wwPDB EM Validation Summary Report (i)

Jan 17, 2023 – 12:30 PM EST

PDB ID	:	8DBS
EMDB ID	:	EMD-27304
Title	:	E. coli ATP synthase imaged in 10mM MgATP State2 "half-up" Fo classified
Authors	:	Sobti, M.; Stewart, A.G.
Deposited on	:	2022-06-14
Resolution	:	3.50 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 (i)) were used in the production of this report:

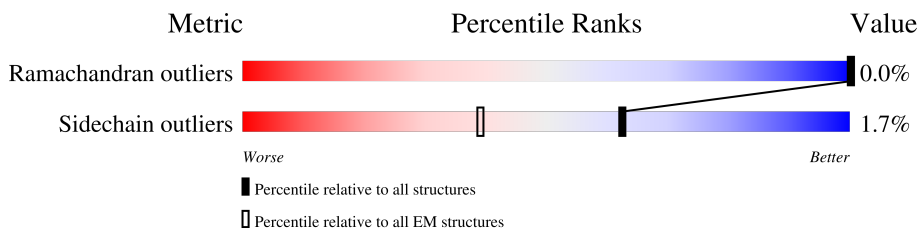|		
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1　Overall quality at a glance　ⓘ

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

The reported resolution of this entry is 3.50 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		0.0%
Sidechain outliers		1.7%

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	508	99%
2	B	513	99%
2	C	513	98%
3	D	460	99%
3	E	460	99%
3	F	460	99%
4	G	284	98%
5	H	101	6% 97%
6	I	77	6% 99%

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Mol	Chain	Length	Quality of chain
6	J	77	8% / 100%
6	L	77	9% / 97%
6	M	77	8% / 99%
6	N	77	14% / 100%
6	O	77	14% / 97%
6	P	77	6% / 100%
6	Q	77	9% / 99%
6	R	77	94% / 5%
6	S	77	14% / 99%
7	W	173	99%
8	X	156	6% / 98%
9	Y	156	99%
10	a	266	97%

2 Entry composition ⓘ

There are 13 unique types of molecules in this entry. The entry contains 36678 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
1	A	508	Total 3826	C 2402	N 676	O 739	S 9	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ALA	CYS	conflict	UNP A0A7U9G3U3
A	90	ALA	CYS	conflict	UNP A0A7U9G3U3
A	193	ALA	CYS	conflict	UNP A0A7U9G3U3
A	243	ALA	CYS	conflict	UNP A0A7U9G3U3
A	409	ALA	PHE	conflict	UNP A0A7U9G3U3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	513	Total 3877	C 2438	N 683	O 746	S 10	0	0
2	C	510	Total 3849	C 2419	N 679	O 742	S 9	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	47	ALA	CYS	conflict	UNP A0A7U9G3U3
B	90	ALA	CYS	conflict	UNP A0A7U9G3U3
B	193	ALA	CYS	conflict	UNP A0A7U9G3U3
B	243	ALA	CYS	conflict	UNP A0A7U9G3U3
C	47	ALA	CYS	conflict	UNP A0A7U9G3U3
C	90	ALA	CYS	conflict	UNP A0A7U9G3U3
C	193	ALA	CYS	conflict	UNP A0A7U9G3U3
C	243	ALA	CYS	conflict	UNP A0A7U9G3U3

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

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	137	ALA	CYS	conflict	UNP A0A192CEZ8
E	137	ALA	CYS	conflict	UNP A0A192CEZ8
F	137	ALA	CYS	conflict	UNP A0A192CEZ8

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

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	5	ASP	GLU	conflict	UNP C3SLA2
G	87	ALA	CYS	conflict	UNP C3SLA2
G	112	ALA	CYS	conflict	UNP C3SLA2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	101	Total 772	C 486	N 133	O 150	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	77	Total 557	C 370	N 88	O 92	S 7	0	0
6	J	77	Total 557	C 370	N 88	O 92	S 7	0	0
6	L	77	Total 557	C 370	N 88	O 92	S 7	0	0

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	156	Total	C	N	O	S	0	0
			1200	751	214	232	3		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	21	ALA	CYS	conflict	UNP A0A829DQ01
X	81	ALA	LYS	conflict	UNP A0A829DQ01
X	82	ALA	ARG	conflict	UNP A0A829DQ01

- Molecule 9 is a protein called ATP synthase subunit b.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	21	ALA	CYS	conflict	UNP D6IFY0

- Molecule 10 is a protein called ATP synthase subunit a.

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

- Molecule 11 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

ATP

Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	A	1	31	10	5	13	3	0
11	B	1	31	10	5	13	3	0
11	C	1	31	10	5	13	3	0
11	D	1	31	10	5	13	3	0
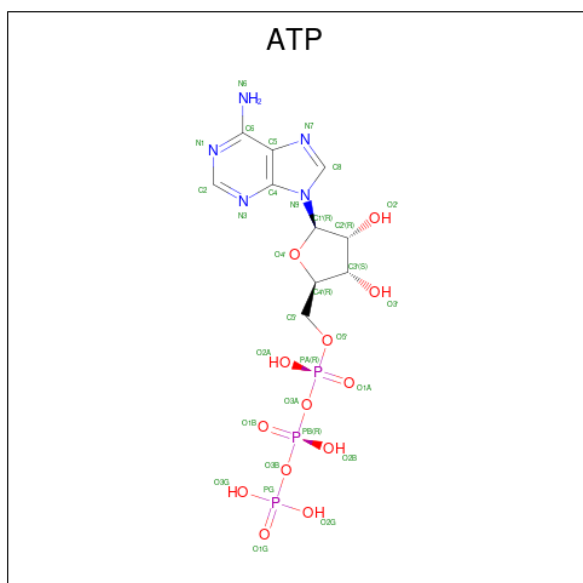
- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
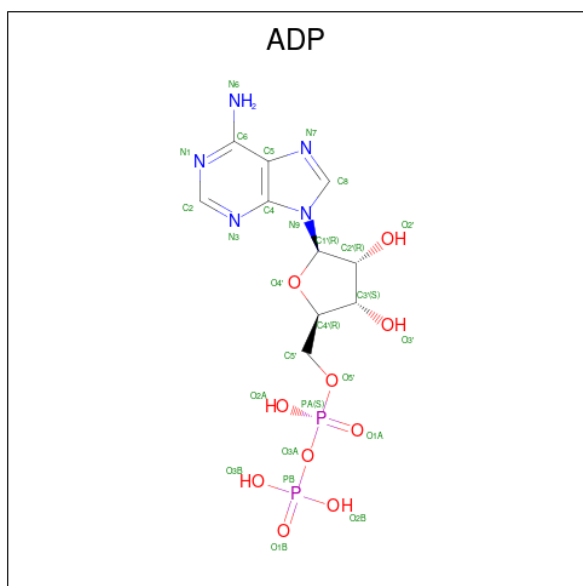
Mol	Chain	Residues	Atoms					AltConf
13	E	1	Total 27	C 10	N 5	O 10	P 2	0
13	F	1	Total 27	C 10	N 5	O 10	P 2	0

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
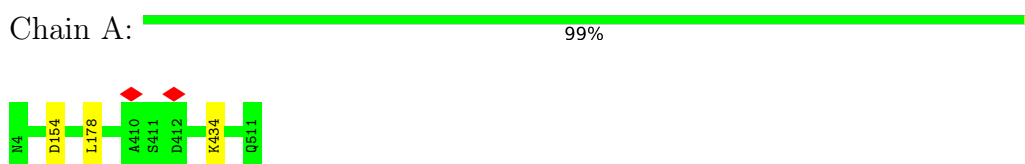
Chain A:

• Molecule 2: ATP synthase subunit alpha
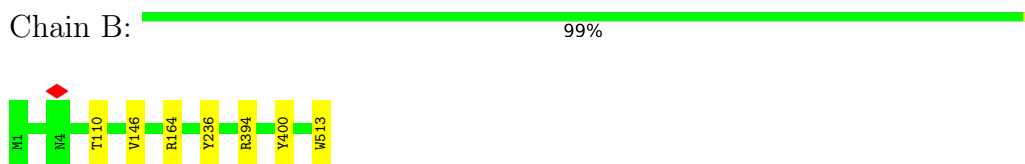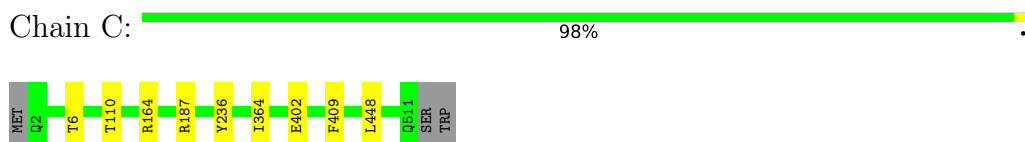
Chain B:

• Molecule 2: ATP synthase subunit alpha

Chain C:

• Molecule 3: ATP synthase subunit beta

Chain D:

• Molecule 3: ATP synthase subunit beta

Chain E:

• Molecule 3: ATP synthase subunit beta

Chain F:

99%
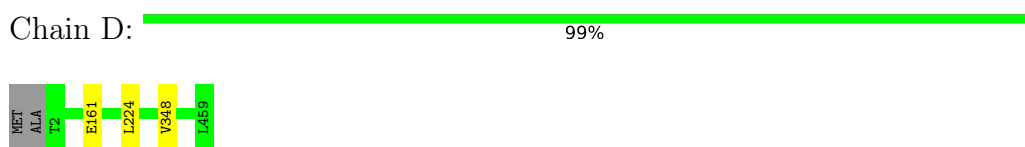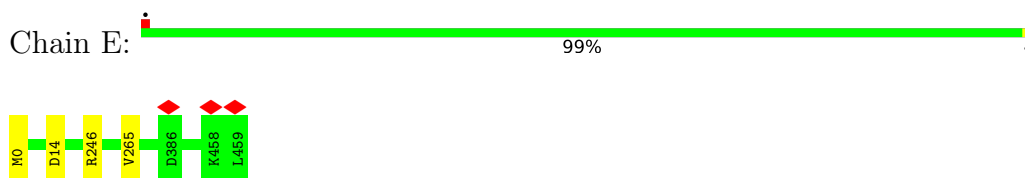
M0 Q19 E181 V265 K458 L459

• Molecule 4: ATP synthase gamma chain

Chain G:

98%

A1 R42 N59 D71 M178 D194 D195 W203 K258 L276 A284
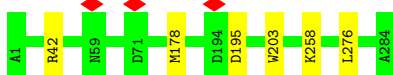
• Molecule 5: ATP synthase epsilon chain
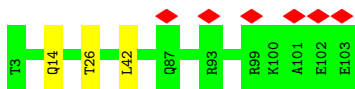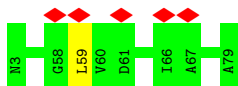
6%

Chain H:

97%

T3 Q14 T26 L42 Q87 R93 R99 K100 A101 E102 E103

• Molecule 6: ATP synthase subunit c

6%

Chain I:

99%

N3 G58 L59 V60 D61 I66 A67 A79

• Molecule 6: ATP synthase subunit c

8%

Chain J:

100%

N3 A24 A39 D44 L59 G69 A79

• Molecule 6: ATP synthase subunit c

9%

Chain L:

97%

N3 L4 N5 L8 A39 D61 A62 I63 A79

• Molecule 6: ATP synthase subunit c

8%

Chain M:

99%

N3 Y10 G32 E37 G38 A39 D61 A77 V78 A79
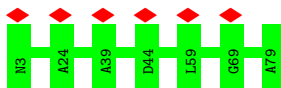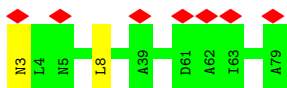
• Molecule 6: ATP synthase subunit c

Chain N:

• Molecule 6: ATP synthase subunit c

Chain O:

• Molecule 6: ATP synthase subunit c

Chain P:

• Molecule 6: ATP synthase subunit c

Chain Q:

• Molecule 6: ATP synthase subunit c

Chain R:

• Molecule 6: ATP synthase subunit c

Chain S:
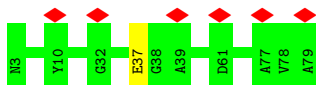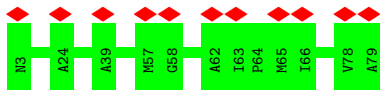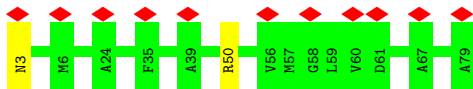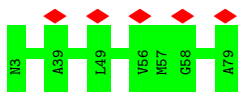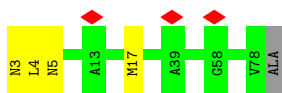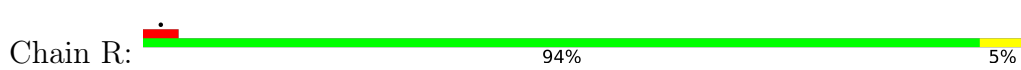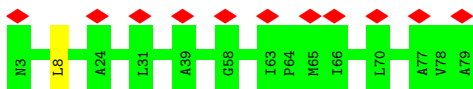
• Molecule 7: ATP synthase subunit delta

Chain W:

E2 K137 K144 D160 L174
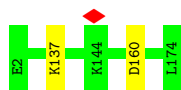
• Molecule 8: ATP synthase subunit b

Chain X:

6%

98%

M1 I12 L16 M30 E34 A50 D55 E137 R138 S139 V140 D141 K151 L156
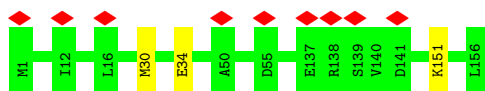
• Molecule 9: ATP synthase subunit b

Chain Y:

99%

M1 F17 L44 R49 K58 A68 L156
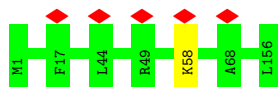
• Molecule 10: ATP synthase subunit a

Chain a:

97%

E4 L19 T37 I41 N42 F47 L52 G53 L54 L55 F56 A67 L125 I129 R140 V147 E177 K203 F256 E269
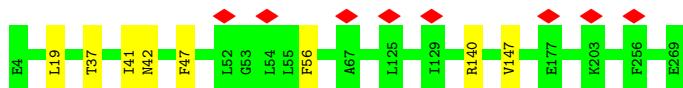
4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23917	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 $(e^-/\text{Å}^2)$	48	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.022	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	379.80798, 379.80798, 379.80798	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.079, 1.079, 1.079	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, 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	0.35	0/3879	0.58	0/5248
2	B	0.28	0/3933	0.49	0/5321
2	C	0.27	0/3903	0.49	0/5280
3	D	0.28	0/3577	0.49	0/4841
3	E	0.27	0/3590	0.48	0/4858
3	F	0.27	0/3590	0.48	0/4858
4	G	0.27	0/2217	0.48	0/2990
5	H	0.25	0/784	0.49	0/1058
6	I	0.27	0/565	0.46	0/764
6	J	0.28	0/565	0.43	0/764
6	L	0.27	0/565	0.45	0/764
6	M	0.28	0/565	0.45	0/764
6	N	0.27	0/565	0.44	0/764
6	O	0.28	0/565	0.46	0/764
6	P	0.28	0/565	0.47	0/764
6	Q	0.28	0/565	0.46	0/764
6	R	0.31	0/560	0.45	0/757
6	S	0.28	0/565	0.47	0/764
7	W	0.26	0/1333	0.47	0/1798
8	X	0.26	0/1208	0.47	0/1623
9	Y	0.27	0/1218	0.46	0/1634
10	a	0.31	0/2164	0.46	0/2955
All	All	0.29	0/37041	0.49	0/50097

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	506/508 (100%)	497 (98%)	9 (2%)	0	100	100
2	B	511/513 (100%)	503 (98%)	8 (2%)	0	100	100
2	C	508/513 (99%)	501 (99%)	7 (1%)	0	100	100
3	D	456/460 (99%)	447 (98%)	9 (2%)	0	100	100
3	E	458/460 (100%)	450 (98%)	8 (2%)	0	100	100
3	F	458/460 (100%)	452 (99%)	5 (1%)	1 (0%)	47	81
4	G	282/284 (99%)	279 (99%)	3 (1%)	0	100	100
5	H	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	I	75/77 (97%)	75 (100%)	0	0	100	100
6	J	75/77 (97%)	75 (100%)	0	0	100	100
6	L	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
6	M	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
6	N	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
6	O	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
6	P	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
6	Q	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
6	R	74/77 (96%)	73 (99%)	1 (1%)	0	100	100
6	S	75/77 (97%)	75 (100%)	0	0	100	100
7	W	171/173 (99%)	169 (99%)	2 (1%)	0	100	100
8	X	154/156 (99%)	148 (96%)	6 (4%)	0	100	100
9	Y	154/156 (99%)	152 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	a	264/266 (99%)	259 (98%)	4 (2%)	1 (0%)	34	72
All	All	4770/4820 (99%)	4695 (98%)	73 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	a	19	LEU
3	F	265	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	397/397 (100%)	394 (99%)	3 (1%)	81	91
2	B	403/403 (100%)	396 (98%)	7 (2%)	60	82
2	C	400/403 (99%)	391 (98%)	9 (2%)	50	77
3	D	379/380 (100%)	376 (99%)	3 (1%)	81	91
3	E	380/380 (100%)	376 (99%)	4 (1%)	73	88
3	F	380/380 (100%)	377 (99%)	3 (1%)	81	91
4	G	236/236 (100%)	230 (98%)	6 (2%)	47	75
5	H	81/81 (100%)	78 (96%)	3 (4%)	34	65
6	I	54/54 (100%)	53 (98%)	1 (2%)	57	80
6	J	54/54 (100%)	54 (100%)	0	100	100
6	L	54/54 (100%)	52 (96%)	2 (4%)	34	65
6	M	54/54 (100%)	53 (98%)	1 (2%)	57	80
6	N	54/54 (100%)	54 (100%)	0	100	100
6	O	54/54 (100%)	52 (96%)	2 (4%)	34	65
6	P	54/54 (100%)	54 (100%)	0	100	100
6	Q	54/54 (100%)	53 (98%)	1 (2%)	57	80
6	R	54/54 (100%)	50 (93%)	4 (7%)	13	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	S	54/54 (100%)	53 (98%)	1 (2%)	57	80
7	W	136/136 (100%)	134 (98%)	2 (2%)	65	84
8	X	119/119 (100%)	116 (98%)	3 (2%)	47	75
9	Y	121/121 (100%)	120 (99%)	1 (1%)	81	91
10	a	233/233 (100%)	226 (97%)	7 (3%)	41	71
All	All	3805/3809 (100%)	3742 (98%)	63 (2%)	62	82

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	458	LYS
9	Y	58	LYS
5	H	14	GLN
8	X	151	LYS
10	a	47	PHE

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

Mol	Chain	Res	Type
4	G	54	HIS
10	a	20	GLN
10	a	42	ASN

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   (i)

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	$\#|Z| > 2$
11	ATP	C	600	12	26,33,33	0.62	0	31,52,52	0.74	1 (3%)
13	ADP	F	500	-	24,29,29	0.96	1 (4%)	29,45,45	1.50	5 (17%)
11	ATP	D	502	12	26,33,33	0.67	0	31,52,52	0.80	2 (6%)
11	ATP	A	600	12	26,33,33	0.76	0	31,52,52	1.19	4 (12%)
13	ADP	E	501	12	24,29,29	0.96	1 (4%)	29,45,45	1.50	4 (13%)
11	ATP	B	600	12	26,33,33	0.62	0	31,52,52	0.74	2 (6%)

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
11	ATP	C	600	12	-	2/18/38/38	0/3/3/3
13	ADP	F	500	-	-	2/12/32/32	0/3/3/3
11	ATP	D	502	12	-	3/18/38/38	0/3/3/3
11	ATP	A	600	12	-	0/18/38/38	0/3/3/3
13	ADP	E	501	12	-	0/12/32/32	0/3/3/3
11	ATP	B	600	12	-	2/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	500	ADP	C5-C4	2.46	1.47	1.40
13	E	501	ADP	C5-C4	2.38	1.47	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	E	501	ADP	PA-O3A-PB	-3.70	120.14	132.83
13	F	500	ADP	N3-C2-N1	-3.61	123.03	128.68
13	E	501	ADP	C3'-C2'-C1'	3.38	106.07	100.98
11	A	600	ATP	O4'-C1'-C2'	-3.23	102.21	106.93
13	E	501	ADP	N3-C2-N1	-3.23	123.64	128.68

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	F	500	ADP	O4'-C4'-C5'-O5'
13	F	500	ADP	C3'-C4'-C5'-O5'
11	D	502	ATP	O4'-C4'-C5'-O5'
11	C	600	ATP	PA-O3A-PB-O1B
11	B	600	ATP	PA-O3A-PB-O1B

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 C 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP F 500

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP D 502

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP A 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP E 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 600

Bond lengths

Bond angles

Torsions

Rings
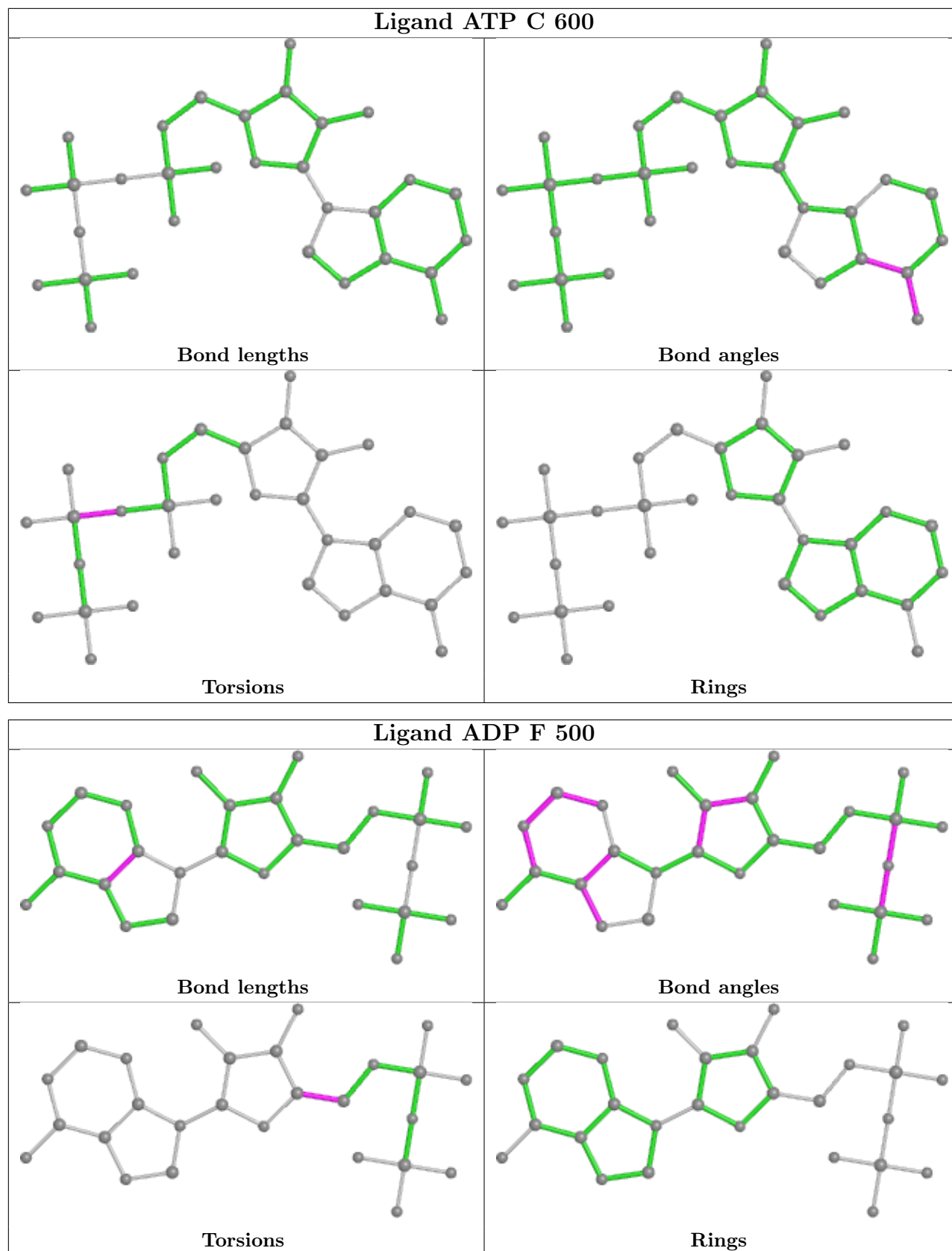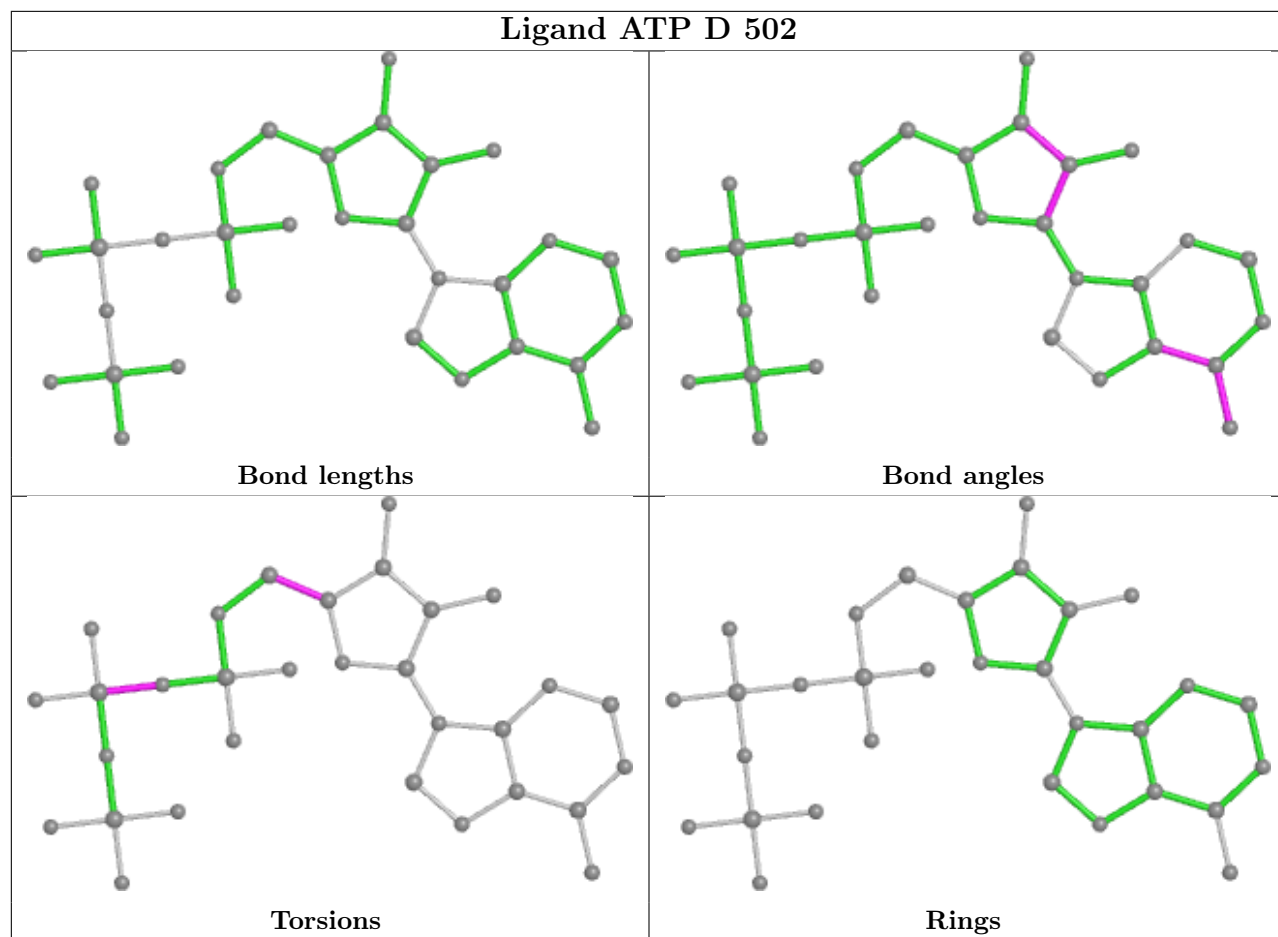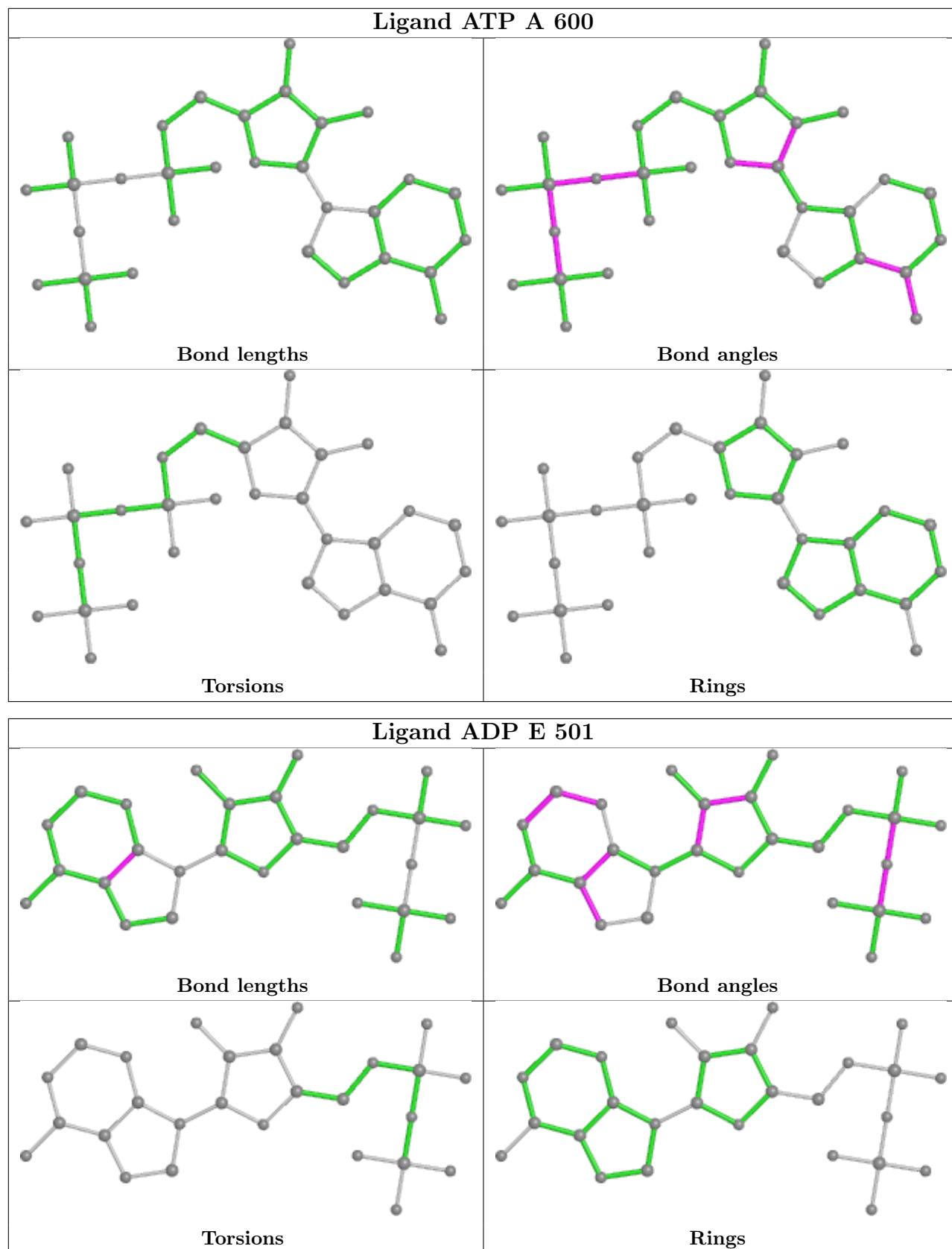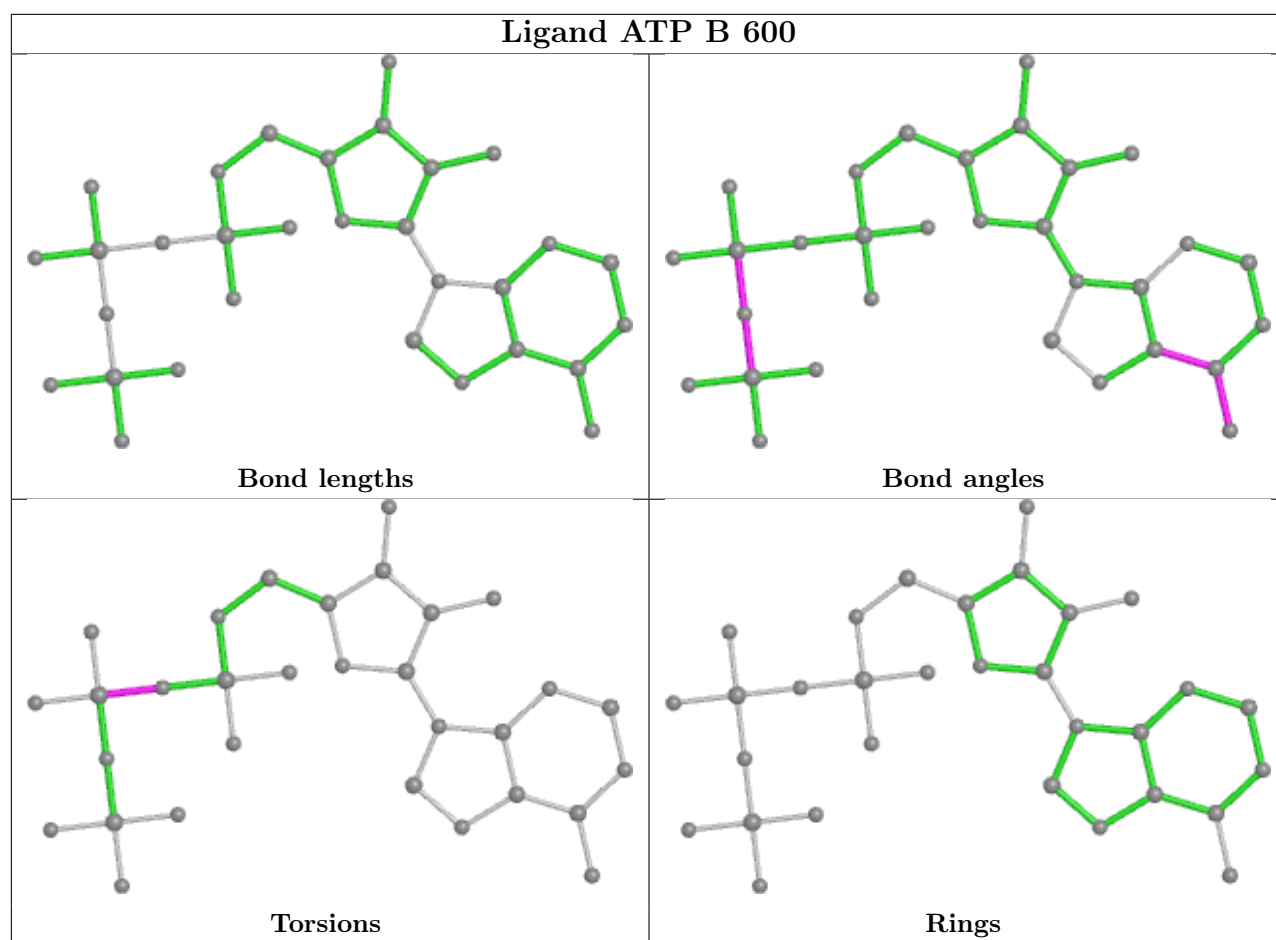
5.7 Other polymers ⓘ

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-27304. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections ⓘ
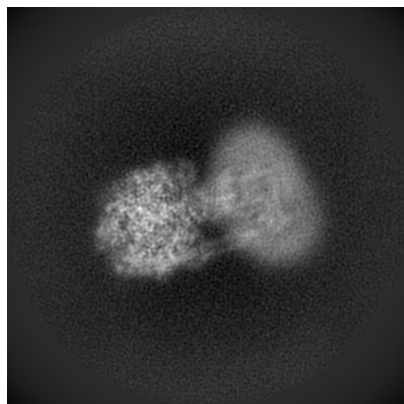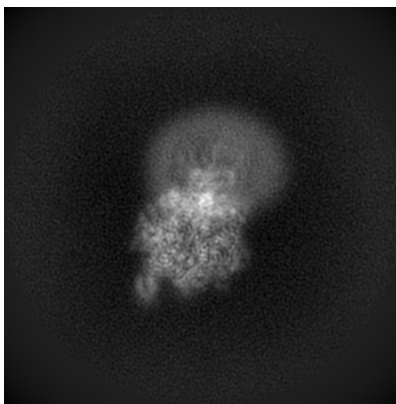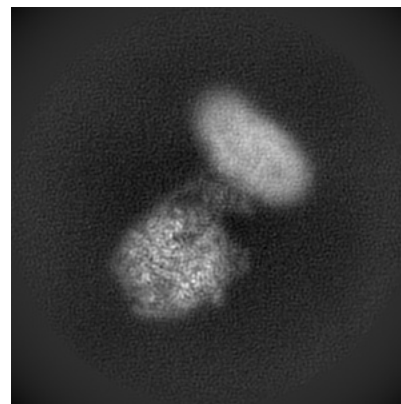
6.1.1 Primary map

| X | Y | Z |

6.1.2 Raw map

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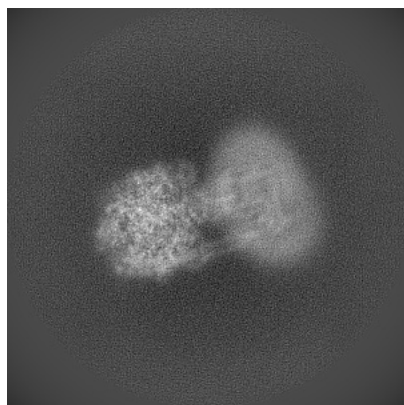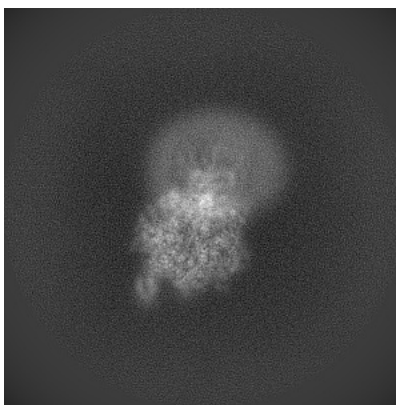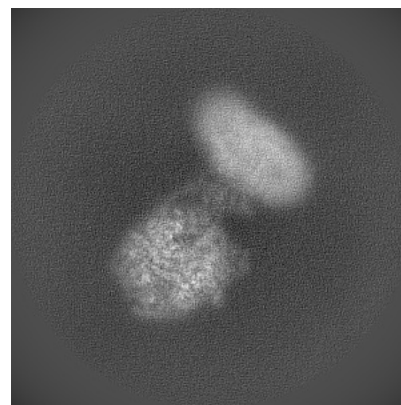
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
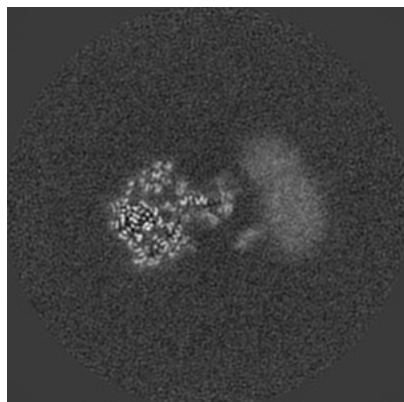
6.2.1 Primary map
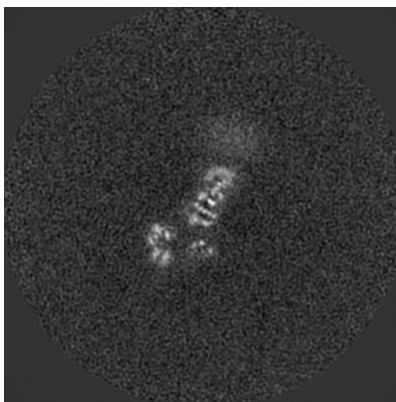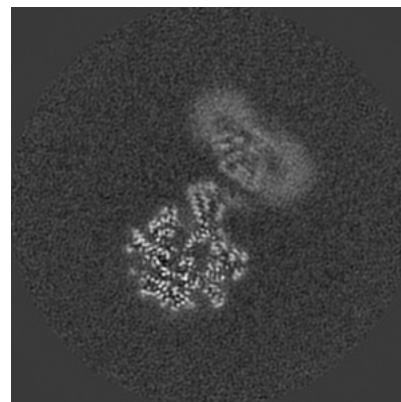
| X Index: 176 | Y Index: 176 | Z Index: 176 |

6.2.2 Raw map
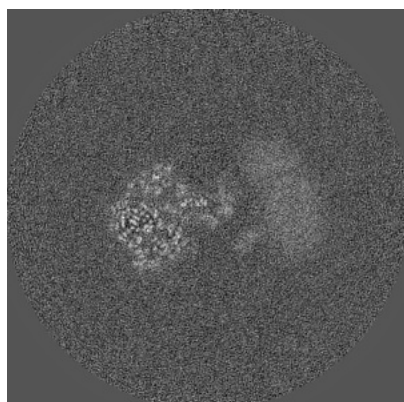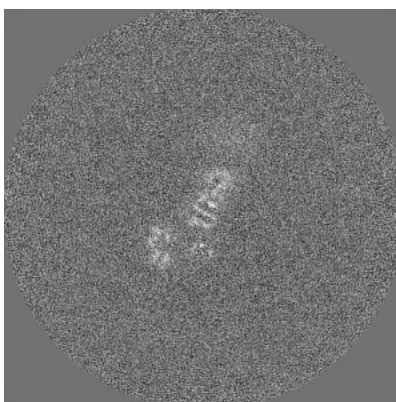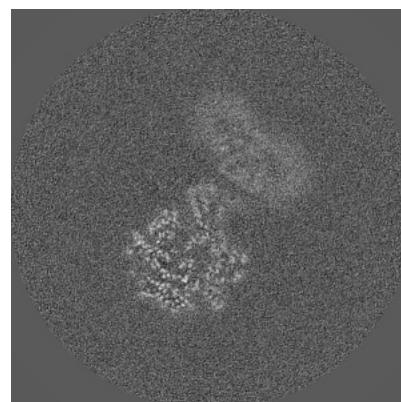
| X Index: 176 | Y Index: 176 | Z Index: 176 |

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

6.3 Largest variance slices (i)

6.3.1 Primary map
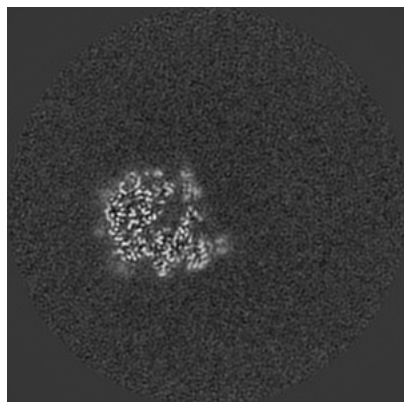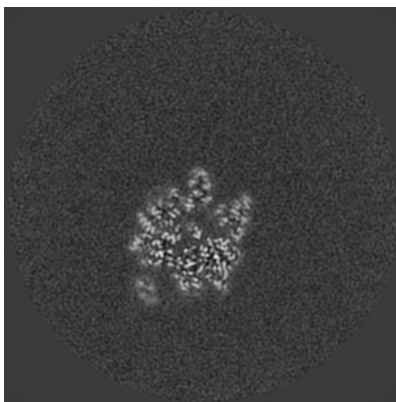
X Index: 148	Y Index: 134	Z Index: 174
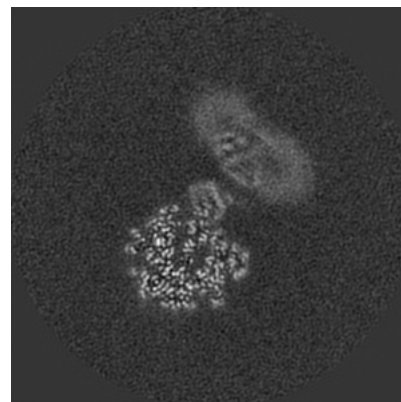
6.3.2 Raw map
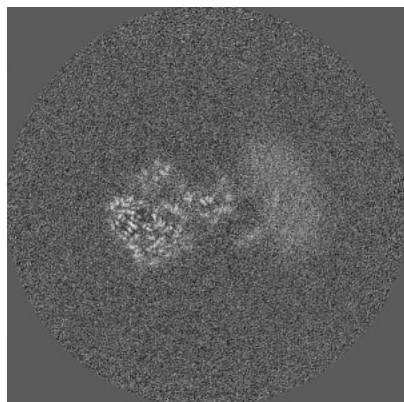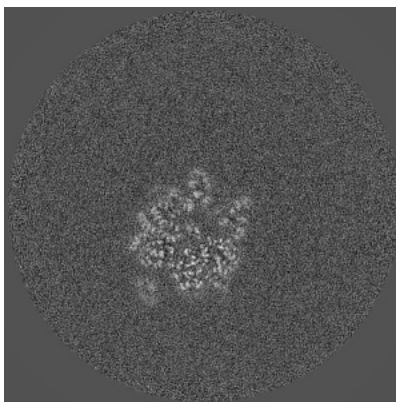
X Index: 178	Y Index: 135	Z Index: 175
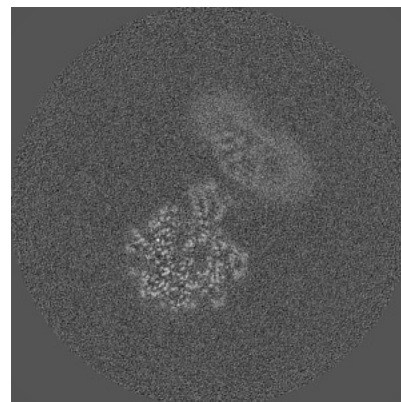
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

| X | Y | Z |
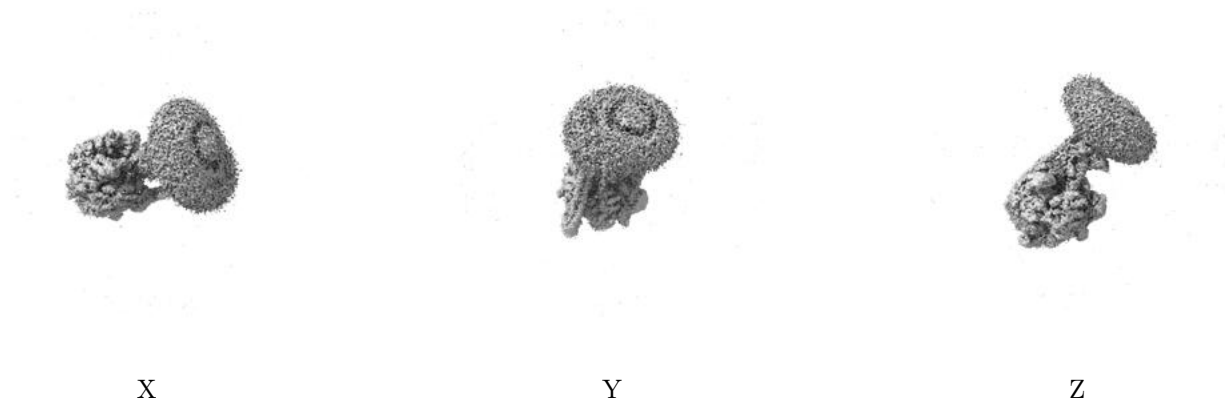
The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

| X | Y | Z |
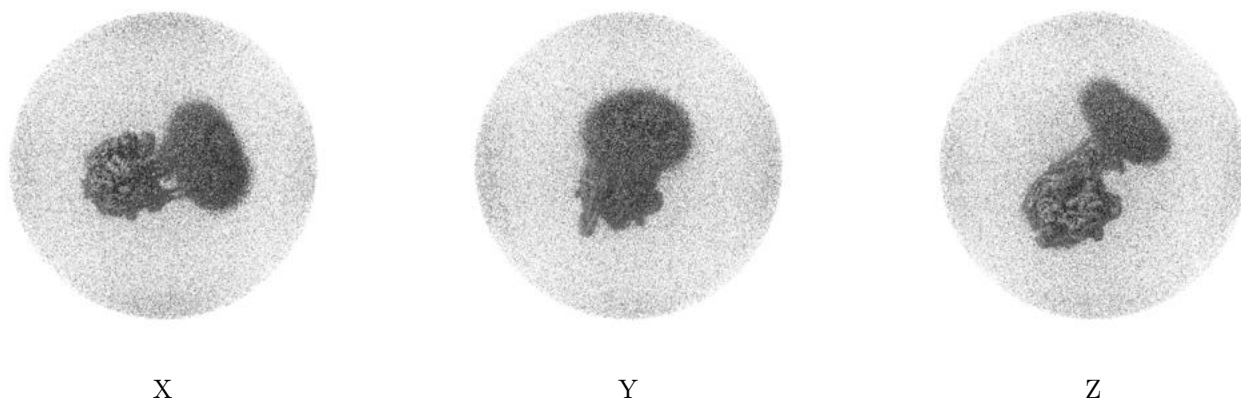
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 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)
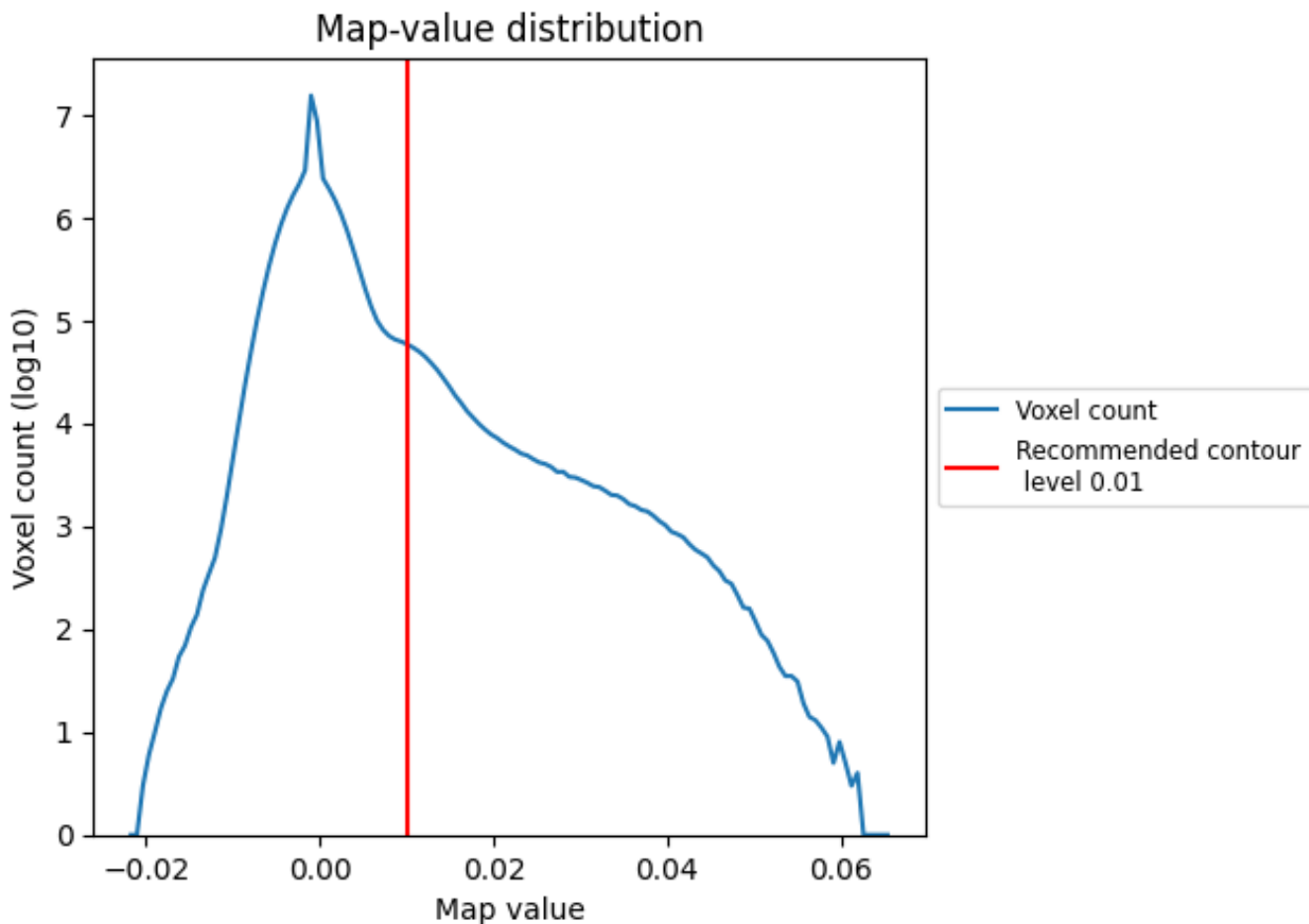
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
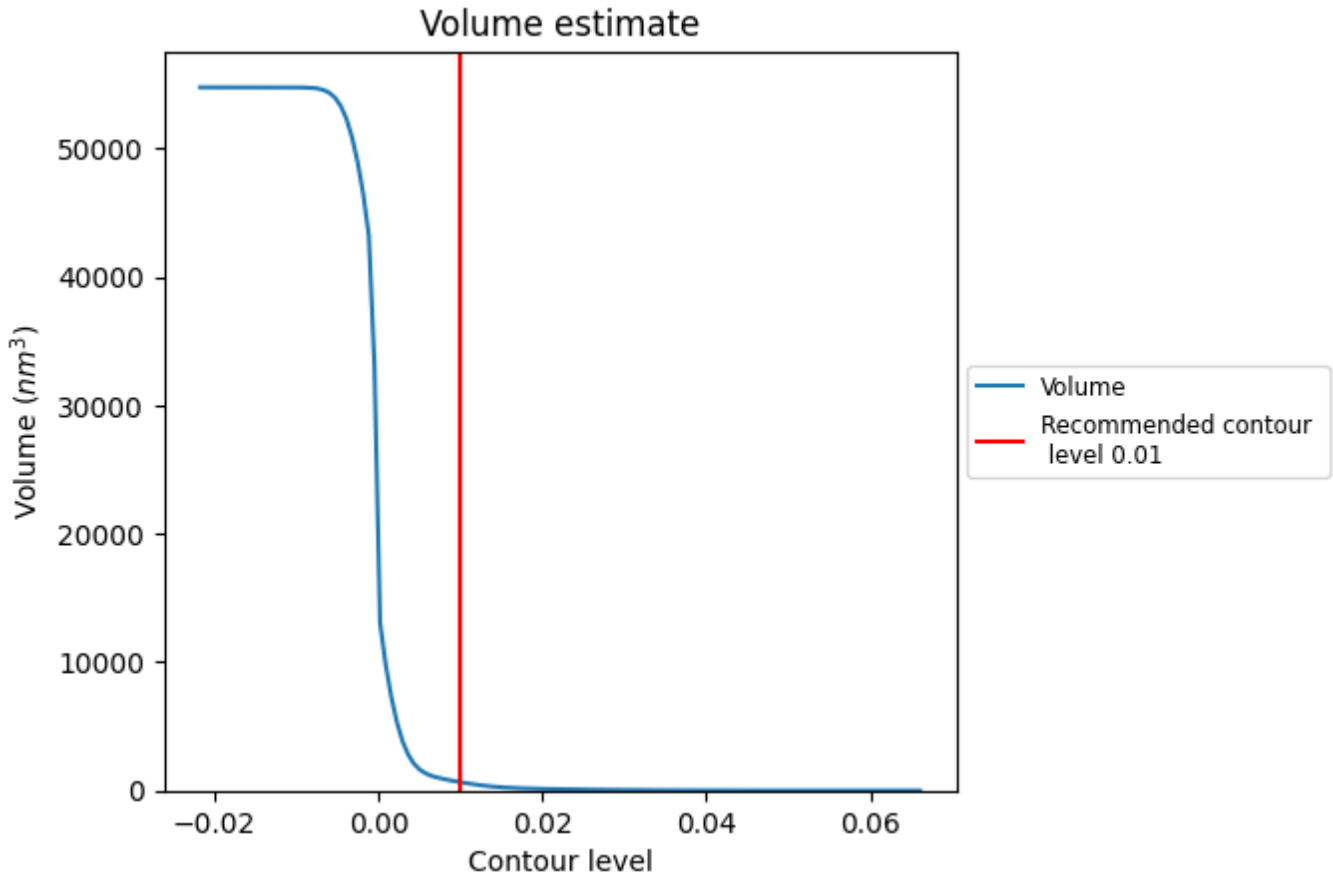
The volume at the recommended contour level is 653 nm^3; this corresponds to an approximate mass of 590 kDa.

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 ⓘ
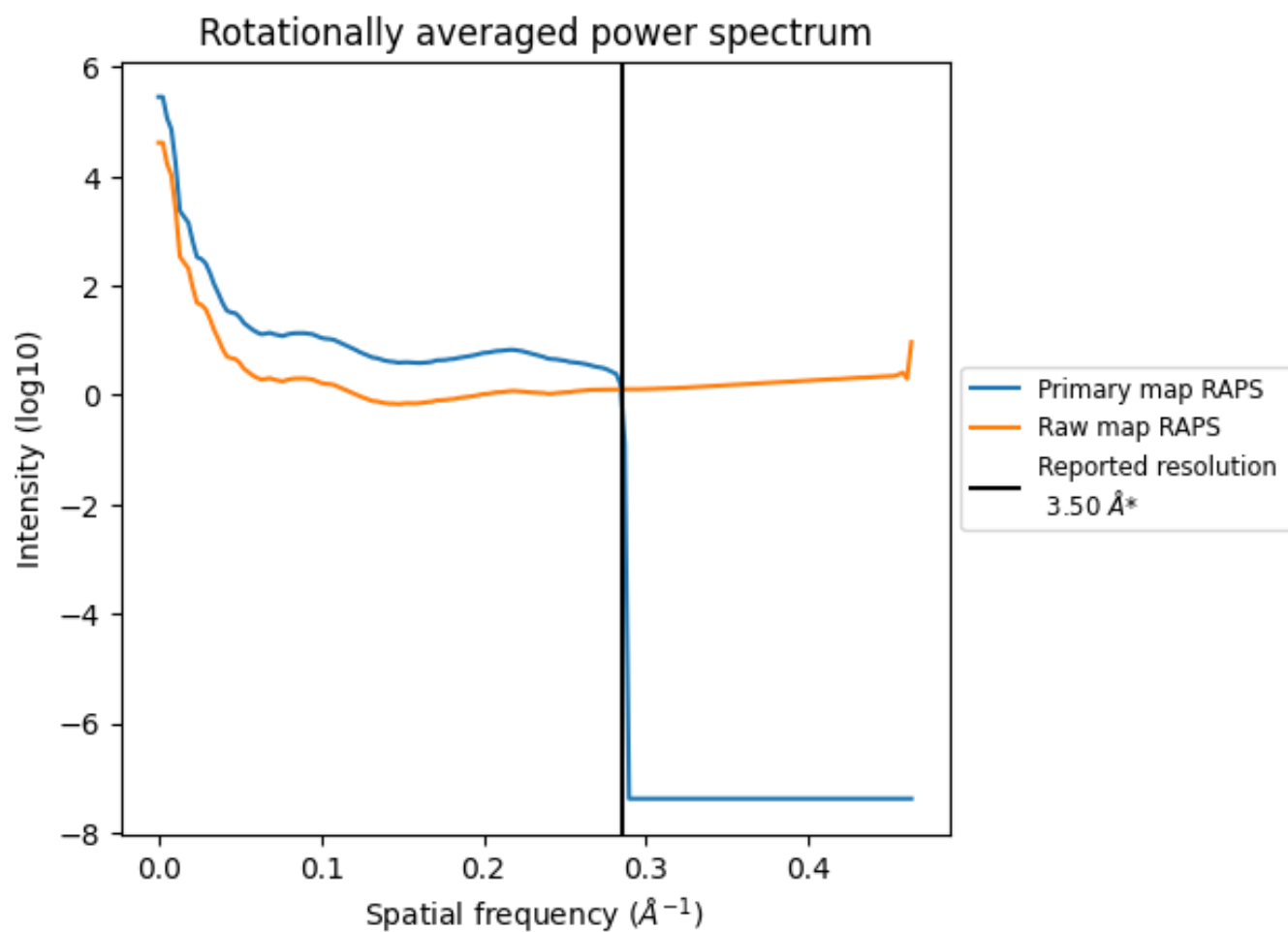
*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8   Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1   FSC ⓘ
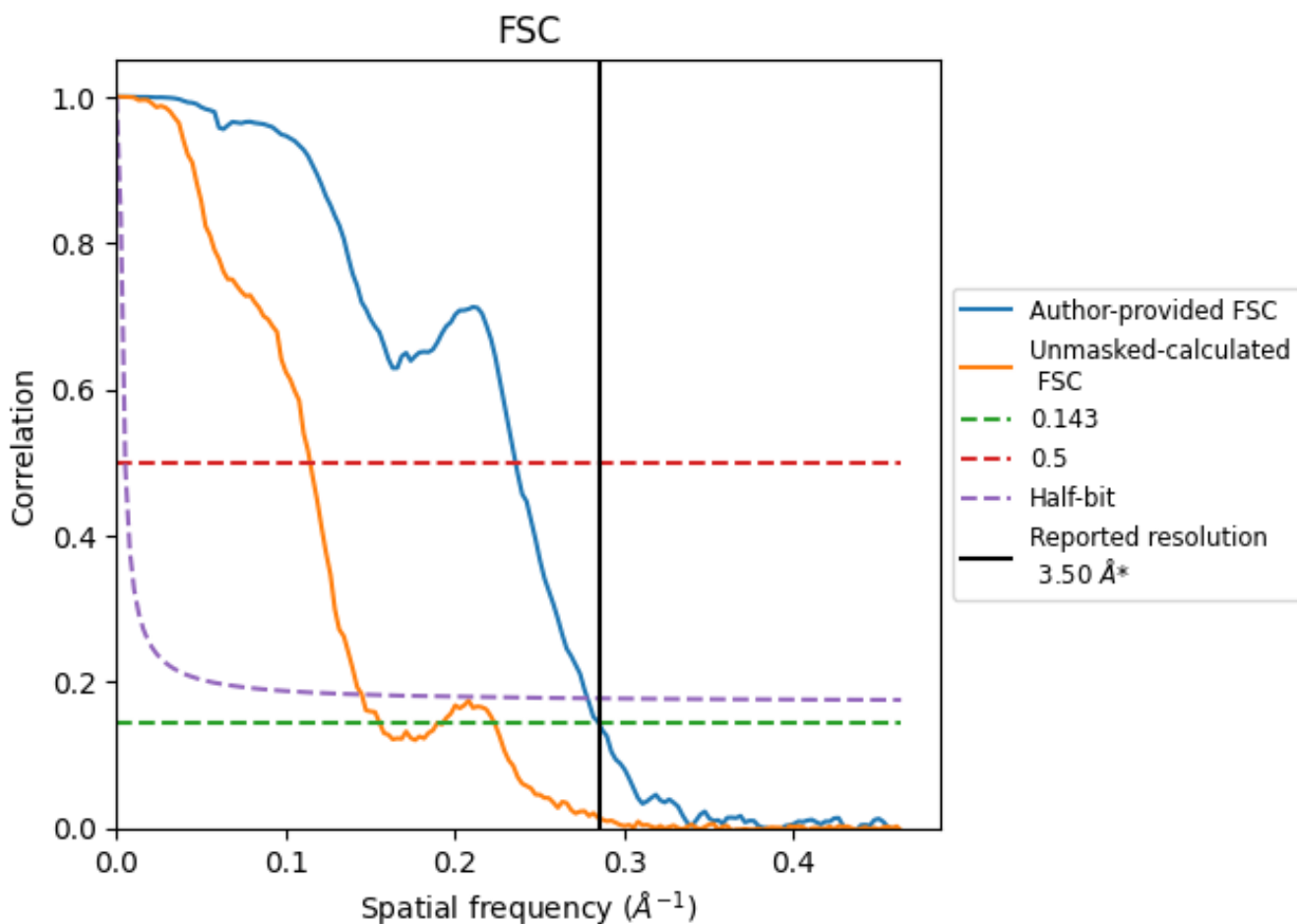
*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2   Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	4.24	3.59
Unmasked-calculated*	6.43	8.74	6.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.43 differs from the reported value 3.5 by more than 10 %

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-27304 and PDB model 8DBS. Per-residue inclusion information can be found in section 3 on page 9.

9.1   Map-model overlay ⓘ

X   Y   Z
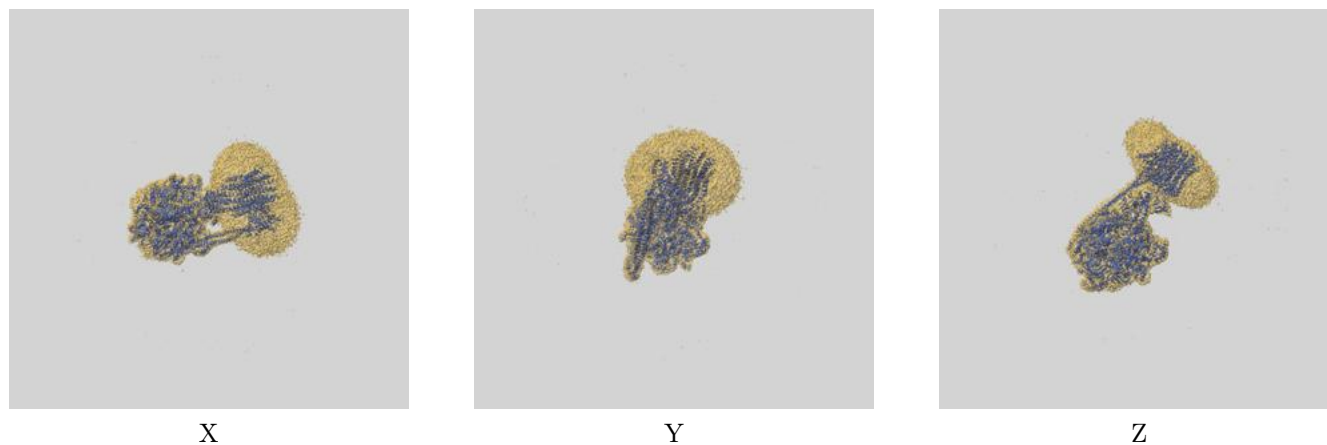
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ

X　　　　　　　　　Y　　　　　　　　　Z
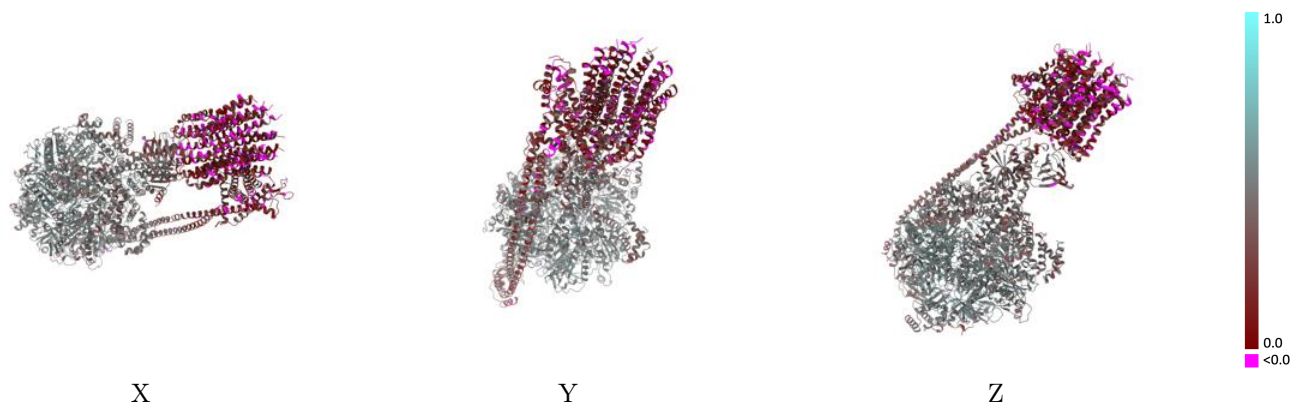
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
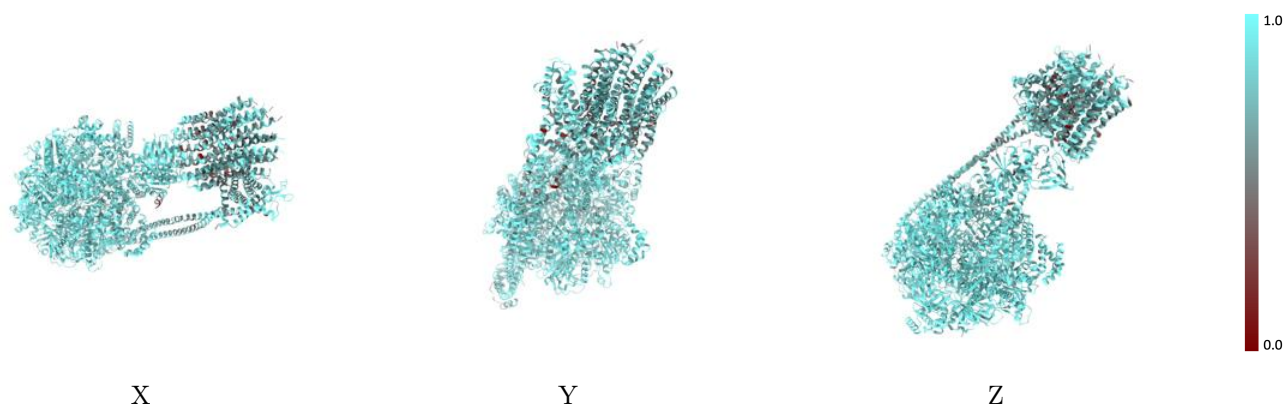
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4　Atom inclusion ⓘ
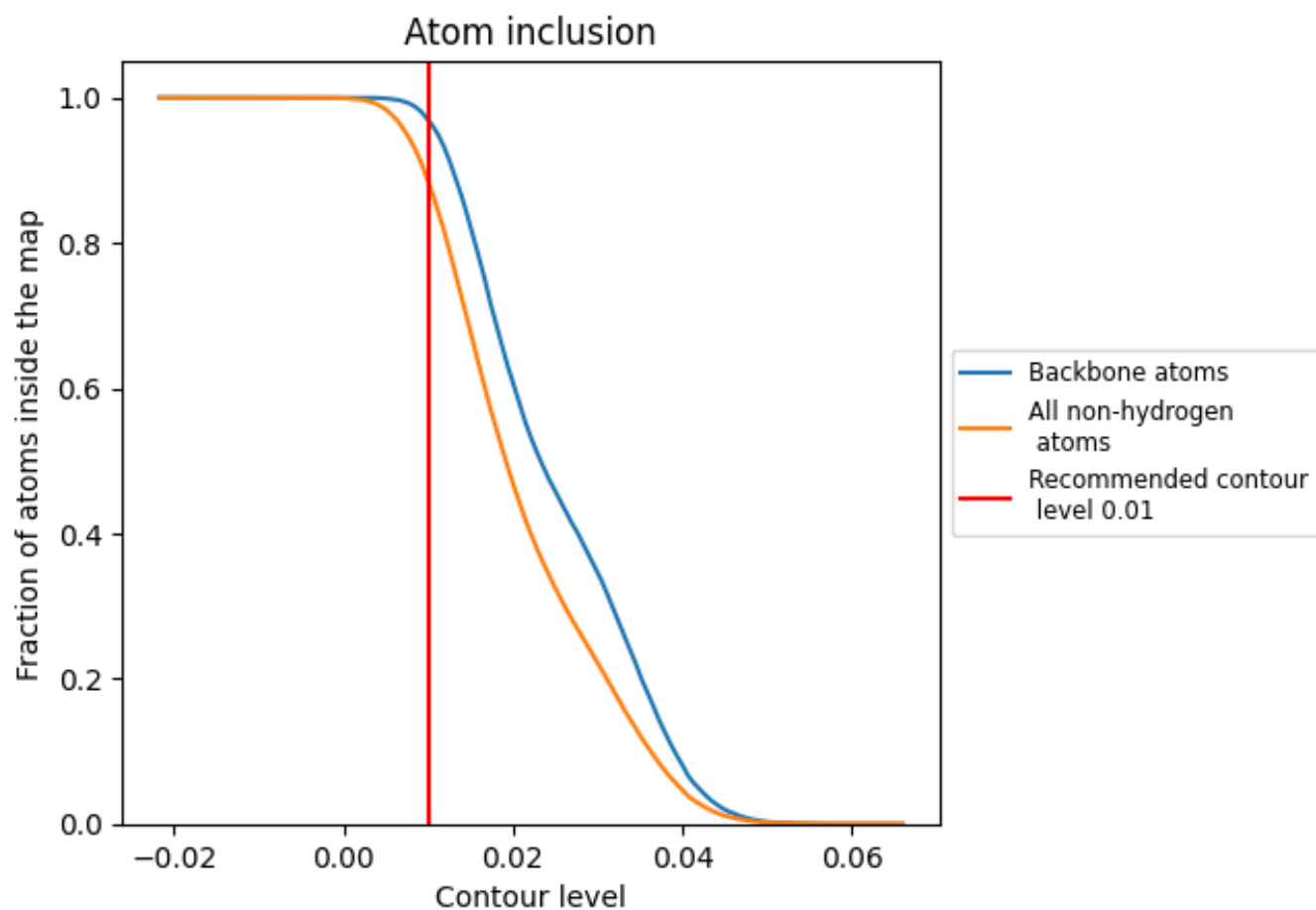
At the recommended contour level, 97% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5   Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8845	0.3900
A	0.9408	0.4830
B	0.9405	0.4810
C	0.9409	0.4810
D	0.9495	0.5110
E	0.9233	0.4760
F	0.9439	0.4910
G	0.8878	0.4050
H	0.8173	0.3580
I	0.7659	0.1450
J	0.7314	0.1200
L	0.7387	0.1070
M	0.7314	0.1130
N	0.7368	0.1010
O	0.7005	0.1260
P	0.7532	0.1550
Q	0.7114	0.1090
R	0.7857	0.1480
S	0.7332	0.1070
W	0.9321	0.4290
X	0.7729	0.2400
Y	0.7963	0.2640
a	0.7926	0.2020

1.0

0.0
<0.0