



# Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 02:24 PM EST

PDB ID : 6N2Z  
EMDB ID : EMD-9334  
Title : Bacillus PS3 ATP synthase class 2  
Authors : Guo, H.; Rubinstein, J.L.  
Deposited on : 2018-11-14  
Resolution : 3.00 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:

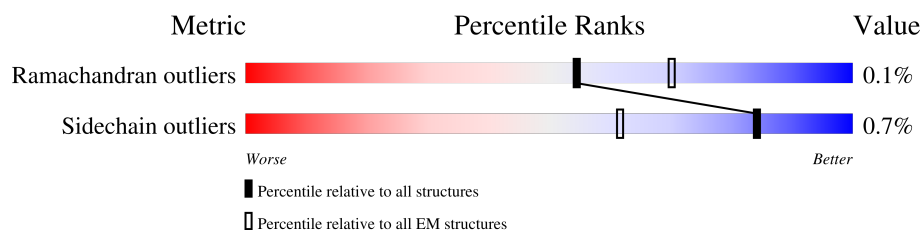
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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.



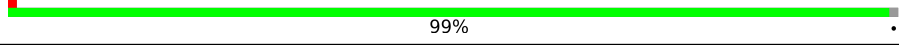
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	b2	168	
2	b1	168	
3	a	237	
4	c0	72	
4	c1	72	
4	c2	72	
4	c3	72	
4	c4	72	
4	c5	72	

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Mol	Chain	Length	Quality of chain
4	c6	72	 97% ..
4	c7	72	 99% .
4	c8	72	 97% ..
4	c9	72	 99% .
5	A	502	 99% .
5	B	502	 98% ..
5	C	502	 97% ..
6	D	473	 99%
6	E	473	 99% ..
6	F	473	 99% ..
7	G	285	 97% .
8	H	133	 92% . 5%
9	I	178	 98% ..

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 35051 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 Bacillus PS3 ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	b2	151	Total	C	N	O	S	0	0
			856	534	164	156	2		

- Molecule 2 is a protein called Bacillus PS3 ATP synthase subunit b.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b1	157	Total	C	N	O	S	0	0
			890	557	167	165	1		

- Molecule 3 is a protein called Bacillus PS3 ATP synthase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	203	Total	C	N	O	S	0	0
			1486	990	238	250	8		

- Molecule 4 is a protein called ATP synthase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c7	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
4	c8	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
4	c9	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
4	c0	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
4	c1	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
4	c2	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
4	c3	71	Total	C	N	O	S	0	0
			507	333	86	87	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	c4	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
4	c5	71	Total	C	N	O	S	0	0
			507	333	86	87	1		
4	c6	71	Total	C	N	O	S	0	0
			507	333	86	87	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	499	Total	C	N	O	S	0	0
			3806	2412	665	720	9		
5	C	494	Total	C	N	O	S	0	0
			3725	2360	652	704	9		
5	A	500	Total	C	N	O	S	0	0
			3833	2427	668	729	9		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	132	PRO	ARG	conflict	UNP A0A0M3VGF9
B	193	SER	CYS	conflict	UNP A0A0M3VGF9
B	463	PHE	TRP	conflict	UNP A0A0M3VGF9
C	132	PRO	ARG	conflict	UNP A0A0M3VGF9
C	193	SER	CYS	conflict	UNP A0A0M3VGF9
C	463	PHE	TRP	conflict	UNP A0A0M3VGF9
A	132	PRO	ARG	conflict	UNP A0A0M3VGF9
A	193	SER	CYS	conflict	UNP A0A0M3VGF9
A	463	PHE	TRP	conflict	UNP A0A0M3VGF9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	470	Total	C	N	O	S	0	0
			3618	2284	627	694	13		
6	F	469	Total	C	N	O	S	0	0
			3578	2261	624	681	12		
6	D	471	Total	C	N	O	S	0	0
			3614	2284	627	690	13		

- Molecule 7 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	284	Total	C	N	O	S	0	0
			2205	1393	386	418	8		

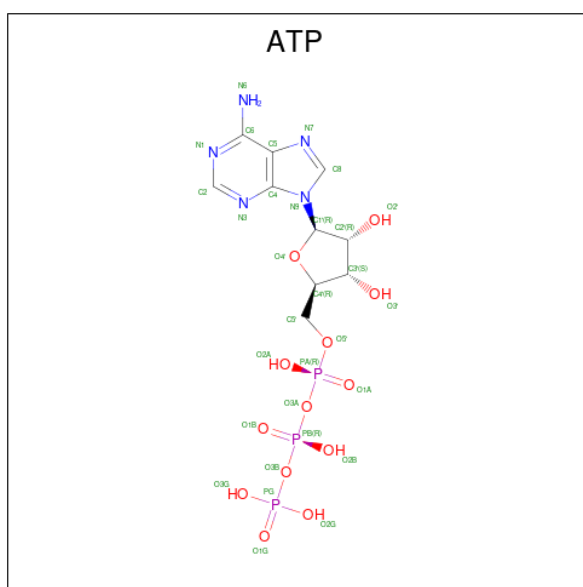
- Molecule 8 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	126	Total	C	N	O	S	0	0
			927	585	169	171	2		

- Molecule 9 is a protein called Bacillus PS3 ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	175	Total	C	N	O		0	0
			1314	840	238	236			

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

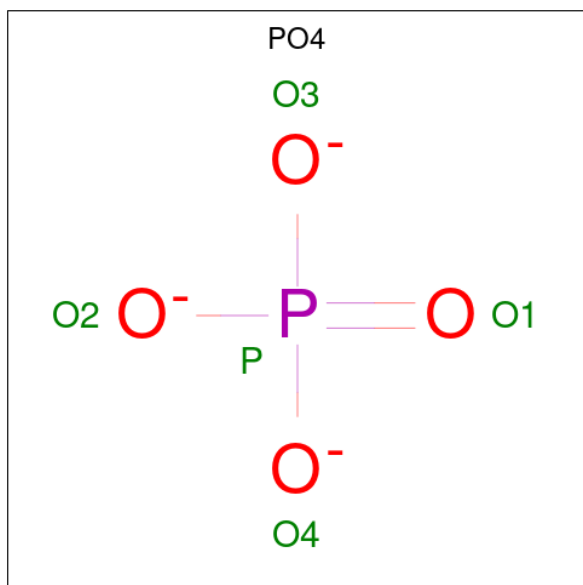


Mol	Chain	Residues	Atoms					AltConf
10	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

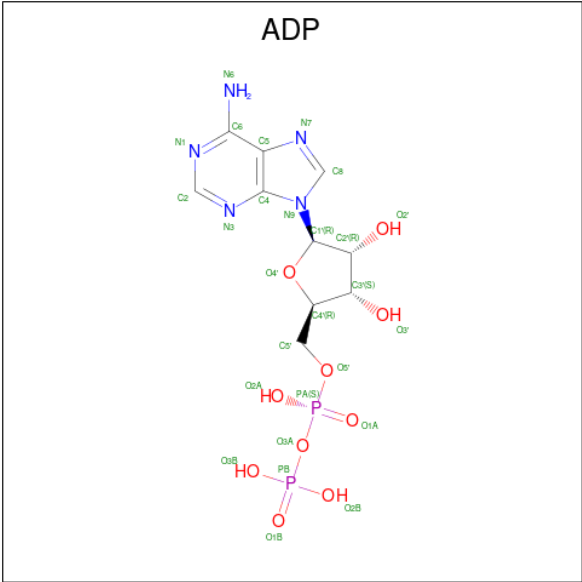
Mol	Chain	Residues	Atoms		AltConf
11	B	1	Total	Mg	0
			1	1	
11	C	1	Total	Mg	0
			1	1	
11	A	1	Total	Mg	0
			1	1	
11	D	1	Total	Mg	0
			1	1	

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



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

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



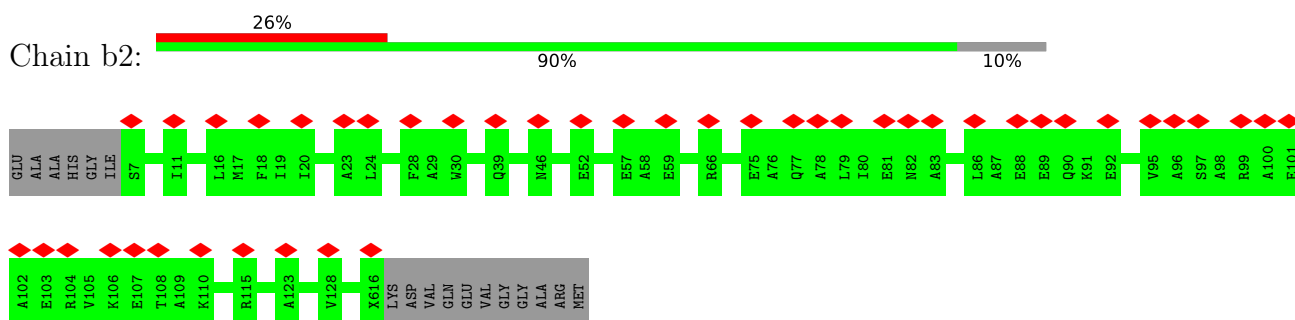
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
13	D	1	27	10	5	10	2	0



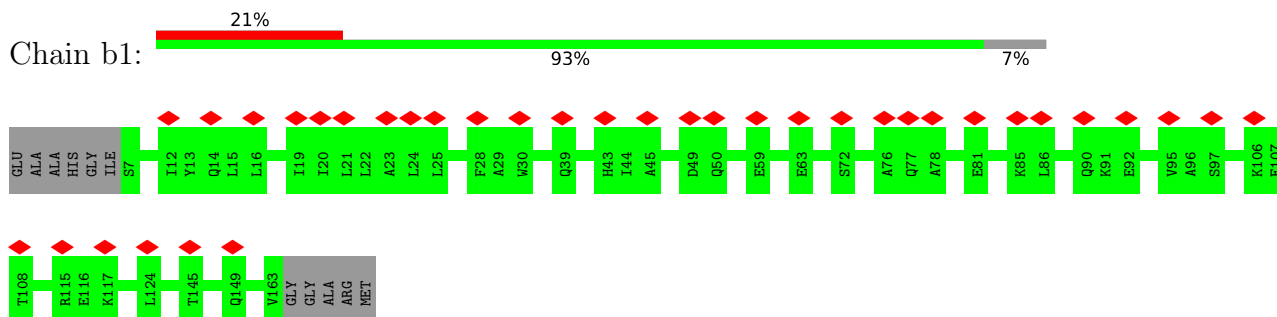
### 3 Residue-property plots [i](#)

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

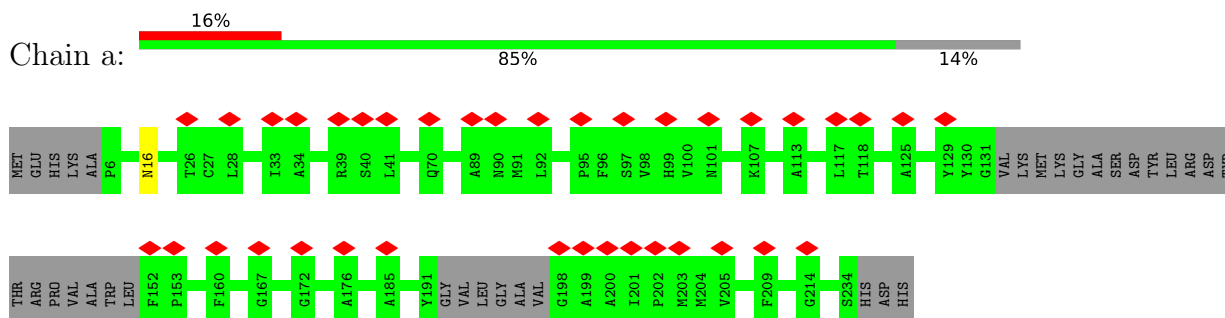
- Molecule 1: Bacillus PS3 ATP synthase subunit b



- Molecule 2: Bacillus PS3 ATP synthase subunit b

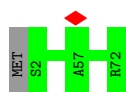


- Molecule 3: Bacillus PS3 ATP synthase subunit a



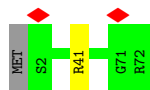
- Molecule 4: ATP synthase subunit c





- Molecule 4: ATP synthase subunit c

Chain c8: 97%



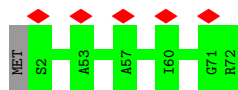
- Molecule 4: ATP synthase subunit c

Chain c9: 99%



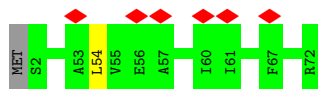
- Molecule 4: ATP synthase subunit c

Chain c0: 99%



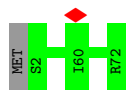
- Molecule 4: ATP synthase subunit c

Chain c1: 97%



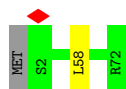
- Molecule 4: ATP synthase subunit c

Chain c2: 99%



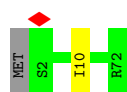
- Molecule 4: ATP synthase subunit c

Chain c3: 97%



- Molecule 4: ATP synthase subunit c

Chain c4:  97%



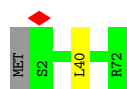
- Molecule 4: ATP synthase subunit c

Chain c5:  99%



- Molecule 4: ATP synthase subunit c

Chain c6:  97%



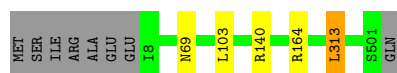
- Molecule 5: ATP synthase subunit alpha

Chain B:  98%



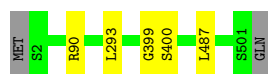
- Molecule 5: ATP synthase subunit alpha

Chain C:  97%



- Molecule 5: ATP synthase subunit alpha

Chain A:  99%



- Molecule 6: ATP synthase subunit beta

Chain E:  99%



- Molecule 6: ATP synthase subunit beta

Chain F:  99% ..



- Molecule 6: ATP synthase subunit beta

Chain D:  99%



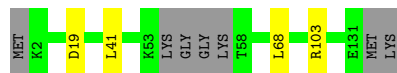
- Molecule 7: ATP synthase gamma chain

Chain G:  97% .



- Molecule 8: ATP synthase epsilon chain

Chain H:  92% . 5%



- Molecule 9: Bacillus PS3 ATP synthase subunit delta

Chain I:  98% ..



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	314448	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 ( $e^-/\text{\AA}^2$ )	0.71	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	132075	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	10.709	Depositor
Minimum map value	-6.071	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.211	Depositor
Recommended contour level	0.4	Depositor
Map size ( $\text{\AA}$ )	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP, PO4, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	b2	0.33	0/777	0.51	0/1074
2	b1	0.28	0/896	0.50	0/1242
3	a	0.32	0/1520	0.61	0/2079
4	c0	0.35	0/513	0.64	0/697
4	c1	0.32	0/513	0.66	1/697 (0.1%)
4	c2	0.34	0/513	0.64	0/697
4	c3	0.36	0/513	0.70	0/697
4	c4	0.35	0/513	0.73	0/697
4	c5	0.35	0/513	0.69	0/697
4	c6	0.35	0/513	0.71	0/697
4	c7	0.37	0/513	0.67	0/697
4	c8	0.37	0/513	0.66	0/697
4	c9	0.34	0/513	0.64	0/697
5	A	0.39	0/3894	0.60	1/5276 (0.0%)
5	B	0.37	0/3867	0.60	1/5241 (0.0%)
5	C	0.37	0/3785	0.60	2/5135 (0.0%)
6	D	0.41	0/3677	0.59	1/4980 (0.0%)
6	E	0.36	0/3681	0.59	0/4987
6	F	0.37	0/3641	0.61	1/4938 (0.0%)
7	G	0.33	0/2238	0.60	2/3031 (0.1%)
8	H	0.29	0/937	0.63	3/1270 (0.2%)
9	I	0.28	0/1329	0.53	0/1800
All	All	0.36	0/35372	0.61	12/48023 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	E	0	1
7	G	0	2
All	All	0	5

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	41	LEU	CA-CB-CG	6.53	130.31	115.30
5	C	313	LEU	CA-CB-CG	5.86	128.79	115.30
5	B	313	LEU	CA-CB-CG	5.84	128.73	115.30
6	D	198	LEU	CA-CB-CG	5.63	128.25	115.30
7	G	216	LEU	CA-CB-CG	5.55	128.08	115.30
4	c1	54	LEU	CA-CB-CG	5.40	127.73	115.30
8	H	19	ASP	CB-CG-OD2	5.19	122.97	118.30
8	H	68	LEU	CA-CB-CG	5.17	127.19	115.30
6	F	46	LEU	CA-CB-CG	5.16	127.16	115.30
7	G	4	LEU	CA-CB-CG	5.05	126.92	115.30
5	C	103	LEU	CA-CB-CG	5.02	126.85	115.30
5	A	293	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	399	GLY	Peptide
5	A	400	SER	Peptide
6	E	394	ASP	Peptide
7	G	135	LEU	Peptide
7	G	136	ASP	Peptide

## 5.2 Too-close contacts [i](#)

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	b2	132/168 (79%)	130 (98%)	2 (2%)	0	100	100
2	b1	155/168 (92%)	154 (99%)	1 (1%)	0	100	100
3	a	197/237 (83%)	186 (94%)	11 (6%)	0	100	100
4	c0	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
4	c1	69/72 (96%)	67 (97%)	2 (3%)	0	100	100
4	c2	69/72 (96%)	69 (100%)	0	0	100	100
4	c3	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
4	c4	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
4	c5	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
4	c6	69/72 (96%)	67 (97%)	2 (3%)	0	100	100
4	c7	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
4	c8	69/72 (96%)	67 (97%)	2 (3%)	0	100	100
4	c9	69/72 (96%)	68 (99%)	1 (1%)	0	100	100
5	A	498/502 (99%)	474 (95%)	24 (5%)	0	100	100
5	B	497/502 (99%)	482 (97%)	15 (3%)	0	100	100
5	C	492/502 (98%)	475 (96%)	17 (4%)	0	100	100
6	D	469/473 (99%)	447 (95%)	21 (4%)	1 (0%)	47	82
6	E	468/473 (99%)	444 (95%)	23 (5%)	1 (0%)	47	82
6	F	467/473 (99%)	445 (95%)	21 (4%)	1 (0%)	47	82
7	G	282/285 (99%)	269 (95%)	12 (4%)	1 (0%)	34	72
8	H	122/133 (92%)	115 (94%)	7 (6%)	0	100	100
9	I	173/178 (97%)	169 (98%)	4 (2%)	0	100	100
All	All	4642/4814 (96%)	4468 (96%)	170 (4%)	4 (0%)	54	85

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
6	F	275	VAL
6	D	275	VAL
6	E	275	VAL
7	G	207	PRO

### 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	b2	26/124 (21%)	26 (100%)	0	100	100
2	b1	29/140 (21%)	29 (100%)	0	100	100
3	a	143/198 (72%)	142 (99%)	1 (1%)	84	94
4	c0	51/52 (98%)	51 (100%)	0	100	100
4	c1	51/52 (98%)	51 (100%)	0	100	100
4	c2	51/52 (98%)	51 (100%)	0	100	100
4	c3	51/52 (98%)	50 (98%)	1 (2%)	55	83
4	c4	51/52 (98%)	50 (98%)	1 (2%)	55	83
4	c5	51/52 (98%)	51 (100%)	0	100	100
4	c6	51/52 (98%)	50 (98%)	1 (2%)	55	83
4	c7	51/52 (98%)	51 (100%)	0	100	100
4	c8	51/52 (98%)	50 (98%)	1 (2%)	55	83
4	c9	51/52 (98%)	51 (100%)	0	100	100
5	A	408/412 (99%)	406 (100%)	2 (0%)	88	96
5	B	402/412 (98%)	395 (98%)	7 (2%)	60	85
5	C	386/412 (94%)	382 (99%)	4 (1%)	76	91
6	D	384/389 (99%)	384 (100%)	0	100	100
6	E	385/389 (99%)	384 (100%)	1 (0%)	92	97
6	F	374/389 (96%)	373 (100%)	1 (0%)	92	97
7	G	234/240 (98%)	232 (99%)	2 (1%)	78	92
8	H	92/108 (85%)	91 (99%)	1 (1%)	73	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	129/146 (88%)	128 (99%)	1 (1%)	81	93
All	All	3502/3879 (90%)	3478 (99%)	24 (1%)	84	94

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	a	16	ASN
4	c8	41	ARG
4	c3	58	LEU
4	c4	10	ILE
4	c6	40	LEU
5	B	90	ARG
5	B	140	ARG
5	B	164	ARG
5	B	283	ARG
5	B	358	ASN
5	B	454	ARG
5	B	496	LYS
5	C	69	ASN
5	C	140	ARG
5	C	164	ARG
5	C	313	LEU
5	A	90	ARG
5	A	487	LEU
6	E	297	LYS
6	F	196	ASN
7	G	85	ARG
7	G	186	ARG
8	H	103	ARG
9	I	115	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
3	a	16	ASN
3	a	90	ASN
3	a	173	ASN
3	a	217	GLN
3	a	231	HIS
4	c8	37	GLN
4	c2	23	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
4	c4	23	ASN
5	B	186	GLN
5	B	189	GLN
5	B	345	GLN
5	B	358	ASN
5	B	422	GLN
5	B	425	HIS
5	C	42	HIS
5	C	69	ASN
5	C	147	GLN
5	C	186	GLN
5	C	189	GLN
5	C	425	HIS
5	A	186	GLN
5	A	189	GLN
5	A	215	HIS
5	A	345	GLN
5	A	397	GLN
5	A	425	HIS
5	A	426	GLN
5	A	488	ASN
6	E	22	HIS
6	E	289	GLN
6	E	304	GLN
6	E	324	HIS
6	E	381	GLN
6	E	412	GLN
6	F	53	HIS
6	F	196	ASN
6	F	289	GLN
6	F	304	GLN
6	D	53	HIS
6	D	217	GLN
6	D	253	ASN
6	D	289	GLN
6	D	304	GLN
6	D	324	HIS
7	G	55	ASN
7	G	143	GLN
7	G	173	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 ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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$
10	ATP	C	600	11	26,33,33	0.91	1 (3%)	31,52,52	1.51	5 (16%)
13	ADP	D	600	11	24,29,29	0.96	1 (4%)	29,45,45	1.33	4 (13%)
12	PO4	F	600	-	4,4,4	0.96	0	6,6,6	0.45	0
10	ATP	A	600	11	26,33,33	0.92	1 (3%)	31,52,52	1.46	5 (16%)
10	ATP	B	600	11	26,33,33	0.92	1 (3%)	31,52,52	1.58	6 (19%)

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
10	ATP	B	600	11	-	5/18/38/38	0/3/3/3
10	ATP	C	600	11	-	4/18/38/38	0/3/3/3
13	ADP	D	600	11	-	1/12/32/32	0/3/3/3
10	ATP	A	600	11	-	2/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	600	ATP	C5-C4	2.38	1.47	1.40
10	C	600	ATP	C5-C4	2.32	1.47	1.40
10	A	600	ATP	C5-C4	2.30	1.47	1.40
13	D	600	ADP	C5-C4	2.27	1.46	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	600	ATP	PB-O3B-PG	-3.79	119.83	132.83
10	C	600	ATP	PB-O3B-PG	-3.47	120.91	132.83
10	B	600	ATP	PA-O3A-PB	-3.43	121.07	132.83
10	C	600	ATP	N3-C2-N1	-3.26	123.59	128.68
10	A	600	ATP	N3-C2-N1	-3.25	123.61	128.68
10	B	600	ATP	N3-C2-N1	-3.15	123.75	128.68
10	B	600	ATP	C3'-C2'-C1'	3.13	105.69	100.98
13	D	600	ADP	N3-C2-N1	-3.13	123.79	128.68
13	D	600	ADP	C3'-C2'-C1'	3.13	105.68	100.98
10	C	600	ATP	PA-O3A-PB	-3.04	122.40	132.83
10	C	600	ATP	C3'-C2'-C1'	3.00	105.49	100.98
10	A	600	ATP	PA-O3A-PB	-2.97	122.62	132.83
10	A	600	ATP	C3'-C2'-C1'	2.83	105.24	100.98
10	A	600	ATP	PB-O3B-PG	-2.72	123.48	132.83
13	D	600	ADP	C4-C5-N7	-2.56	106.73	109.40
10	A	600	ATP	C4-C5-N7	-2.51	106.78	109.40
10	B	600	ATP	C4-C5-N7	-2.44	106.86	109.40
10	C	600	ATP	C4-C5-N7	-2.36	106.94	109.40
10	B	600	ATP	O2A-PA-O1A	2.15	122.87	112.24
13	D	600	ADP	PA-O3A-PB	-2.12	125.56	132.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	600	ATP	C5'-O5'-PA-O2A
10	B	600	ATP	C5'-O5'-PA-O3A
10	B	600	ATP	O4'-C4'-C5'-O5'
10	C	600	ATP	C5'-O5'-PA-O2A
13	D	600	ADP	O4'-C4'-C5'-O5'
10	B	600	ATP	C3'-C4'-C5'-O5'
10	A	600	ATP	O4'-C4'-C5'-O5'
10	C	600	ATP	C5'-O5'-PA-O3A

*Continued on next page...*

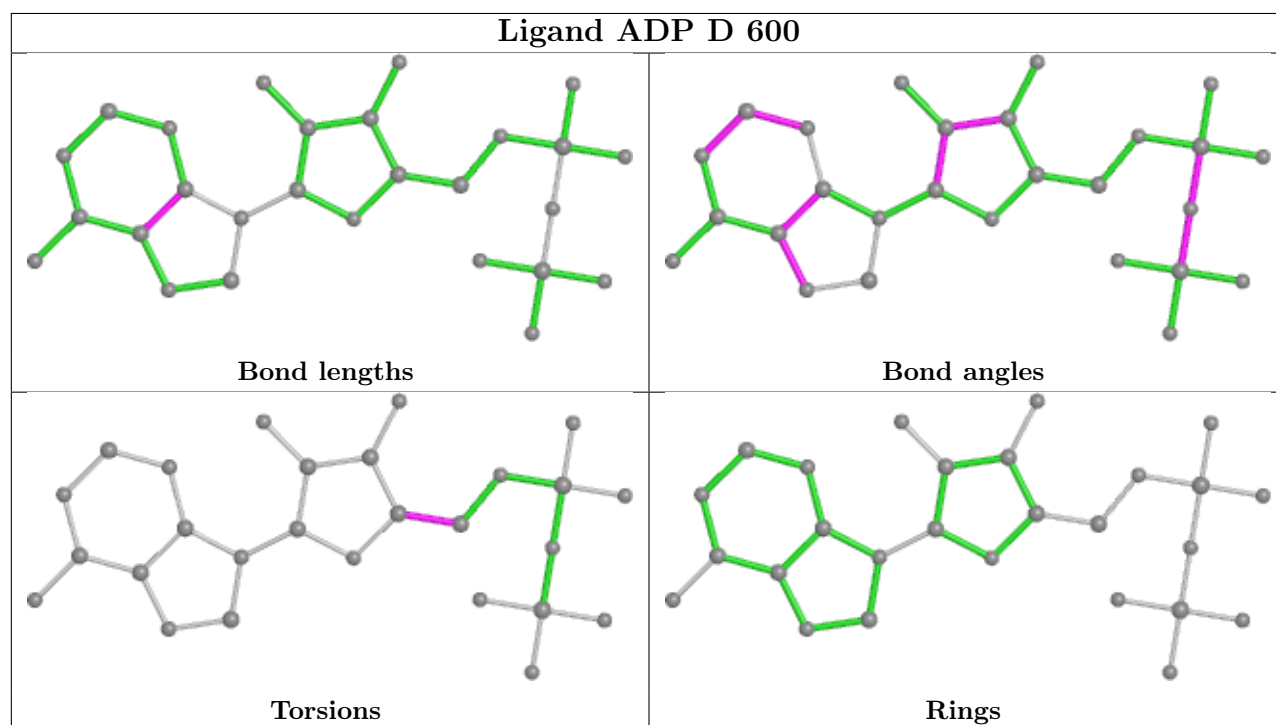
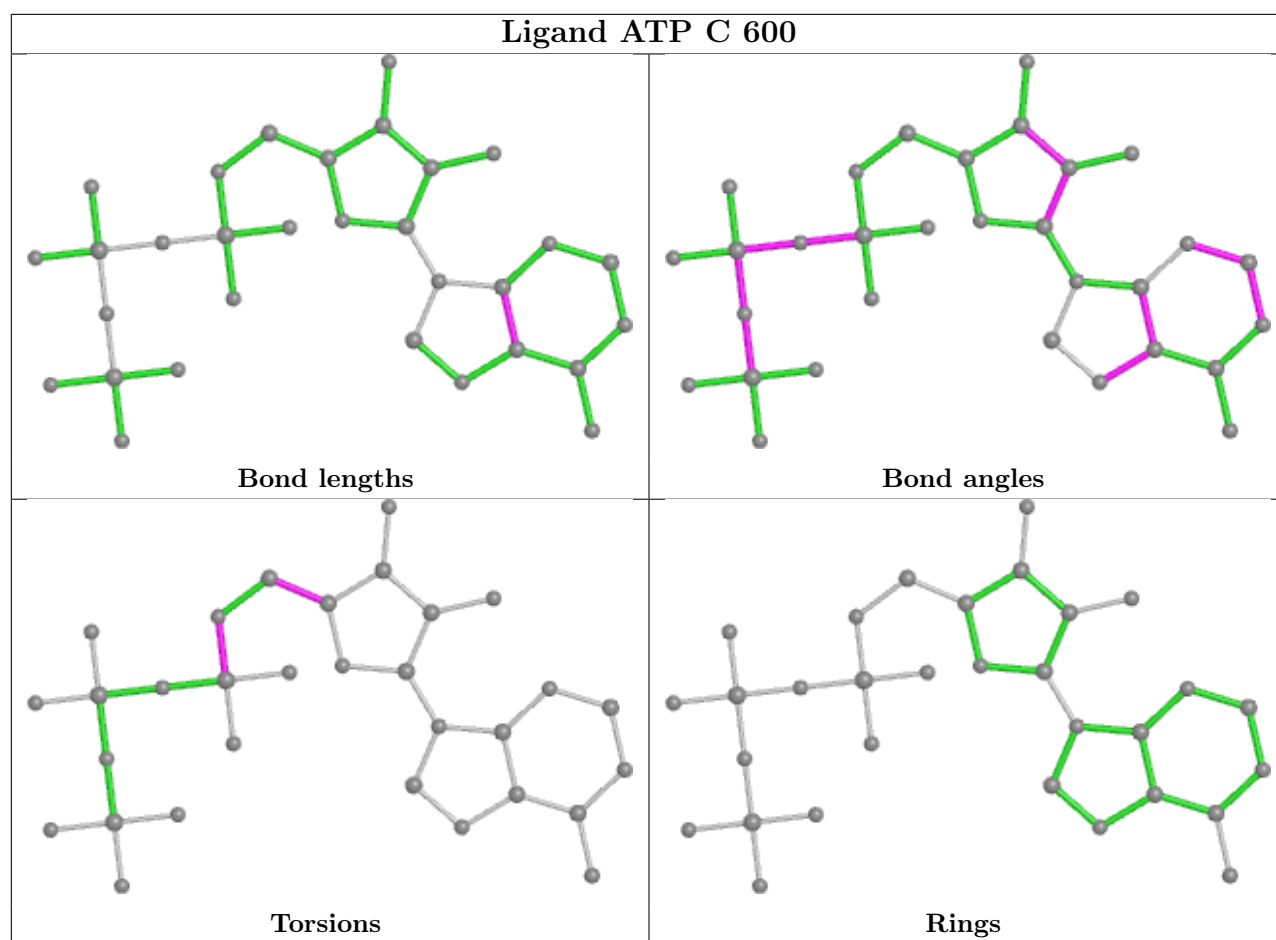
*Continued from previous page...*

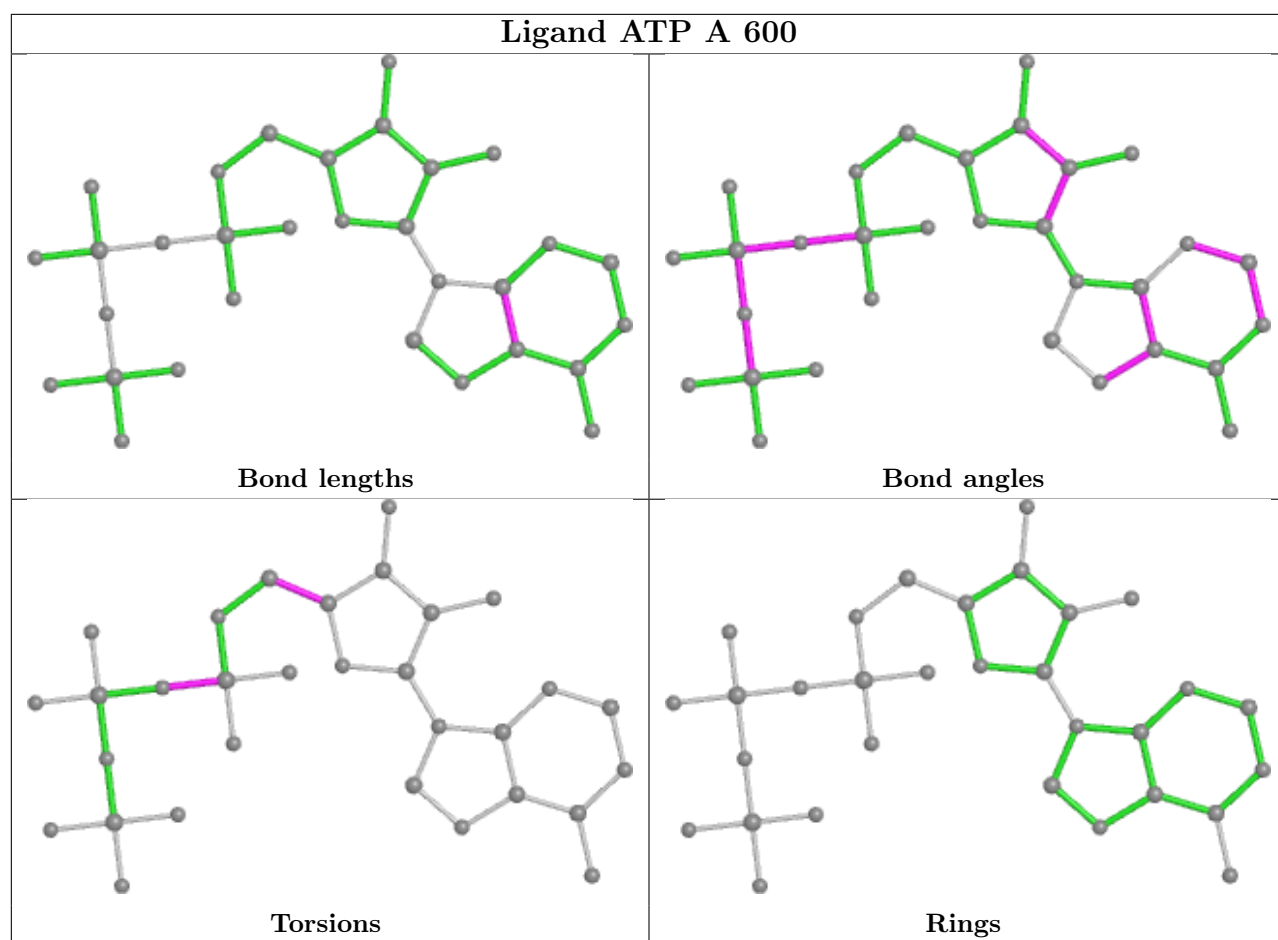
Mol	Chain	Res	Type	Atoms
10	A	600	ATP	PB-O3A-PA-O2A
10	B	600	ATP	C4'-C5'-O5'-PA
10	C	600	ATP	C5'-O5'-PA-O1A
10	C	600	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

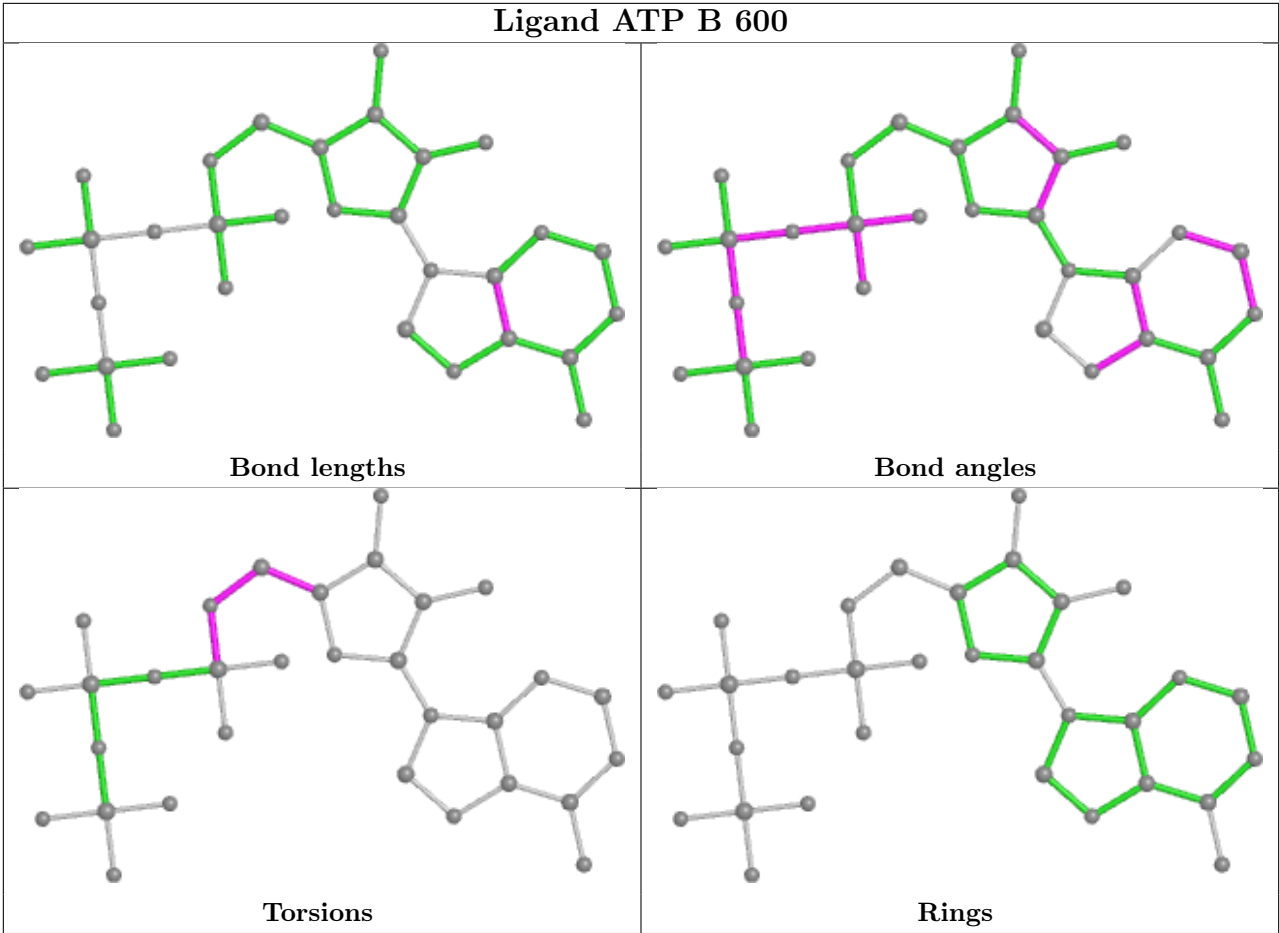
No monomer is involved in short contacts.

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 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	b2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b2	140:ILE	C	600:UNK	N	11.21

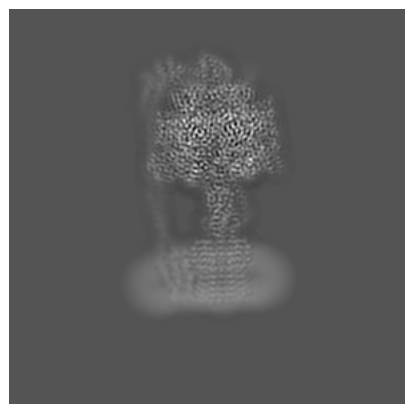
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9334. These allow visual inspection of the internal detail of the map and identification of artifacts.

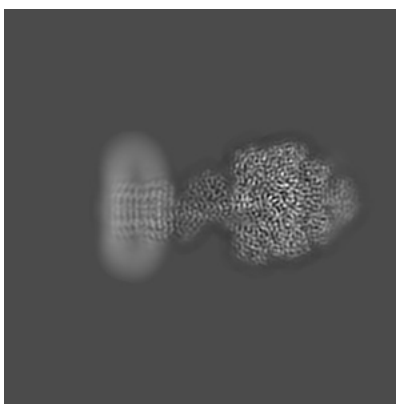
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

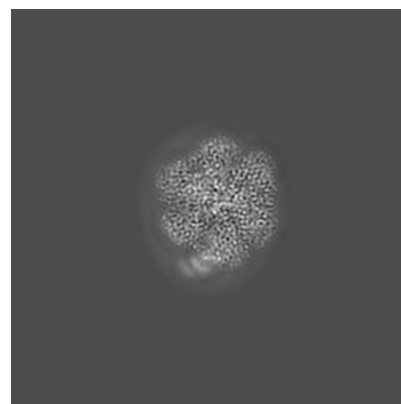
#### 6.1.1 Primary map



X

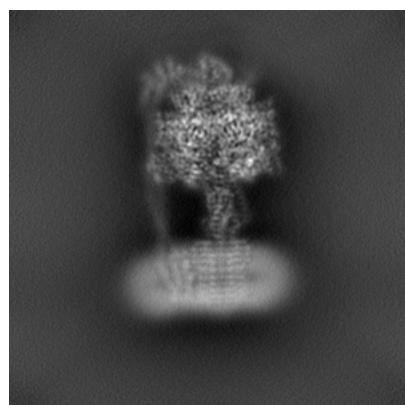


Y

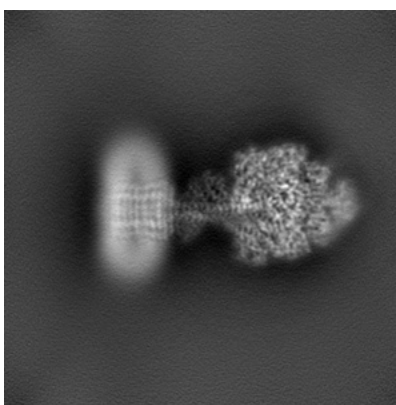


Z

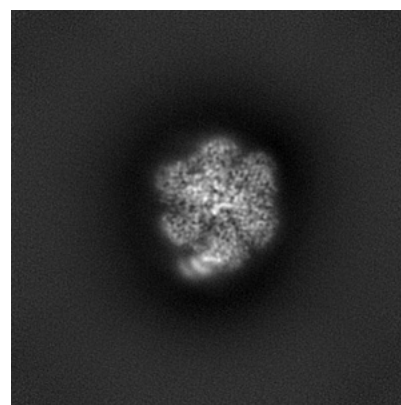
#### 6.1.2 Raw map



X



Y



Z

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

## 6.2 Central slices [i](#)

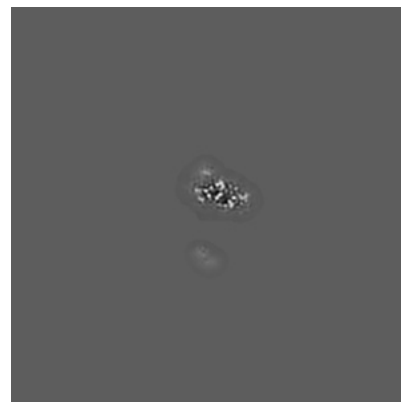
### 6.2.1 Primary map



X Index: 160

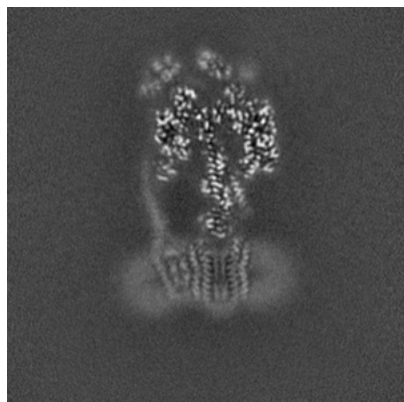


Y Index: 160

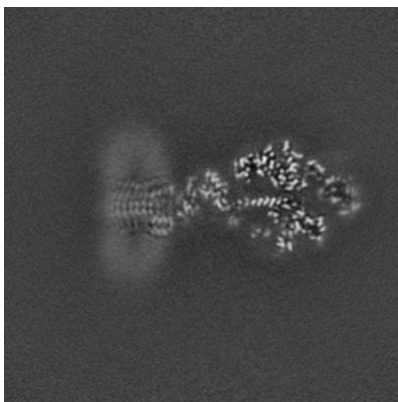


Z Index: 160

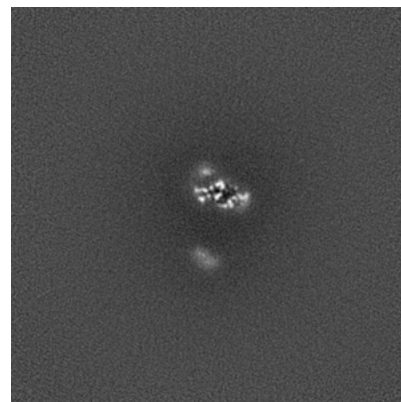
### 6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

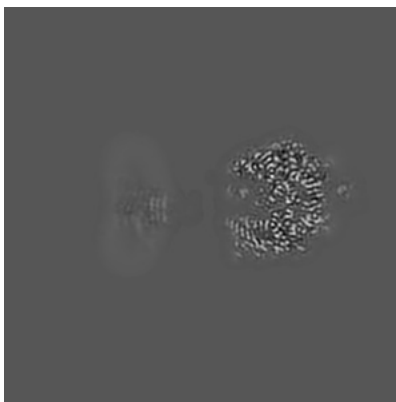
The images above show central slices of the map in three orthogonal directions.

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

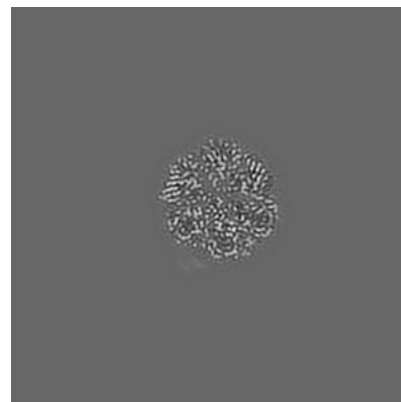
### 6.3.1 Primary map



X Index: 163

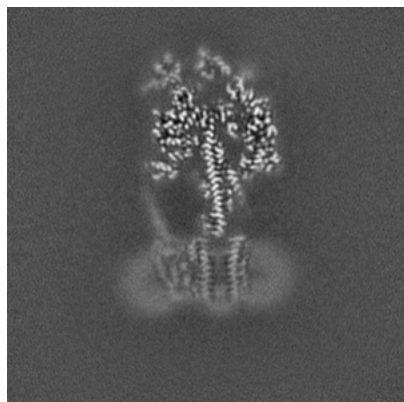


Y Index: 147

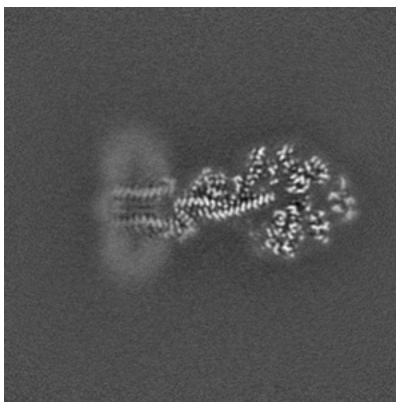


Z Index: 226

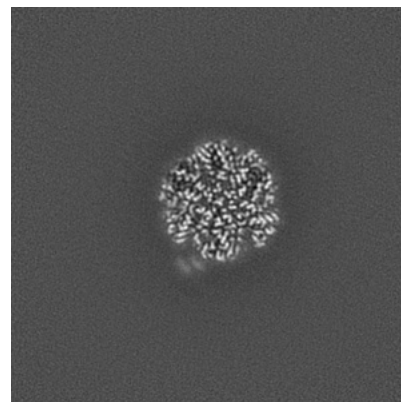
### 6.3.2 Raw map



X Index: 163



Y Index: 169

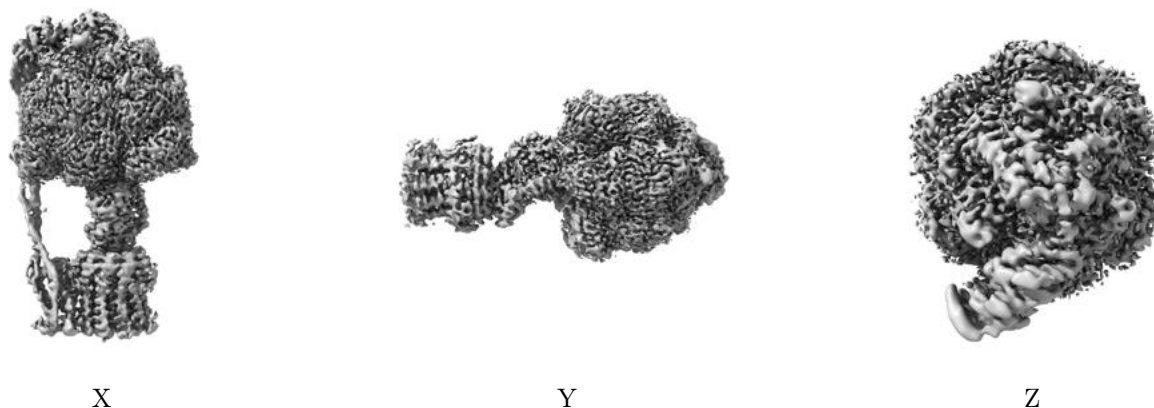


Z Index: 230

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

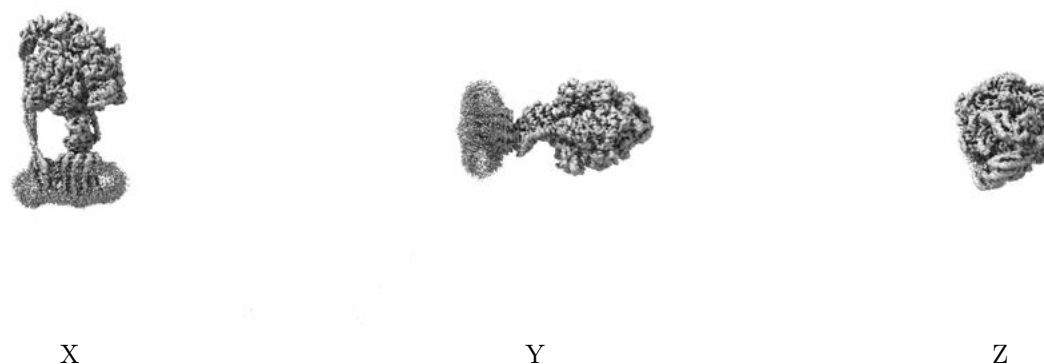
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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



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.

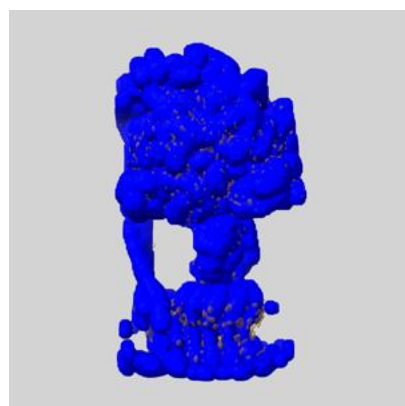
## 6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

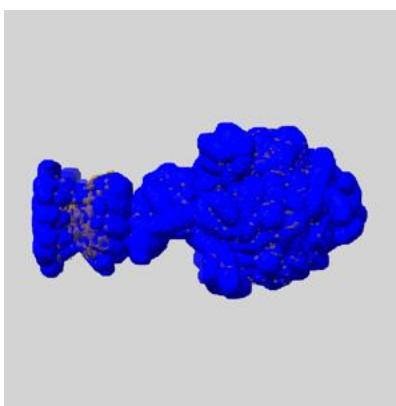
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

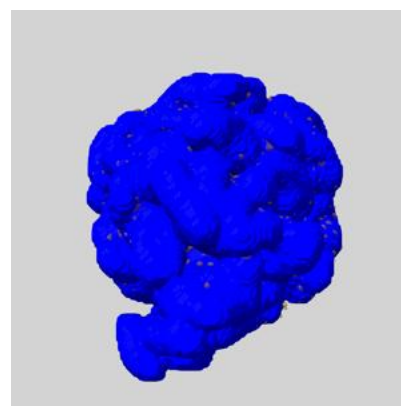
### 6.5.1 emd\_9334\_msk\_1.map [i](#)



X



Y

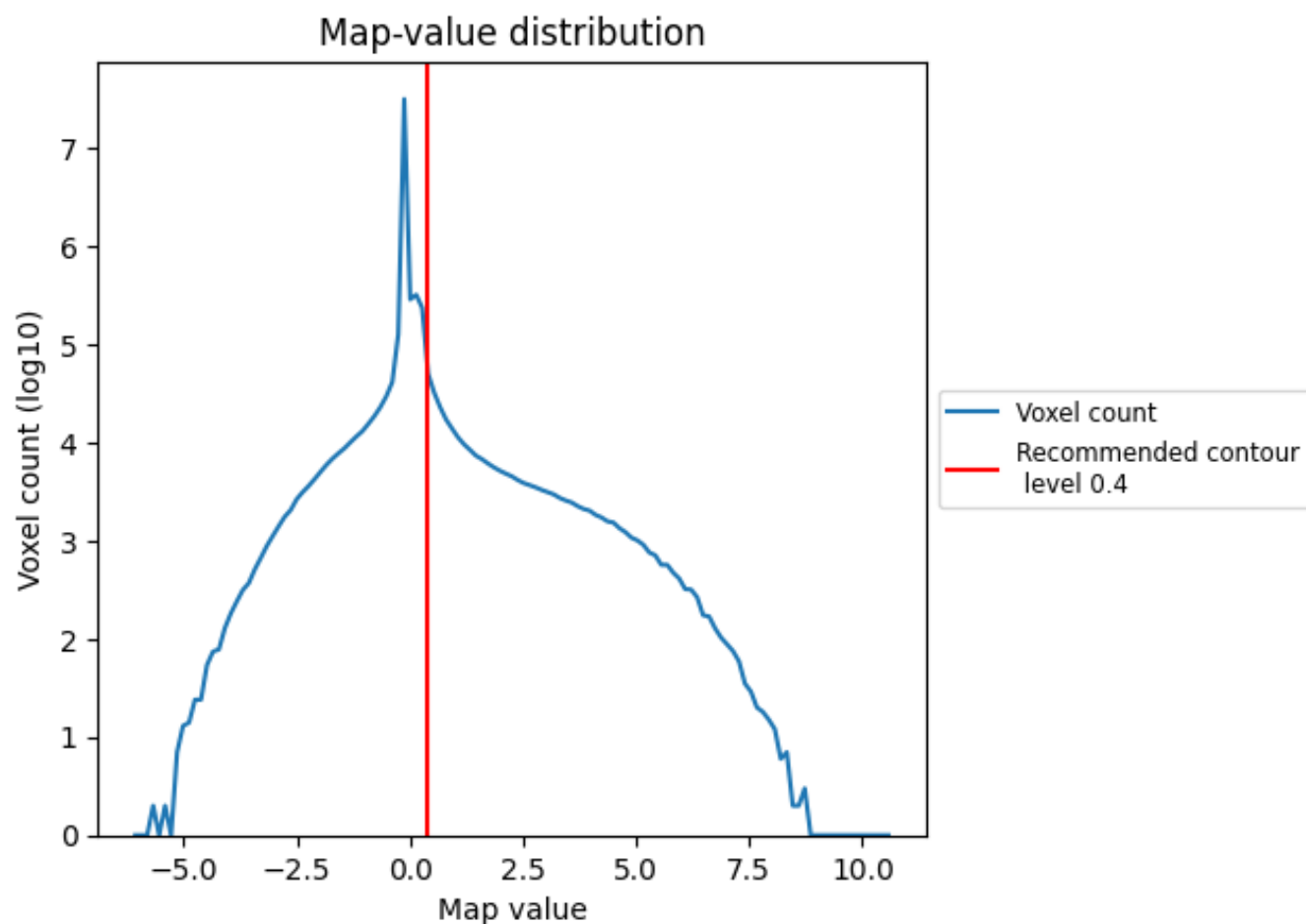


Z

## 7 Map analysis [i](#)

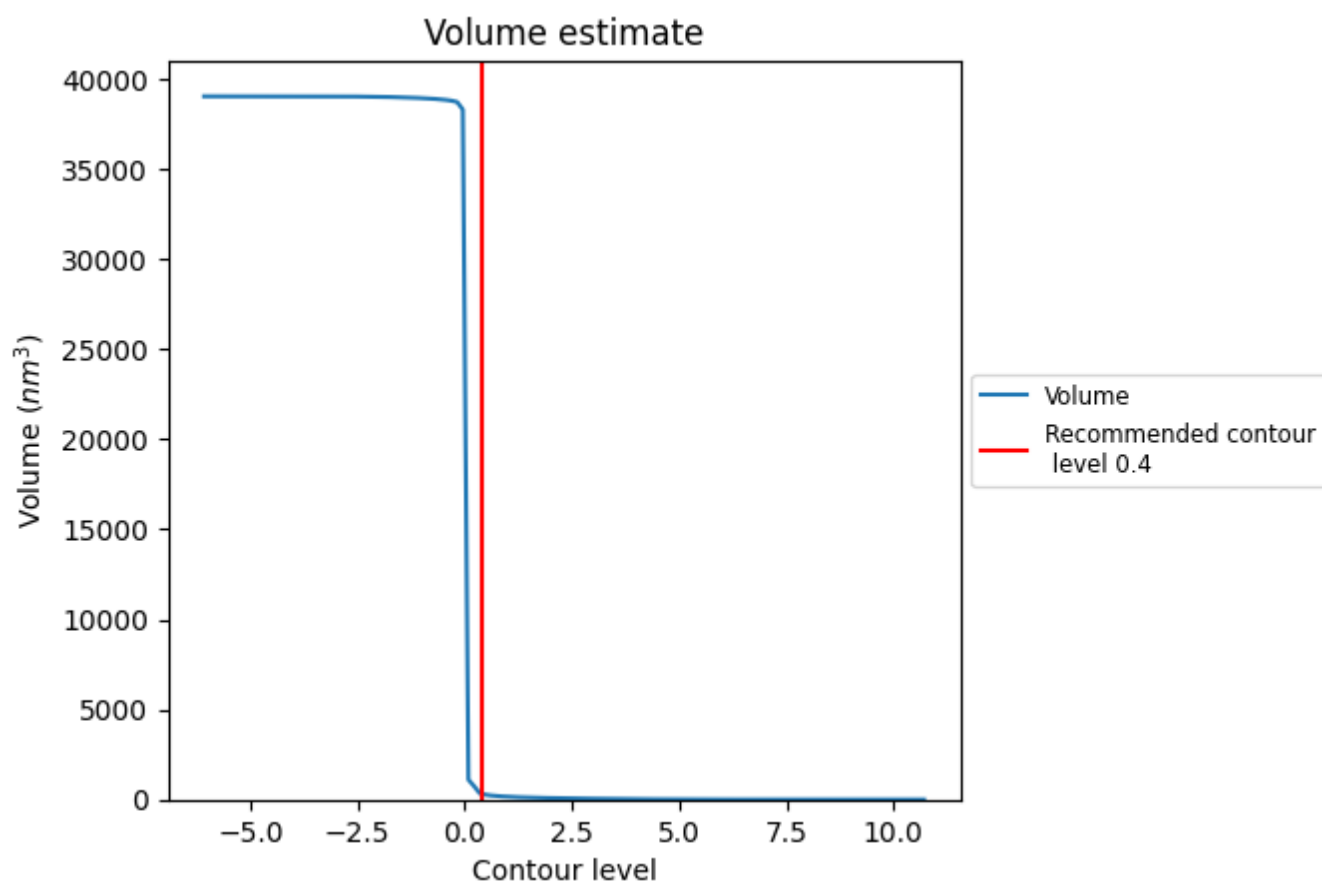
This section contains the results of statistical analysis of the map.

### 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](#)

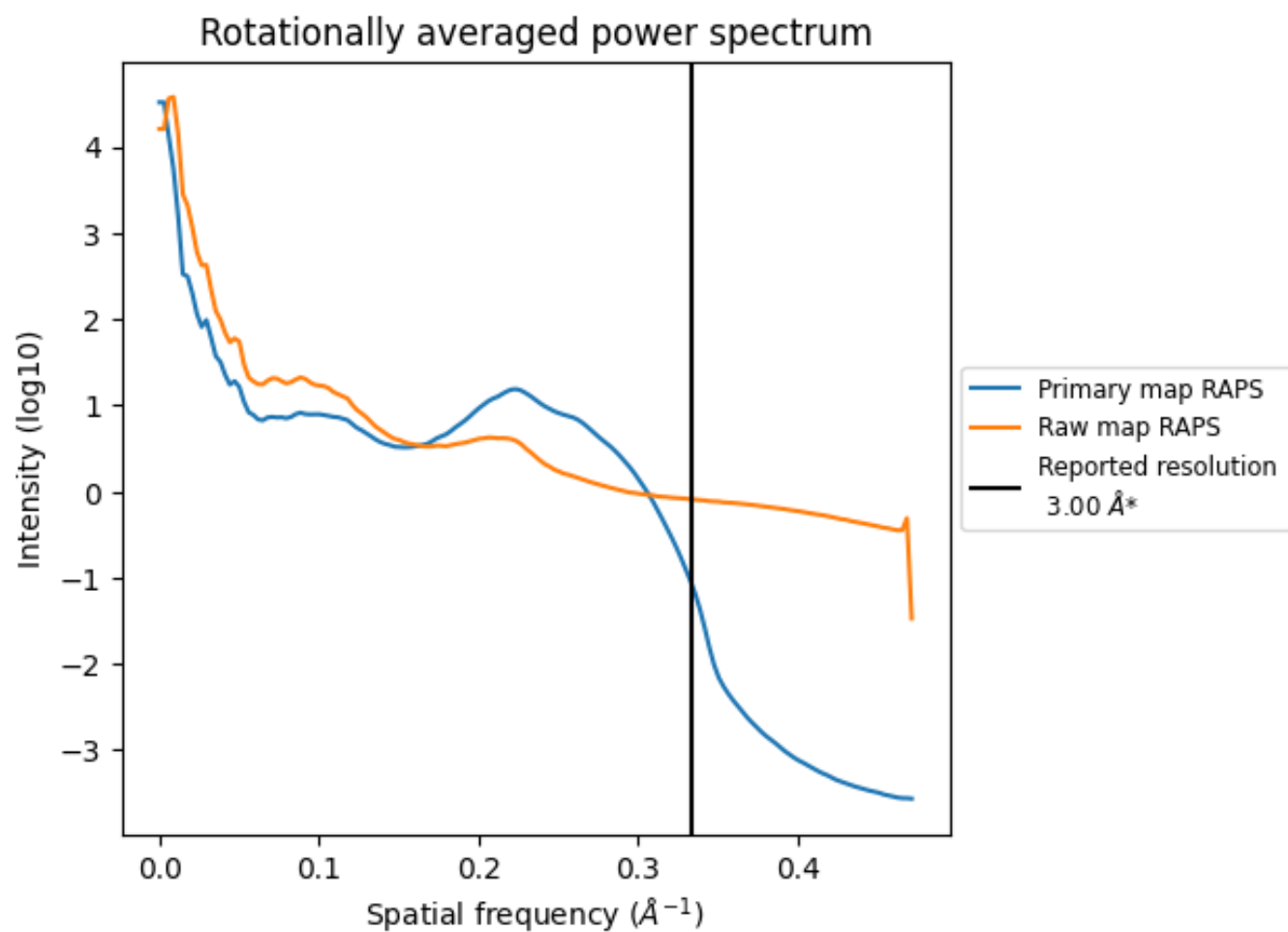


The volume at the recommended contour level is 322  $\text{nm}^3$ ; this corresponds to an approximate mass of 291 kDa.

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 ⓘ

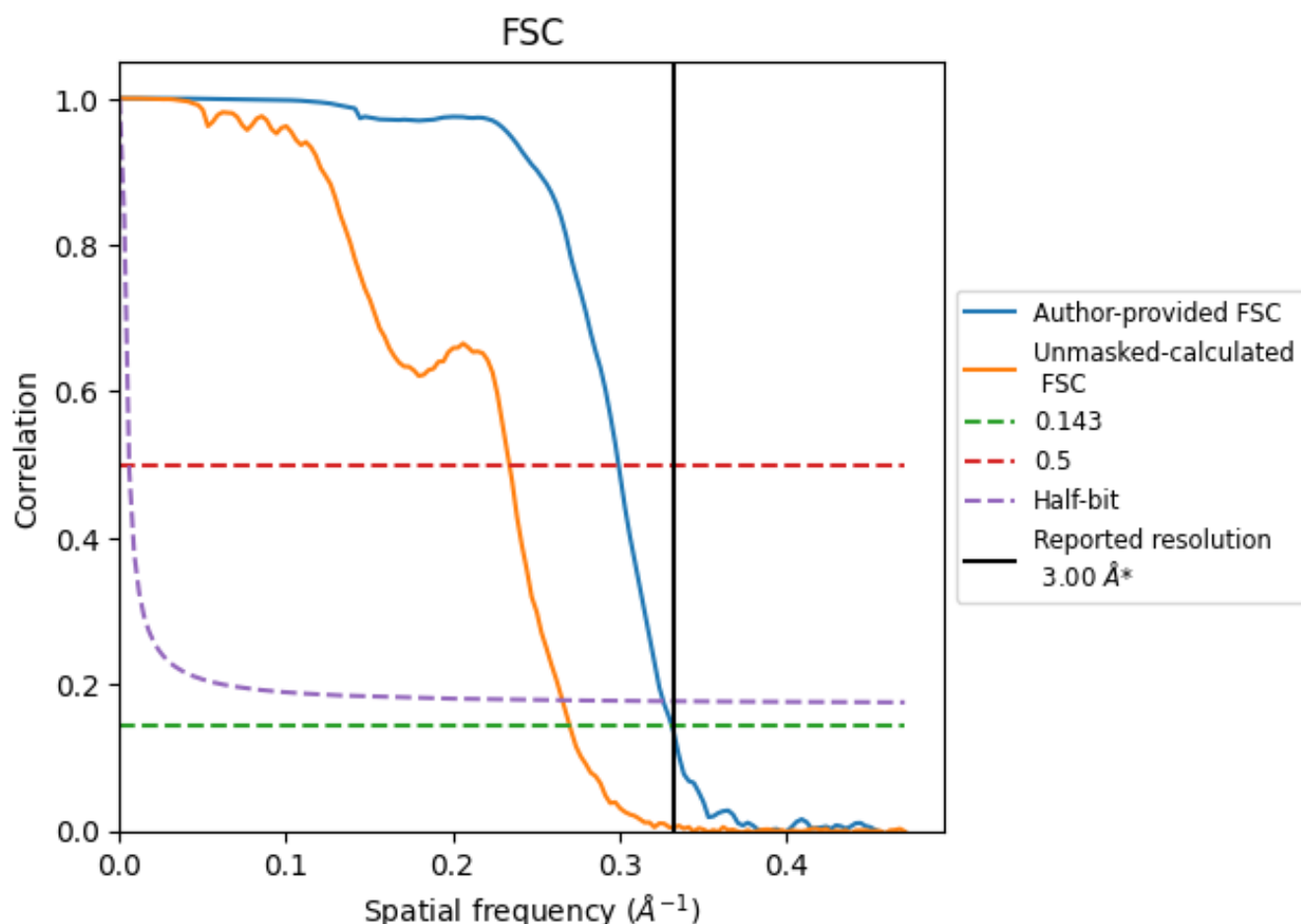


\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

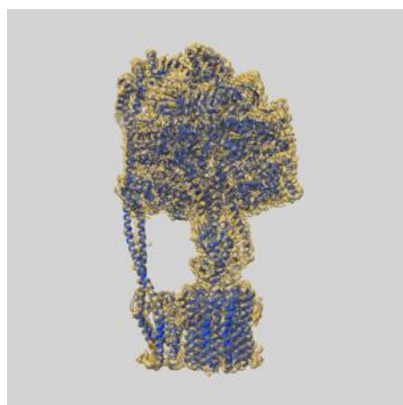
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.01	3.34	3.06
Unmasked-calculated*	3.70	4.27	3.76

\*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 3.70 differs from the reported value 3.0 by more than 10 %

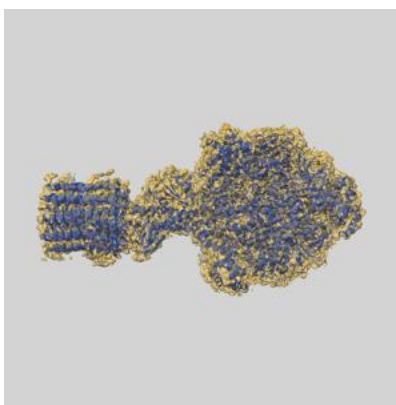
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9334 and PDB model 6N2Z. Per-residue inclusion information can be found in section [3](#) on page [9](#).

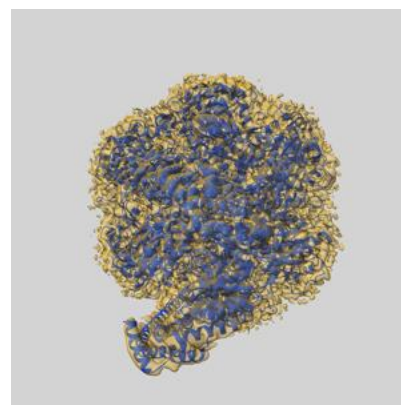
### 9.1 Map-model overlay [i](#)



X



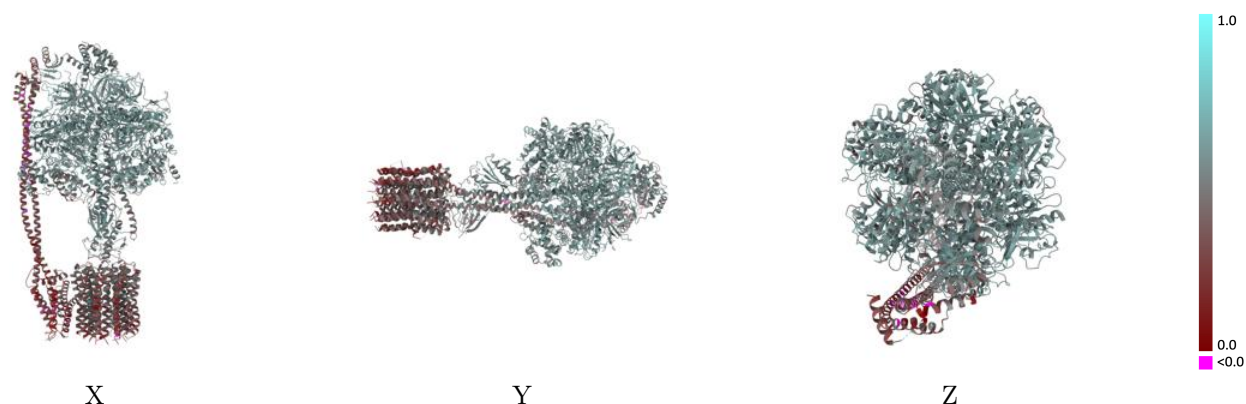
Y



Z

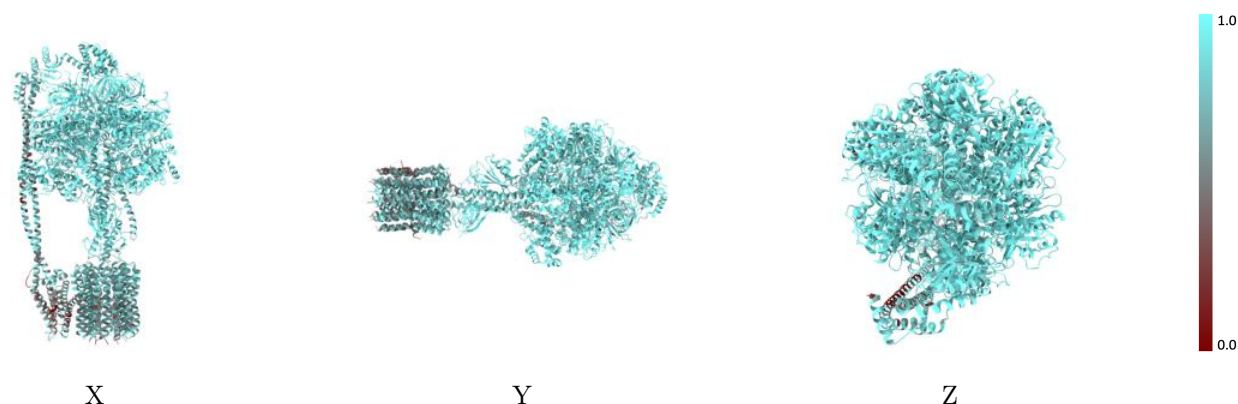
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



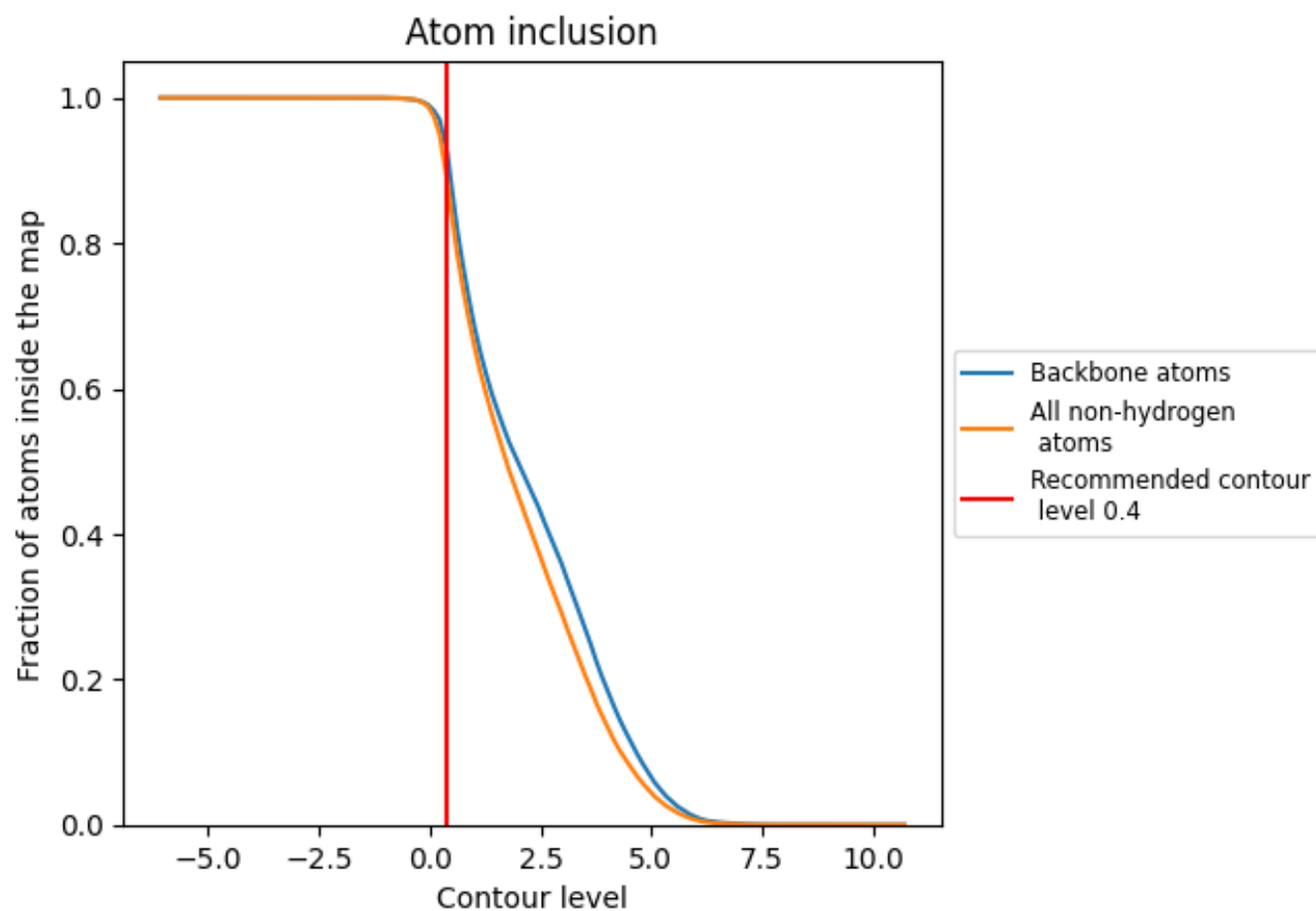
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8852	 0.5030
A	 0.9578	 0.5770
B	 0.9479	 0.5570
C	 0.9435	 0.5620
D	 0.9634	 0.5810
E	 0.9524	 0.5690
F	 0.9542	 0.5620
G	 0.9212	 0.5430
H	 0.9030	 0.5030
I	 0.9050	 0.5010
a	 0.5970	 0.2460
b1	 0.6490	 0.2160
b2	 0.6141	 0.2360
c0	 0.7008	 0.3380
c1	 0.6727	 0.3200
c2	 0.7309	 0.3680
c3	 0.7490	 0.3810
c4	 0.7410	 0.3800
c5	 0.7570	 0.3870
c6	 0.7631	 0.3770
c7	 0.7610	 0.4000
c8	 0.7570	 0.3850
c9	 0.7269	 0.3560

