wwPDB EM Validation Summary Report (i)

May 18, 2024 – 05:01 PM EDT

PDB ID	:	7L1R
EMDB ID	:	EMD-23116
Title	:	PS3 F1-ATPase Hydrolysis Dwell
Authors	:	Sobti, M.; Ueno, H.; Noji, H.; Stewart, A.G.
Deposited on	:	2020-12-15
Resolution	:	3.10 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:

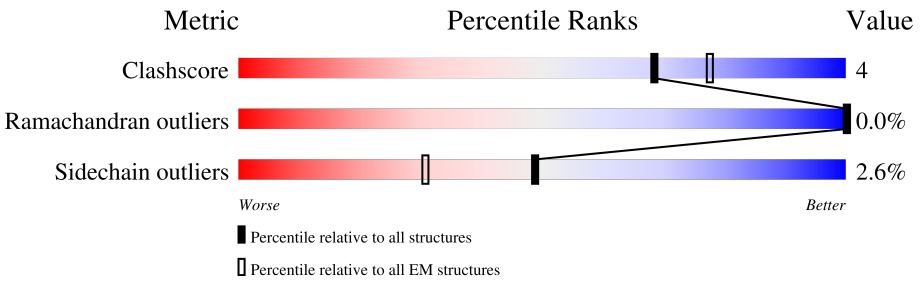
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.10 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	A	510	8% 80% 12% • 7%
1	B	510	6% 83% 10% • 7%
1	C	510	• 85% 7% • 7%
2	D	484	• 91% 6% •
2	E	484	7% 91% 5% • •
2	F	484	5% 94% • •
3	G	285	29% 88% 10% ••

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 24199 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	474	3636	2303	637	687	9	0	0
1	B	475	3643	2308	638	688	9	0	0
1	C	476	3649	2311	639	690	9	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP A0A0M3VGF9
A	-6	SER	-	expression tag	UNP A0A0M3VGF9
A	-5	HIS	-	expression tag	UNP A0A0M3VGF9
A	-4	HIS	-	expression tag	UNP A0A0M3VGF9
A	-3	HIS	-	expression tag	UNP A0A0M3VGF9
A	-2	HIS	-	expression tag	UNP A0A0M3VGF9
A	-1	HIS	-	expression tag	UNP A0A0M3VGF9
A	0	HIS	-	expression tag	UNP A0A0M3VGF9
A	1	GLY	-	expression tag	UNP A0A0M3VGF9
A	193	SER	CYS	conflict	UNP A0A0M3VGF9
A	463	PHE	TRP	conflict	UNP A0A0M3VGF9
B	-7	MET	-	expression tag	UNP A0A0M3VGF9
B	-6	SER	-	expression tag	UNP A0A0M3VGF9
B	-5	HIS	-	expression tag	UNP A0A0M3VGF9
B	-4	HIS	-	expression tag	UNP A0A0M3VGF9
B	-3	HIS	-	expression tag	UNP A0A0M3VGF9
B	-2	HIS	-	expression tag	UNP A0A0M3VGF9
B	-1	HIS	-	expression tag	UNP A0A0M3VGF9
B	0	HIS	-	expression tag	UNP A0A0M3VGF9
B	1	GLY	-	expression tag	UNP A0A0M3VGF9
B	193	SER	CYS	conflict	UNP A0A0M3VGF9
B	463	PHE	TRP	conflict	UNP A0A0M3VGF9
C	-7	MET	-	expression tag	UNP A0A0M3VGF9
C	-6	SER	-	expression tag	UNP A0A0M3VGF9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	expression tag	UNP A0A0M3VGF9
C	-4	HIS	-	expression tag	UNP A0A0M3VGF9
C	-3	HIS	-	expression tag	UNP A0A0M3VGF9
C	-2	HIS	-	expression tag	UNP A0A0M3VGF9
C	-1	HIS	-	expression tag	UNP A0A0M3VGF9
C	0	HIS	-	expression tag	UNP A0A0M3VGF9
C	1	GLY	-	expression tag	UNP A0A0M3VGF9
C	193	SER	CYS	conflict	UNP A0A0M3VGF9
C	463	PHE	TRP	conflict	UNP A0A0M3VGF9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	470	3621	2285	627	696	13	0	0
2	E	470	3622	2285	627	696	14	0	0
2	F	471	3629	2290	628	697	14	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	MET	-	expression tag	UNP A0A0M4U1P9
D	-9	HIS	-	expression tag	UNP A0A0M4U1P9
D	-8	HIS	-	expression tag	UNP A0A0M4U1P9
D	-7	HIS	-	expression tag	UNP A0A0M4U1P9
D	-6	HIS	-	expression tag	UNP A0A0M4U1P9
D	-5	HIS	-	expression tag	UNP A0A0M4U1P9
D	-4	HIS	-	expression tag	UNP A0A0M4U1P9
D	-3	HIS	-	expression tag	UNP A0A0M4U1P9
D	-2	HIS	-	expression tag	UNP A0A0M4U1P9
D	-1	HIS	-	expression tag	UNP A0A0M4U1P9
D	0	HIS	-	expression tag	UNP A0A0M4U1P9
D	190	ASP	GLU	conflict	UNP A0A0M4U1P9
E	-10	MET	-	expression tag	UNP A0A0M4U1P9
E	-9	HIS	-	expression tag	UNP A0A0M4U1P9
E	-8	HIS	-	expression tag	UNP A0A0M4U1P9
E	-7	HIS	-	expression tag	UNP A0A0M4U1P9
E	-6	HIS	-	expression tag	UNP A0A0M4U1P9
E	-5	HIS	-	expression tag	UNP A0A0M4U1P9
E	-4	HIS	-	expression tag	UNP A0A0M4U1P9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	HIS	-	expression tag	UNP A0A0M4U1P9
E	-2	HIS	-	expression tag	UNP A0A0M4U1P9
E	-1	HIS	-	expression tag	UNP A0A0M4U1P9
E	0	HIS	-	expression tag	UNP A0A0M4U1P9
E	190	ASP	GLU	conflict	UNP A0A0M4U1P9
F	-10	MET	-	expression tag	UNP A0A0M4U1P9
F	-9	HIS	-	expression tag	UNP A0A0M4U1P9
F	-8	HIS	-	expression tag	UNP A0A0M4U1P9
F	-7	HIS	-	expression tag	UNP A0A0M4U1P9
F	-6	HIS	-	expression tag	UNP A0A0M4U1P9
F	-5	HIS	-	expression tag	UNP A0A0M4U1P9
F	-4	HIS	-	expression tag	UNP A0A0M4U1P9
F	-3	HIS	-	expression tag	UNP A0A0M4U1P9
F	-2	HIS	-	expression tag	UNP A0A0M4U1P9
F	-1	HIS	-	expression tag	UNP A0A0M4U1P9
F	0	HIS	-	expression tag	UNP A0A0M4U1P9
F	190	ASP	GLU	conflict	UNP A0A0M4U1P9

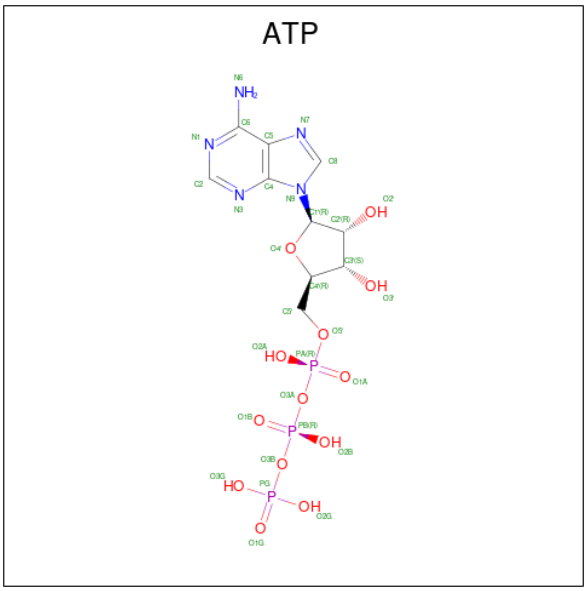
- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	282	2211	1393	388	420	10	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	112	CYS	SER	conflict	UNP A0A0M4TPJ7
G	215	CYS	ILE	conflict	UNP A0A0M4TPJ7

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



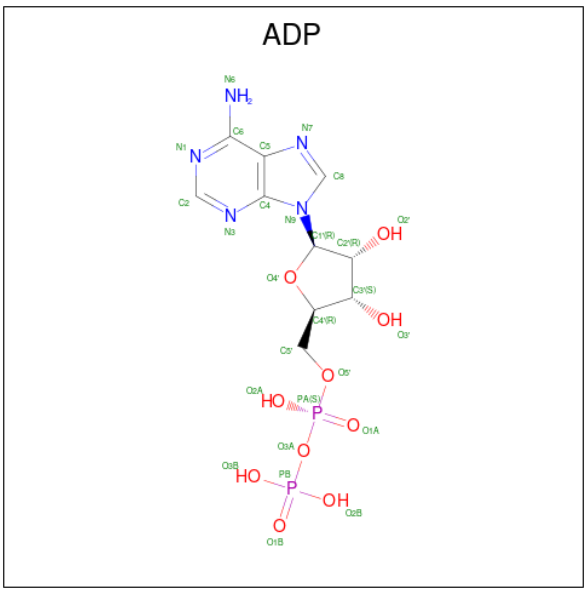
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

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



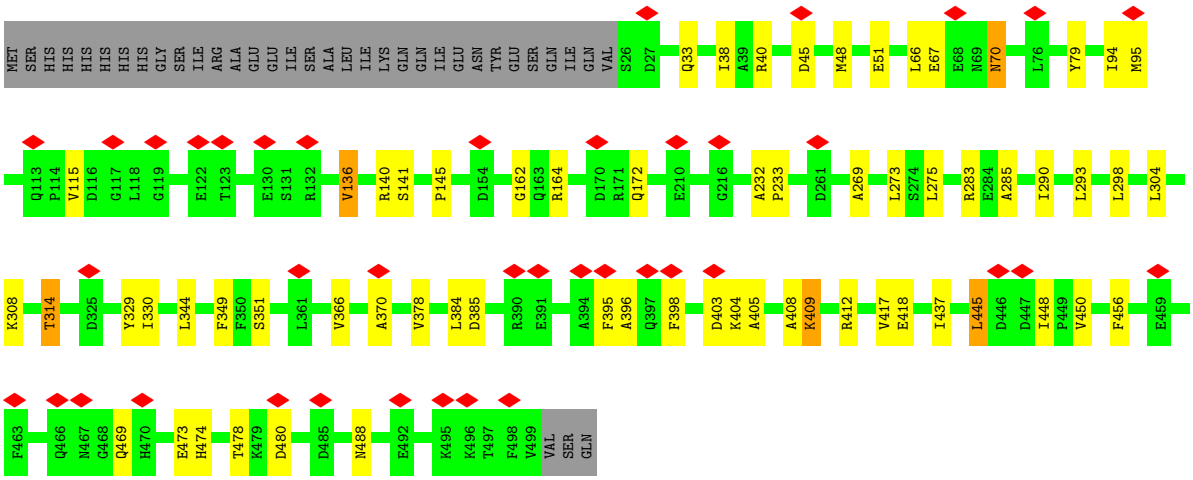
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	E	1	27	10	5	10	2	0

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.

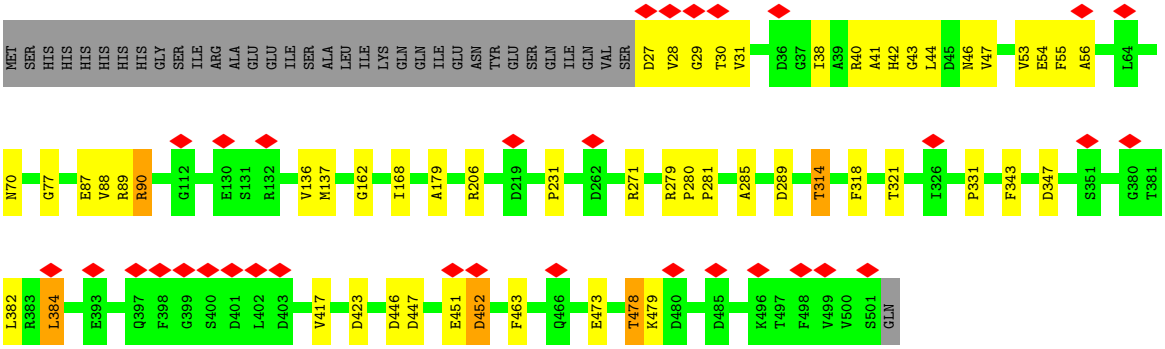
• Molecule 1: ATP synthase subunit alpha

Chain A:



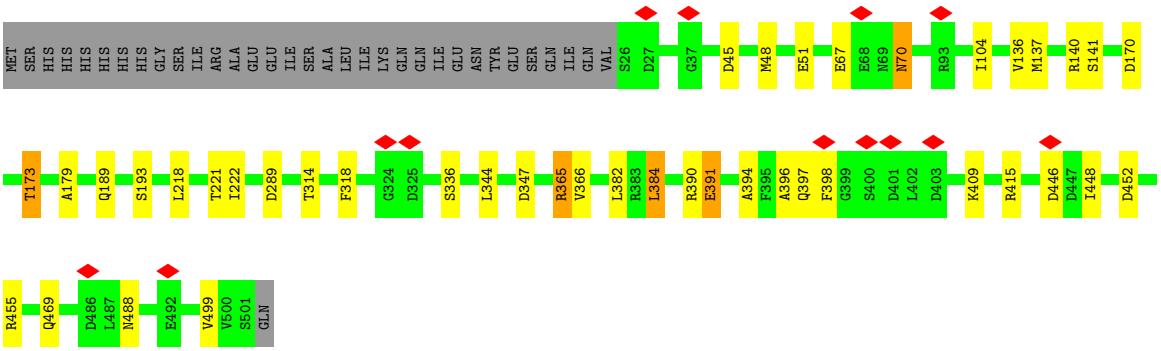
• Molecule 1: ATP synthase subunit alpha

Chain B:



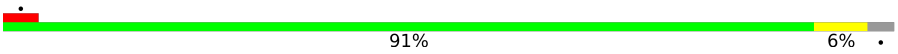
• Molecule 1: ATP synthase subunit alpha

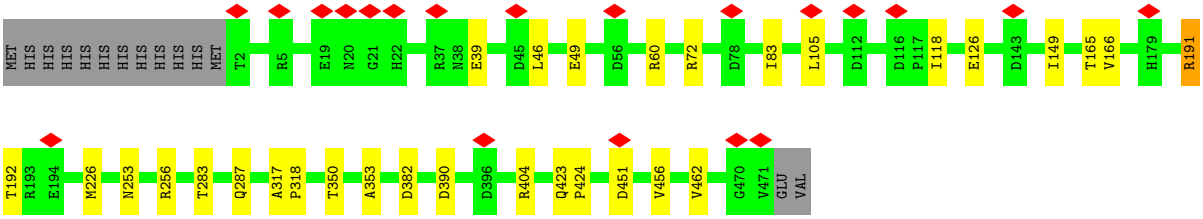
Chain C:



- Molecule 2: ATP synthase subunit beta

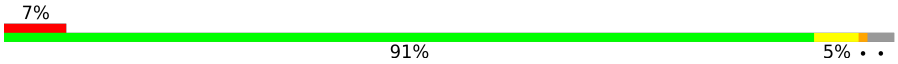
Chain D:

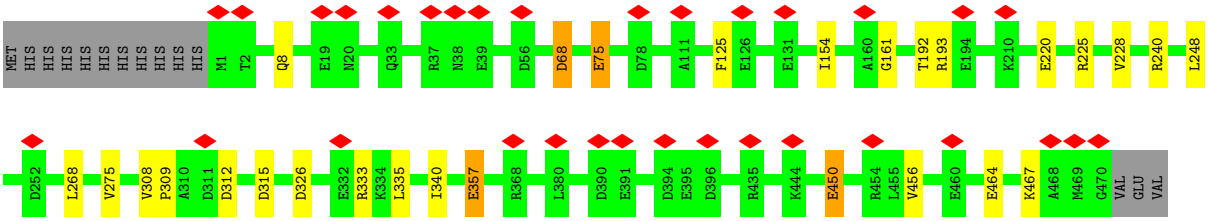




- Molecule 2: ATP synthase subunit beta

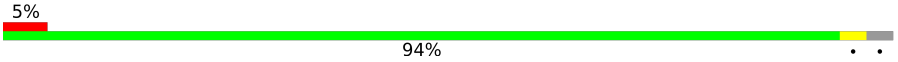
Chain E:

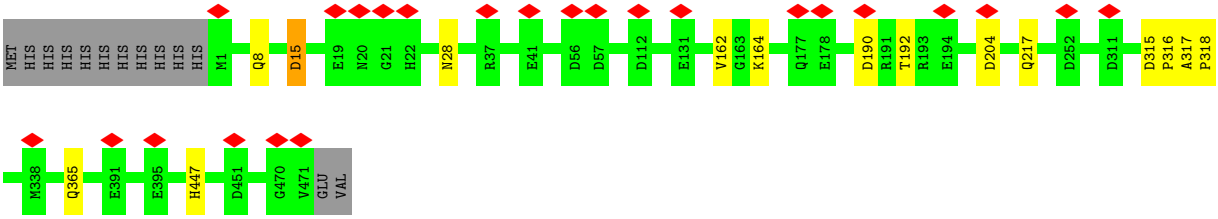




- Molecule 2: ATP synthase subunit beta

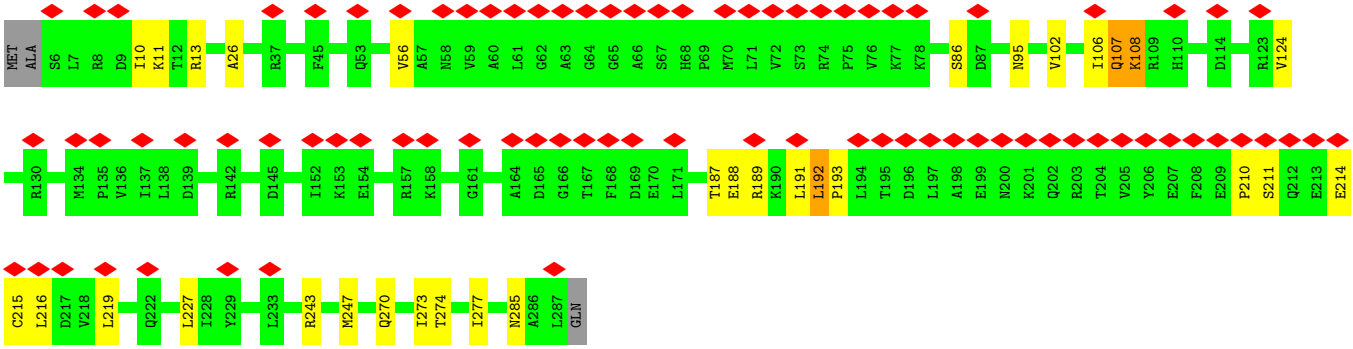
Chain F:





- Molecule 3: ATP synthase gamma chain

Chain G:


MET ALA S6 L7 R8 D9 I10 K11 T12 R13 A26 R37 F45 Q53 V56 A57 N58 V59 A60 L61 G62 A63 G64 G65 A66 S67 H68 P69 M70 L71 V72 S73 R74 P75 V76 K77 K78 S86 D87 N95 V102 I106 Q107 K108 R109 H110 D114 R123 V124
R130 M134 P135 V136 I137 L138 D139 R142 D145 T152 K153 E154 R157 K158 G161 A164 D165 G166 T167 F168 D169 E170 L171 T187 E188 R189 K190 L191 L192 P193 L194 T195 D196 L197 A198 E199 N200 K201 Q202 R203 T204 V205 Y206 E207 F208 E209 P210 S211 Q212 E213 E214
C215 L216 D217 V218 L219 Q222 L227 I228 Y229 L233 R243 M247 Q270 I273 T274 I277 N285 A286 L287 GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	340916	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	2.095	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	215.04, 215.04, 215.04	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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: 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	A	0.57	0/3695	0.93	0/5004
1	B	0.58	0/3702	0.93	0/5014
1	C	0.56	0/3708	0.85	0/5022
2	D	0.54	0/3684	0.83	0/4991
2	E	0.53	0/3685	0.81	0/4991
2	F	0.53	0/3692	0.82	0/5001
3	G	0.54	0/2244	0.80	0/3036
All	All	0.55	0/24410	0.86	0/33059

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	A	3636	0	3710	49	0
1	B	3643	0	3718	40	0
1	C	3649	0	3724	37	0
2	D	3621	0	3631	24	0
2	E	3622	0	3634	20	0
2	F	3629	0	3643	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	2211	0	2257	20	0
4	A	31	0	12	2	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	1	0
4	F	31	0	12	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	E	27	0	12	0	0
All	All	24199	0	24389	186	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 4.

The worst 5 of 186 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)
4:F:500:ATP:H8	4:F:500:ATP:H5'1	1.38	0.89
1:B:55:PHE:HA	1:B:88:VAL:HA	1.57	0.86
2:E:275:VAL:H	3:G:274:THR:HG22	1.41	0.86
4:F:500:ATP:H5'1	4:F:500:ATP:C8	2.11	0.85
2:D:191:ARG:CG	2:D:191:ARG:HH21	1.91	0.84

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	A	472/510 (92%)	453 (96%)	19 (4%)	0	100	100
1	B	473/510 (93%)	456 (96%)	16 (3%)	1 (0%)	47	79
1	C	474/510 (93%)	461 (97%)	13 (3%)	0	100	100
2	D	468/484 (97%)	451 (96%)	17 (4%)	0	100	100
2	E	468/484 (97%)	455 (97%)	13 (3%)	0	100	100
2	F	469/484 (97%)	453 (97%)	16 (3%)	0	100	100
3	G	280/285 (98%)	273 (98%)	7 (2%)	0	100	100
All	All	3104/3267 (95%)	3002 (97%)	101 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	281	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/419 (92%)	375 (97%)	11 (3%)	43	73
1	B	387/419 (92%)	375 (97%)	12 (3%)	40	70
1	C	388/419 (93%)	379 (98%)	9 (2%)	50	77
2	D	386/400 (96%)	377 (98%)	9 (2%)	50	77
2	E	386/400 (96%)	376 (97%)	10 (3%)	46	74
2	F	387/400 (97%)	383 (99%)	4 (1%)	76	90
3	G	238/240 (99%)	227 (95%)	11 (5%)	27	59
All	All	2558/2697 (95%)	2492 (97%)	66 (3%)	49	74

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	102	VAL
3	G	108	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	285	ASN
1	C	173	THR
1	C	70	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	33	GLN
2	F	8	GLN
2	E	33	GLN
2	F	217	GLN
1	B	397	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 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
4	ATP	F	500	5	26,33,33	0.71	0	31,52,52	0.95	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ATP	B	600	5	26,33,33	0.71	0	31,52,52	0.85	1 (3%)
6	ADP	E	501	5	24,29,29	0.70	0	29,45,45	0.84	1 (3%)
4	ATP	C	600	5	26,33,33	0.74	0	31,52,52	0.98	2 (6%)
4	ATP	D	500	5	26,33,33	0.74	0	31,52,52	1.07	3 (9%)
4	ATP	A	600	5	26,33,33	0.72	0	31,52,52	0.97	1 (3%)

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
4	ATP	F	500	5	-	3/18/38/38	0/3/3/3
4	ATP	B	600	5	-	1/18/38/38	0/3/3/3
6	ADP	E	501	5	-	1/12/32/32	0/3/3/3
4	ATP	C	600	5	-	1/18/38/38	0/3/3/3
4	ATP	D	500	5	-	1/18/38/38	0/3/3/3
4	ATP	A	600	5	-	1/18/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	500	ATP	PB-O3B-PG	-2.77	123.33	132.83
4	D	500	ATP	PA-O3A-PB	-2.66	123.69	132.83
4	C	600	ATP	C5-C6-N6	2.32	123.87	120.35
4	B	600	ATP	C5-C6-N6	2.31	123.86	120.35
4	A	600	ATP	C5-C6-N6	2.28	123.81	120.35

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	500	ATP	O4'-C4'-C5'-O5'
4	B	600	ATP	O4'-C4'-C5'-O5'
4	C	600	ATP	O4'-C4'-C5'-O5'
4	F	500	ATP	PA-O3A-PB-O1B
4	F	500	ATP	PA-O3A-PB-O2B

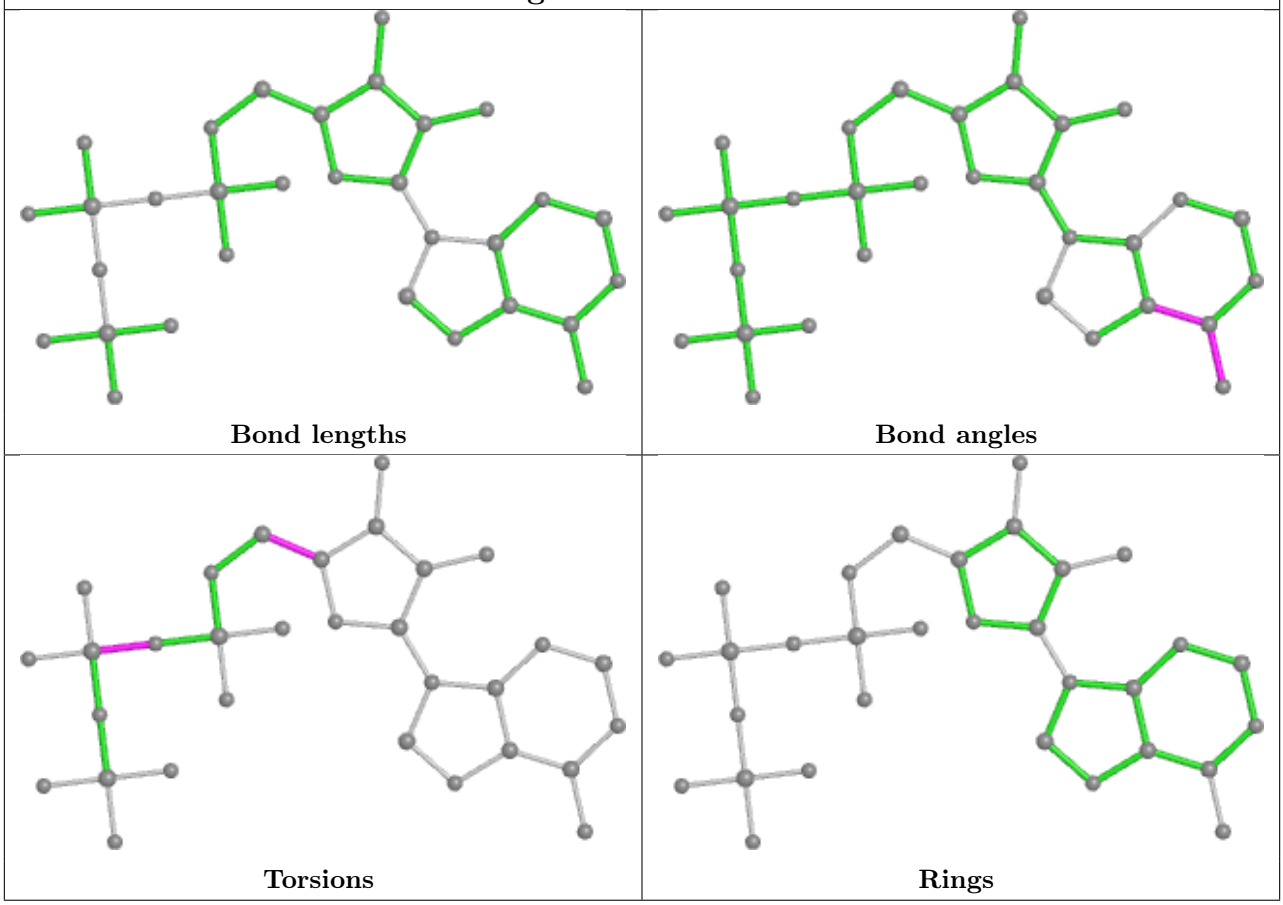
There are no ring outliers.

3 monomers are involved in 7 short contacts:

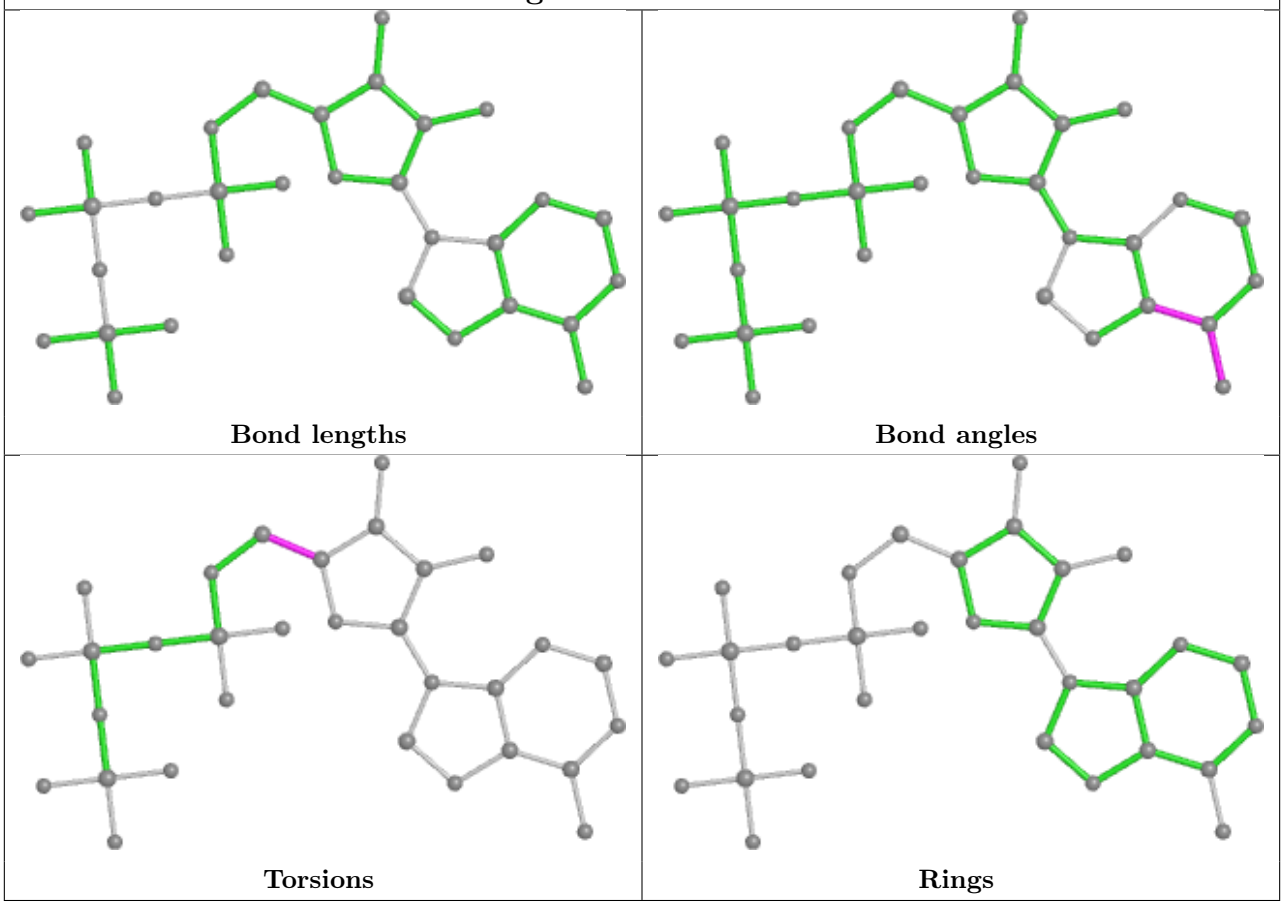
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	500	ATP	4	0
4	D	500	ATP	1	0
4	A	600	ATP	2	0

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.

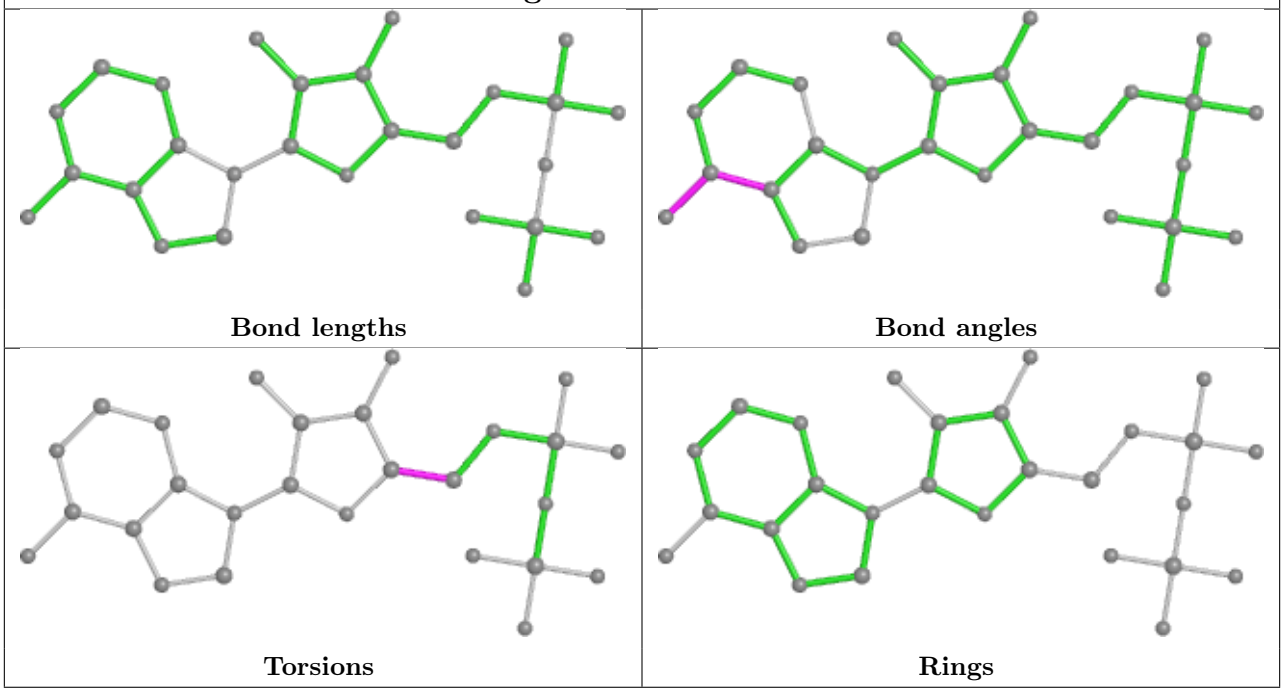
Ligand ATP F 500



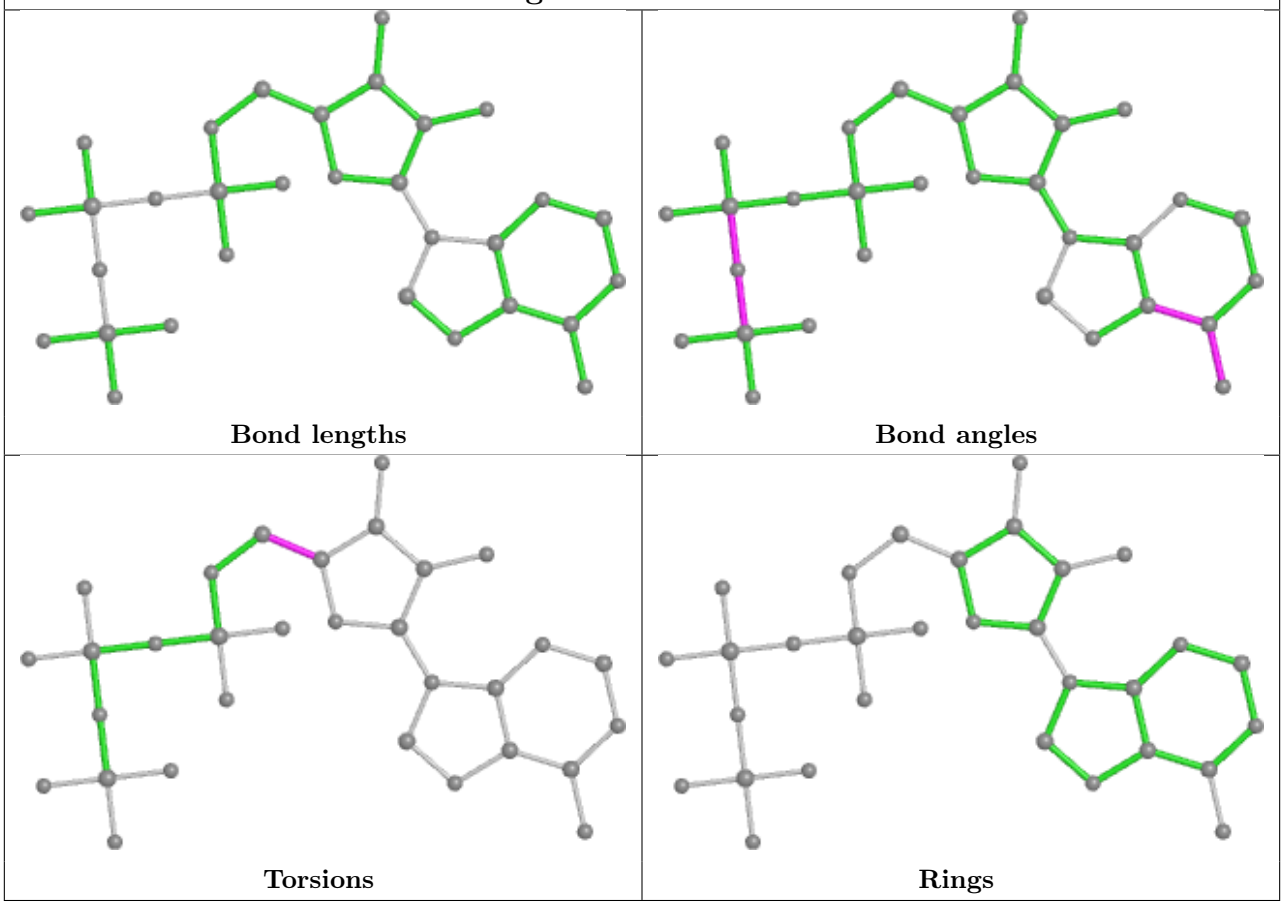
Ligand ATP B 600



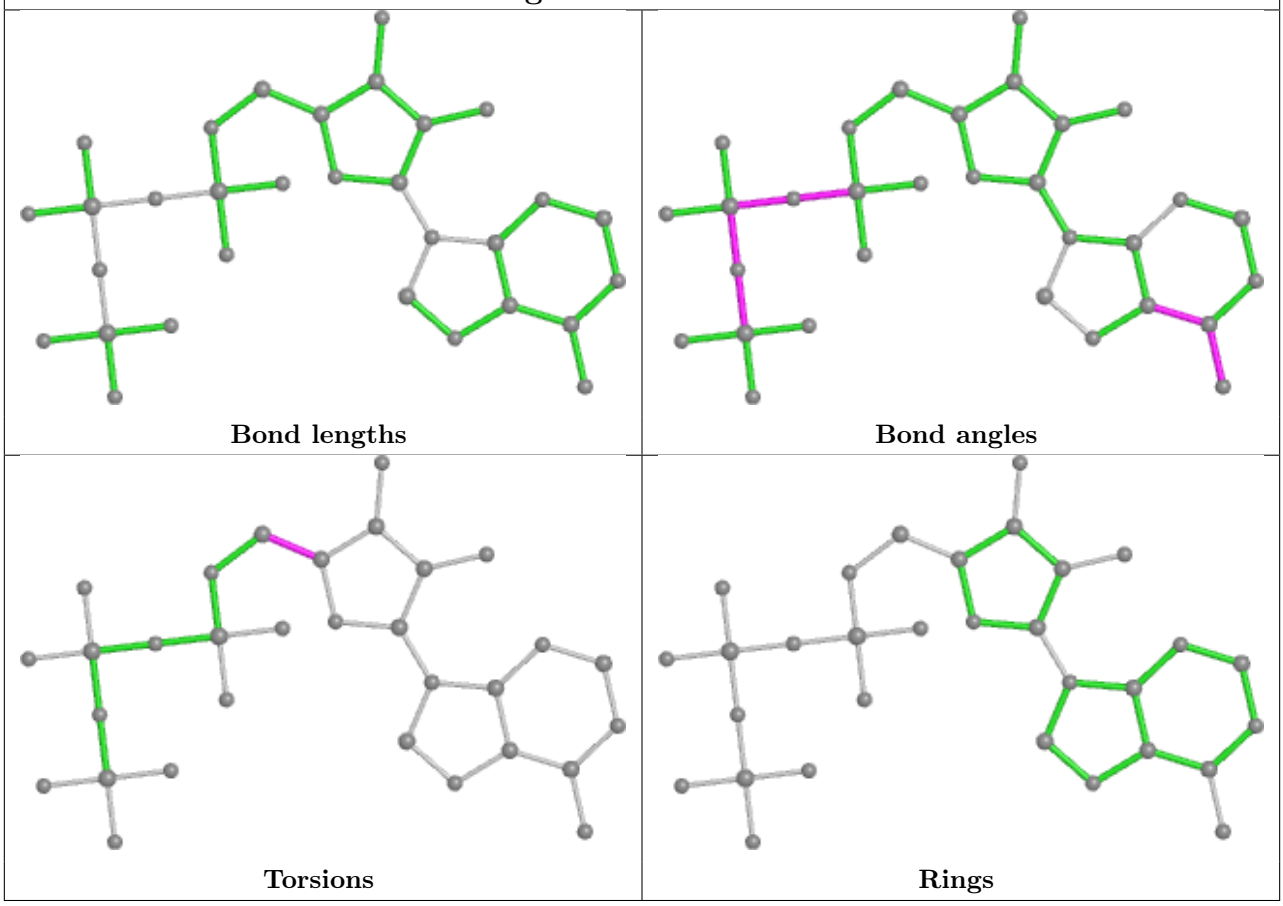
Ligand ADP E 501

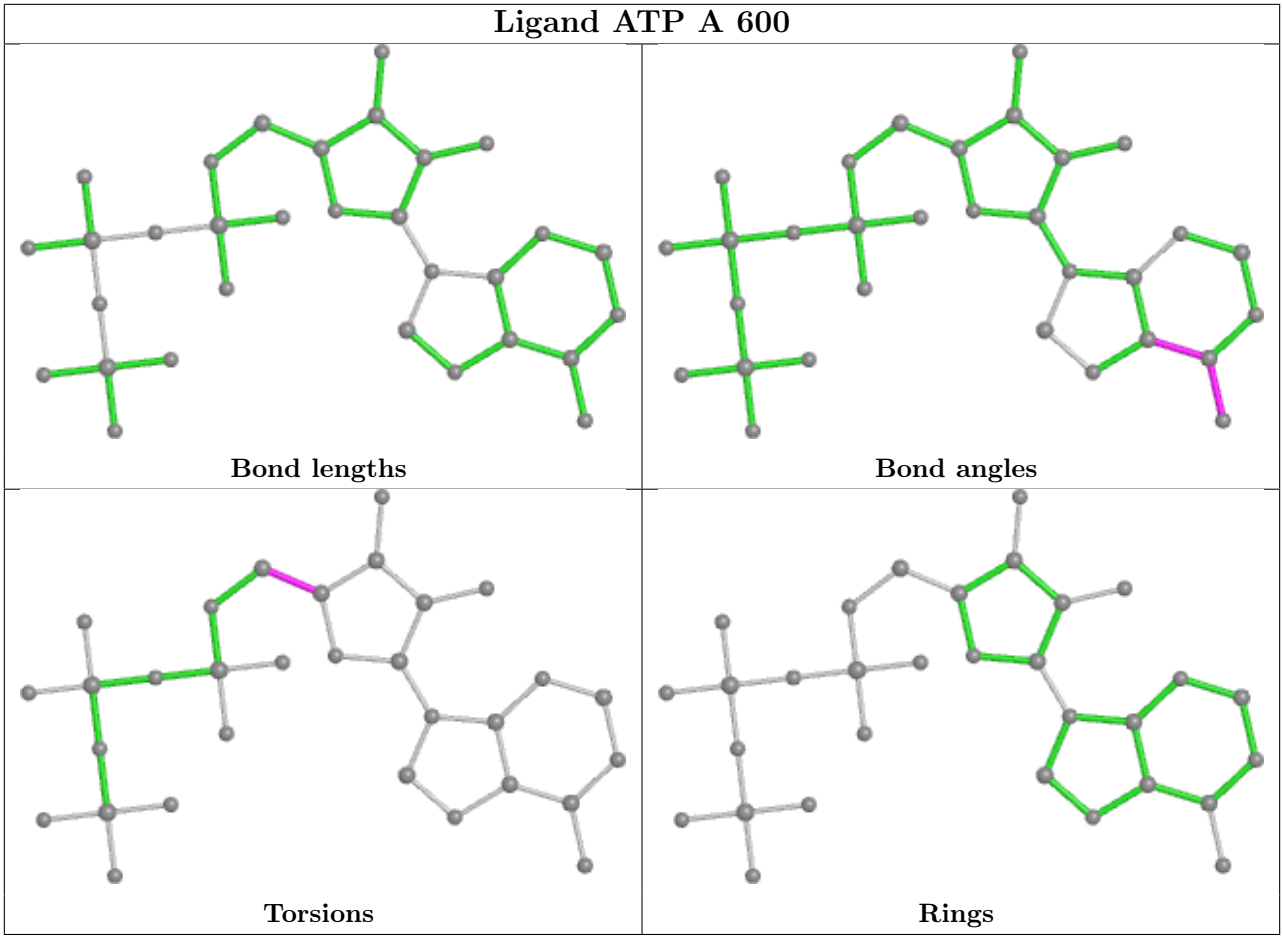


Ligand ATP C 600



Ligand ATP D 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.

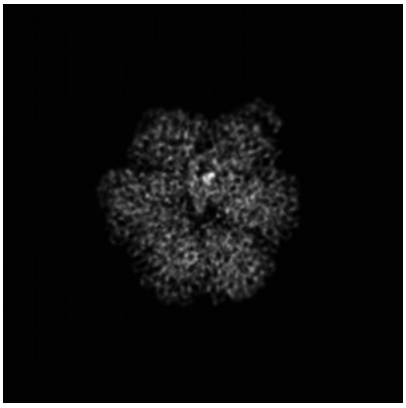
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23116. These allow visual inspection of the internal detail of the map and identification of artifacts.

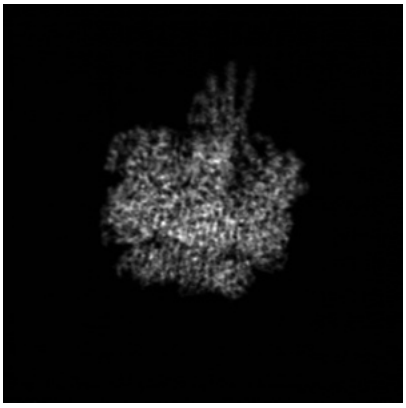
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

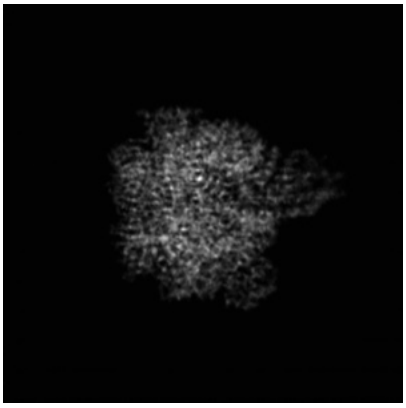
6.1.1 Primary map



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: 128

Y Index: 128

Z Index: 128

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: 125

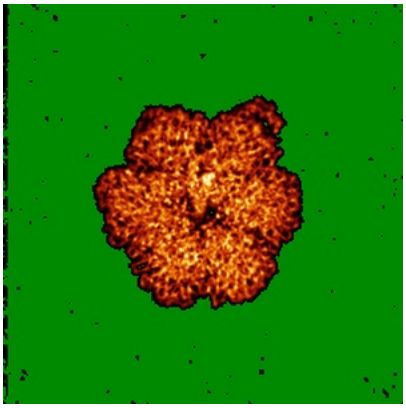
Y Index: 149

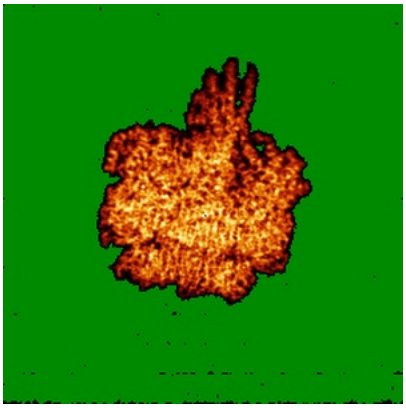
Z Index: 136

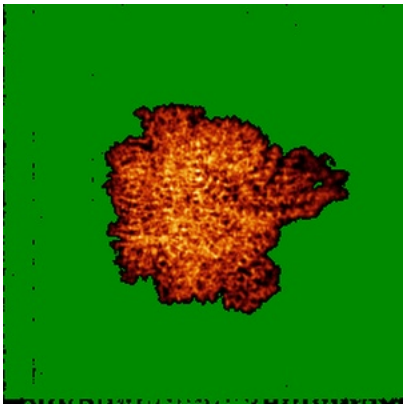
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

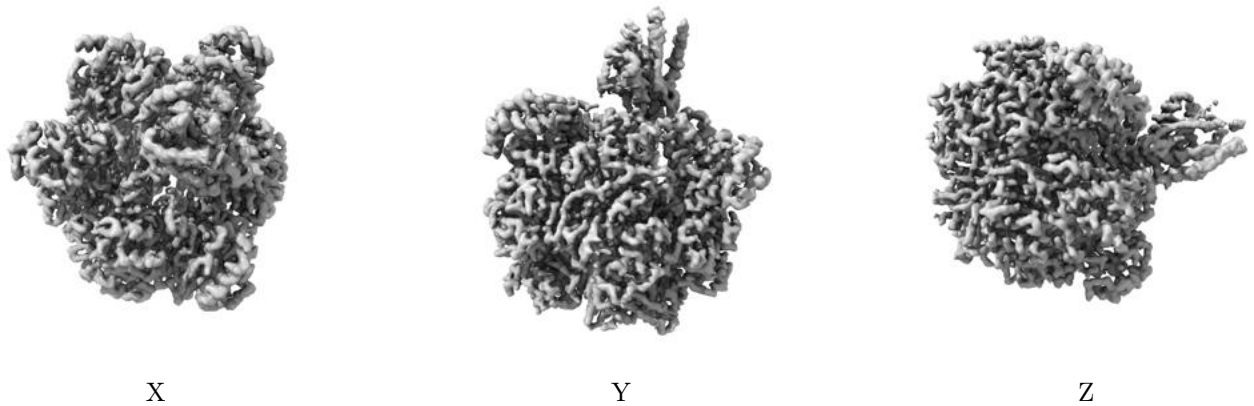

Y


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



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

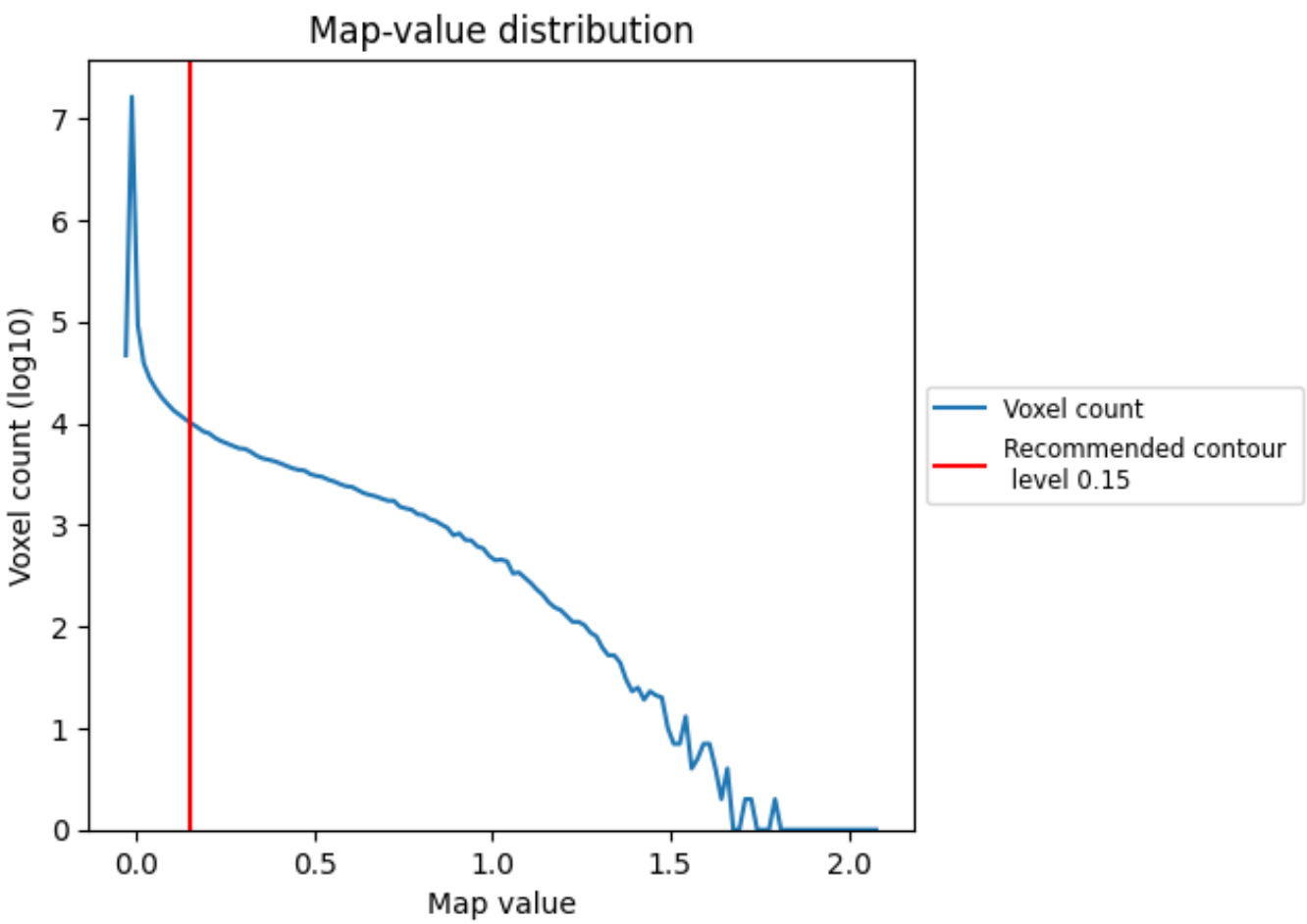
6.6 Mask visualisation (i)

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

7 Map analysis (i)

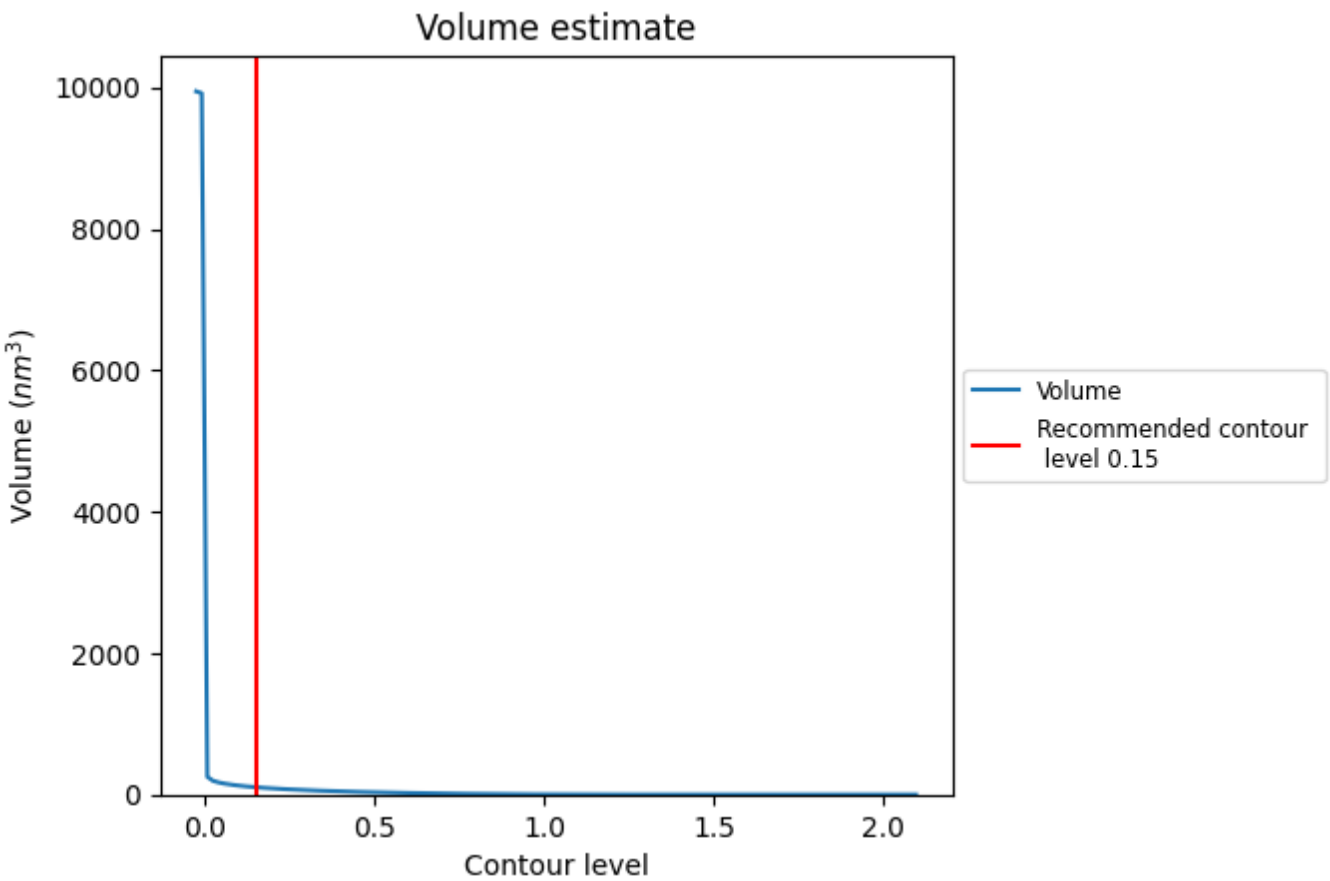
This section contains the results of statistical analysis of the map.

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.

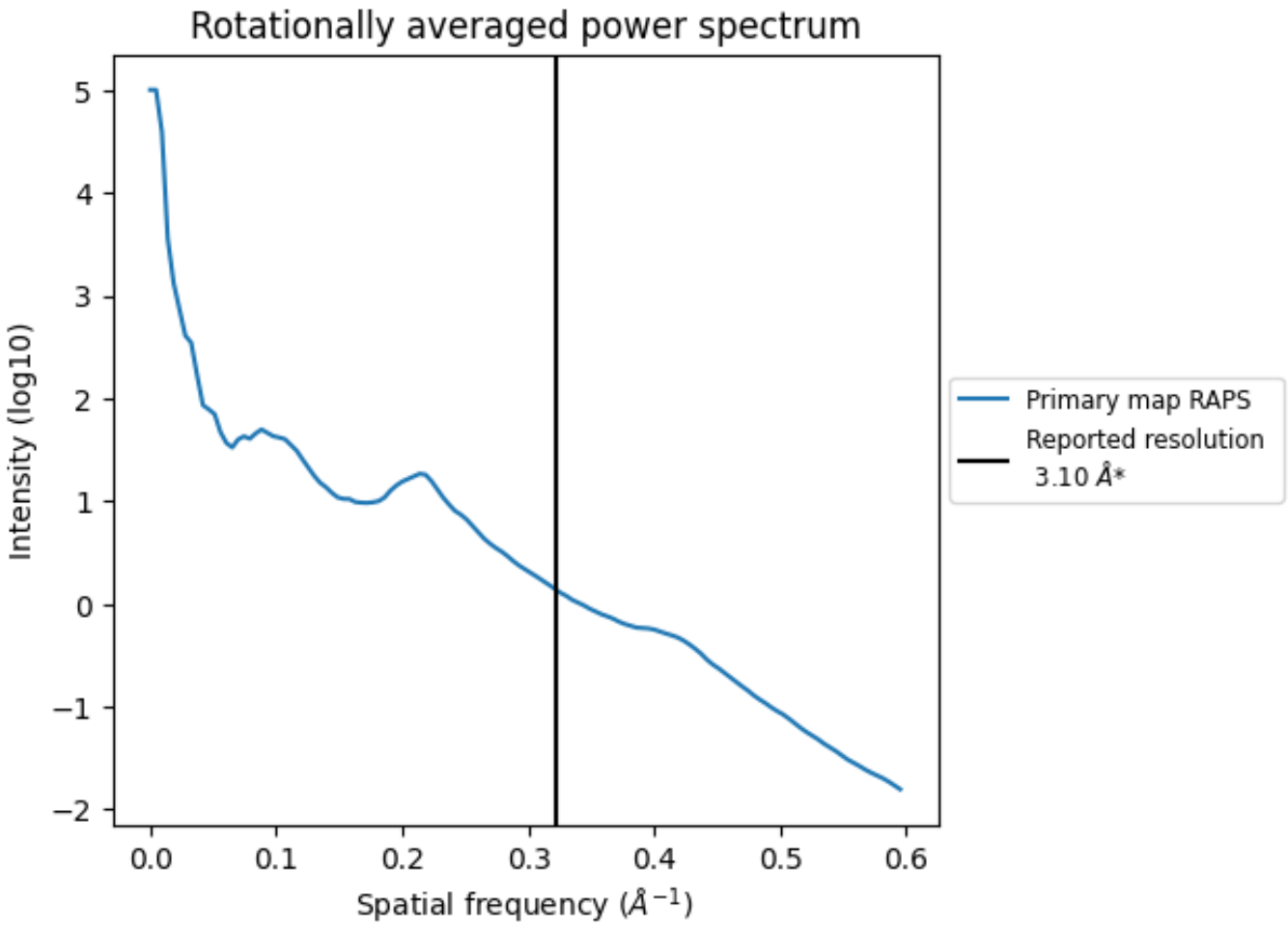
7.2 Volume estimate (i)



The volume at the recommended contour level is 103 nm^3; this corresponds to an approximate mass of 93 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 0.323 Å^{-1}

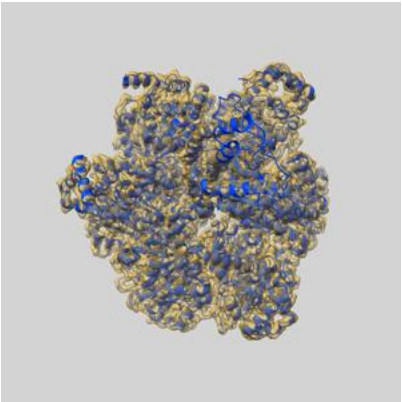
8 Fourier-Shell correlation (i)

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

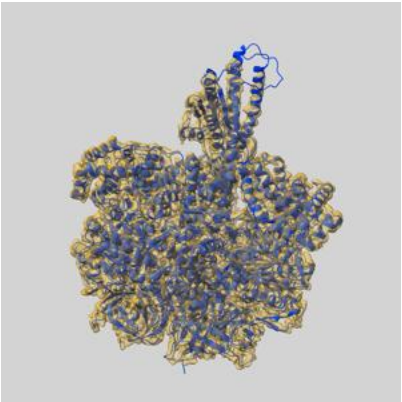
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-23116 and PDB model 7L1R. Per-residue inclusion information can be found in section 3 on page 8.

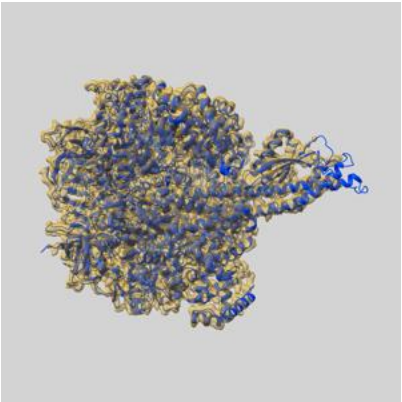
9.1 Map-model overlay (i)



X



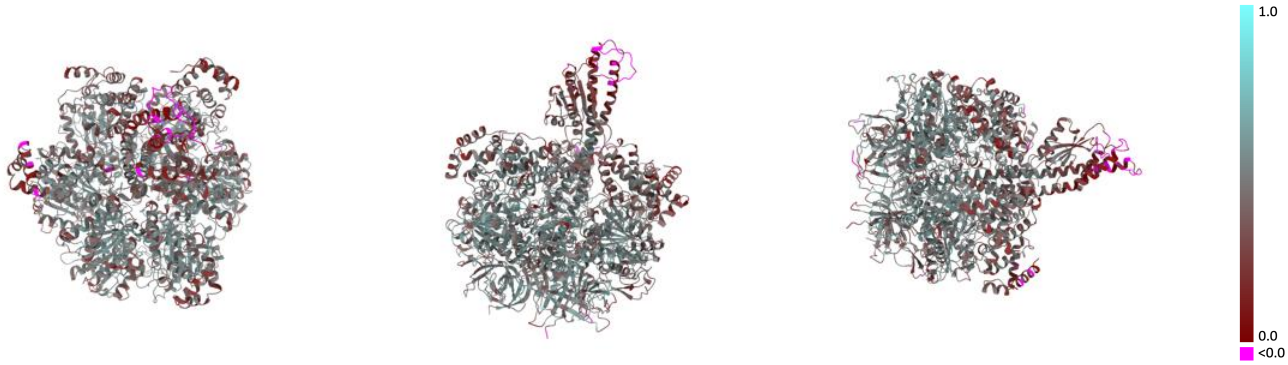
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

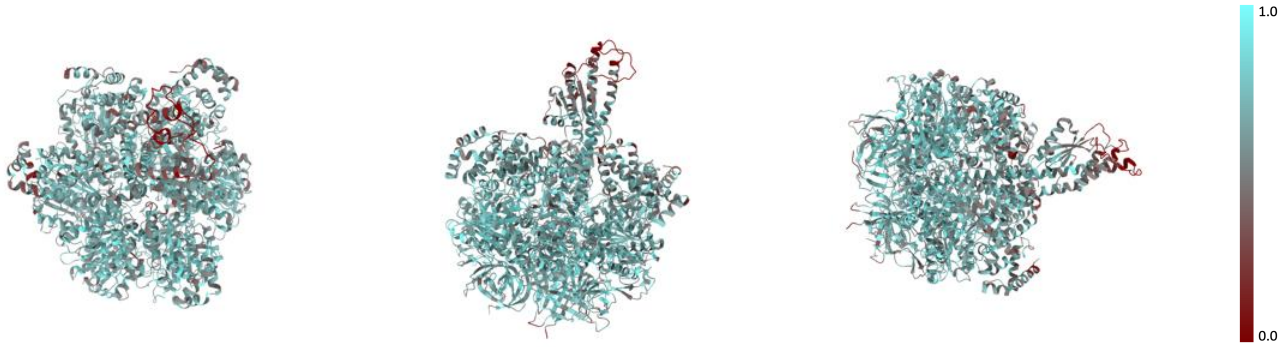
9.2 Q-score mapped to coordinate model (i)



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.

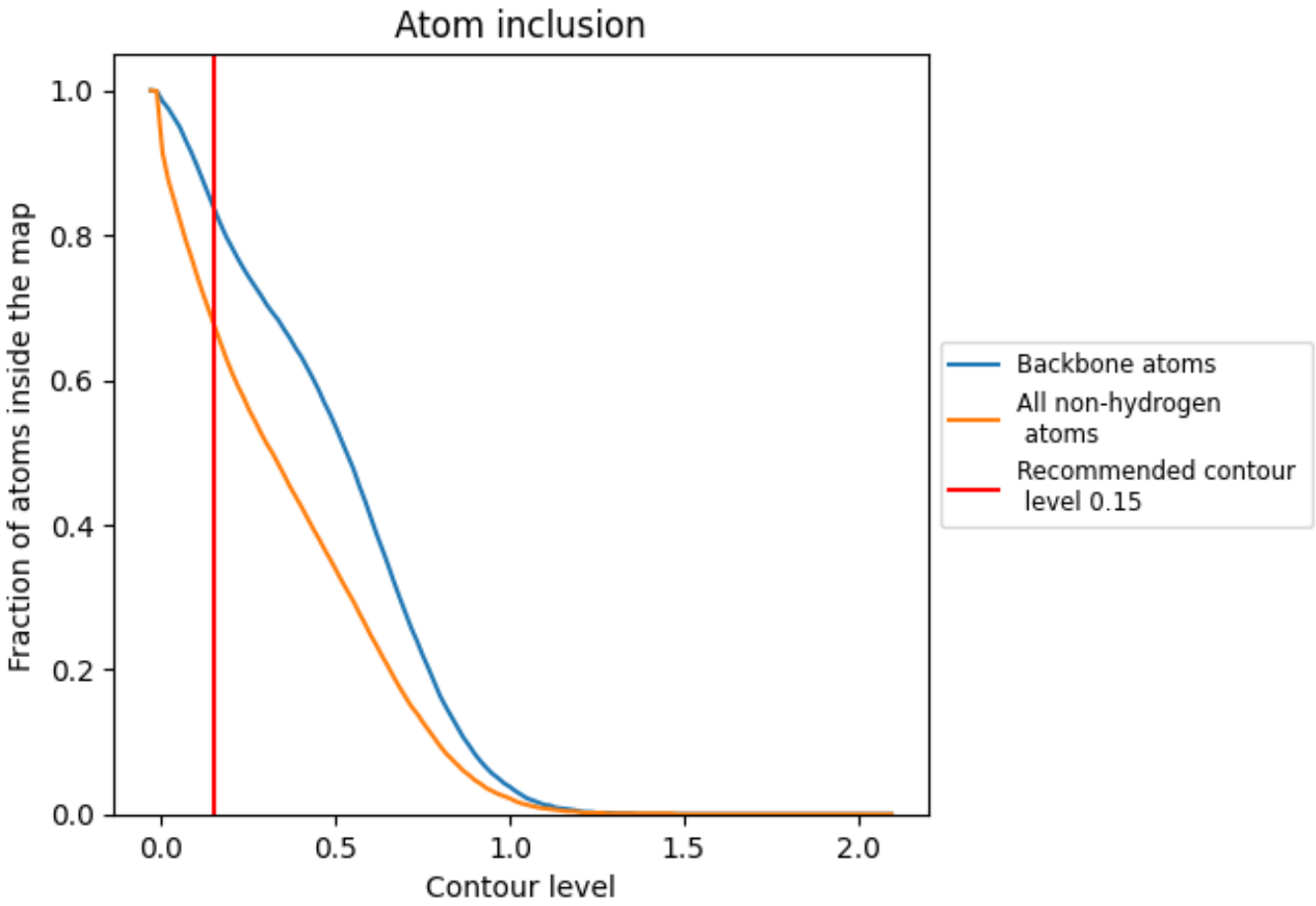
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 68% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6800	0.4440
A	0.6730	0.4170
B	0.6810	0.4290
C	0.7230	0.4780
D	0.7160	0.4820
E	0.6800	0.4590
F	0.7010	0.4840
G	0.5180	0.3030