W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Dec 18, 2022 – 11:50 pm GMT

PDB ID	:	7NJR
EMDB ID	:	EMD-12412
Title	:	Mycobacterium smegmatis ATP synthase state 3b
Authors	:	Montgomery, M.G.; Petri, J.; Spikes, T.E.; Walker, J.E.
Deposited on	:	2021-02-17
Resolution	:	2.56 Å(reported)

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.56 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	Percentile Ranks	Value
Ramachandran outliers		0.1%
Sidechain outliers		0.2%

Worse   *Better*

▌ Percentile relative to all structures

▯ Percentile relative to all EM structures
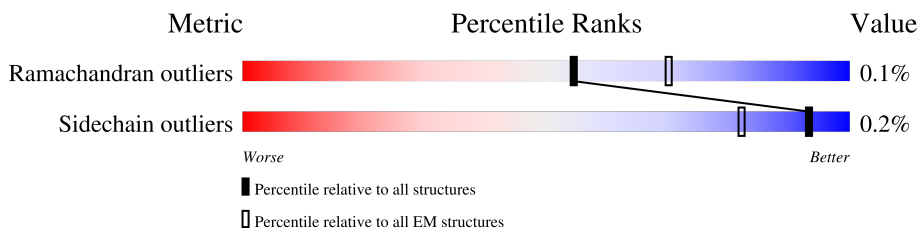
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	548	93% 7%
1	B	548	92% 8%
1	C	548	95% 5%
2	D	475	98%
2	E	475	97%
2	F	475	98%
3	G	307	5% 97%
4	H	121	15% 98%
5	L	86	97%

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Mol	Chain	Length	Quality of chain
5	M	86	98%
5	N	86	98%
5	O	86	6% 98%
5	P	86	99%
5	Q	86	98%
5	R	86	98%
5	S	86	98%
5	T	86	98%
6	a	252	5% 94% 6%
7	b	180	14% 81% 19%
8	d	445	13% 98%

2 Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 74659 atoms, of which 37393 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
1	A	511	Total 7732	C 2428	H 3867	N 668	O 759	S 10	0	0
1	B	505	Total 7638	C 2398	H 3823	N 659	O 748	S 10	0	0
1	C	521	Total 7921	C 2487	H 3967	N 684	O 773	S 10	1	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	468	Total 7162	C 2265	H 3573	N 616	O 695	S 13	2	0
2	E	464	Total 7087	C 2243	H 3533	N 609	O 689	S 13	0	0
2	F	468	Total 7144	C 2260	H 3564	N 614	O 693	S 13	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	297	Total 4567	C 1418	H 2290	N 412	O 441	S 6	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	H	118	Total 1802	C 565	H 891	N 161	O 184	S 1	0	0

- Molecule 5 is a protein called ATP synthase subunit c.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	L	84	Total 1192	C 387	H 603	N 96	O 104	S 2	0	0
5	M	84	Total 1192	C 387	H 603	N 96	O 104	S 2	0	0
5	N	84	Total 1192	C 387	H 603	N 96	O 104	S 2	0	0
5	O	84	Total 1192	C 387	H 603	N 96	O 104	S 2	0	0
5	P	85	Total 1204	C 391	H 607	N 97	O 107	S 2	0	0
5	Q	84	Total 1192	C 387	H 603	N 96	O 104	S 2	0	0
5	R	84	Total 1192	C 387	H 603	N 96	O 104	S 2	0	0
5	S	84	Total 1192	C 387	H 603	N 96	O 104	S 2	0	0
5	T	84	Total 1192	C 387	H 603	N 96	O 104	S 2	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	a	238	Total 3767	C 1252	H 1916	N 292	O 301	S 6	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	b	145	Total 2172	C 667	H 1095	N 194	O 214	S 2	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	171	HIS	-	expression tag	UNP A0R204
b	172	HIS	-	expression tag	UNP A0R204
b	173	HIS	-	expression tag	UNP A0R204
b	174	HIS	-	expression tag	UNP A0R204
b	175	HIS	-	expression tag	UNP A0R204
b	176	HIS	-	expression tag	UNP A0R204
b	177	HIS	-	expression tag	UNP A0R204
b	178	HIS	-	expression tag	UNP A0R204
b	179	HIS	-	expression tag	UNP A0R204

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Chain	Residue	Modelled	Actual	Comment	Reference
b	180	HIS	-	expression tag	UNP A0R204

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	d	438	Total	C	H	N	O	S	0	0
			6656	2034	3371	597	649	5		

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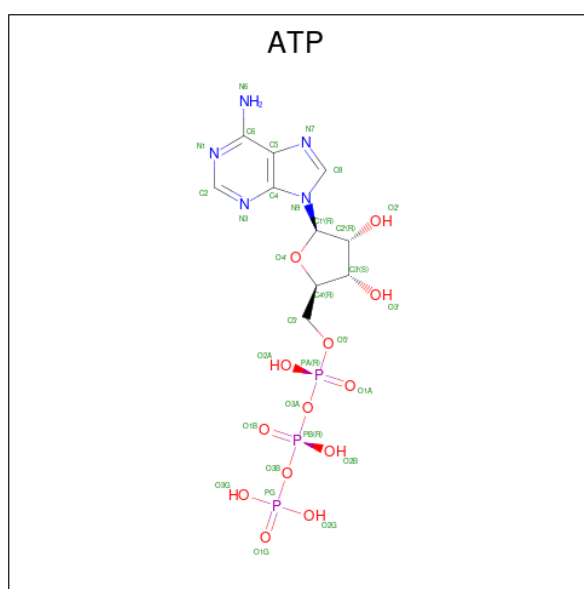
ATP

Mol	Chain	Residues	Atoms						AltConf
9	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
9	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
9	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
9	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mg	0
			1	1	

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

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
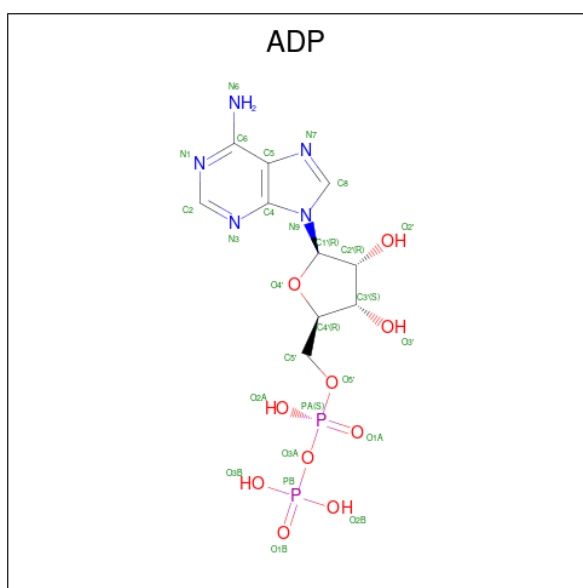
Mol	Chain	Residues	Atoms						AltConf
11	D	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
11	E	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		AltConf
12	A	3	Total 3	O 3	0
12	B	3	Total 3	O 3	0
12	C	3	Total 3	O 3	0

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Mol	Chain	Residues	Atoms		AltConf
12	D	4	Total 4	O 4	0
12	F	3	Total 3	O 3	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

Chain A:
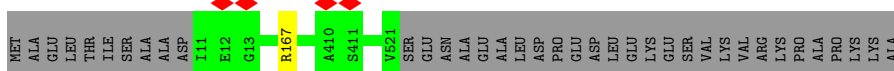
- Molecule 1: ATP synthase subunit alpha

Chain B:
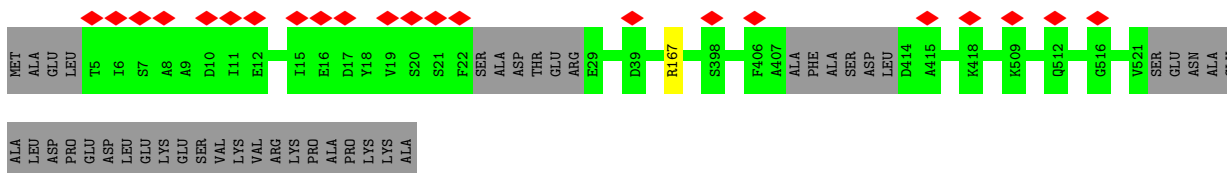
- Molecule 1: ATP synthase subunit alpha

Chain C:

- Molecule 2: ATP synthase subunit beta

Chain D:
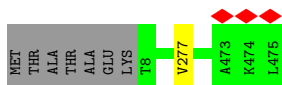
- Molecule 2: ATP synthase subunit beta

Chain E:

MET THR ALA THR ALA GLU LYS T8 **V277** D392 E393 E396 D448 E469 S470 L471 GLY ALA LYS LEU

• Molecule 2: ATP synthase subunit beta

Chain F: 98%

MET THR ALA THR ALA GLU LYS T8 **V277** K474 L475
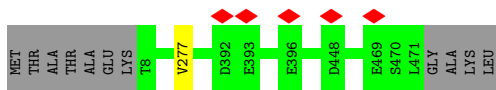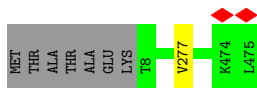
• Molecule 3: ATP synthase gamma chain

Chain G: 5%   97%

MET ALA A3 R44 D64 Q73 E143 D167 E168 G169 D170 D171 A172 G173 G176 G212 E213 V214 GLU THR GLY PRO ARG T220 E229 A304 GLY SER LYS
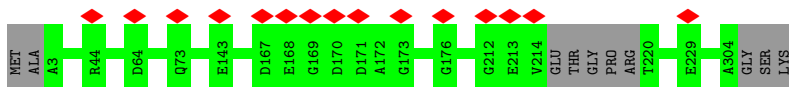
• Molecule 4: ATP synthase epsilon chain

Chain H: 15%   98%

MET ALA D3 E56 G57 E58 D59 D60 E74 E89 I90 D91 A92 D93 A94 A95 K96 E97 D98 A99 A100 S101 D102 D103 E104 I120 ASP
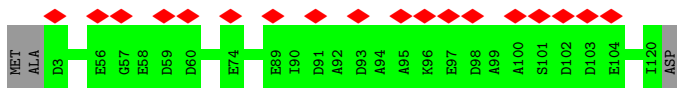
• Molecule 5: ATP synthase subunit c

Chain L: 97%

MET ASP L3 **R45** Q86
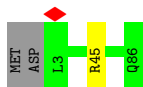
• Molecule 5: ATP synthase subunit c

Chain M: 98%
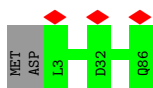
MET ASP L3 D32 Q86

• Molecule 5: ATP synthase subunit c

Chain N: 98%
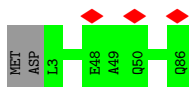
MET ASP L3 E48 A49 Q50 Q86
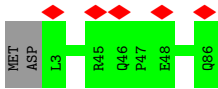
• Molecule 5: ATP synthase subunit c

6%

Chain O:
98%

MET ASP L3 R45 Q46 P47 E48 Q86

• Molecule 5: ATP synthase subunit c

Chain P:
99%

MET D2 E48 Q86

• Molecule 5: ATP synthase subunit c

Chain Q:
98%

MET ASP L3 E48 Q86

• Molecule 5: ATP synthase subunit c

Chain R:
98%

MET ASP L3 Q86

• Molecule 5: ATP synthase subunit c

Chain S:
98%

MET ASP L3 E48 Q86

• Molecule 5: ATP synthase subunit c

Chain T:
98%

MET ASP L3 Q86
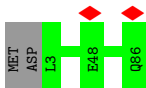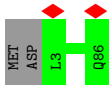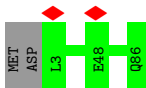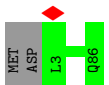
• Molecule 6: ATP synthase subunit a

5%

Chain a:
94%
6%

MET LEU ALA ALA GLU GLU GLY ALA A10 I11 H12 M25 A36 T54 A116 D117 G118 A119 H166 F169 E177 F224 E246 L247 ASP HIS GLU ASP HIS
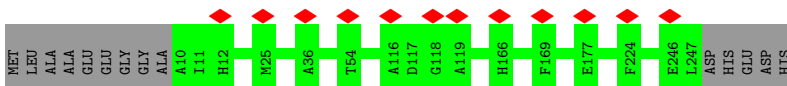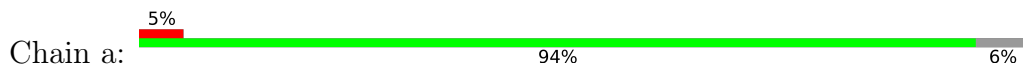
• Molecule 7: ATP synthase subunit b

Chain b:

14%

81% 19%

MET GLY GLU PHE SER ALA THR ILE LEU ALA ALA SER GLN ALA ALA GLU GLU GLY GLY GLY S22 A62 R72 E76 A79 E86 R108 E113 K114 R115 S119 Q124 T125 L126 A129 D130 L133 G137 D138 Q139 L144 E145 D149 L155

V162 D163 V164 N165 S166 GLY GLY THR GLN HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS
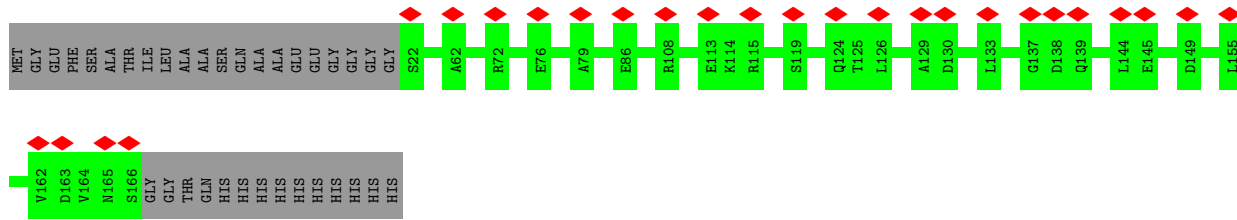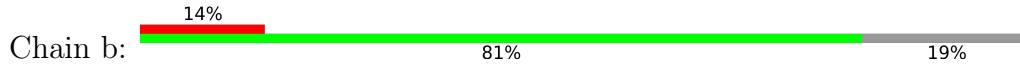
• Molecule 8: ATP synthase subunit b-delta

Chain d:

13%

98%

M1 E46 K49 A52 E70 E81 K99 L108 M109 R110 R115 G120 A123 E124 K128 E131 A138 Q141 Q156 S161 V162 VAL ILE ASP THR ALA ALA T169 S170 R171 A174 G192 G193 A196 D197 N220 K221 H222 E225

P226 T227 D228 D229 S230 K233 V234 R235 L236 L237 E238 R239 L240 L241 S242 D243 K244 A247 R254 T255 A256 V257 S258 E264 S265 N266 E284 G287 E288 E294 R301 D304 R308 K329 R334 P335 G336 R353 R371 A383 D412 L443 P444

ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28438	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 $(e^-/\text{Å}^2)$	59.86	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0146	Depositor
Map size (Å)	415.0, 415.0, 415.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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, 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	0.28	0/3925	0.49	0/5314
1	B	0.28	0/3872	0.49	0/5240
1	C	0.28	0/4018	0.49	0/5436
2	D	0.29	0/3659	0.50	0/4961
2	E	0.28	0/3619	0.50	0/4908
2	F	0.30	0/3645	0.51	0/4942
3	G	0.27	0/2306	0.53	0/3117
4	H	0.26	0/922	0.54	0/1252
5	L	0.28	0/600	0.47	0/814
5	M	0.29	0/600	0.47	0/814
5	N	0.28	0/600	0.47	0/814
5	O	0.28	0/600	0.45	0/814
5	P	0.28	0/608	0.47	0/825
5	Q	0.28	0/600	0.45	0/814
5	R	0.28	0/600	0.46	0/814
5	S	0.28	0/600	0.44	0/814
5	T	0.27	0/600	0.45	0/814
6	a	0.26	0/1905	0.42	0/2602
7	b	0.25	0/1086	0.46	0/1467
8	d	0.24	0/3314	0.48	0/4488
All	All	0.28	0/37679	0.49	0/51064

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 ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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	509/548 (93%)	499 (98%)	10 (2%)	0	100	100
1	B	499/548 (91%)	487 (98%)	12 (2%)	0	100	100
1	C	516/548 (94%)	502 (97%)	14 (3%)	0	100	100
2	D	468/475 (98%)	461 (98%)	6 (1%)	1 (0%)	47	58
2	E	462/475 (97%)	450 (97%)	11 (2%)	1 (0%)	47	58
2	F	466/475 (98%)	455 (98%)	10 (2%)	1 (0%)	47	58
3	G	293/307 (95%)	290 (99%)	3 (1%)	0	100	100
4	H	116/121 (96%)	113 (97%)	3 (3%)	0	100	100
5	L	82/86 (95%)	75 (92%)	7 (8%)	0	100	100
5	M	82/86 (95%)	77 (94%)	5 (6%)	0	100	100
5	N	82/86 (95%)	73 (89%)	9 (11%)	0	100	100
5	O	82/86 (95%)	75 (92%)	7 (8%)	0	100	100
5	P	83/86 (96%)	77 (93%)	6 (7%)	0	100	100
5	Q	82/86 (95%)	80 (98%)	2 (2%)	0	100	100
5	R	82/86 (95%)	78 (95%)	4 (5%)	0	100	100
5	S	82/86 (95%)	77 (94%)	5 (6%)	0	100	100
5	T	82/86 (95%)	78 (95%)	4 (5%)	0	100	100
6	a	236/252 (94%)	221 (94%)	15 (6%)	0	100	100
7	b	143/180 (79%)	138 (96%)	5 (4%)	0	100	100
8	d	434/445 (98%)	425 (98%)	9 (2%)	0	100	100
All	All	4881/5148 (95%)	4731 (97%)	147 (3%)	3 (0%)	54	65

WORLDWIDE
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PROTEIN DATA BANK

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	277	VAL
2	F	277	VAL
2	D	277	VAL

5.3.2   Protein sidechains ⓘ

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	411/441 (93%)	410 (100%)	1 (0%)	93	97
1	B	406/441 (92%)	405 (100%)	1 (0%)	93	97
1	C	420/441 (95%)	419 (100%)	1 (0%)	93	97
2	D	384/388 (99%)	384 (100%)	0	100	100
2	E	381/388 (98%)	381 (100%)	0	100	100
2	F	383/388 (99%)	383 (100%)	0	100	100
3	G	231/238 (97%)	231 (100%)	0	100	100
4	H	94/96 (98%)	94 (100%)	0	100	100
5	L	54/56 (96%)	53 (98%)	1 (2%)	57	71
5	M	54/56 (96%)	54 (100%)	0	100	100
5	N	54/56 (96%)	54 (100%)	0	100	100
5	O	54/56 (96%)	54 (100%)	0	100	100
5	P	55/56 (98%)	55 (100%)	0	100	100
5	Q	54/56 (96%)	54 (100%)	0	100	100
5	R	54/56 (96%)	54 (100%)	0	100	100
5	S	54/56 (96%)	54 (100%)	0	100	100
5	T	54/56 (96%)	54 (100%)	0	100	100
6	a	191/200 (96%)	191 (100%)	0	100	100
7	b	111/134 (83%)	111 (100%)	0	100	100
8	d	342/347 (99%)	339 (99%)	3 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3841/4006 (96%)	3834 (100%)	7 (0%)	93 97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	L	45	ARG
8	d	110	ARG
8	d	353	ARG
8	d	308	ARG
1	C	167	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	399	GLN
6	a	229	GLN
7	b	136	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 5 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	$\#|Z| > 2$
9	ATP	A	600	10	26,33,33	0.67	0	31,52,52	1.08	3 (9%)
9	ATP	F	600	10	26,33,33	0.68	0	31,52,52	1.05	2 (6%)
11	ADP	E	600	-	24,29,29	0.94	1 (4%)	29,45,45	1.56	4 (13%)
9	ATP	C	600	10	26,33,33	0.68	0	31,52,52	1.10	3 (9%)
9	ATP	B	600	10	26,33,33	0.67	0	31,52,52	1.10	3 (9%)
11	ADP	D	600	10	24,29,29	0.94	1 (4%)	29,45,45	1.33	3 (10%)

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	A	600	10	-	0/18/38/38	0/3/3/3
9	ATP	F	600	10	-	2/18/38/38	0/3/3/3
11	ADP	E	600	-	-	1/12/32/32	0/3/3/3
9	ATP	C	600	10	-	0/18/38/38	0/3/3/3
9	ATP	B	600	10	-	0/18/38/38	0/3/3/3
11	ADP	D	600	10	-	5/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E	600	ADP	C5-C4	2.36	1.47	1.40
11	D	600	ADP	C5-C4	2.18	1.46	1.40

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	E	600	ADP	PA-O3A-PB	-3.88	119.52	132.83
11	E	600	ADP	C3'-C2'-C1'	3.71	106.56	100.98
11	D	600	ADP	N3-C2-N1	-3.68	122.92	128.68
11	E	600	ADP	N3-C2-N1	-3.57	123.10	128.68
11	D	600	ADP	PA-O3A-PB	-3.39	121.19	132.83

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	600	ADP	C5'-O5'-PA-O3A
9	F	600	ATP	PA-O3A-PB-O1B
11	D	600	ADP	C5'-O5'-PA-O1A
11	D	600	ADP	C5'-O5'-PA-O2A
11	D	600	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP A 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP F 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP E 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP C 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 600

Bond lengths

Bond angles

Torsions

Rings
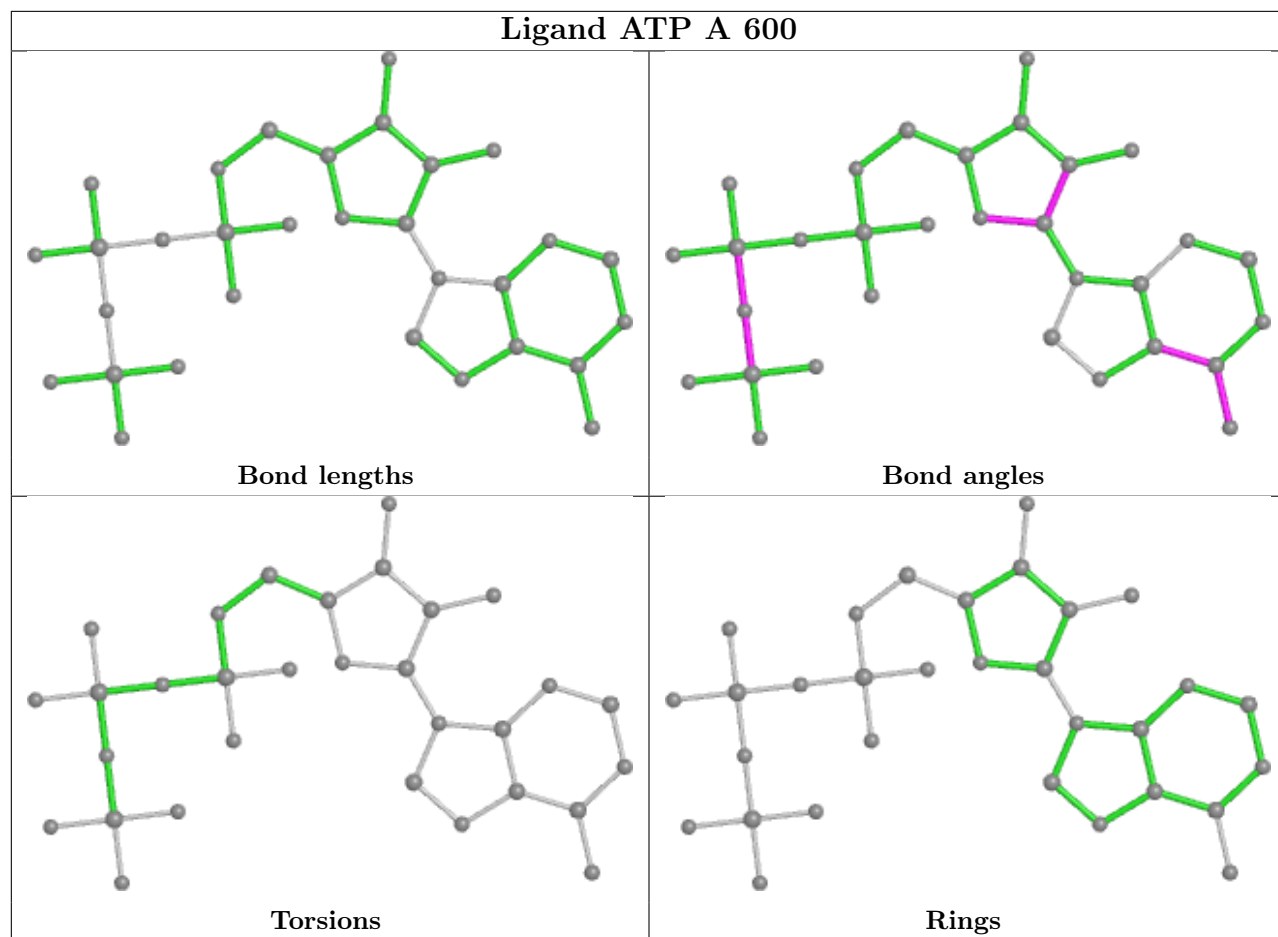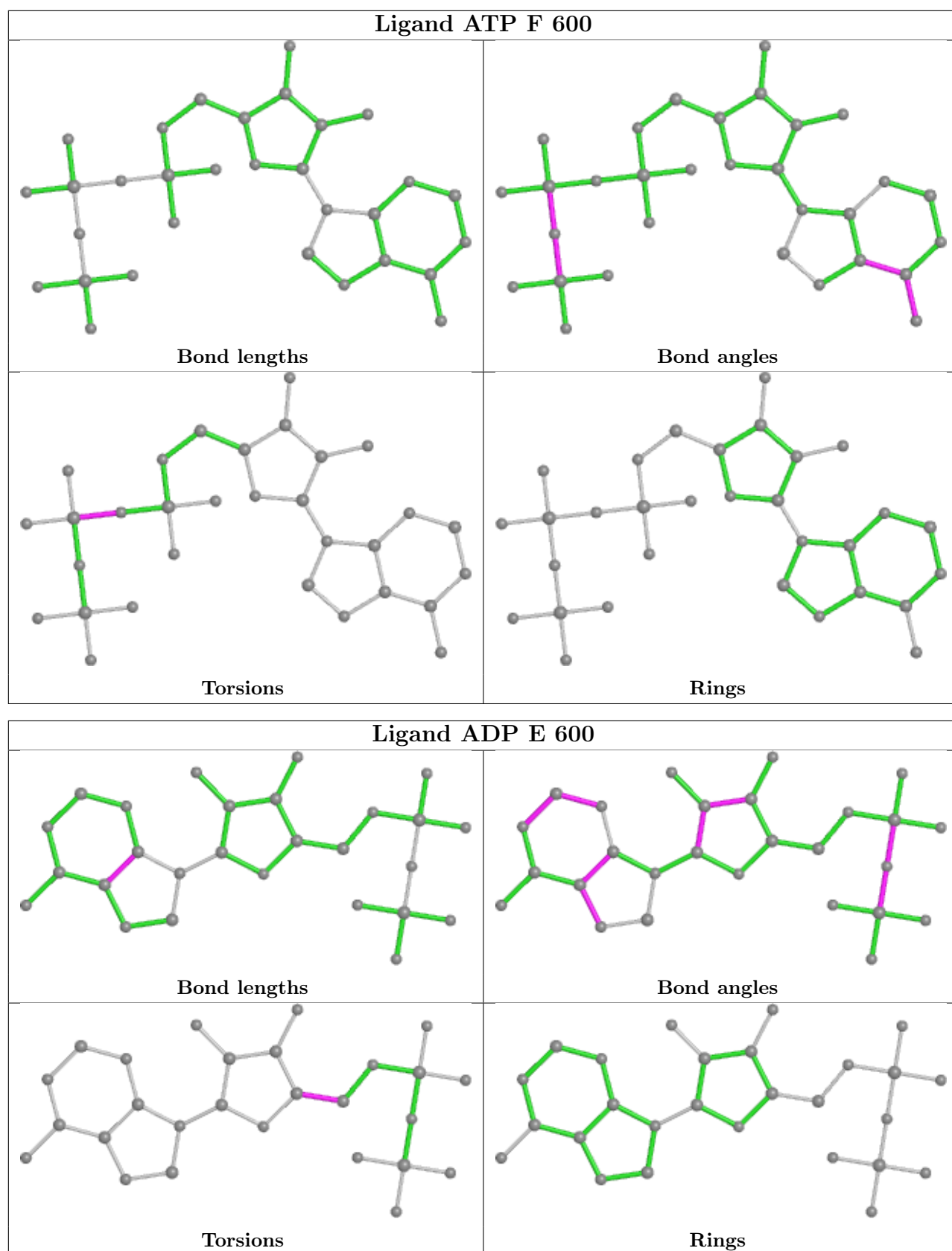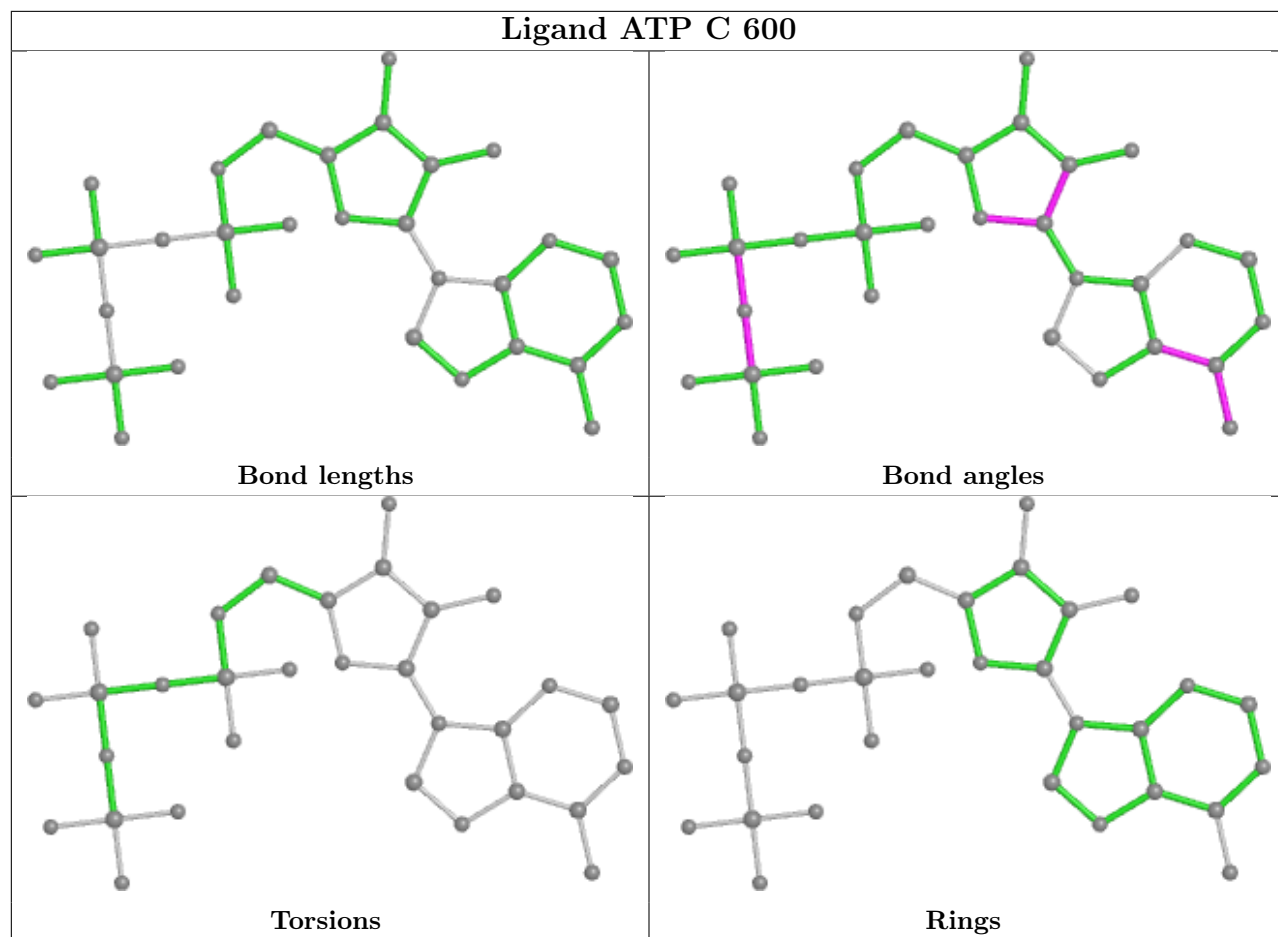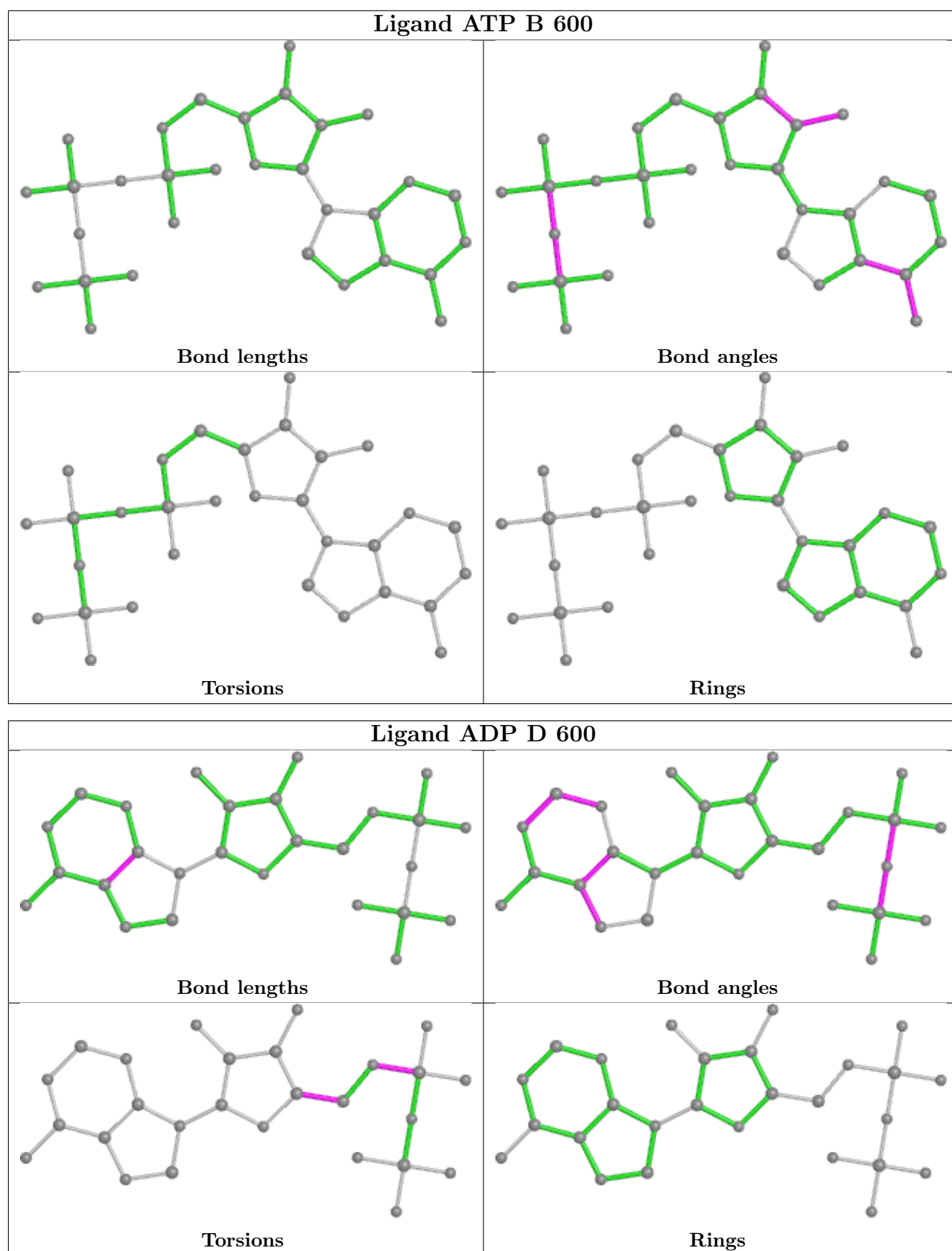
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-12412. 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 ⓘ

6.1.1 Primary map

| X | Y | Z |
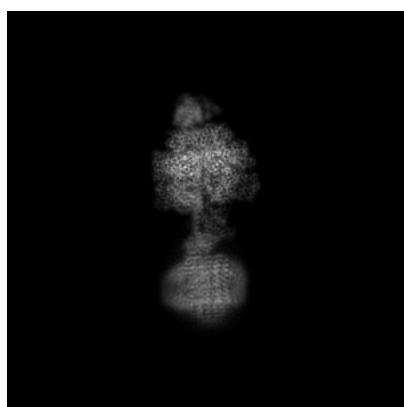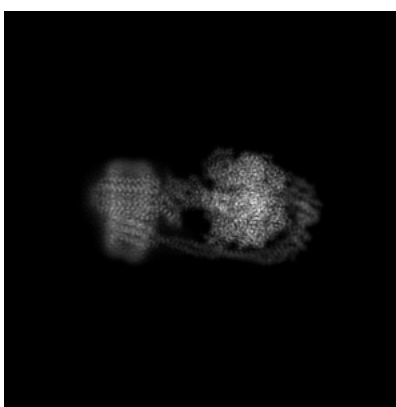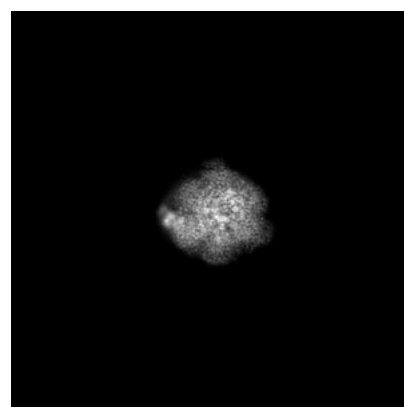
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
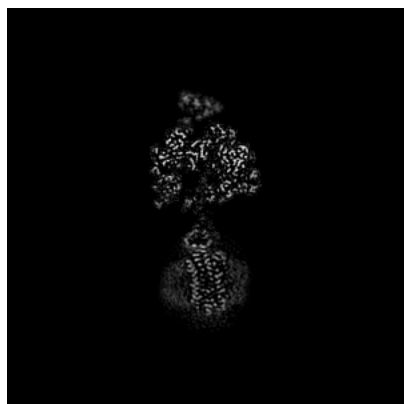
6.2.1 Primary map

| X Index: 250 | Y Index: 250 | Z Index: 250 |
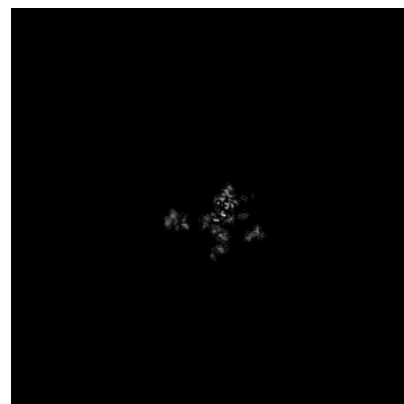
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices ⓘ
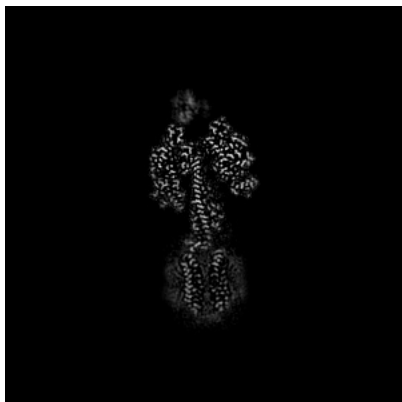
6.3.1   Primary map
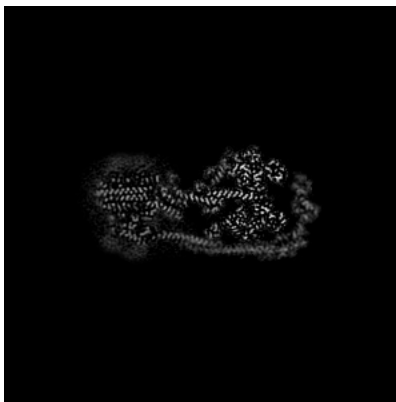
| X Index: 264 | Y Index: 238 | Z Index: 310 |
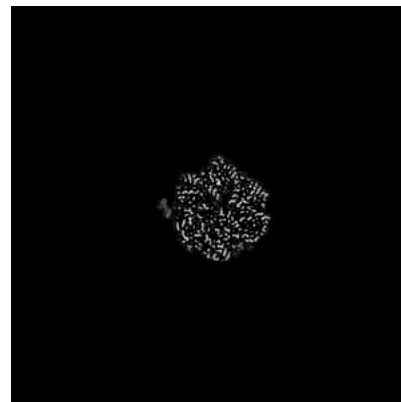
The images above show the largest variance slices of the map in three orthogonal directions.

6.4   Orthogonal surface views ⓘ
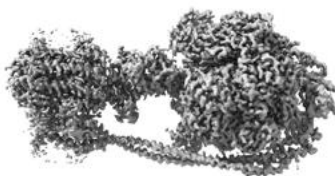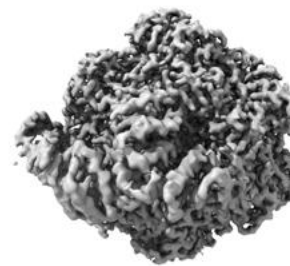
6.4.1   Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.0146. 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 ⓘ

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

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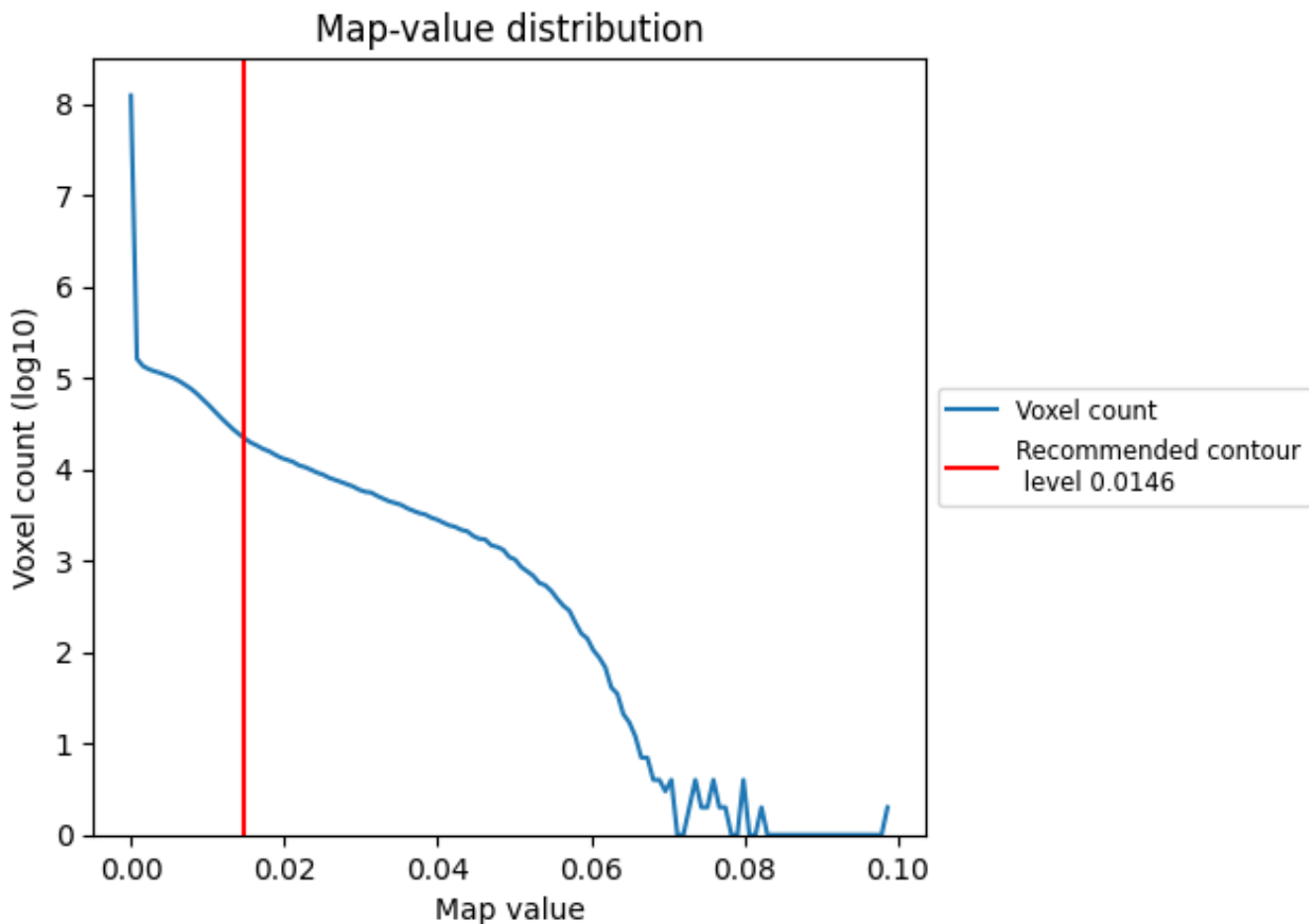
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
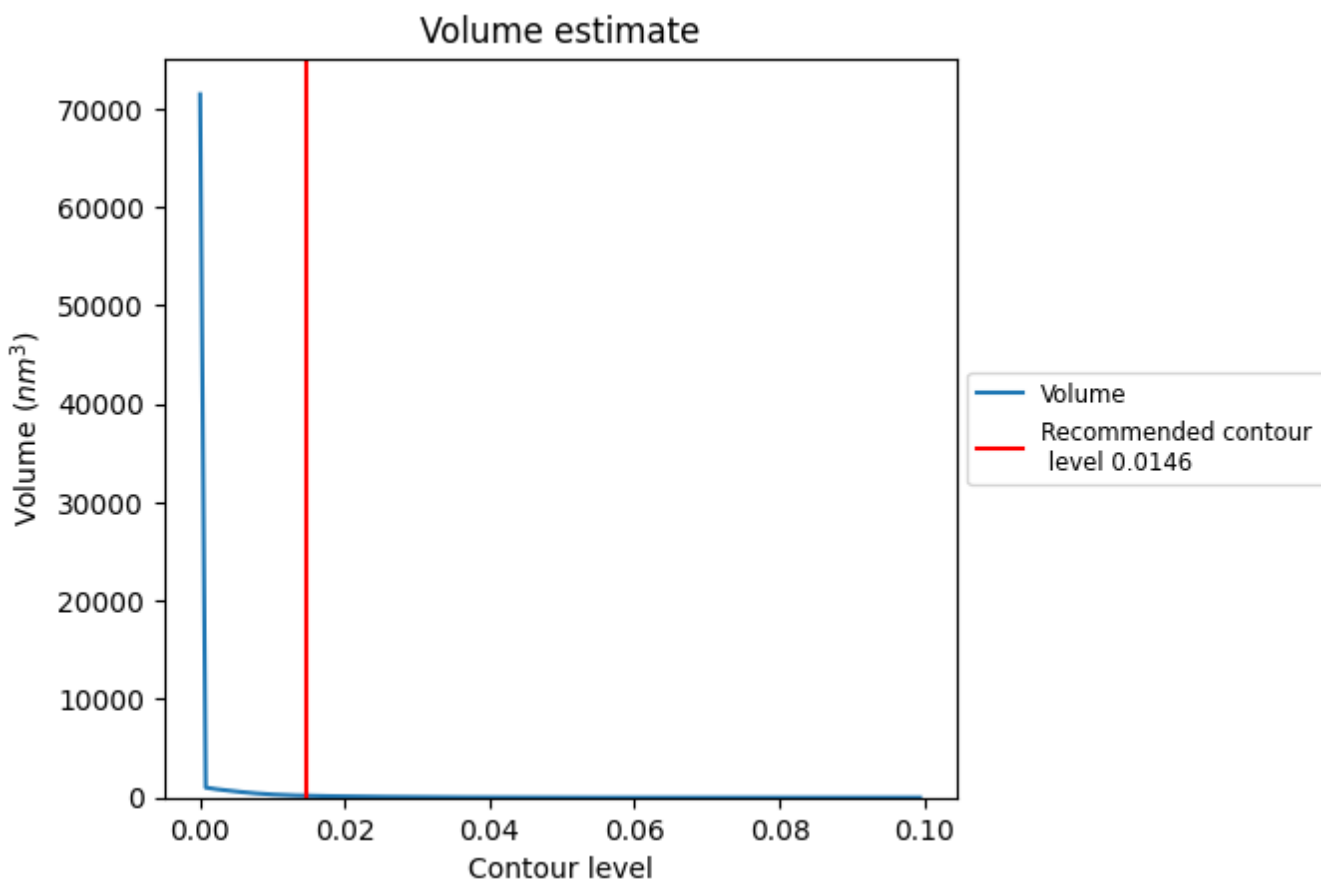
The volume at the recommended contour level is 187 nm^3; this corresponds to an approximate mass of 169 kDa.

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)
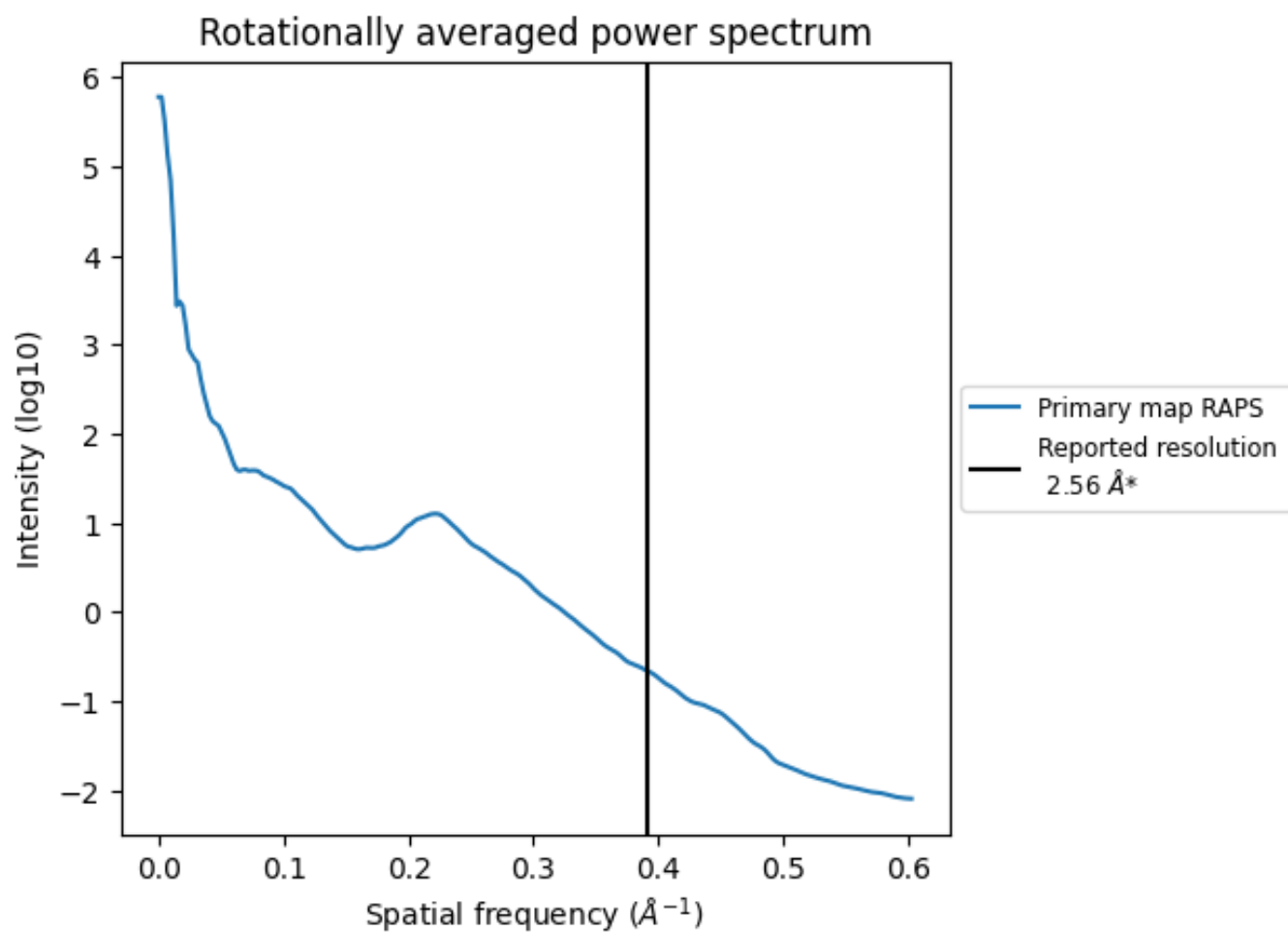
*Reported resolution corresponds to spatial frequency of 0.391 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

9　Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-12412 and PDB model 7NJR. Per-residue inclusion information can be found in section 3 on page 9.

9.1　Map-model overlay ⓘ
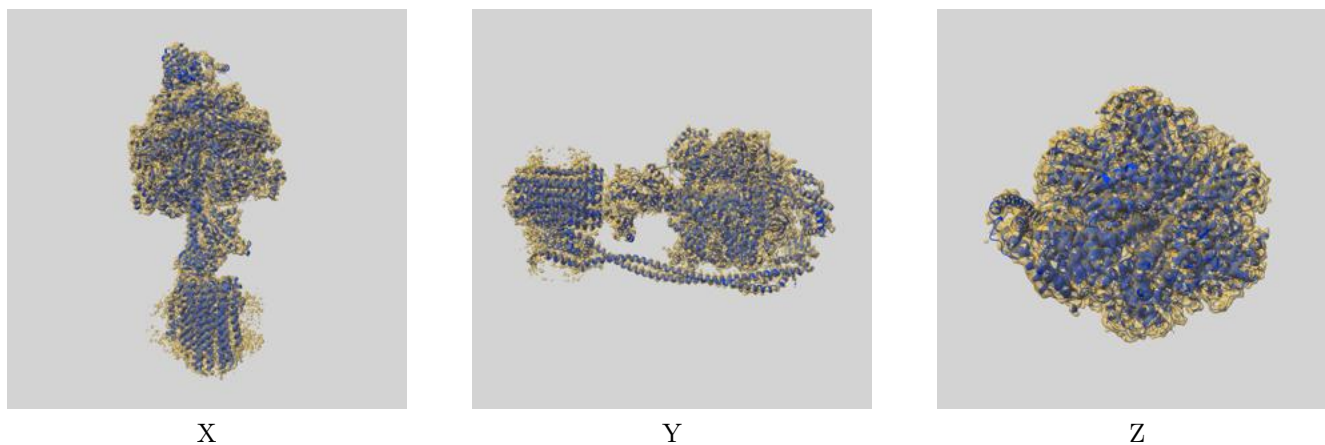
| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.0146 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 ⓘ

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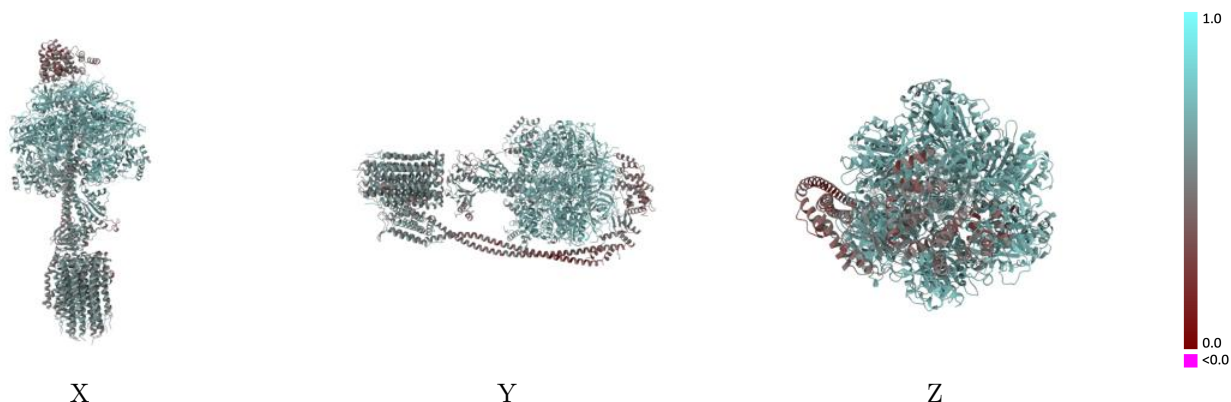
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
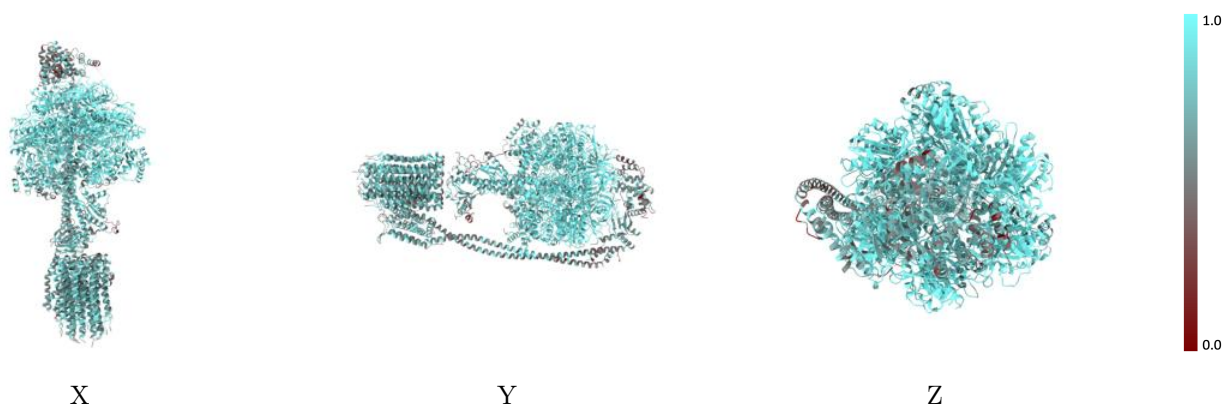
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0146).

9.4 Atom inclusion ⓘ
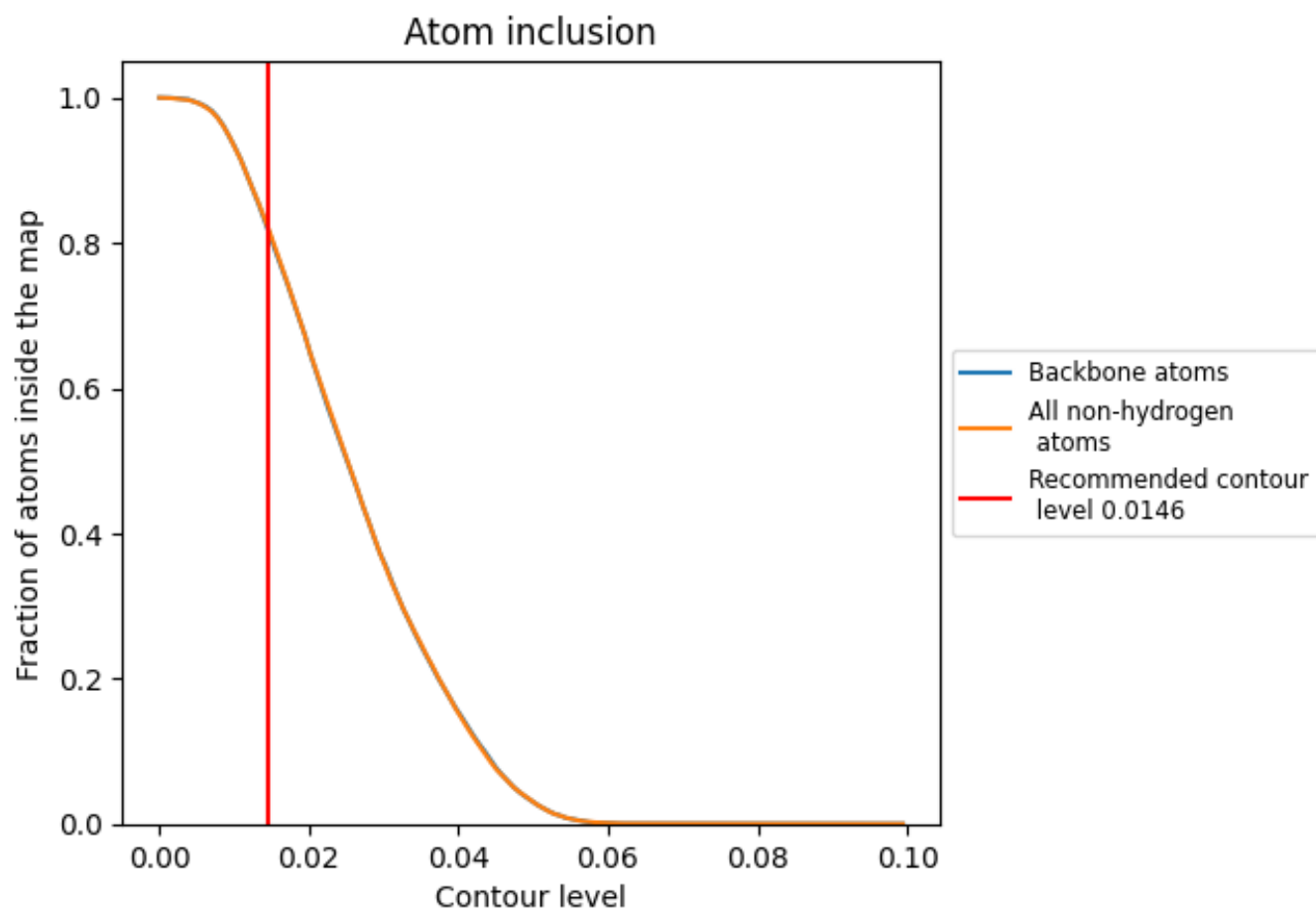
At the recommended contour level, 82% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0146) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8188	0.5990
A	0.9118	0.6550
B	0.8697	0.6400
C	0.8950	0.6530
D	0.9272	0.6740
E	0.8948	0.6520
F	0.9366	0.6760
G	0.7938	0.5820
H	0.6697	0.5190
L	0.7500	0.5510
M	0.7483	0.5550
N	0.7260	0.5330
O	0.7106	0.5350
P	0.7247	0.5360
Q	0.7175	0.5420
R	0.7089	0.5550
S	0.7209	0.5460
T	0.7534	0.5510
a	0.6796	0.5320
b	0.6074	0.3980
d	0.6187	0.4180

1.0

0.0
<0.0