



## Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 12:59 PM EST

PDB ID : 7L1Q  
EMDB ID : EMD-23115  
Title : PS3 F1-ATPase Binding/TS Dwell  
Authors : Sobti, M.; Ueno, H.; Noji, H.; Stewart, A.G.  
Deposited on : 2020-12-15  
Resolution : 3.40 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43  
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 : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

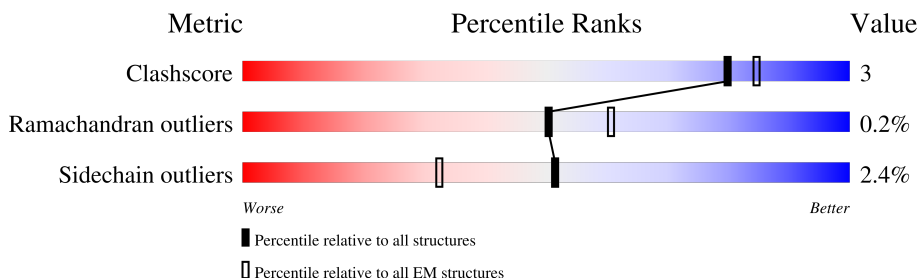
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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  $\geq 3$ , 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  $\leq 5\%$ . 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	
1	B	510	
1	C	510	
2	D	484	
2	E	484	
2	F	484	
3	G	285	

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 24204 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	Total	C	N	O	S	0	0
			3636	2303	637	687	9		
1	B	475	Total	C	N	O	S	0	0
			3643	2308	638	688	9		
1	C	476	Total	C	N	O	S	0	0
			3649	2311	639	690	9		

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
2	D	470	Total	C	N	O	S	0	0
			3621	2285	627	696	13		
2	E	470	Total	C	N	O	S	0	0
			3622	2285	627	696	14		
2	F	471	Total	C	N	O	S	0	0
			3629	2290	628	697	14		

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

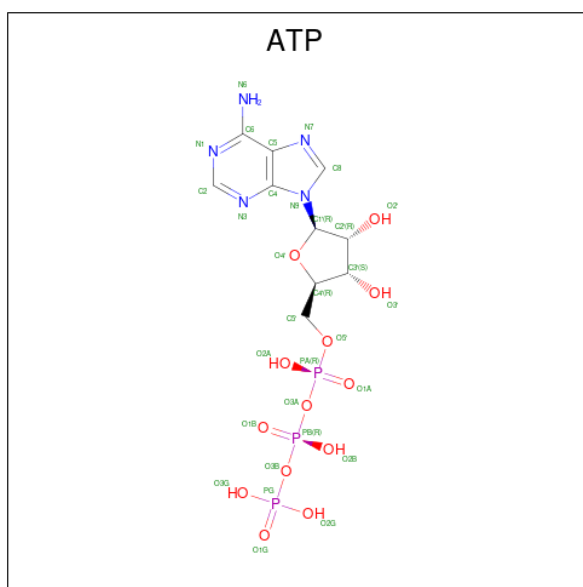
- Molecule 3 is a protein called ATP synthase gamma chain.

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



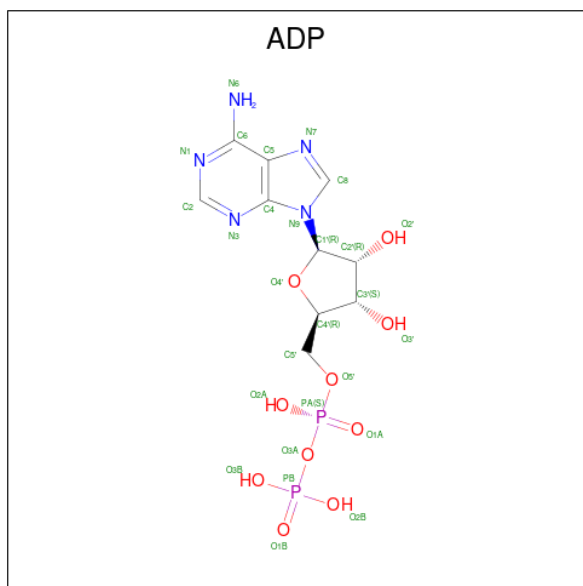
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
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	

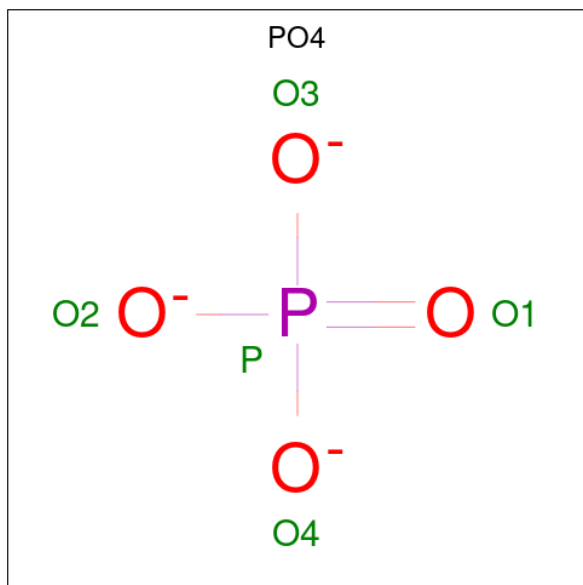
- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

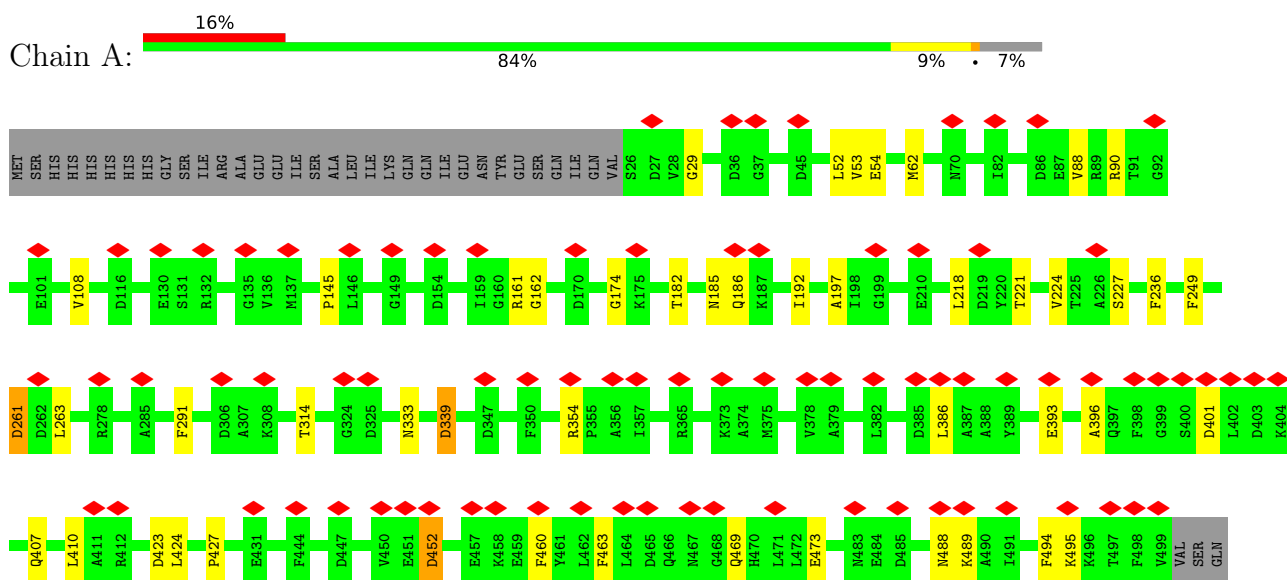


Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
7	D	1	5	4	1	0

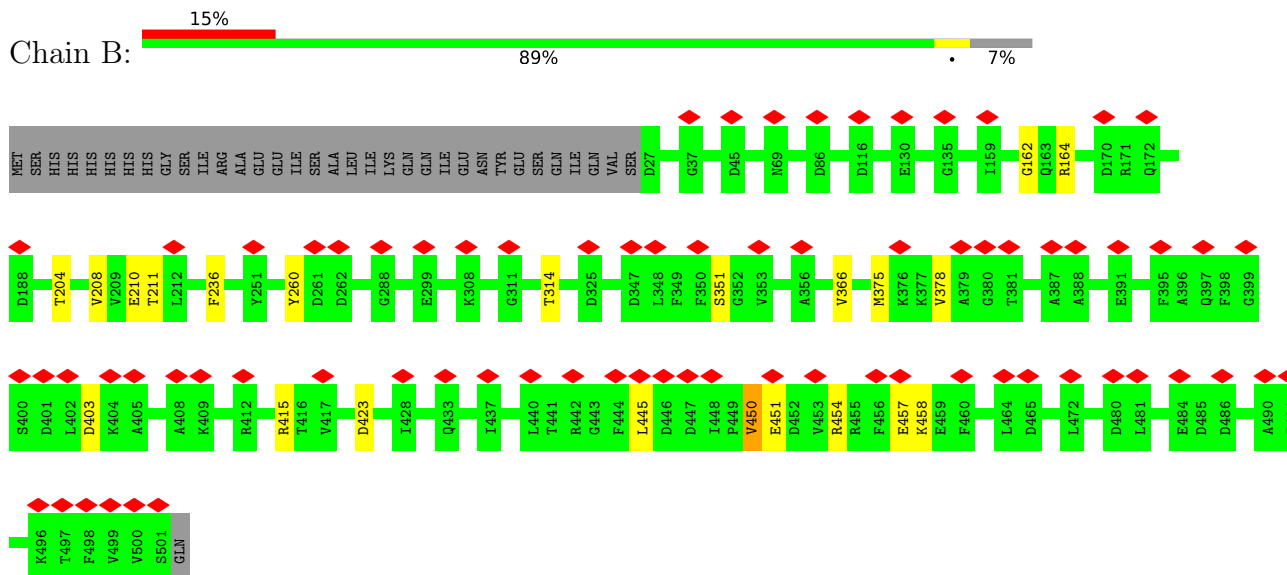
### 3 Residue-property plots

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

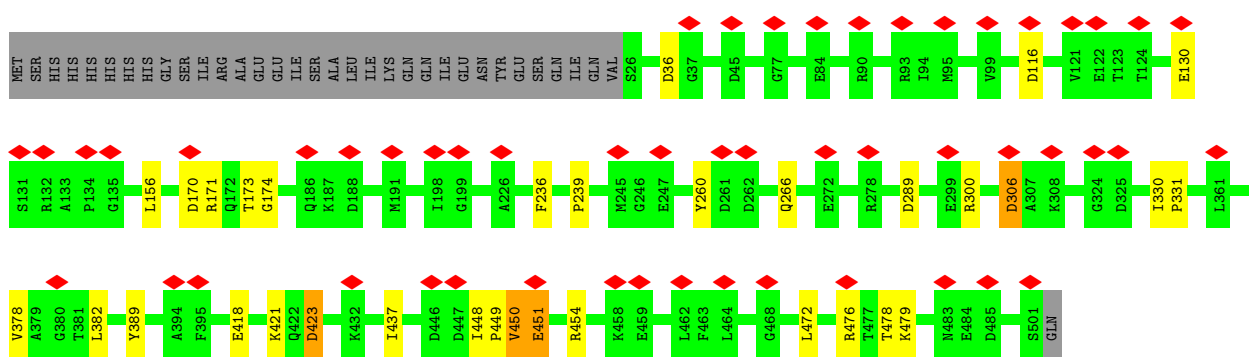
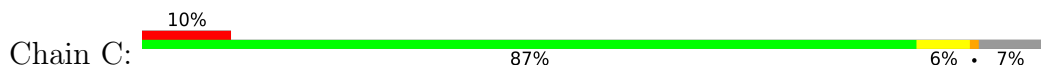


- Molecule 1: ATP synthase subunit alpha

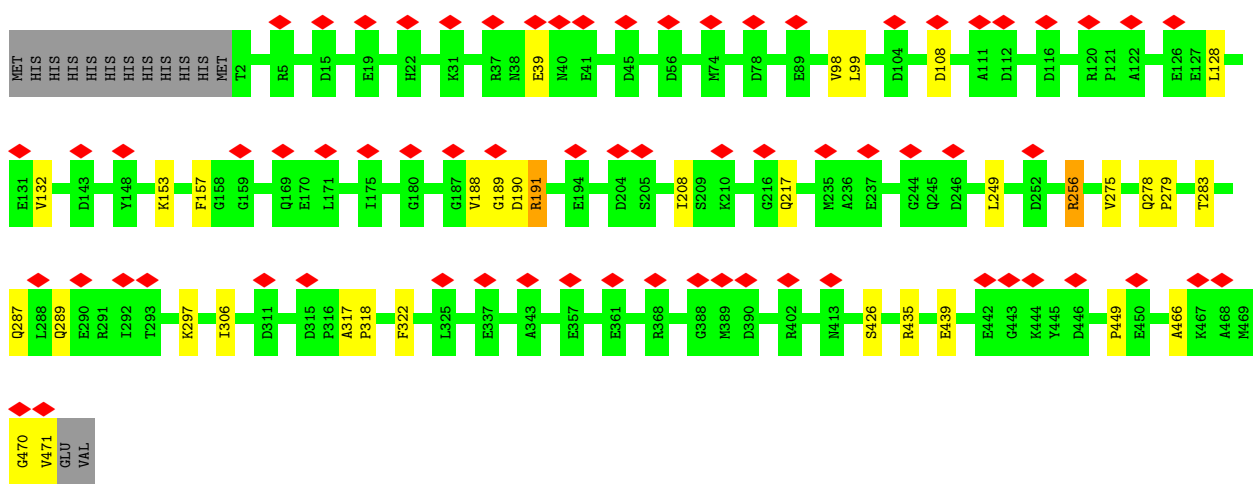
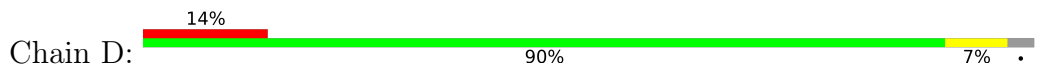


- Molecule 1: ATP synthase subunit alpha

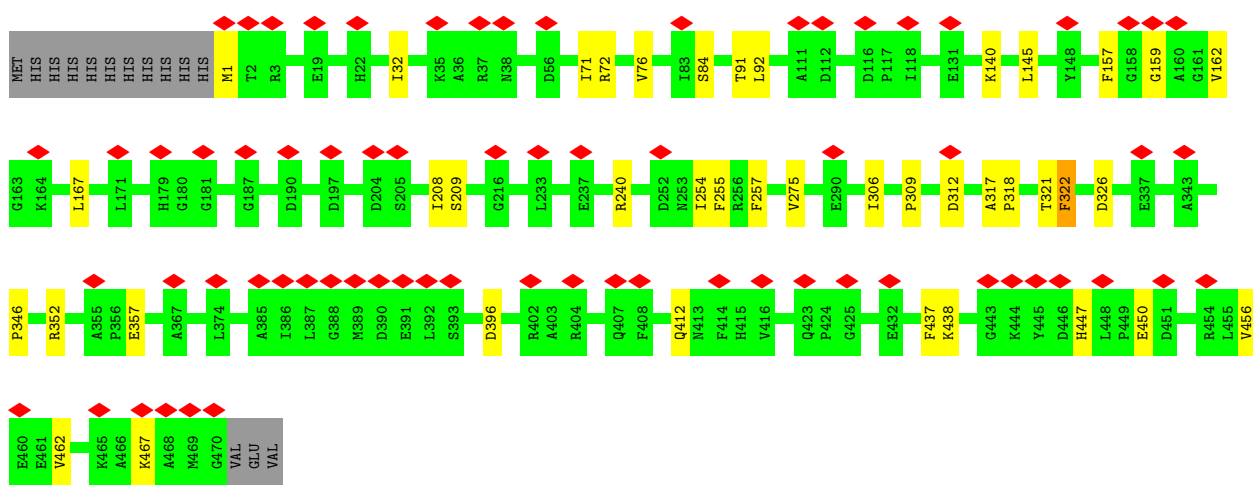
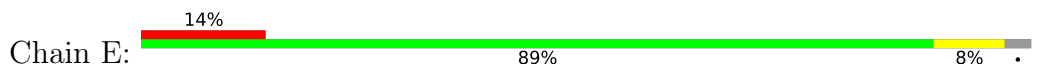




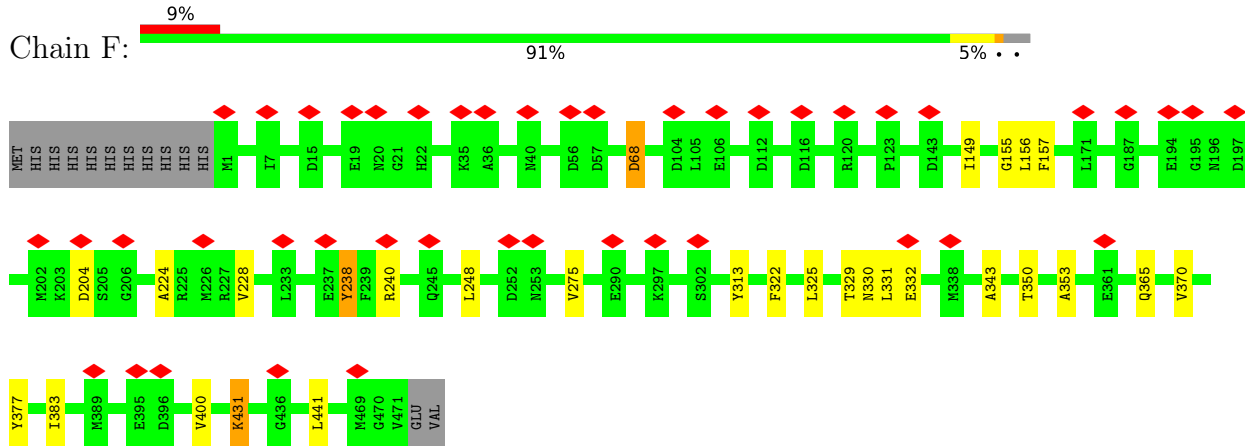
• Molecule 2: ATP synthase subunit beta



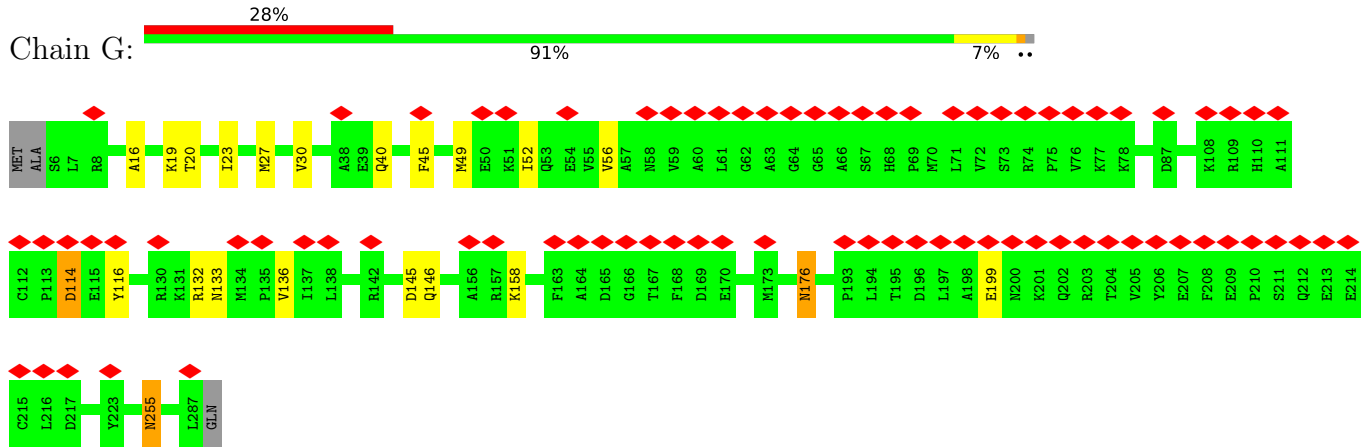
• Molecule 2: ATP synthase subunit beta



• Molecule 2: ATP synthase subunit beta



• Molecule 3: ATP synthase gamma chain



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	482550	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 ( $e^-/\text{\AA}^2$ )	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	1.855	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.049	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, PO4, ADP, ATP

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	0.39	0/3695	0.66	0/5004
1	B	0.39	0/3702	0.66	0/5014
1	C	0.41	0/3708	0.65	0/5022
2	D	0.39	0/3684	0.66	0/4991
2	E	0.39	0/3685	0.66	0/4991
2	F	0.40	0/3692	0.66	0/5001
3	G	0.37	0/2244	0.61	0/3036
All	All	0.39	0/24410	0.66	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	33	0
1	B	3643	0	3718	12	0
1	C	3649	0	3724	17	0
2	D	3621	0	3631	17	0
2	E	3622	0	3634	22	0
2	F	3629	0	3642	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	2211	0	2257	11	0
4	A	31	0	12	4	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	E	31	0	12	0	0
4	F	31	0	12	2	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	D	27	0	12	0	0
7	D	5	0	0	1	0
All	All	24204	0	24388	129	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 3.

All (129) 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)
1:A:185:ASN:HB2	1:A:427:PRO:HB2	1.70	0.71
2:D:189:GLY:O	2:D:256:ARG:NH1	2.25	0.69
1:B:450:VAL:HG13	1:B:451:GLU:H	1.56	0.69
1:A:185:ASN:O	1:A:185:ASN:ND2	2.28	0.67
2:F:370:VAL:HG23	2:F:441:LEU:HD11	1.77	0.66
1:A:354:ARG:HD3	4:A:600:ATP:N1	2.13	0.64
3:G:19:LYS:O	3:G:23:ILE:HG12	1.99	0.63
1:C:454:ARG:HH21	1:C:454:ARG:HG3	1.64	0.62
1:C:418:GLU:HG3	1:C:450:VAL:HG12	1.82	0.60
2:E:318:PRO:O	2:E:322:PHE:HB2	2.02	0.60
2:E:357:GLU:OE2	2:E:357:GLU:N	2.35	0.59
1:C:156:LEU:HD21	1:C:382:LEU:HD23	1.85	0.58
1:B:450:VAL:HG13	1:B:451:GLU:N	2.20	0.57
1:A:174:GLY:HA2	4:A:600:ATP:H5'1	1.86	0.57
1:A:460:PHE:HB2	1:A:494:PHE:CE2	2.40	0.57
2:E:357:GLU:H	2:E:357:GLU:CD	2.09	0.56
2:E:32:ILE:HG12	2:E:76:VAL:HG12	1.89	0.54
2:D:435:ARG:O	2:D:439:GLU:HG2	2.09	0.53
3:G:114:ASP:OD1	3:G:114:ASP:N	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:157:PHE:CE1	2:D:306:ILE:HD12	2.44	0.52
2:D:278:GLN:HB2	2:D:279:PRO:HD2	1.92	0.52
1:C:423:ASP:OD1	1:C:423:ASP:N	2.38	0.51
1:B:375:MET:HA	1:B:378:VAL:HG22	1.92	0.51
2:E:456:VAL:HG21	2:E:462:VAL:HG22	1.92	0.51
1:B:208:VAL:O	1:B:211:THR:N	2.44	0.51
4:F:500:ATP:H5'1	4:F:500:ATP:C8	2.46	0.51
2:E:255:PHE:CE1	2:E:309:PRO:HG3	2.45	0.51
2:E:32:ILE:CG1	2:E:76:VAL:HG12	2.42	0.50
1:A:185:ASN:HB2	1:A:427:PRO:CB	2.39	0.50
1:A:423:ASP:OD2	1:A:423:ASP:N	2.41	0.50
3:G:52:ILE:O	3:G:56:VAL:HG22	2.12	0.50
1:A:339:ASP:OD2	1:A:339:ASP:N	2.42	0.49
1:C:171:ARG:CZ	1:C:171:ARG:HB3	2.41	0.49
2:D:39:GLU:OE1	2:D:39:GLU:N	2.38	0.49
2:F:331:LEU:HA	2:F:343:ALA:O	2.12	0.49
1:A:401:ASP:OD2	1:A:401:ASP:N	2.46	0.48
2:F:68:ASP:OD2	2:F:68:ASP:N	2.47	0.48
2:D:39:GLU:H	2:D:39:GLU:CD	2.17	0.48
1:B:351:SER:O	1:B:351:SER:OG	2.30	0.48
1:C:306:ASP:OD1	1:C:306:ASP:N	2.45	0.48
2:D:283:THR:O	2:D:287:GLN:HG2	2.14	0.47
2:F:224:ALA:O	2:F:228:VAL:HG23	2.13	0.47
1:C:116:ASP:N	1:C:116:ASP:OD1	2.48	0.47
1:B:454:ARG:HG2	1:B:454:ARG:HH21	1.78	0.47
3:G:255:ASN:HD22	3:G:255:ASN:N	2.12	0.47
2:D:466:ALA:O	2:D:470:GLY:N	2.48	0.47
3:G:132:ARG:O	3:G:133:ASN:HB2	2.15	0.47
1:B:366:VAL:HG12	1:B:366:VAL:O	2.15	0.47
1:A:407:GLN:O	1:A:410:LEU:N	2.49	0.46
1:A:452:ASP:OD1	1:A:452:ASP:N	2.48	0.46
2:E:157:PHE:CE1	2:E:306:ILE:HB	2.51	0.46
1:A:218:LEU:HA	1:A:221:THR:HG22	1.97	0.46
1:A:489:LYS:HD2	1:A:489:LYS:N	2.30	0.46
2:F:350:THR:O	2:F:350:THR:OG1	2.31	0.46
1:C:454:ARG:HG3	1:C:454:ARG:NH2	2.28	0.45
1:A:463:PHE:CD2	1:A:494:PHE:HB2	2.52	0.45
2:E:254:ILE:O	2:E:257:PHE:HB3	2.16	0.45
2:E:467:LYS:HB2	2:E:467:LYS:HE2	1.48	0.45
1:C:330:ILE:HB	1:C:331:PRO:HD3	1.99	0.45
2:F:155:GLY:HA3	2:F:325:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:GLY:H	1:B:314:THR:HB	1.81	0.45
4:F:500:ATP:H5'1	4:F:500:ATP:H8	1.81	0.45
3:G:136:VAL:HG23	3:G:136:VAL:O	2.17	0.44
2:D:191:ARG:NH2	7:D:501:PO4:O3	2.51	0.44
1:B:208:VAL:C	1:B:210:GLU:N	2.71	0.44
1:A:108:VAL:O	1:A:224:VAL:HA	2.18	0.44
1:A:291:PHE:HA	1:A:333:ASN:HD21	1.83	0.44
1:C:478:THR:O	1:C:479:LYS:HB2	2.18	0.44
1:A:424:LEU:HD13	4:A:600:ATP:C5	2.53	0.44
1:A:192:ILE:HG21	1:A:249:PHE:CE1	2.53	0.44
1:C:239:PRO:HB3	1:C:260:TYR:CD1	2.52	0.44
2:E:140:LYS:HE2	2:E:412:GLN:HB3	1.99	0.44
1:A:407:GLN:O	1:A:410:LEU:HB2	2.17	0.43
2:F:238:TYR:CD2	2:F:238:TYR:C	2.91	0.43
2:D:157:PHE:CZ	2:D:306:ILE:HD12	2.53	0.43
2:E:71:ILE:HG22	2:E:72:ARG:N	2.33	0.43
2:E:167:LEU:HD12	2:E:167:LEU:HA	1.77	0.43
2:D:317:ALA:HB3	2:D:318:PRO:HD3	1.99	0.43
2:D:153:LYS:HE2	2:D:289:GLN:O	2.19	0.43
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.80	0.43
1:B:423:ASP:OD2	1:B:423:ASP:N	2.39	0.43
1:A:182:THR:O	1:A:186:GLN:HG2	2.19	0.43
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.85	0.42
1:A:162:GLY:H	1:A:314:THR:HB	1.83	0.42
2:D:188:VAL:HG13	2:D:188:VAL:O	2.19	0.42
1:A:145:PRO:O	1:A:161:ARG:NH1	2.52	0.42
1:B:403:ASP:OD1	1:B:403:ASP:N	2.50	0.42
2:E:159:GLY:O	2:E:162:VAL:HG22	2.18	0.42
2:E:145:LEU:HD13	2:E:346:PRO:HB3	2.01	0.42
2:F:156:LEU:HD23	2:F:329:THR:HB	2.02	0.42
2:D:449:PRO:HD3	2:D:471:VAL:HG11	2.01	0.42
2:E:317:ALA:O	2:E:321:THR:HG23	2.20	0.42
1:A:29:GLY:O	1:A:88:VAL:HG12	2.20	0.42
1:A:495:LYS:HE2	1:A:495:LYS:HB3	1.87	0.42
2:F:313:TYR:N	2:F:313:TYR:CD2	2.88	0.42
2:E:71:ILE:HG22	2:E:72:ARG:H	1.84	0.42
2:E:92:LEU:HD23	2:E:92:LEU:HA	1.89	0.42
3:G:45:PHE:O	3:G:49:MET:HG2	2.19	0.42
1:C:130:GLU:HA	1:C:300:ARG:HH22	1.85	0.42
1:C:421:LYS:HB2	1:C:454:ARG:HD3	2.02	0.42
1:C:448:ILE:HA	1:C:449:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLU:HA	1:A:396:ALA:HB2	2.01	0.41
1:A:469:GLN:O	1:A:473:GLU:HG2	2.20	0.41
3:G:16:ALA:O	3:G:20:THR:HG23	2.20	0.41
1:A:424:LEU:HD13	4:A:600:ATP:C4	2.56	0.41
1:C:472:LEU:O	1:C:476:ARG:HG3	2.21	0.41
3:G:27:MET:HA	3:G:30:VAL:HG12	2.03	0.41
3:G:199:GLU:H	3:G:199:GLU:CD	2.24	0.41
2:E:208:ILE:HG23	2:E:209:SER:N	2.35	0.41
2:D:190:ASP:O	2:D:217:GLN:NE2	2.52	0.41
2:F:377:TYR:HE1	2:F:400:VAL:HG23	1.84	0.41
2:E:326:ASP:OD2	2:E:352:ARG:NE	2.45	0.41
2:F:332:GLU:OE2	2:F:332:GLU:HA	2.20	0.41
2:E:438:LYS:HE2	2:E:438:LYS:HB3	1.99	0.41
2:D:297:LYS:HD2	2:D:297:LYS:N	2.36	0.41
2:F:157:PHE:HB2	2:F:330:ASN:HD22	1.85	0.41
2:F:431:LYS:HD2	2:F:431:LYS:O	2.20	0.41
2:E:456:VAL:HG21	2:E:462:VAL:CG2	2.49	0.41
2:D:98:VAL:HG13	2:D:99:LEU:HG	2.03	0.40
1:A:197:ALA:HA	1:A:261:ASP:OD2	2.21	0.40
2:F:383:ILE:HD12	2:F:383:ILE:HA	1.98	0.40
1:A:53:VAL:CG1	1:A:88:VAL:HG22	2.51	0.40
1:B:415:ARG:HH11	1:B:415:ARG:HG3	1.85	0.40
1:C:451:GLU:H	1:C:451:GLU:HG3	1.39	0.40
1:A:263:LEU:HD23	1:A:263:LEU:HA	1.83	0.40
1:C:378:VAL:HG12	1:C:437:ILE:HG22	2.03	0.40
2:F:149:ILE:HG12	2:F:353:ALA:HB2	2.03	0.40
3:G:176:ASN:N	3:G:176:ASN:OD1	2.55	0.40
1:A:407:GLN:HA	1:A:410:LEU:HD12	2.03	0.40

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%)	456 (97%)	16 (3%)	0	100	100
1	B	473/510 (93%)	450 (95%)	22 (5%)	1 (0%)	47	78
1	C	474/510 (93%)	458 (97%)	15 (3%)	1 (0%)	47	78
2	D	468/484 (97%)	452 (97%)	15 (3%)	1 (0%)	47	78
2	E	468/484 (97%)	449 (96%)	18 (4%)	1 (0%)	47	78
2	F	469/484 (97%)	445 (95%)	23 (5%)	1 (0%)	47	78
3	G	280/285 (98%)	274 (98%)	6 (2%)	0	100	100
All	All	3104/3267 (95%)	2984 (96%)	115 (4%)	5 (0%)	50	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	450	VAL
2	F	275	VAL
2	E	275	VAL
1	C	174	GLY
2	D	275	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	A	386/419 (92%)	377 (98%)	9 (2%)	50	74
1	B	387/419 (92%)	380 (98%)	7 (2%)	59	79
1	C	388/419 (93%)	377 (97%)	11 (3%)	43	70
2	D	386/400 (96%)	377 (98%)	9 (2%)	50	74
2	E	386/400 (96%)	376 (97%)	10 (3%)	46	72
2	F	387/400 (97%)	379 (98%)	8 (2%)	53	76
3	G	238/240 (99%)	230 (97%)	8 (3%)	37	65
All	All	2558/2697 (95%)	2496 (98%)	62 (2%)	51	74

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	62	MET
1	A	90	ARG
1	A	227	SER
1	A	236	PHE
1	A	261	ASP
1	A	339	ASP
1	A	452	ASP
1	A	488	ASN
1	B	164	ARG
1	B	204	THR
1	B	236	PHE
1	B	260	TYR
1	B	445	LEU
1	B	457	GLU
1	B	458	LYS
1	C	36	ASP
1	C	170	ASP
1	C	173	THR
1	C	236	PHE
1	C	266	GLN
1	C	289	ASP
1	C	306	ASP
1	C	389	TYR
1	C	423	ASP
1	C	450	VAL
1	C	451	GLU
2	D	108	ASP
2	D	128	LEU
2	D	132	VAL
2	D	191	ARG
2	D	208	ILE
2	D	249	LEU
2	D	256	ARG
2	D	322	PHE
2	D	426	SER
2	E	1	MET
2	E	84	SER
2	E	91	THR
2	E	240	ARG
2	E	312	ASP
2	E	322	PHE
2	E	396	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	E	437	PHE
2	E	447	HIS
2	E	450	GLU
2	F	68	ASP
2	F	204	ASP
2	F	238	TYR
2	F	240	ARG
2	F	248	LEU
2	F	322	PHE
2	F	365	GLN
2	F	431	LYS
3	G	40	GLN
3	G	114	ASP
3	G	116	TYR
3	G	145	ASP
3	G	146	GLN
3	G	158	LYS
3	G	176	ASN
3	G	255	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	185	ASN
1	A	407	GLN
1	A	469	GLN
1	A	474	HIS
1	B	143	HIS
1	B	470	HIS
1	C	407	GLN
1	C	488	ASN
2	D	33	GLN
2	D	196	ASN
2	D	217	GLN
2	D	365	GLN
2	E	33	GLN
2	E	177	GLN
2	E	200	HIS
2	E	381	GLN
2	F	33	GLN
2	F	119	HIS
2	F	289	GLN

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Mol	Chain	Res	Type
2	F	304	GLN
2	F	324	HIS
2	F	330	ASN
3	G	255	ASN
3	G	266	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 13 ligands modelled in this entry, 6 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	$\# Z  > 2$
7	PO4	D	501	5	4,4,4	0.92	0	6,6,6	0.42	0
4	ATP	B	600	5	26,33,33	0.98	1 (3%)	31,52,52	1.47	4 (12%)
4	ATP	C	602	5	26,33,33	0.75	0	31,52,52	1.27	4 (12%)
6	ADP	D	500	5	24,29,29	0.99	1 (4%)	29,45,45	1.35	5 (17%)
4	ATP	E	501	5	26,33,33	0.69	0	31,52,52	1.06	2 (6%)
4	ATP	F	500	5	26,33,33	0.73	0	31,52,52	1.10	3 (9%)
4	ATP	A	600	5	26,33,33	0.99	1 (3%)	31,52,52	1.97	7 (22%)

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	B	600	5	-	6/18/38/38	0/3/3/3
4	ATP	C	602	5	-	4/18/38/38	0/3/3/3
6	ADP	D	500	5	-	3/12/32/32	0/3/3/3
4	ATP	E	501	5	-	1/18/38/38	0/3/3/3
4	ATP	F	500	5	-	2/18/38/38	0/3/3/3
4	ATP	A	600	5	-	4/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	ATP	C5-C4	2.71	1.48	1.40
6	D	500	ADP	C5-C4	2.59	1.47	1.40
4	B	600	ATP	C5-C4	2.56	1.47	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	ATP	PA-O3A-PB	-4.71	116.65	132.83
4	A	600	ATP	C3'-C2'-C1'	4.44	107.67	100.98
4	B	600	ATP	PB-O3B-PG	-4.05	118.94	132.83
4	A	600	ATP	O4'-C1'-C2'	-3.93	101.18	106.93
4	C	602	ATP	PA-O3A-PB	-3.66	120.28	132.83
6	D	500	ADP	N3-C2-N1	-3.53	123.16	128.68
4	A	600	ATP	N3-C2-N1	-3.44	123.31	128.68
4	B	600	ATP	N3-C2-N1	-3.30	123.53	128.68
4	F	500	ATP	PA-O3A-PB	-3.22	121.77	132.83
4	E	501	ATP	PB-O3B-PG	-3.19	121.88	132.83
4	A	600	ATP	C4-C5-N7	-3.12	106.15	109.40
4	A	600	ATP	O3'-C3'-C2'	-2.97	102.22	111.82
4	A	600	ATP	PB-O3B-PG	-2.89	122.89	132.83
4	C	602	ATP	PB-O3B-PG	-2.87	122.97	132.83
4	C	602	ATP	O4'-C1'-C2'	-2.73	102.94	106.93
4	E	501	ATP	C5-C6-N6	2.71	124.47	120.35
6	D	500	ADP	PA-O3A-PB	-2.70	123.56	132.83
6	D	500	ADP	O3B-PB-O2B	2.41	116.86	107.64
6	D	500	ADP	C4-C5-N7	-2.41	106.89	109.40
4	C	602	ATP	C5-C6-N6	2.39	123.99	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	500	ATP	PB-O3B-PG	-2.28	125.01	132.83
4	F	500	ATP	C5-C6-N6	2.28	123.81	120.35
4	B	600	ATP	PA-O3A-PB	-2.25	125.12	132.83
6	D	500	ADP	C2-N1-C6	2.16	122.45	118.75
4	B	600	ATP	C4-C5-N7	-2.04	107.27	109.40

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	ATP	C5'-O5'-PA-O1A
4	A	600	ATP	C5'-O5'-PA-O2A
4	A	600	ATP	O4'-C4'-C5'-O5'
4	C	602	ATP	C5'-O5'-PA-O1A
4	C	602	ATP	O4'-C4'-C5'-O5'
4	C	602	ATP	C3'-C4'-C5'-O5'
6	D	500	ADP	C5'-O5'-PA-O3A
4	B	600	ATP	O4'-C4'-C5'-O5'
4	B	600	ATP	C4'-C5'-O5'-PA
4	C	602	ATP	C5'-O5'-PA-O3A
6	D	500	ADP	C5'-O5'-PA-O2A
4	B	600	ATP	C3'-C4'-C5'-O5'
4	B	600	ATP	PB-O3A-PA-O2A
4	F	500	ATP	O4'-C4'-C5'-O5'
4	E	501	ATP	O4'-C4'-C5'-O5'
6	D	500	ADP	O4'-C4'-C5'-O5'
4	A	600	ATP	C5'-O5'-PA-O3A
4	F	500	ATP	C5'-O5'-PA-O3A
4	B	600	ATP	PG-O3B-PB-O1B
4	B	600	ATP	PG-O3B-PB-O2B

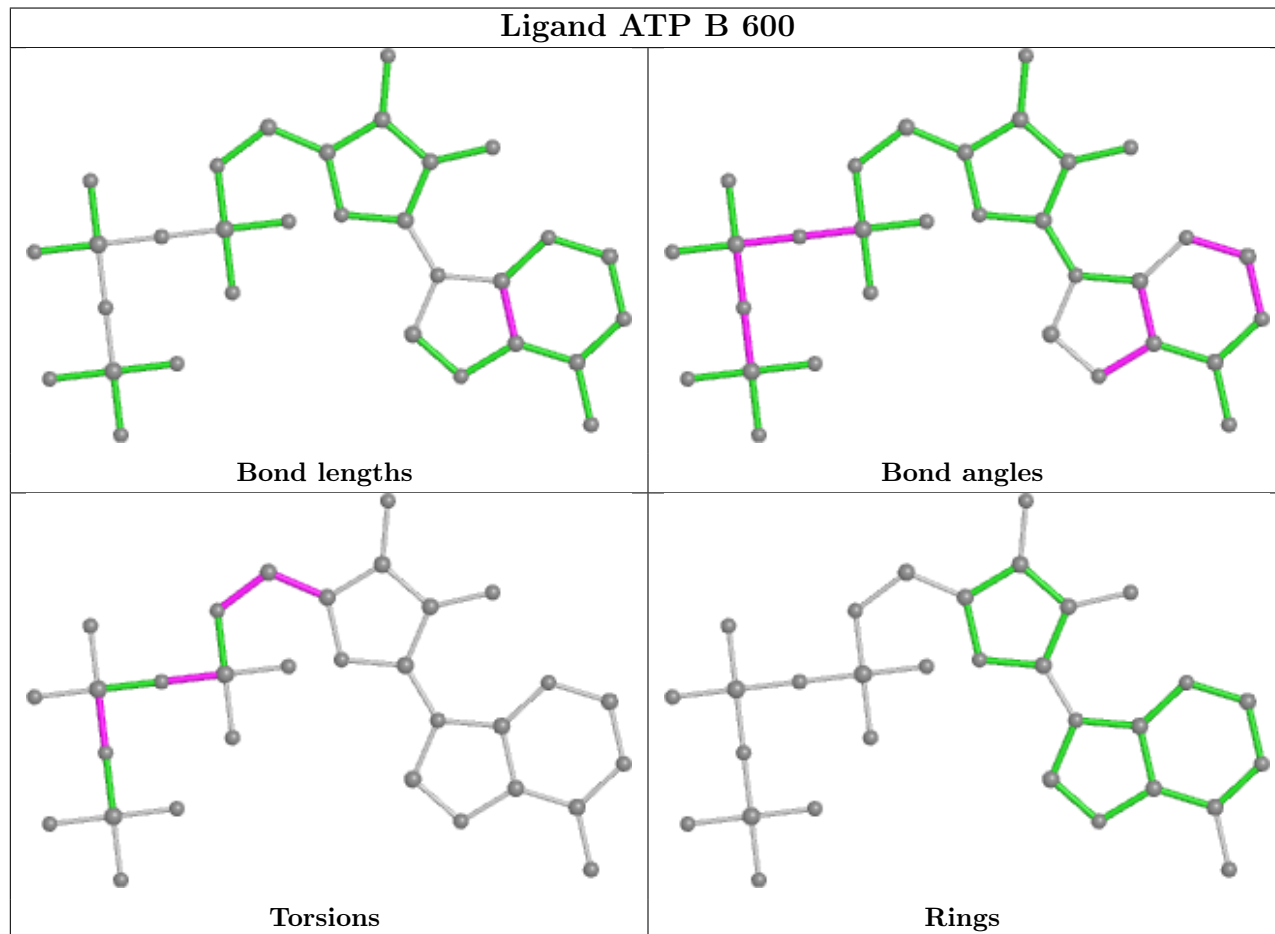
There are no ring outliers.

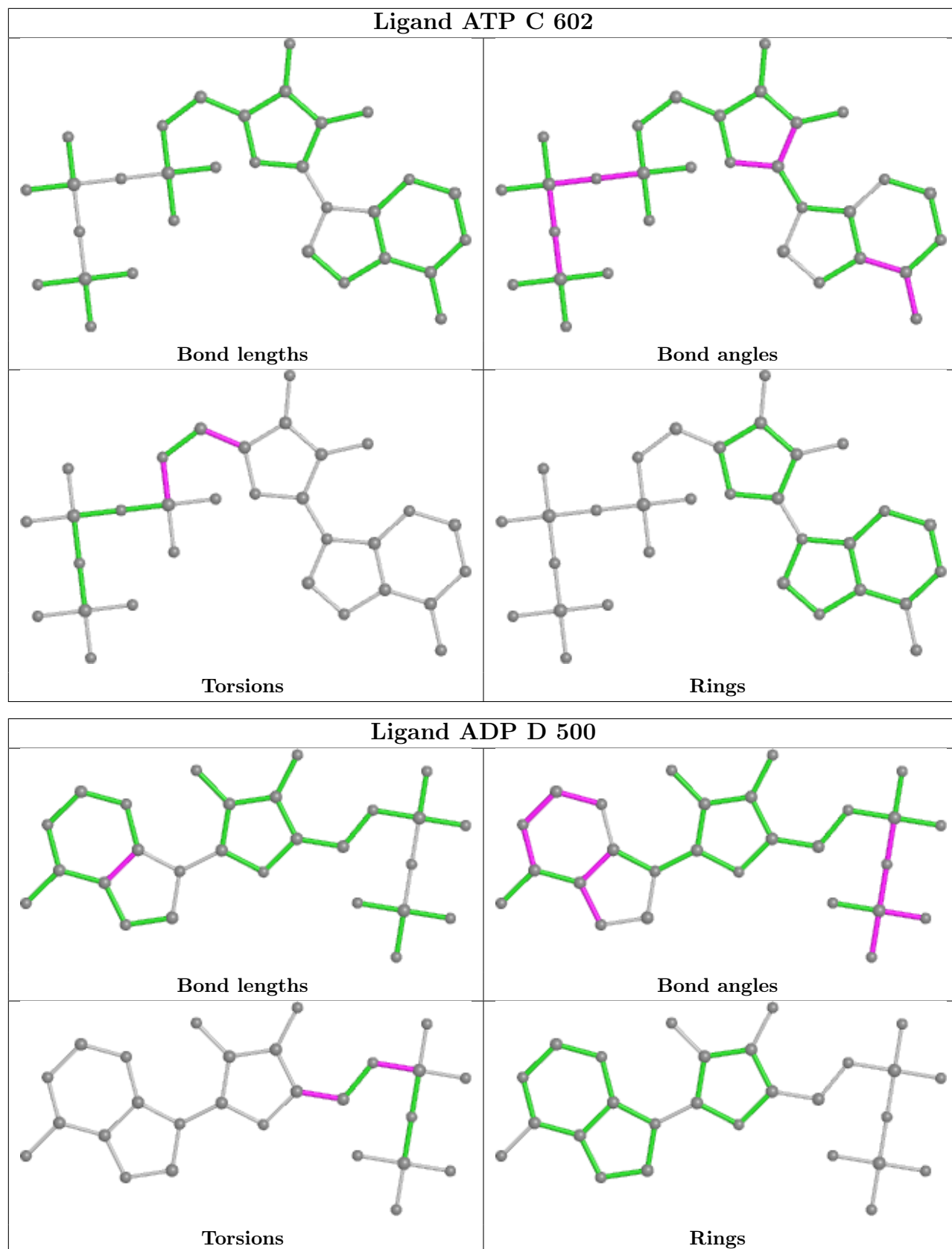
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	501	PO4	1	0
4	F	500	ATP	2	0
4	A	600	ATP	4	0

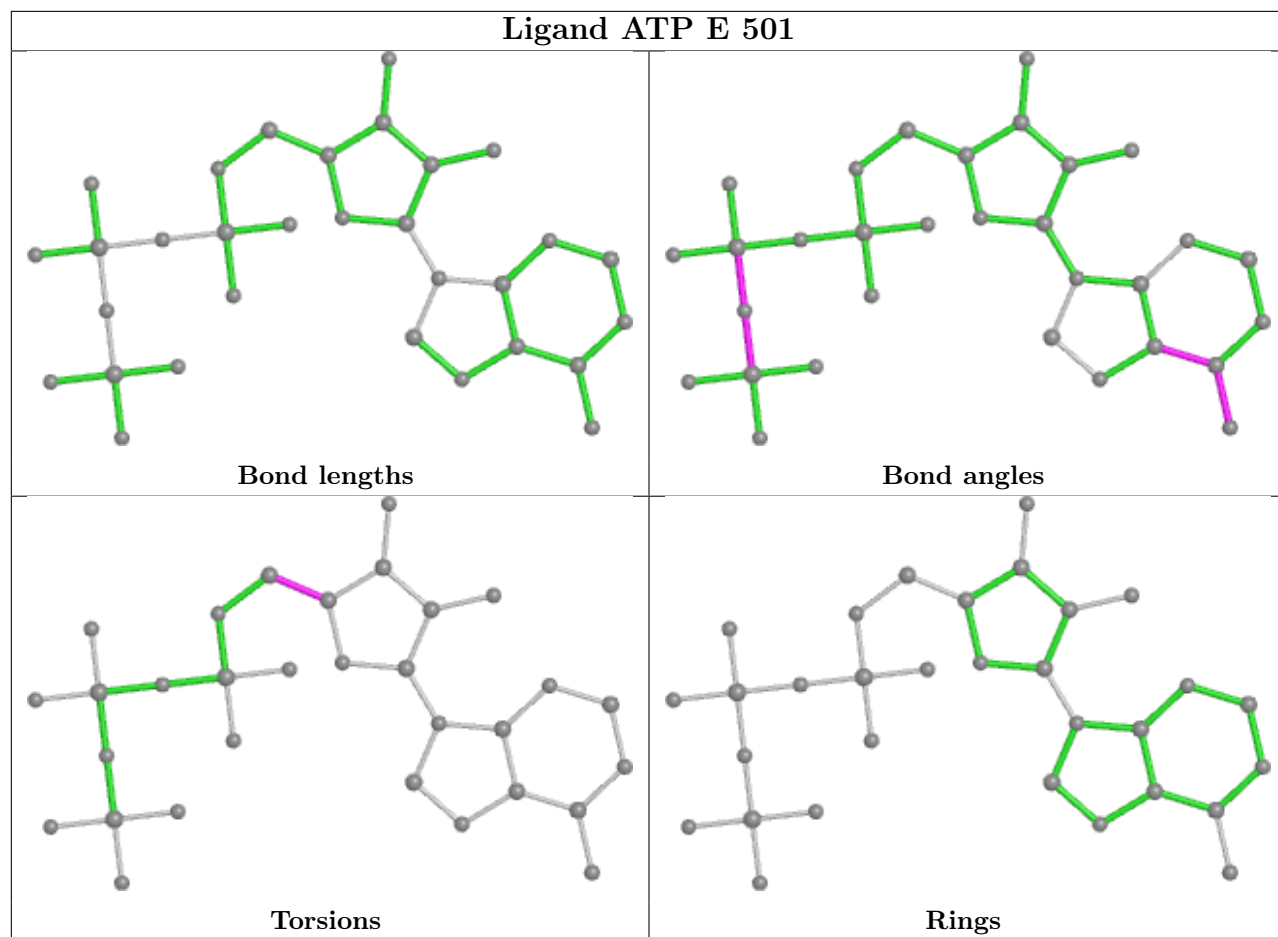
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

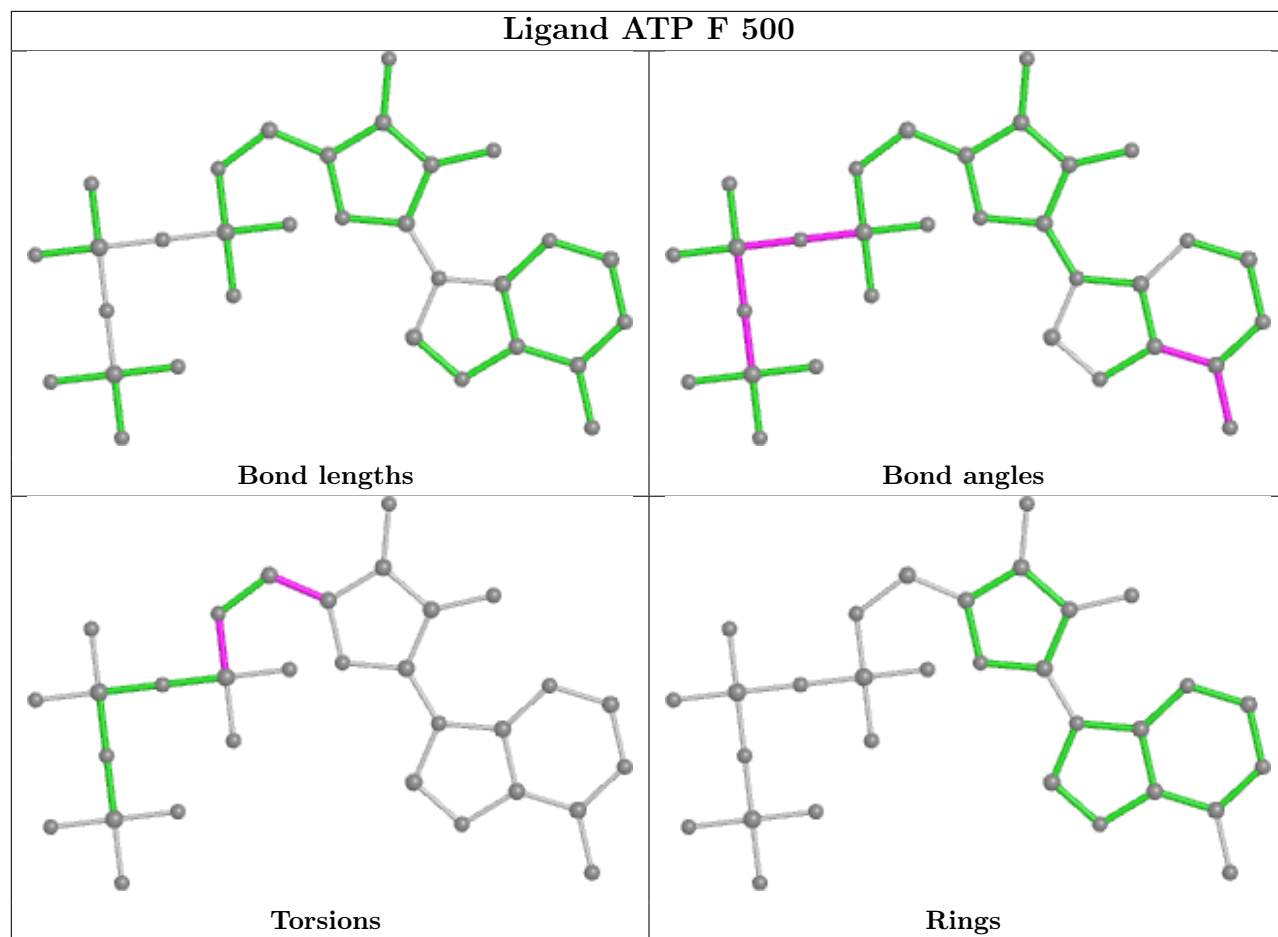
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

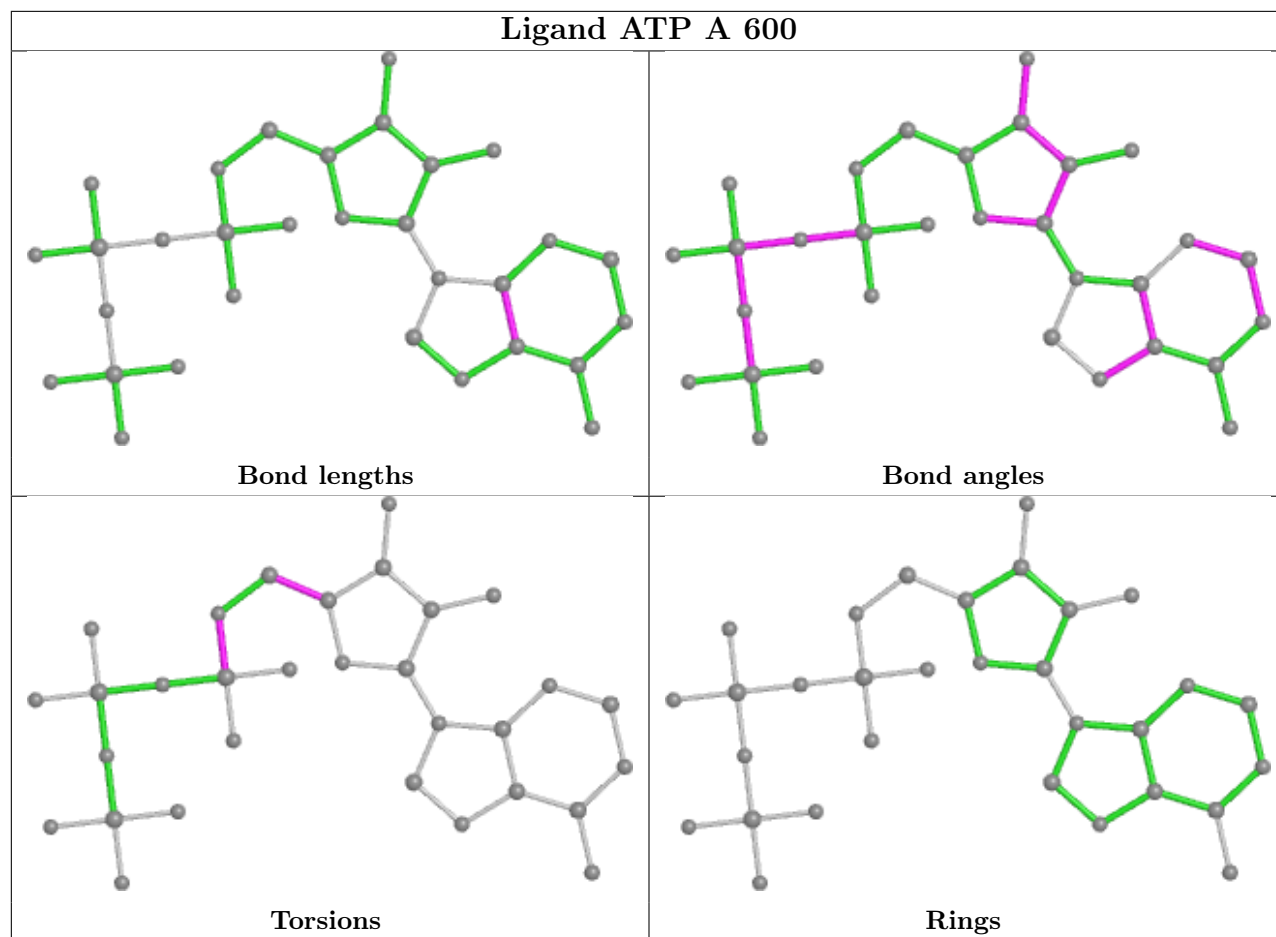












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

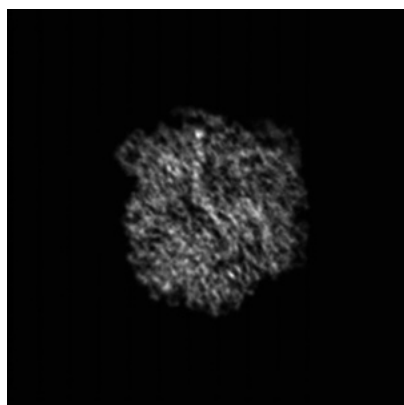
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23115. These allow visual inspection of the internal detail of the map and identification of artifacts.

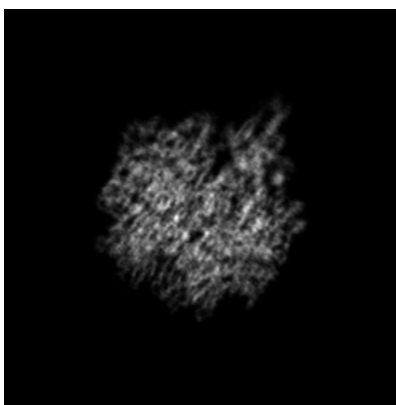
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

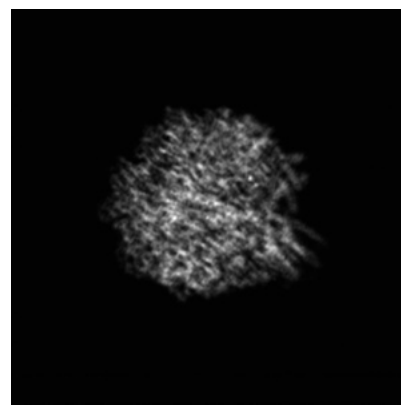
#### 6.1.1 Primary map



X



Y



Z

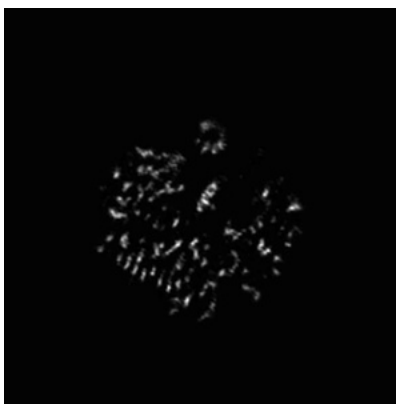
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

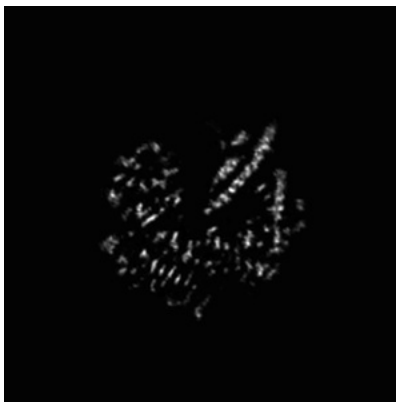
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

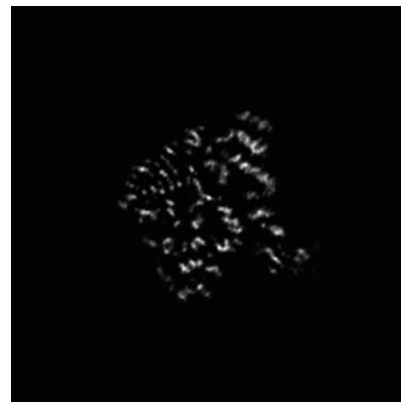
### 6.3.1 Primary map



X Index: 113



Y Index: 122

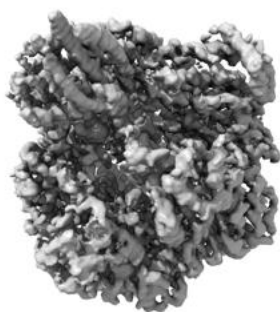


Z Index: 162

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

## 6.4 Orthogonal surface views [i](#)

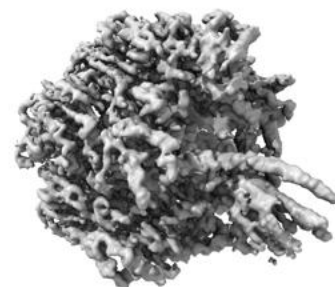
### 6.4.1 Primary map



X



Y



Z

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.

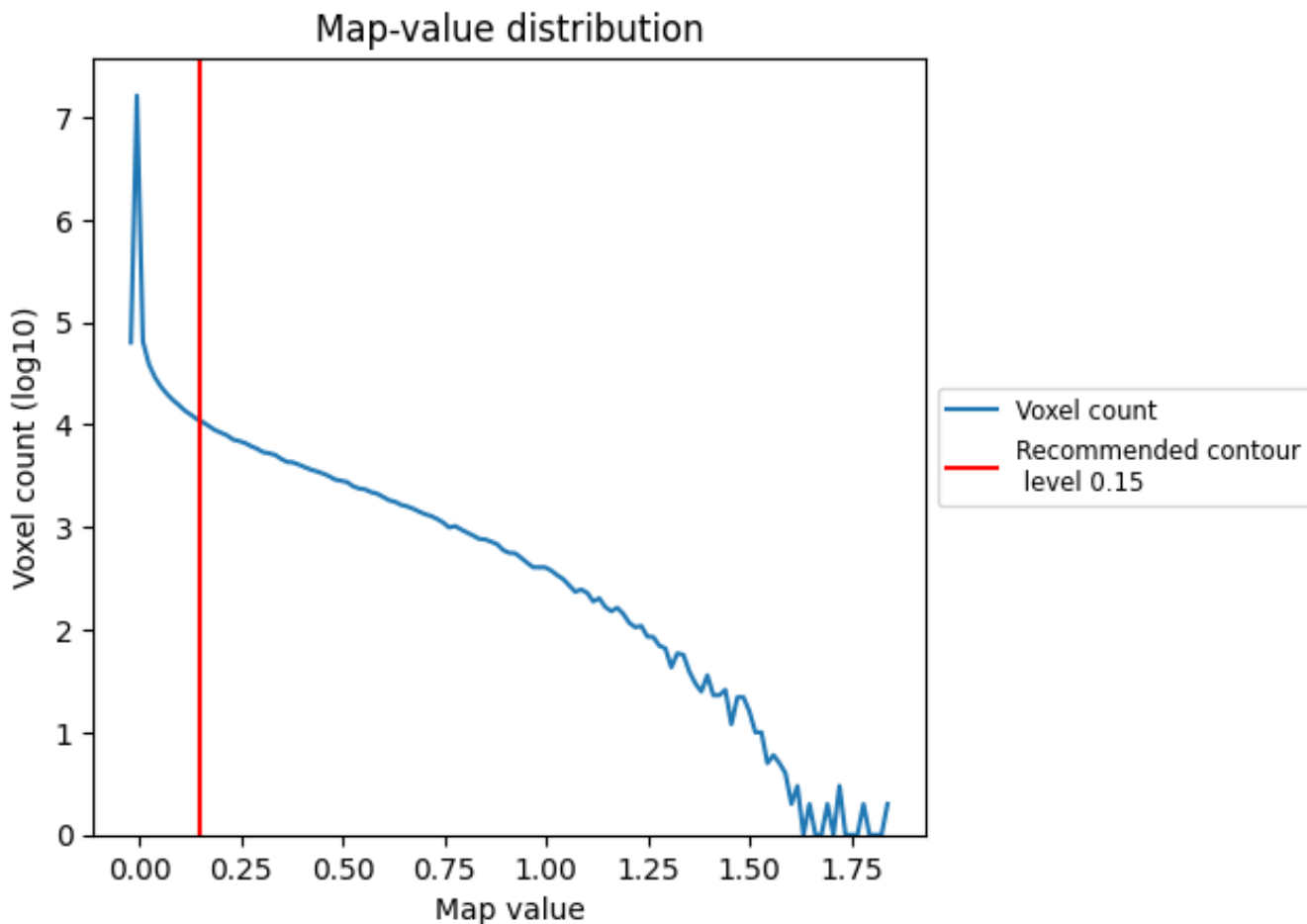
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

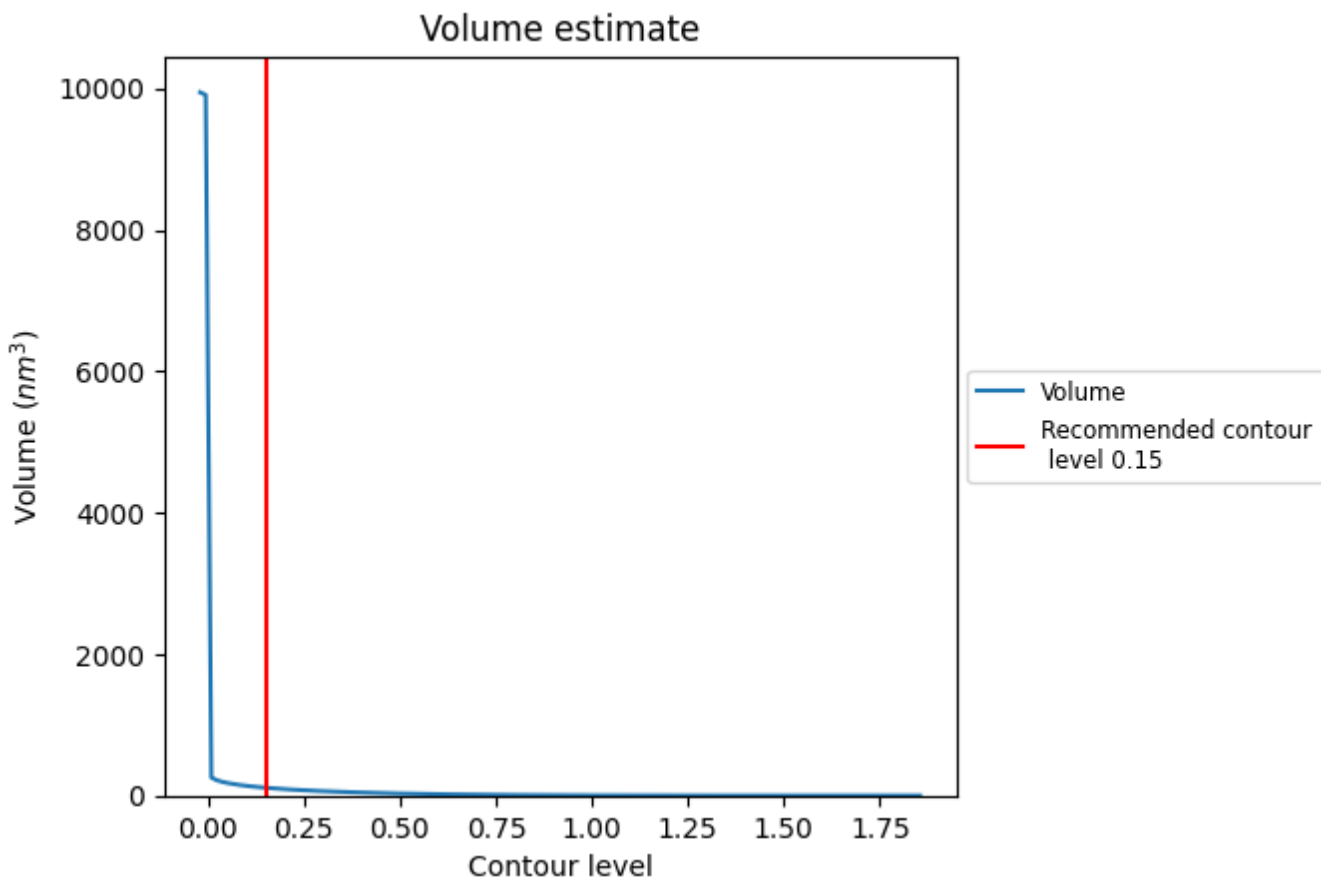
This section contains the results of statistical analysis of the map.

### 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](#)

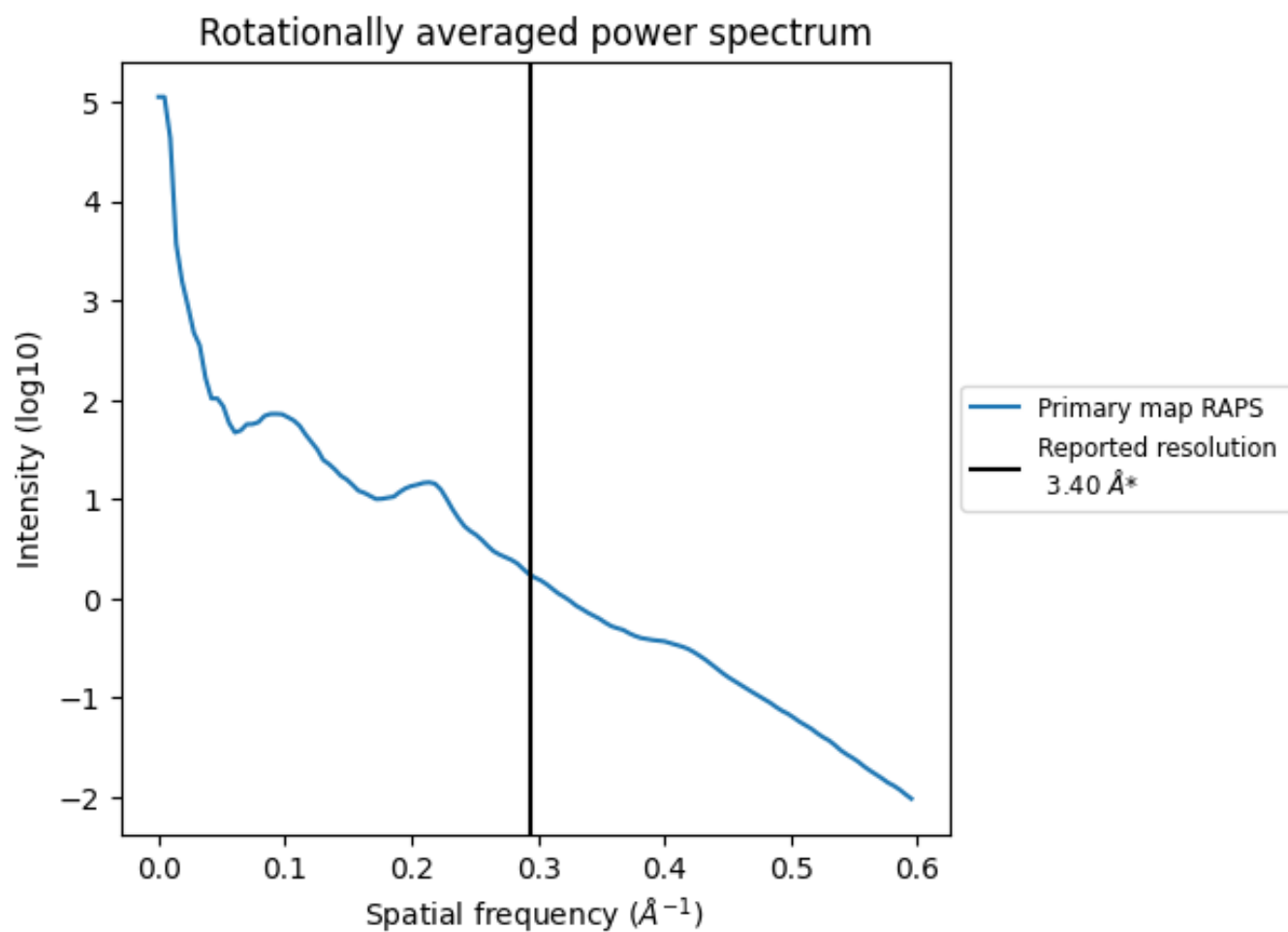


The volume at the recommended contour level is 111  $\text{nm}^3$ ; this corresponds to an approximate mass of 100 kDa.

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 0.294 Å<sup>-1</sup>

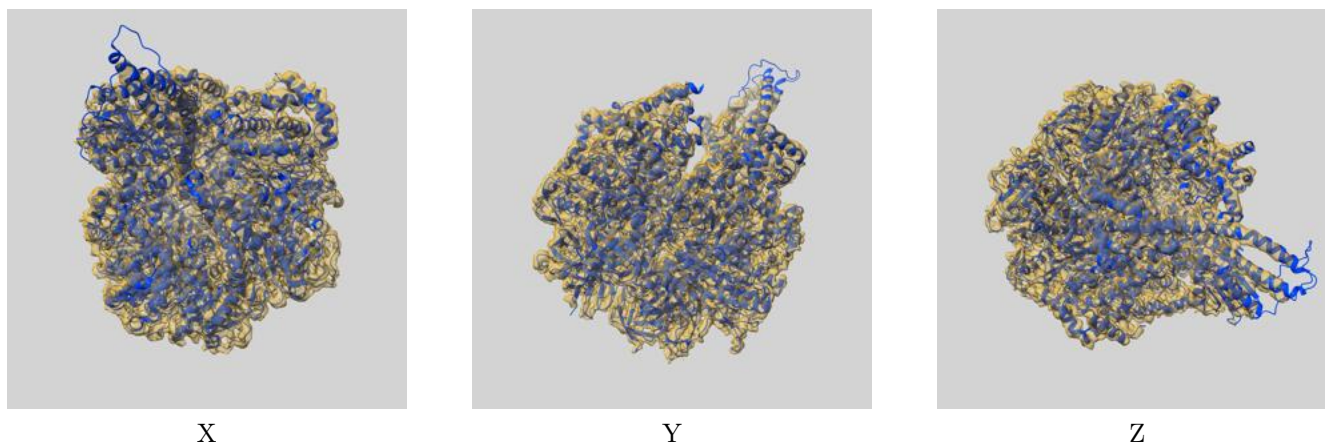
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

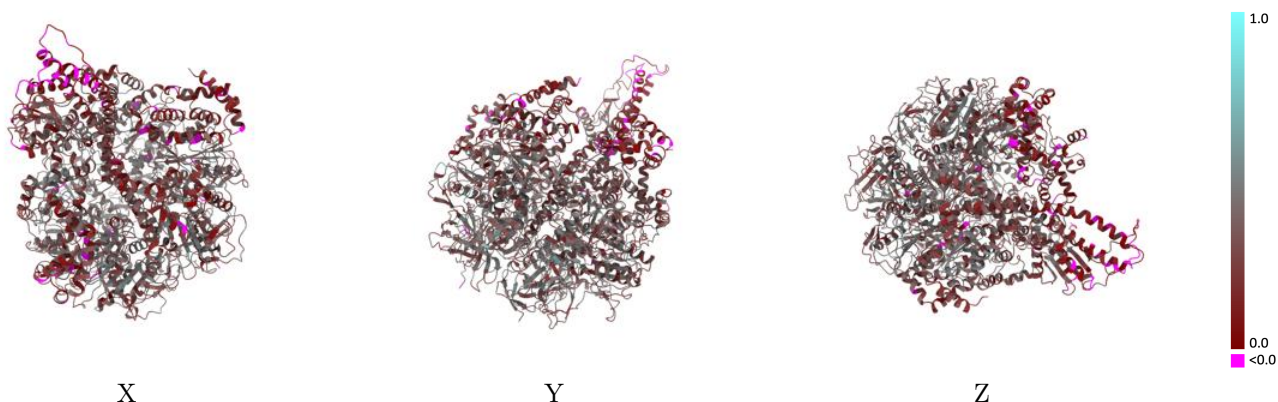
This section contains information regarding the fit between EMDB map EMD-23115 and PDB model 7L1Q. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlay [i](#)



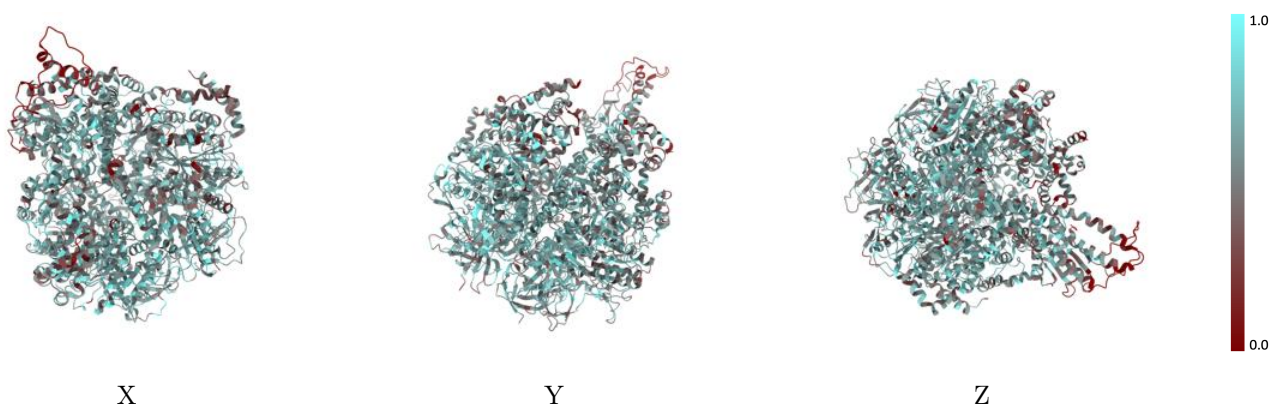
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



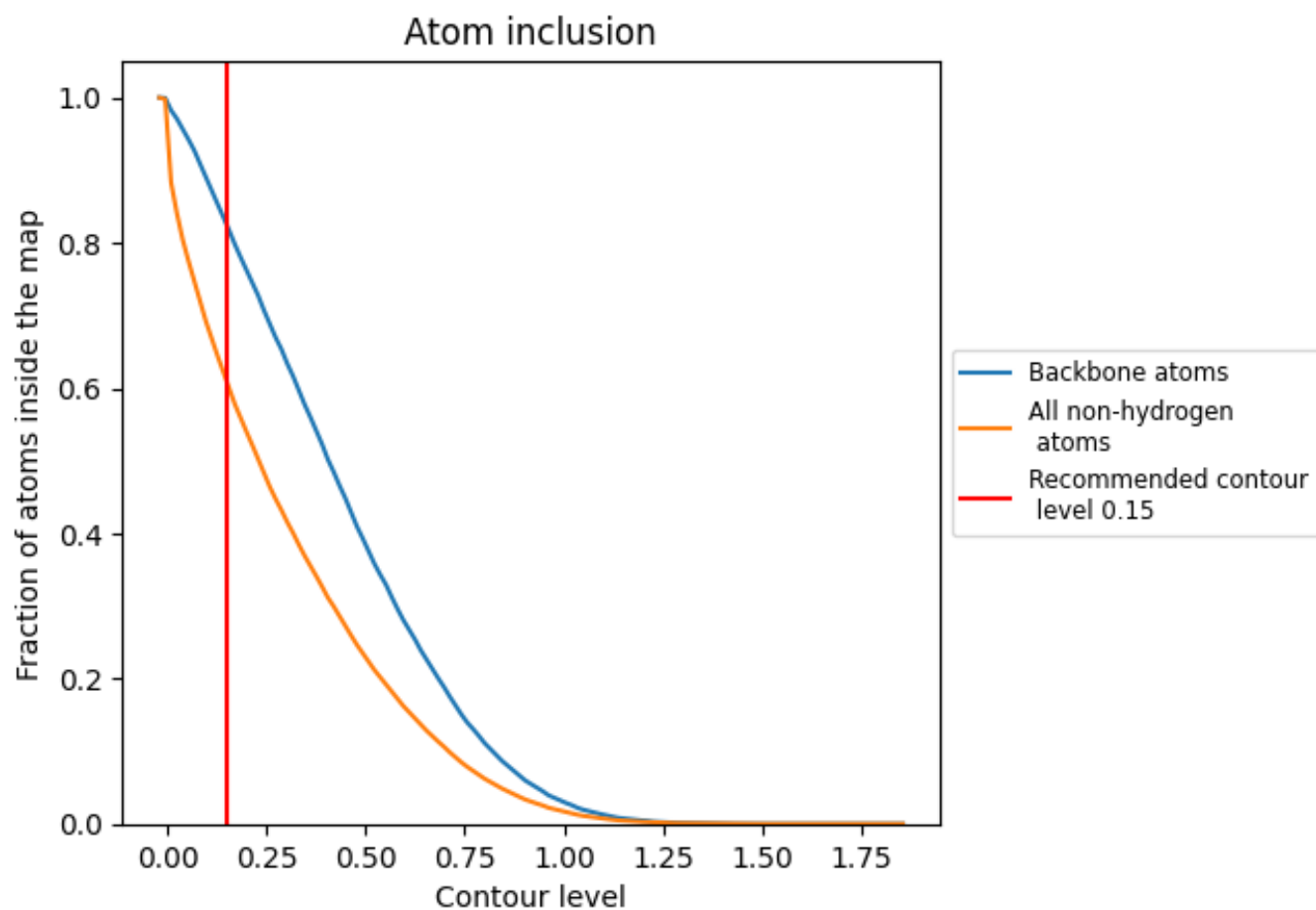
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6088	 0.3290
A	 0.5949	 0.3140
B	 0.6184	 0.3220
C	 0.6379	 0.3650
D	 0.6118	 0.3470
E	 0.6040	 0.3250
F	 0.6531	 0.3670
G	 0.4968	 0.2180

