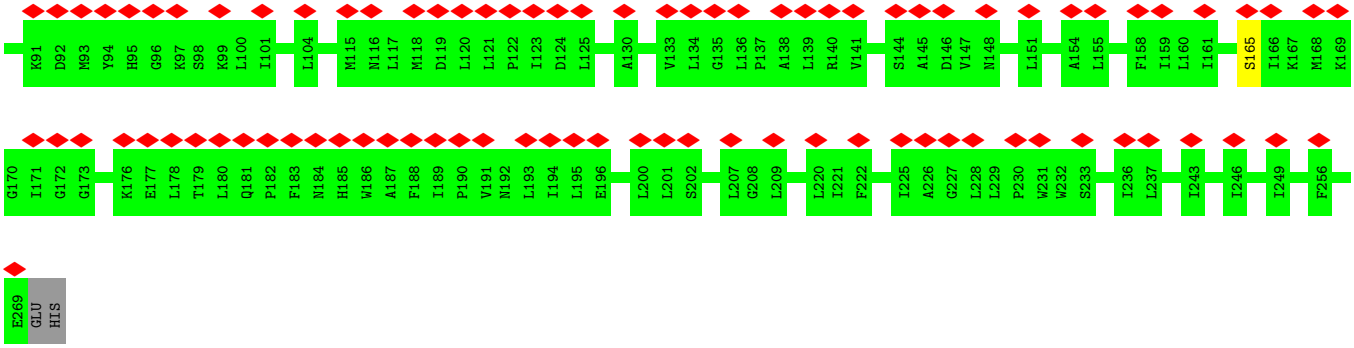


• Molecule 8: ATP synthase subunit a

Chain a:






K91
D92
M93
Y94
H95
G96
K97
S98
K99
L100
I101
L104
M115
N116
L117
M118
D119
L120
L121
P122
I123
D124
L125
A130
V133
L134
G135
L136
P137
A138
L139
R140
V141
S144
A145
D146
V147
N148
L151
A154
L155
F158
I159
L160
I161
S165
I166
K167
M168
K169
G170
I171
G172
G173
K176
E177
L178
T179
L180
Q181
P182
F183
N184
H185
W186
A187
F188
I189
P190
V191
N192
L193
I194
L195
E196
L200
L201
S202
I207
G208
L209
I220
I221
F222
T225
A226
G227
L228
L229
P230
W231
W232
S233
T236
L237
I243
I246
I249
F256

E269
GLU
HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35243	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 ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.087	Depositor
Minimum map value	-0.033	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0178	Depositor
Map size (Å)	377.65, 377.65, 377.65	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.079, 1.079, 1.079	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, PO4, 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	W	0.33	0/1333	0.48	0/1798
2	A	0.39	0/3886	0.48	0/5257
2	B	0.43	0/3926	0.51	0/5312
2	C	0.43	0/3925	0.52	0/5311
3	X	0.32	0/1218	0.48	0/1634
3	Y	0.34	0/1218	0.49	0/1634
4	H	0.37	0/1049	0.52	0/1415
5	G	0.39	0/2217	0.50	0/2990
6	D	0.41	0/3590	0.50	0/4858
6	E	0.42	0/3590	0.52	0/4858
6	F	0.45	0/3577	0.53	0/4841
7	I	0.32	0/565	0.49	0/764
7	J	0.34	0/565	0.51	0/764
7	L	0.31	0/565	0.50	0/764
7	M	0.35	0/565	0.52	0/764
7	N	0.30	0/565	0.46	0/764
7	O	0.30	0/565	0.48	0/764
7	P	0.30	0/565	0.48	0/764
7	Q	0.32	0/565	0.50	0/764
7	R	0.32	0/560	0.47	0/757
7	S	0.32	0/565	0.51	0/764
8	a	0.34	0/2164	0.49	0/2955
All	All	0.39	0/37338	0.51	0/50496

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	W	1320	0	1345	13	0
2	A	3832	0	3876	37	0
2	B	3871	0	3915	42	0
2	C	3869	0	3910	29	0
3	X	1210	0	1264	16	0
3	Y	1210	0	1264	19	0
4	H	1034	0	1041	13	0
5	G	2186	0	2238	16	0
6	D	3533	0	3547	38	0
6	E	3533	0	3548	37	0
6	F	3520	0	3530	26	0
7	I	557	0	598	9	0
7	J	557	0	598	8	0
7	L	557	0	598	12	0
7	M	557	0	598	7	0
7	N	557	0	598	11	0
7	O	557	0	598	11	0
7	P	557	0	598	11	0
7	Q	557	0	598	11	0
7	R	552	0	593	16	0
7	S	557	0	598	24	0
8	a	2104	0	2196	0	0
9	A	31	0	12	1	0
9	B	31	0	12	0	0
9	C	31	0	12	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
10	F	1	0	0	0	0
11	D	27	0	12	1	0
11	E	27	0	12	0	0
11	F	27	0	12	0	0
12	D	5	0	0	0	0
All	All	36971	0	37721	356	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 356 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)
7:Q:28:ILE:HD11	7:Q:61:ASP:OD2	1.70	0.91
3:X:47:ALA:HB2	3:Y:50:ALA:HB1	1.55	0.87
7:Q:63:ILE:HG23	7:Q:64:PRO:HD3	1.58	0.84
7:N:57:MET:SD	7:N:61:ASP:OD2	2.36	0.83
7:R:60:VAL:HG22	7:S:28:ILE:HG23	1.62	0.82

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	W	171/177 (97%)	167 (98%)	4 (2%)	0	100	100
2	A	506/513 (99%)	493 (97%)	13 (3%)	0	100	100
2	B	511/513 (100%)	497 (97%)	14 (3%)	0	100	100
2	C	510/513 (99%)	498 (98%)	12 (2%)	0	100	100
3	X	154/156 (99%)	152 (99%)	2 (1%)	0	100	100
3	Y	154/156 (99%)	154 (100%)	0	0	100	100
4	H	134/139 (96%)	132 (98%)	2 (2%)	0	100	100
5	G	282/287 (98%)	278 (99%)	4 (1%)	0	100	100
6	D	458/471 (97%)	438 (96%)	20 (4%)	0	100	100
6	E	458/471 (97%)	440 (96%)	17 (4%)	1 (0%)	47	77
6	F	456/471 (97%)	443 (97%)	13 (3%)	0	100	100
7	I	75/79 (95%)	75 (100%)	0	0	100	100
7	J	75/79 (95%)	73 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	L	75/79 (95%)	74 (99%)	1 (1%)	0	100	100
7	M	75/79 (95%)	74 (99%)	1 (1%)	0	100	100
7	N	75/79 (95%)	74 (99%)	1 (1%)	0	100	100
7	O	75/79 (95%)	74 (99%)	1 (1%)	0	100	100
7	P	75/79 (95%)	73 (97%)	2 (3%)	0	100	100
7	Q	75/79 (95%)	73 (97%)	2 (3%)	0	100	100
7	R	74/79 (94%)	72 (97%)	2 (3%)	0	100	100
7	S	75/79 (95%)	74 (99%)	1 (1%)	0	100	100
8	a	264/271 (97%)	257 (97%)	7 (3%)	0	100	100
All	All	4807/4928 (98%)	4685 (98%)	121 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	E	265	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	W	136/140 (97%)	136 (100%)	0	100	100
2	A	398/407 (98%)	393 (99%)	5 (1%)	69	82
2	B	402/407 (99%)	392 (98%)	10 (2%)	47	72
2	C	402/407 (99%)	393 (98%)	9 (2%)	52	74
3	X	121/122 (99%)	116 (96%)	5 (4%)	30	61
3	Y	121/122 (99%)	112 (93%)	9 (7%)	13	40
4	H	108/110 (98%)	108 (100%)	0	100	100
5	G	236/238 (99%)	232 (98%)	4 (2%)	60	78
6	D	380/389 (98%)	376 (99%)	4 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	E	380/389 (98%)	377 (99%)	3 (1%)	81	89
6	F	379/389 (97%)	374 (99%)	5 (1%)	69	82
7	I	54/56 (96%)	54 (100%)	0	100	100
7	J	54/56 (96%)	54 (100%)	0	100	100
7	L	54/56 (96%)	54 (100%)	0	100	100
7	M	54/56 (96%)	54 (100%)	0	100	100
7	N	54/56 (96%)	54 (100%)	0	100	100
7	O	54/56 (96%)	54 (100%)	0	100	100
7	P	54/56 (96%)	54 (100%)	0	100	100
7	Q	54/56 (96%)	54 (100%)	0	100	100
7	R	54/56 (96%)	54 (100%)	0	100	100
7	S	54/56 (96%)	54 (100%)	0	100	100
8	a	233/237 (98%)	227 (97%)	6 (3%)	46	71
All	All	3836/3917 (98%)	3776 (98%)	60 (2%)	64	79

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	X	139	SER
8	a	30	ASP
6	F	68	VAL
8	a	5	ASN
8	a	165	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	353	HIS
8	a	32	GLN
7	L	5	ASN
8	a	245	HIS
3	Y	80	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
9	ATP	B	600	10	26,33,33	0.93	1 (3%)	31,52,52	1.72	5 (16%)
12	PO4	D	501	10	4,4,4	1.16	0	6,6,6	0.43	0
11	ADP	D	500	10	24,29,29	0.97	1 (4%)	29,45,45	1.54	4 (13%)
9	ATP	A	600	10	26,33,33	0.93	1 (3%)	31,52,52	1.74	5 (16%)
9	ATP	C	600	10	26,33,33	0.93	1 (3%)	31,52,52	1.72	5 (16%)
11	ADP	E	500	-	24,29,29	0.96	1 (4%)	29,45,45	1.51	4 (13%)
11	ADP	F	500	10	24,29,29	0.88	0	29,45,45	1.14	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
9	ATP	B	600	10	-	0/18/38/38	0/3/3/3
11	ADP	D	500	10	-	1/12/32/32	0/3/3/3
9	ATP	A	600	10	-	2/18/38/38	0/3/3/3
9	ATP	C	600	10	-	0/18/38/38	0/3/3/3
11	ADP	E	500	-	-	4/12/32/32	0/3/3/3
11	ADP	F	500	10	-	4/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E	500	ADP	C5-C4	2.31	1.47	1.40
11	D	500	ADP	C5-C4	2.27	1.46	1.40
9	A	600	ATP	C5-C4	2.18	1.46	1.40
9	B	600	ATP	C5-C4	2.12	1.46	1.40
9	C	600	ATP	C5-C4	2.08	1.46	1.40

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	600	ATP	PB-O3B-PG	-4.85	116.20	132.83
9	C	600	ATP	PA-O3A-PB	-4.71	116.65	132.83
9	A	600	ATP	PA-O3A-PB	-4.69	116.74	132.83
9	A	600	ATP	PB-O3B-PG	-4.29	118.09	132.83
9	C	600	ATP	PB-O3B-PG	-4.20	118.42	132.83

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	F	500	ADP	C5'-O5'-PA-O3A
11	E	500	ADP	C5'-O5'-PA-O1A
11	E	500	ADP	O4'-C4'-C5'-O5'
11	E	500	ADP	C3'-C4'-C5'-O5'
9	A	600	ATP	PA-O3A-PB-O1B

There are no ring outliers.

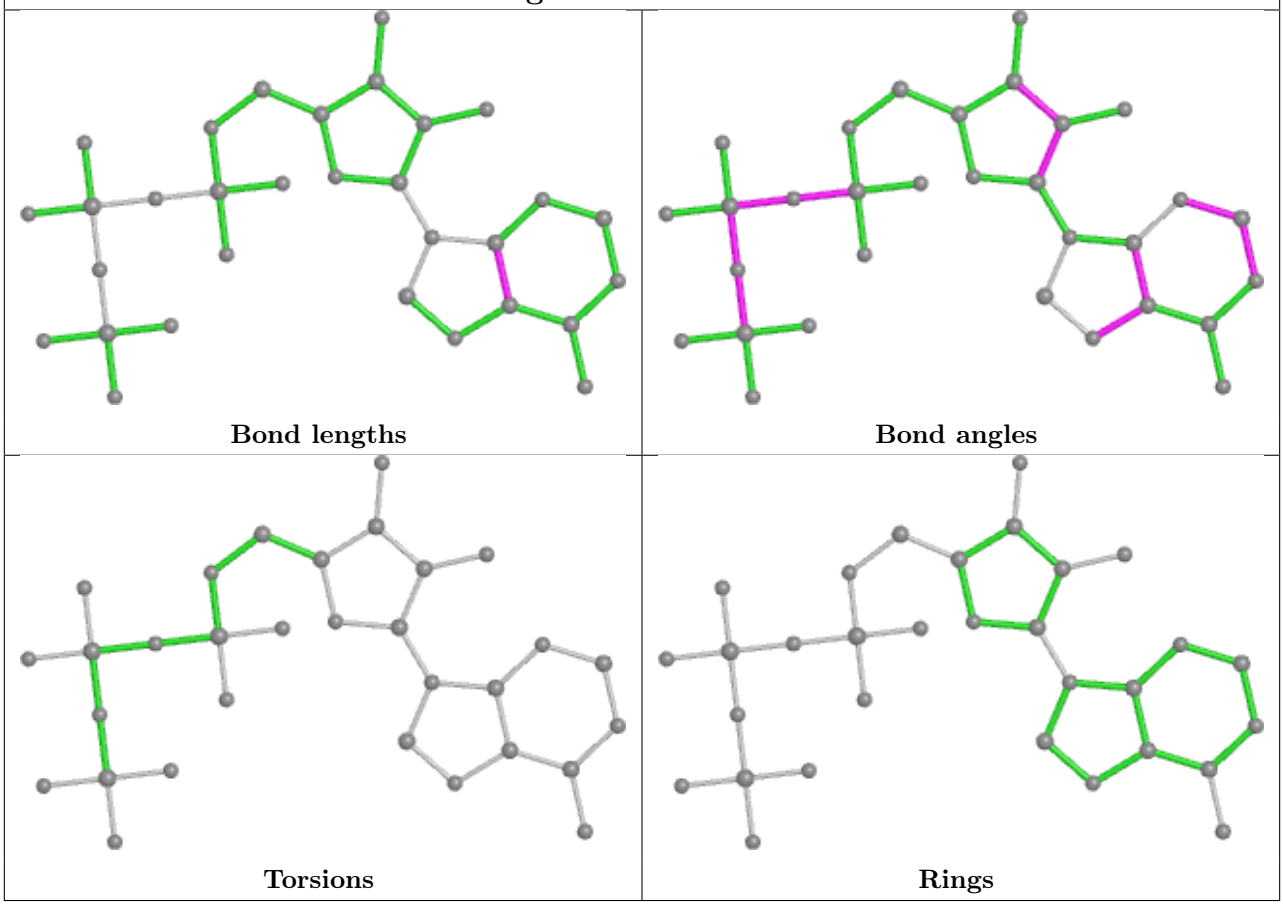
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	500	ADP	1	0
9	A	600	ATP	1	0

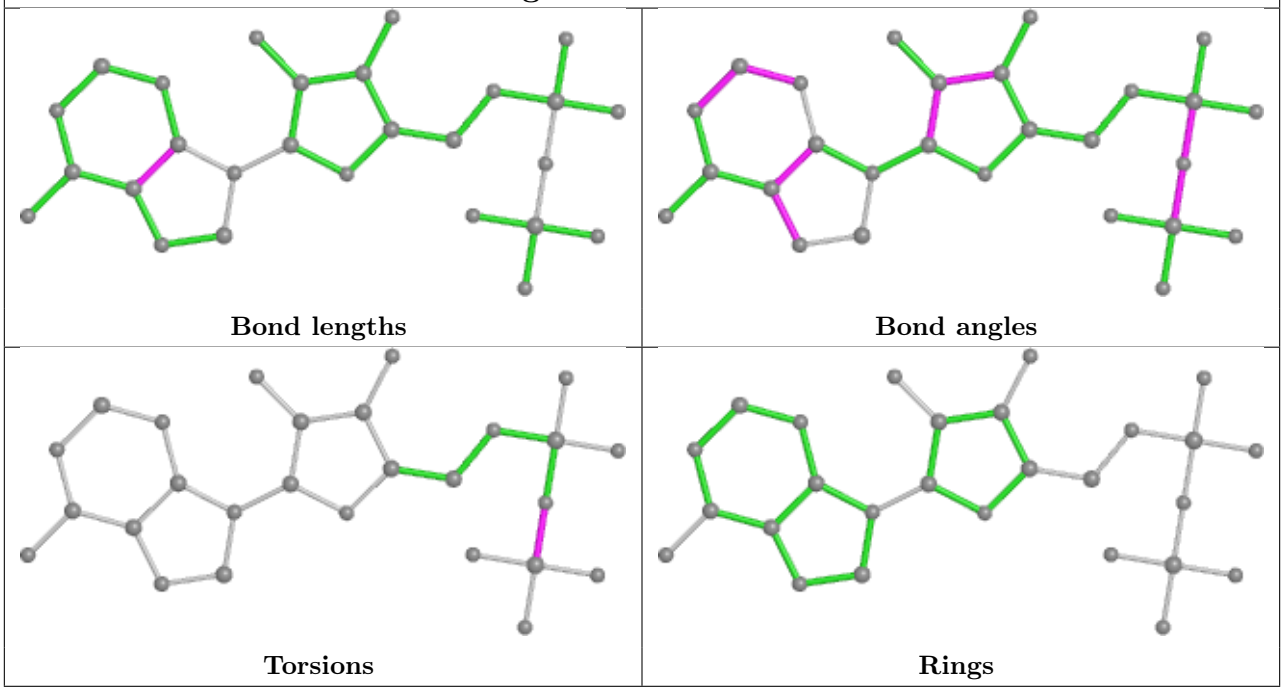
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

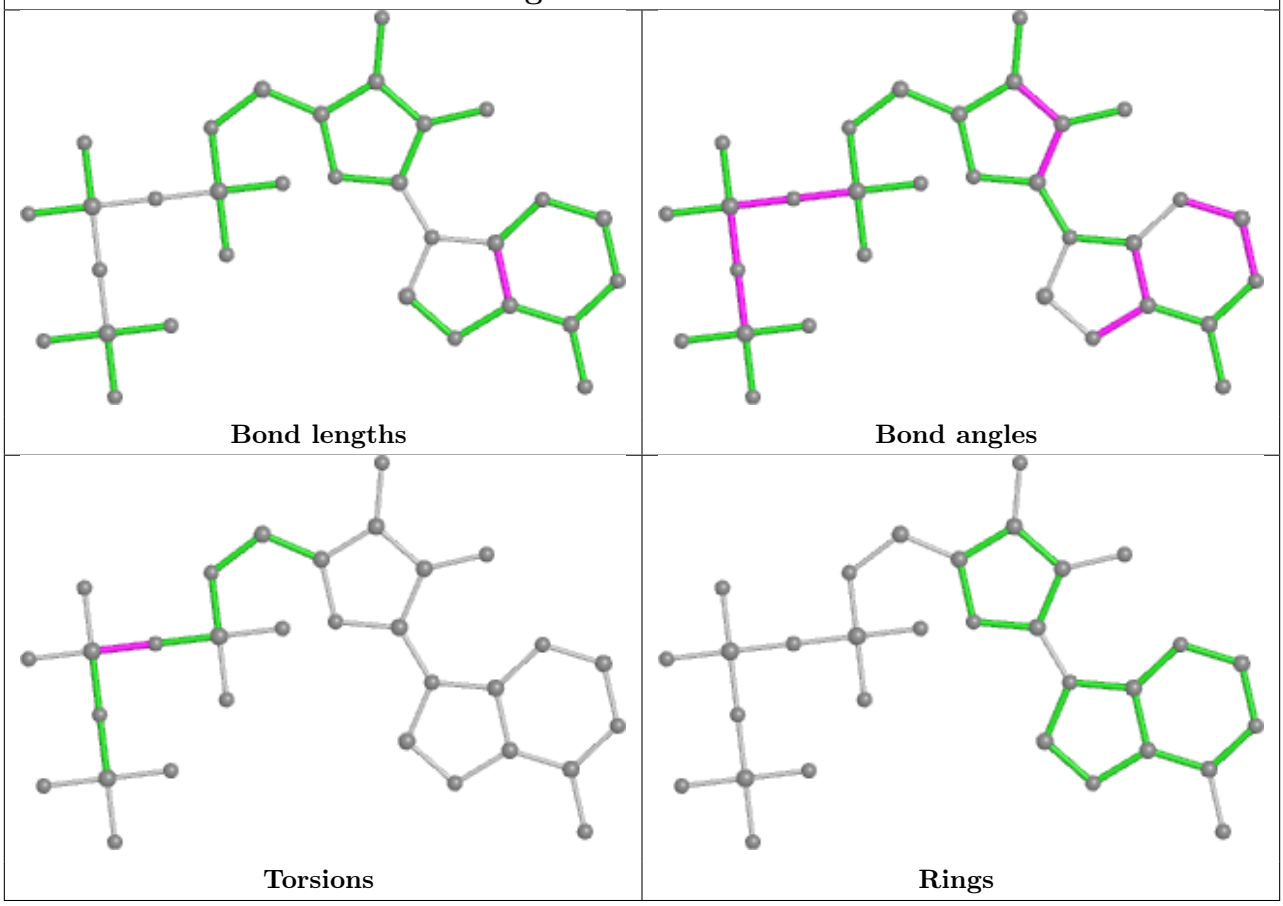
Ligand ATP B 600



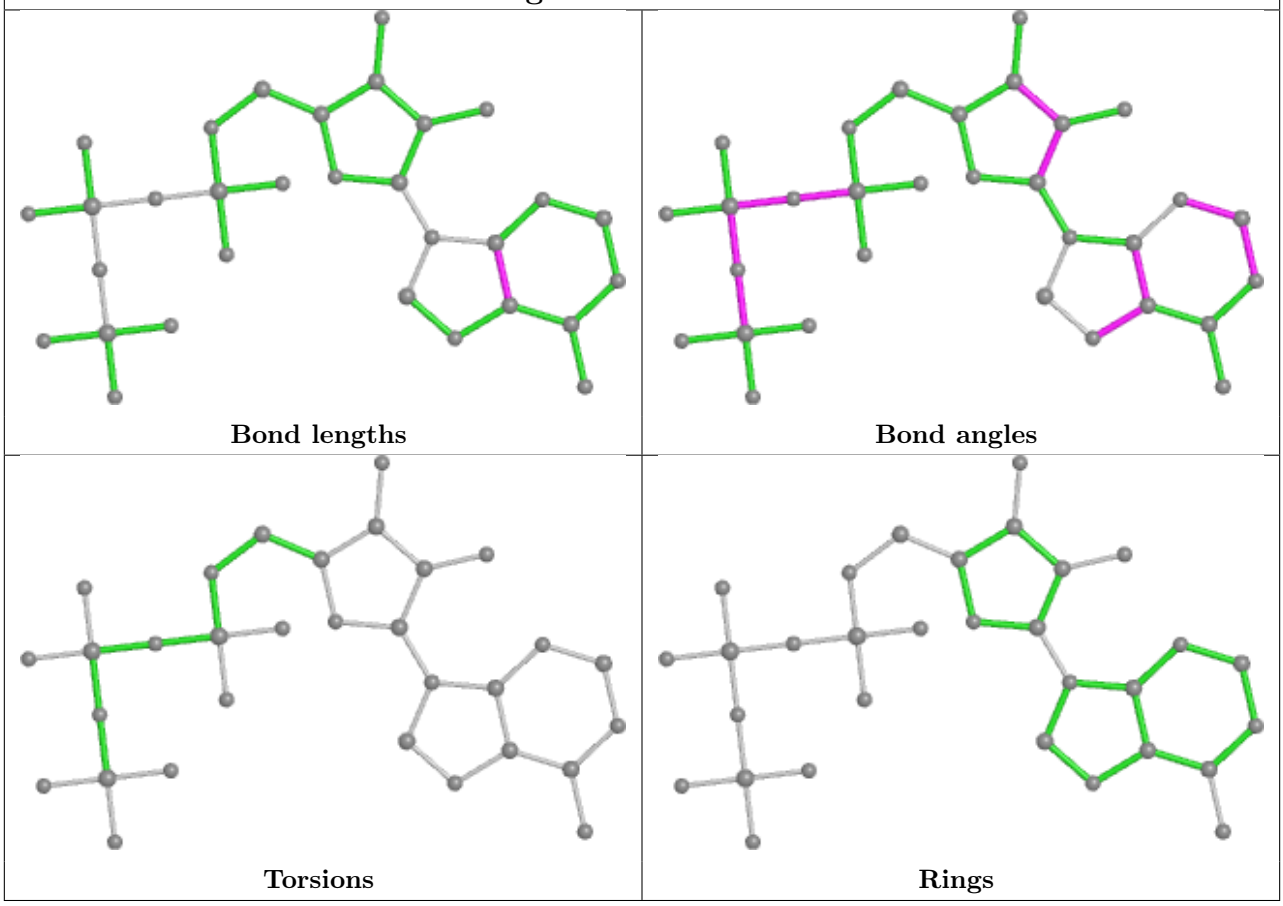
Ligand ADP D 500



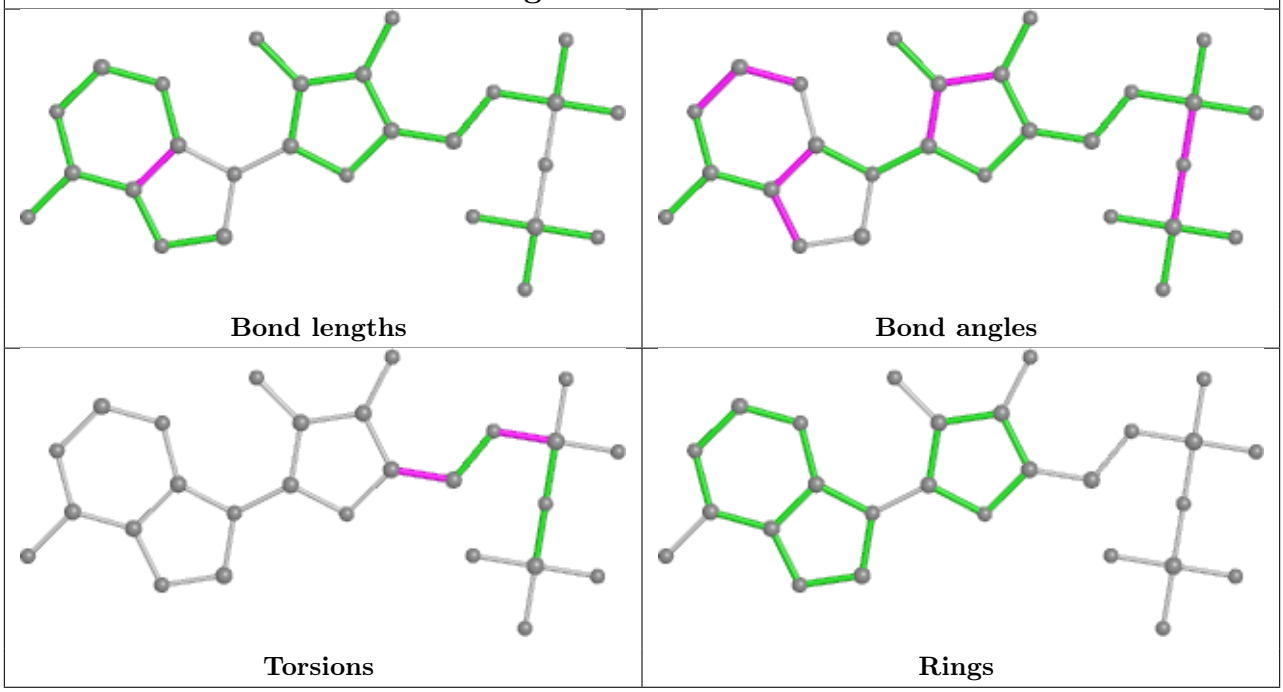
Ligand ATP A 600

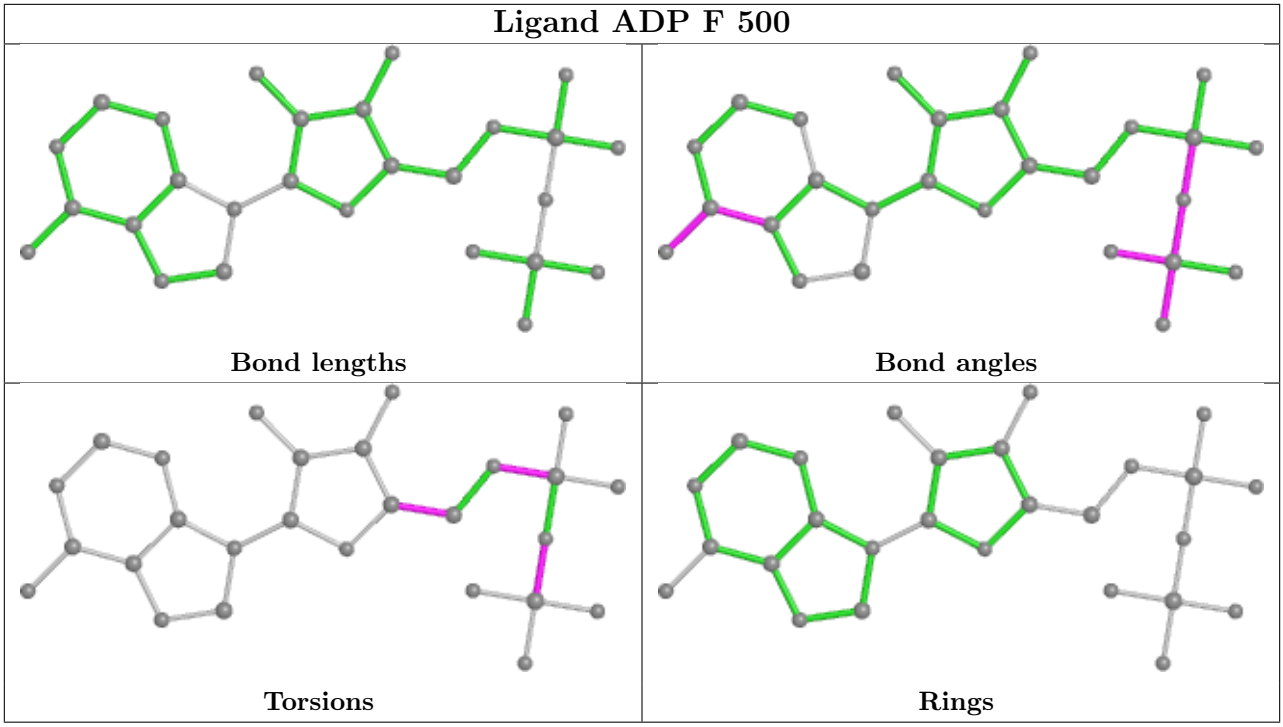


Ligand ATP C 600



Ligand ADP E 500





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

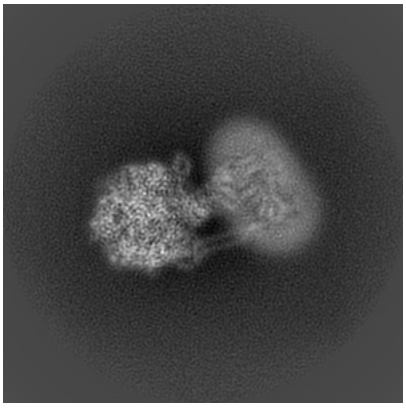
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20168. These allow visual inspection of the internal detail of the map and identification of artifacts.

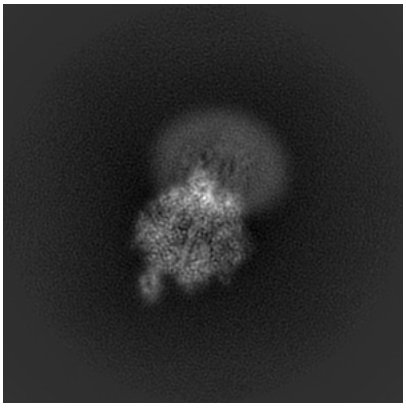
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

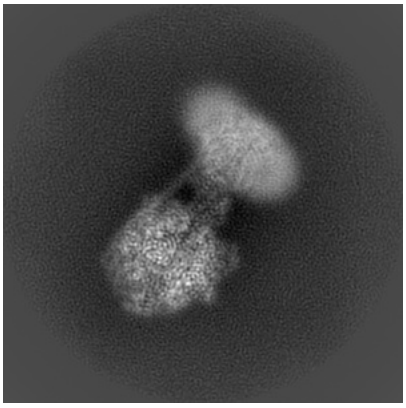
6.1.1 Primary map



X



Y

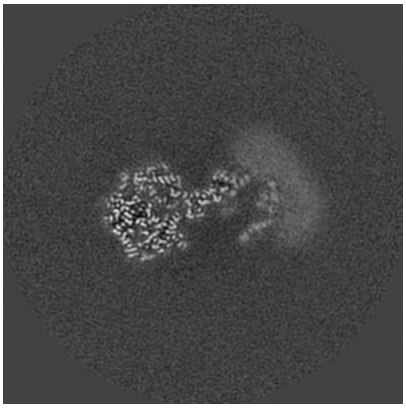


Z

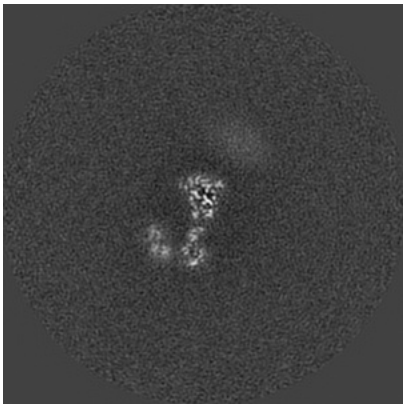
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

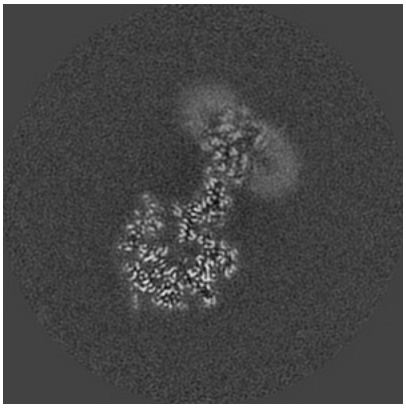
6.2.1 Primary map



X Index: 175



Y Index: 175

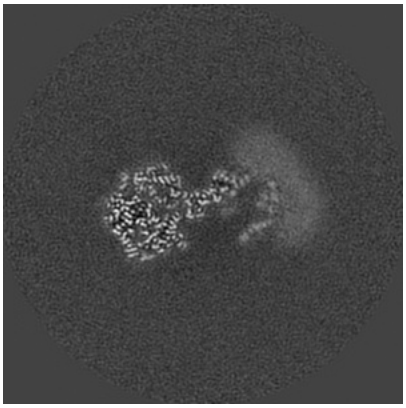


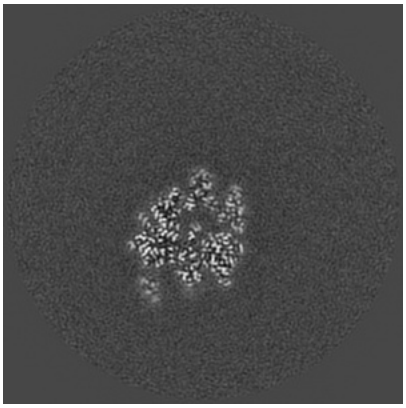
Z Index: 175

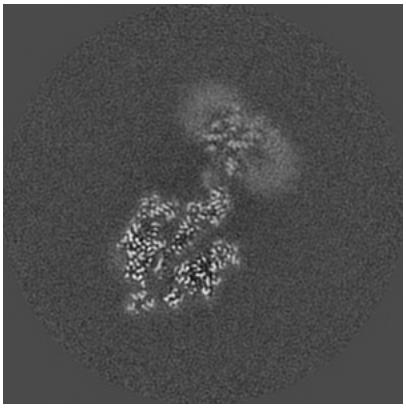
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 175

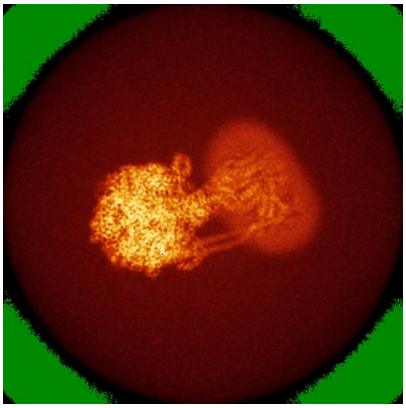

Y Index: 132

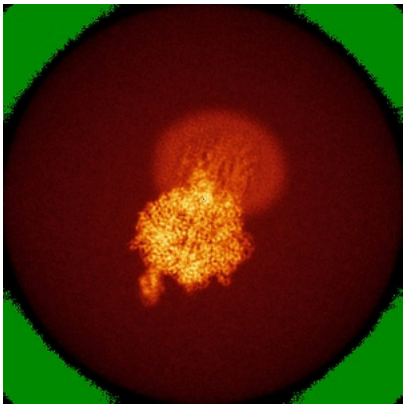

Z Index: 168

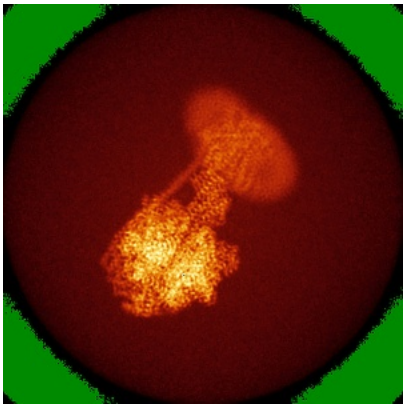
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0178. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

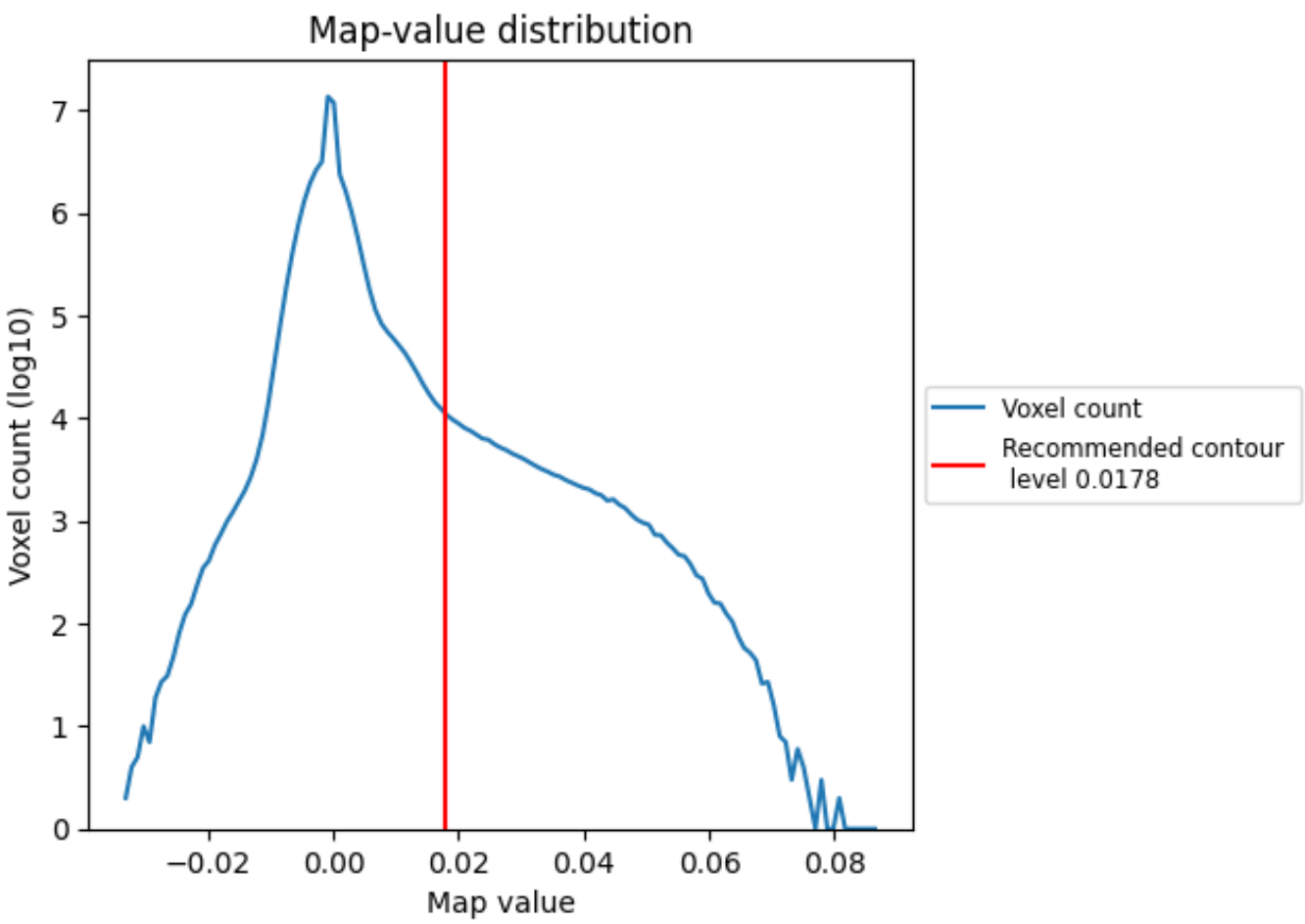
6.6 Mask visualisation (i)

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

7 Map analysis (i)

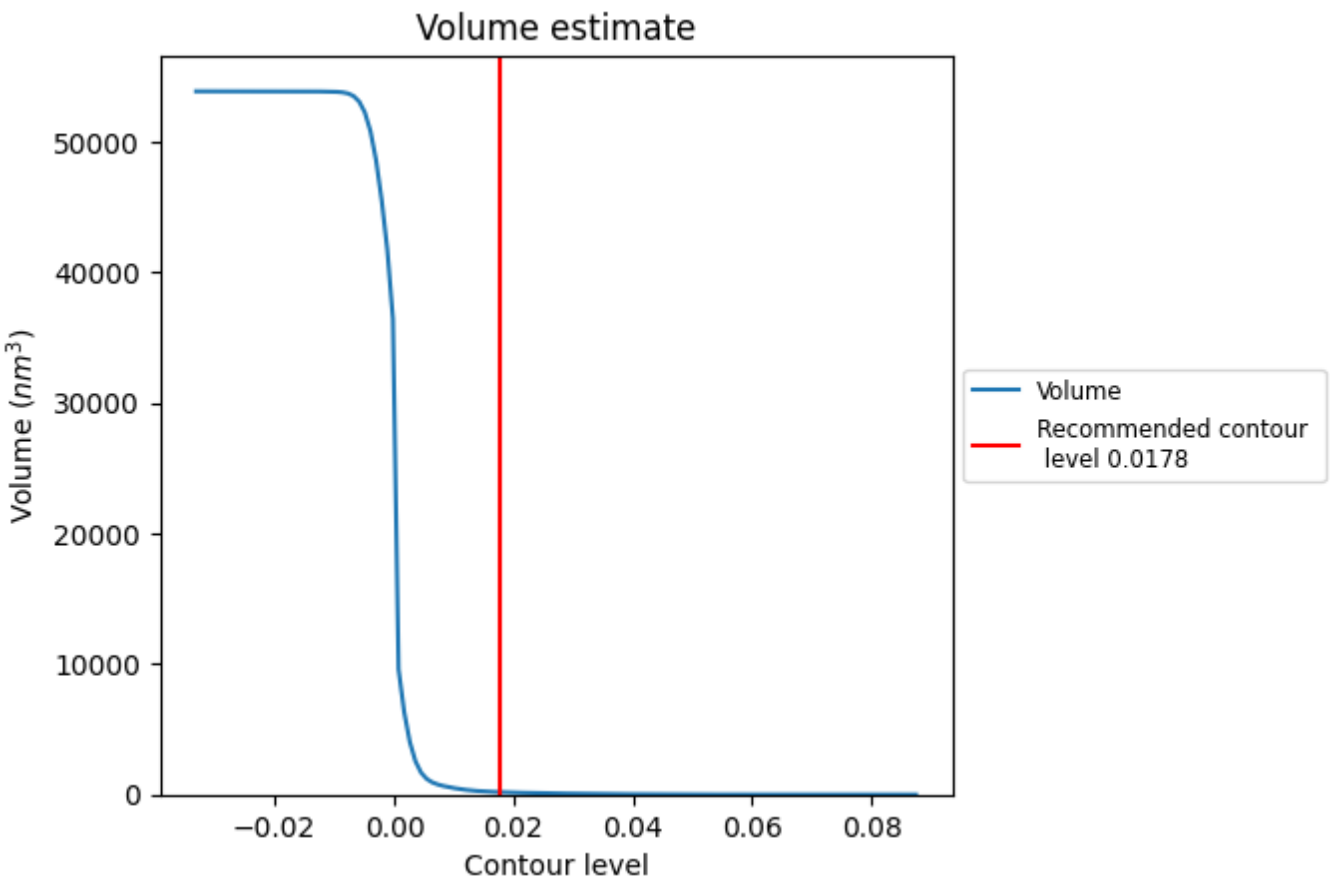
This section contains the results of statistical analysis of the map.

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.

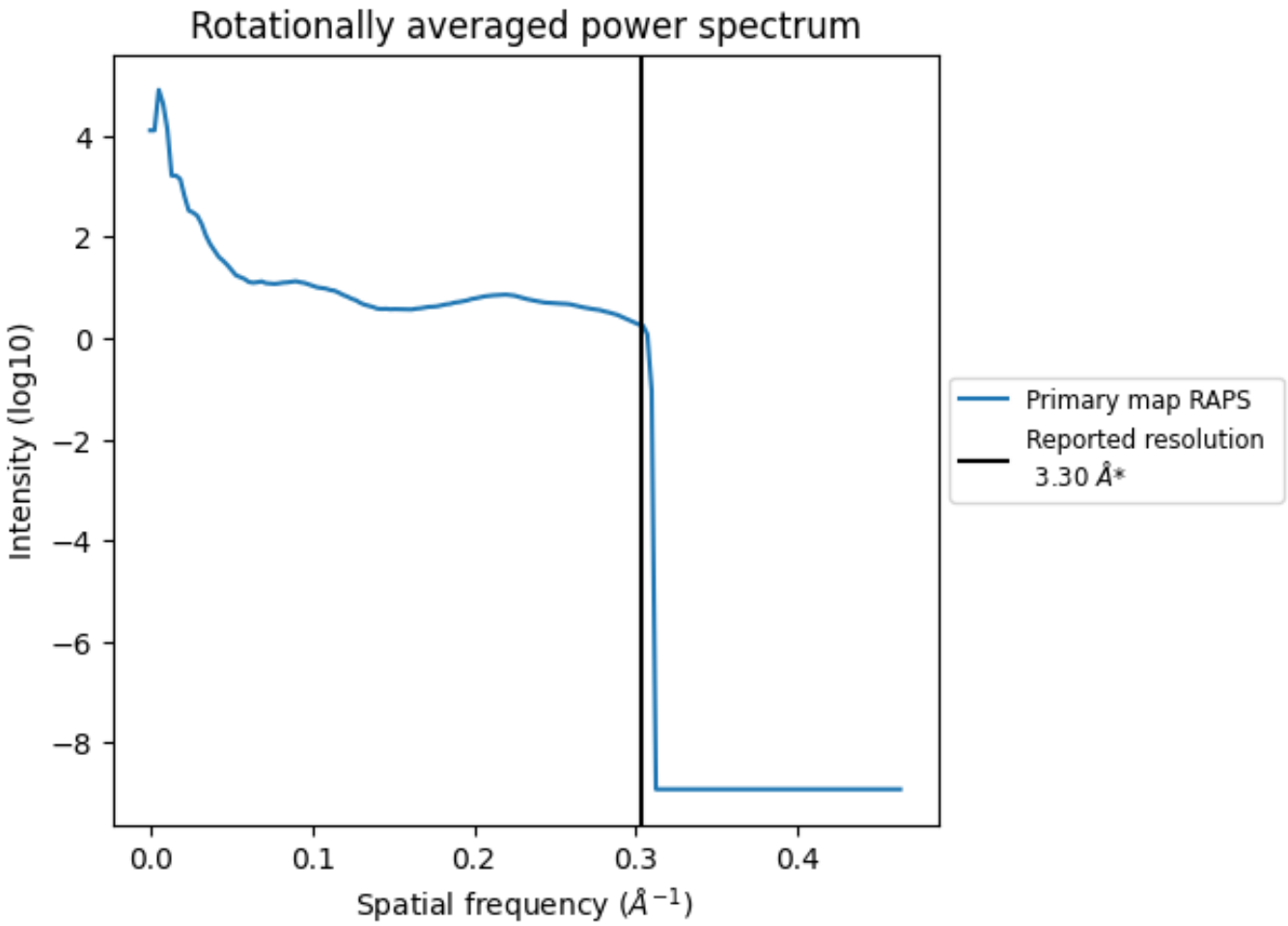
7.2 Volume estimate (i)



The volume at the recommended contour level is 184 nm^3; this corresponds to an approximate mass of 166 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 0.303 Å^{-1}

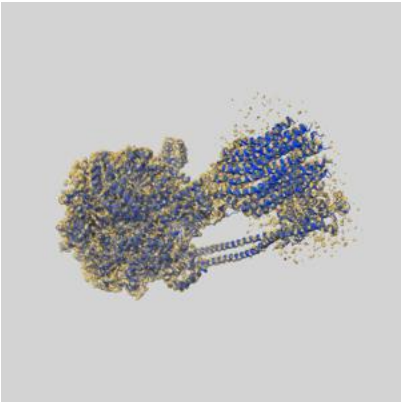
8 Fourier-Shell correlation (i)

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

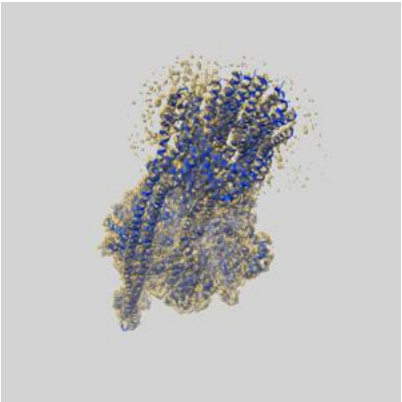
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20168 and PDB model 6OQS. Per-residue inclusion information can be found in section 3 on page 10.

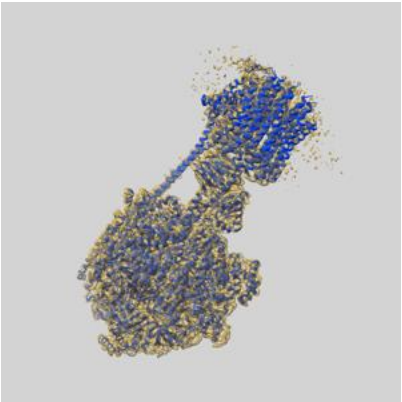
9.1 Map-model overlay (i)



X



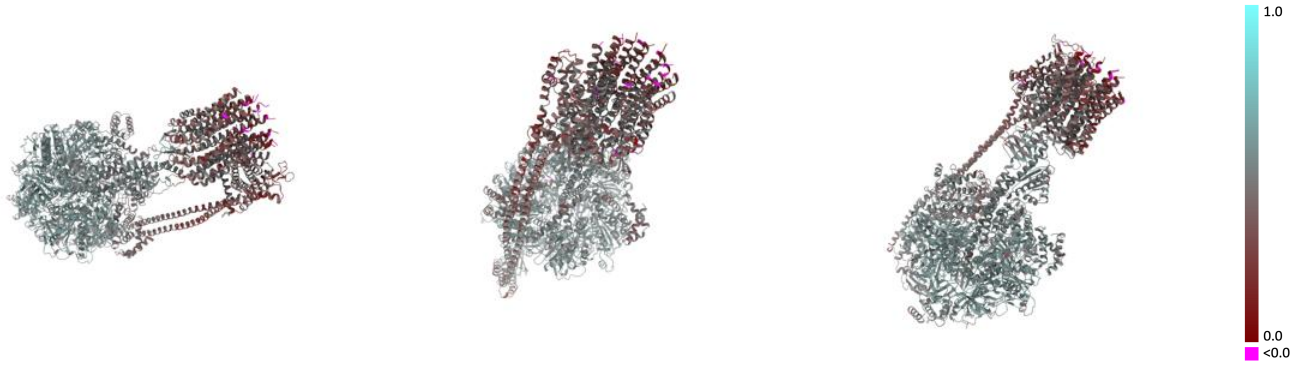
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0178 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

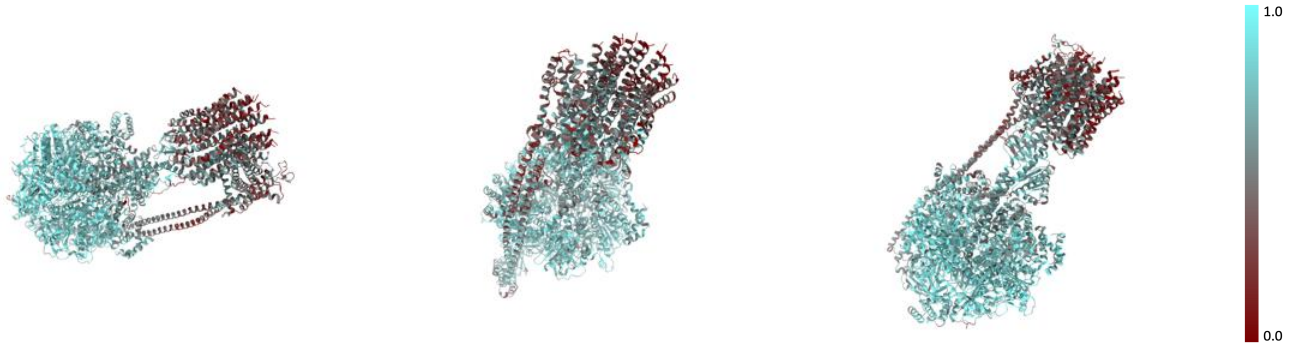
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

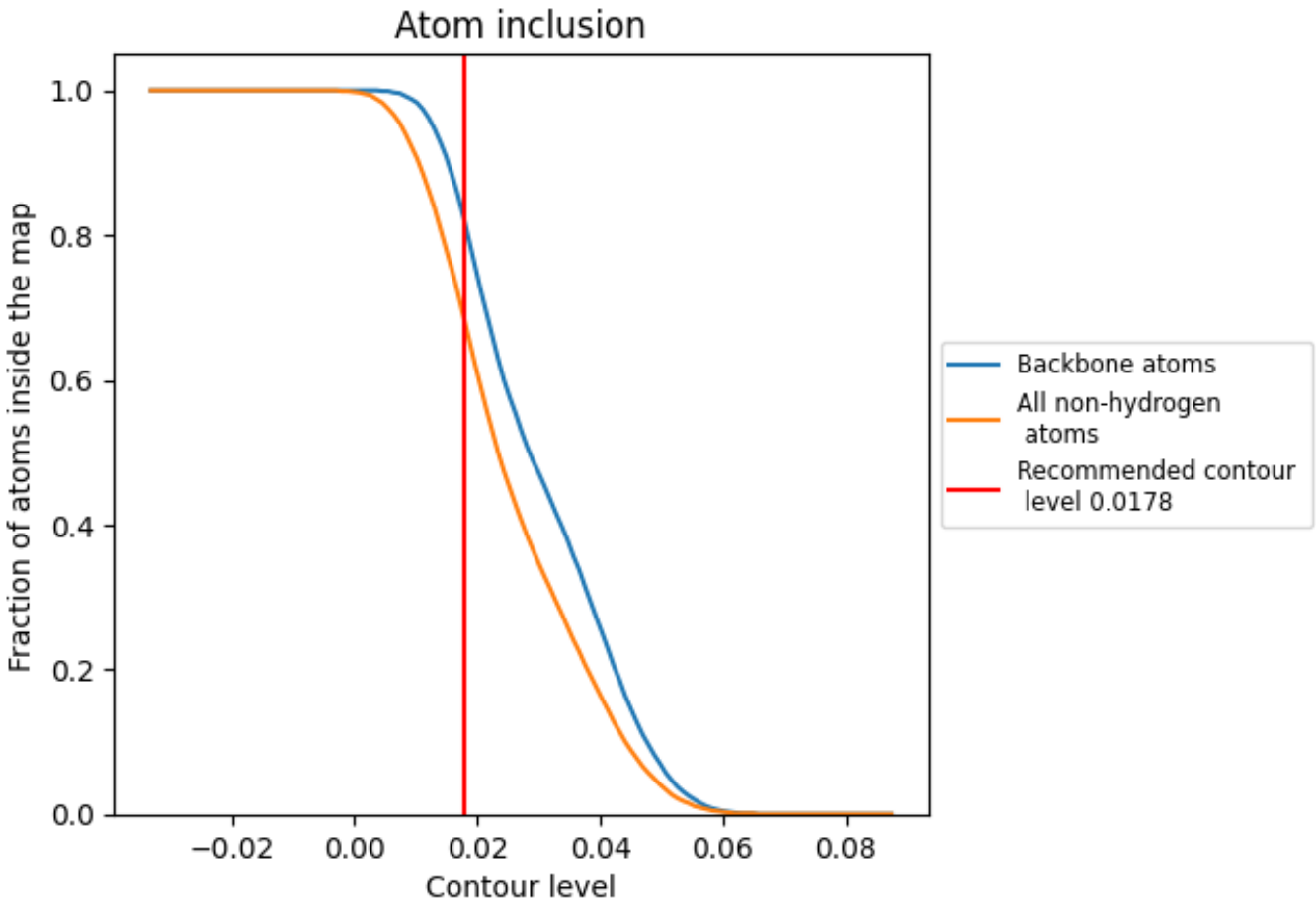
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0178).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 69% 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 (0.0178) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6870	0.4900
A	0.7950	0.5300
B	0.7780	0.5220
C	0.8260	0.5530
D	0.7880	0.5490
E	0.7920	0.5410
F	0.8300	0.5590
G	0.6820	0.5080
H	0.6120	0.4940
I	0.3560	0.3240
J	0.5350	0.4210
L	0.5080	0.4220
M	0.4750	0.3930
N	0.3940	0.3650
O	0.3300	0.3410
P	0.3210	0.3330
Q	0.4320	0.3670
R	0.4720	0.3930
S	0.4050	0.3710
W	0.7550	0.4980
X	0.4850	0.3810
Y	0.4910	0.3750
a	0.4080	0.3510