



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:47 PM UTC

PDB ID : 6AVO / pdb_00006avo
EMDB ID : EMD-7010
Title : Cryo-EM structure of human immunoproteasome with a novel noncompetitive inhibitor that selectively inhibits activated lymphocytes
Authors : Li, H.; Santos, R.; Bai, L.
Deposited on : 2017-09-04
Resolution : 3.80 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

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>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

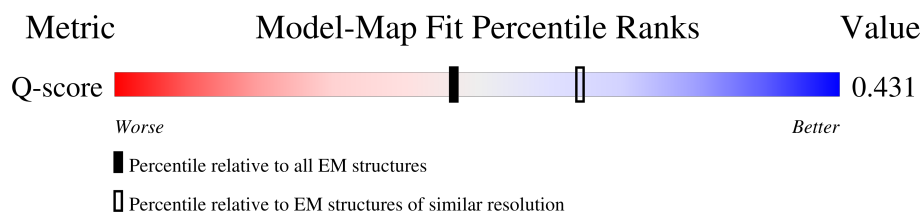
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	10198 (3.30 - 4.30)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 47715 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 Proteasome subunit beta type-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	199	Total	C	N	O	S	0	0
			1493	939	254	291	9		
1	F	199	Total	C	N	O	S	0	0
			1493	939	254	291	9		

- Molecule 2 is a protein called Proteasome subunit beta type-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	219	Total	C	N	O	S	0	0
			1609	1010	286	305	8		
2	E	219	Total	C	N	O	S	0	0
			1609	1010	286	305	8		

- Molecule 3 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	201	Total	C	N	O	S	0	0
			1563	977	273	298	15		
3	D	201	Total	C	N	O	S	0	0
			1563	977	273	298	15		

- Molecule 4 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	234	Total	C	N	O	S	1	0
			1817	1140	324	342	11		
4	L	234	Total	C	N	O	S	3	0
			1841	1153	332	345	11		

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	233	Total	C	N	O	S	0	0
			1753	1100	289	353	11		
5	M	233	Total	C	N	O	S	0	0
			1748	1100	292	345	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	232	Total	C	N	O	S	2	0
			1749	1092	312	340	5		
6	N	232	Total	C	N	O	S	0	0
			1754	1098	309	342	5		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	239	Total	C	N	O	S	4	0
			1888	1198	325	353	12		
7	Q	239	Total	C	N	O	S	1	0
			1851	1175	314	350	12		

- Molecule 8 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	240	Total	C	N	O	S	2	0
			1850	1172	313	352	13		
8	R	240	Total	C	N	O	S	1	0
			1817	1149	304	350	14		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	240	Total	C	N	O	S	2	0
			1843	1168	313	351	11		
9	Z	240	Total	C	N	O	S	2	0
			1860	1182	320	347	11		

- Molecule 10 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	230	Total	C	N	O	S	0	0
			1741	1111	293	331	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	230	Total	C	N	O	S	3	0
			1788	1145	301	336	6		

- Molecule 11 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	213	Total	C	N	O	S	1	0
			1642	1041	280	310	11		
11	X	213	Total	C	N	O	S	2	0
			1636	1038	277	310	11		

- Molecule 12 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	196	Total	C	N	O	S	2	0
			1567	1006	266	285	10		
12	V	196	Total	C	N	O	S	3	0
			1581	1015	270	286	10		

- Molecule 13 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	204	Total	C	N	O	S	2	0
			1599	1018	267	295	19		
13	Y	204	Total	C	N	O	S	2	0
			1604	1022	268	294	20		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	216	Total	C	N	O	S	1	0
			1692	1067	291	322	12		
14	a	216	Total	C	N	O	S	1	0
			1684	1062	290	320	12		

- Molecule 15 is N 1 -{2-[(1,1'-biphenyl)-3-carbonyl]amino}ethyl}-N 4 -tert-butyl-N 2 -(3-phenylpropanoyl)-L-aspartamide (CCD ID: BZ7) (formula: C₃₂H₃₈N₄O₄).



Mol	Chain	Residues	Atoms				AltConf
15	C	1	Total 40	C 32	N 4	O 4	0
15	D	1	Total 40	C 32	N 4	O 4	0

MolProbit failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75017	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.261	Depositor
Minimum map value	-0.153	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0383	Depositor
Map size (Å)	307.2, 307.2, 307.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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
15	BZ7	C	301	-	42,42,42	2.94	13 (30%)	56,56,56	1.18	3 (5%)
15	BZ7	D	301	-	42,42,42	2.94	14 (33%)	56,56,56	1.18	3 (5%)

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
15	BZ7	C	301	-	-	16/37/37/37	0/3/3/3
15	BZ7	D	301	-	-	16/37/37/37	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	301	BZ7	CAE-CAD	8.32	1.53	1.38
15	D	301	BZ7	CAE-CAD	8.31	1.53	1.38
15	D	301	BZ7	CAB-CAC	7.25	1.53	1.38
15	C	301	BZ7	CAB-CAC	7.22	1.53	1.38
15	D	301	BZ7	CAF-CAA	6.80	1.53	1.38
15	C	301	BZ7	CAF-CAA	6.77	1.53	1.38
15	D	301	BZ7	CG-ND2	6.72	1.45	1.34
15	C	301	BZ7	CG-ND2	6.70	1.45	1.34
15	D	301	BZ7	CAI-N	5.51	1.45	1.34
15	C	301	BZ7	CAI-N	5.49	1.45	1.34
15	D	301	BZ7	CBA-NAZ	5.33	1.45	1.33
15	C	301	BZ7	CBA-NAZ	5.32	1.45	1.33
15	D	301	BZ7	C-NAN	5.11	1.45	1.33
15	C	301	BZ7	C-NAN	5.08	1.45	1.33
15	D	301	BZ7	CAA-CAB	-3.98	1.32	1.38
15	C	301	BZ7	CAA-CAB	-3.95	1.32	1.38
15	C	301	BZ7	CAD-CAC	-3.46	1.32	1.38
15	D	301	BZ7	CAD-CAC	-3.45	1.32	1.38
15	D	301	BZ7	CAF-CAE	-2.83	1.32	1.38
15	C	301	BZ7	CAF-CAE	-2.78	1.32	1.38
15	D	301	BZ7	O-C	-2.32	1.18	1.23
15	C	301	BZ7	O-C	-2.32	1.19	1.23
15	C	301	BZ7	OD1-CG	-2.20	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	301	BZ7	OAK-CAI	-2.20	1.18	1.23
15	D	301	BZ7	OAK-CAI	-2.19	1.18	1.23
15	D	301	BZ7	OD1-CG	-2.15	1.19	1.23
15	D	301	BZ7	CAS-ND2	-2.01	1.45	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	D	301	BZ7	CAS-ND2-CG	-4.82	119.97	126.14
15	C	301	BZ7	CAS-ND2-CG	-4.81	119.97	126.14
15	D	301	BZ7	CB-CG-ND2	3.35	120.01	115.87
15	C	301	BZ7	CB-CG-ND2	3.31	119.96	115.87
15	C	301	BZ7	CAH-CAI-N	2.35	120.01	115.86
15	D	301	BZ7	CAH-CAI-N	2.33	119.97	115.86

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	C	301	BZ7	CBF-CBG-CBI-CBJ
15	C	301	BZ7	CBH-CBG-CBI-CBN
15	D	301	BZ7	CBF-CBG-CBI-CBJ
15	D	301	BZ7	CBH-CBG-CBI-CBN
15	C	301	BZ7	CBF-CBG-CBI-CBN
15	C	301	BZ7	CBH-CBG-CBI-CBJ
15	D	301	BZ7	CBF-CBG-CBI-CBN
15	D	301	BZ7	CBH-CBG-CBI-CBJ
15	D	301	BZ7	CAY-CAX-NAN-C
15	C	301	BZ7	NAZ-CBA-CBC-CBD
15	C	301	BZ7	CAY-CAX-NAN-C
15	C	301	BZ7	OBB-CBA-CBC-CBD
15	D	301	BZ7	NAZ-CBA-CBC-CBD
15	D	301	BZ7	OBB-CBA-CBC-CBD
15	C	301	BZ7	NAZ-CBA-CBC-CBH
15	C	301	BZ7	OBB-CBA-CBC-CBH
15	D	301	BZ7	OBB-CBA-CBC-CBH
15	D	301	BZ7	NAZ-CBA-CBC-CBH
15	C	301	BZ7	N-CA-CB-CG
15	D	301	BZ7	N-CA-CB-CG
15	C	301	BZ7	CAX-CAY-NAZ-CBA
15	C	301	BZ7	C-CA-CB-CG
15	D	301	BZ7	C-CA-CB-CG

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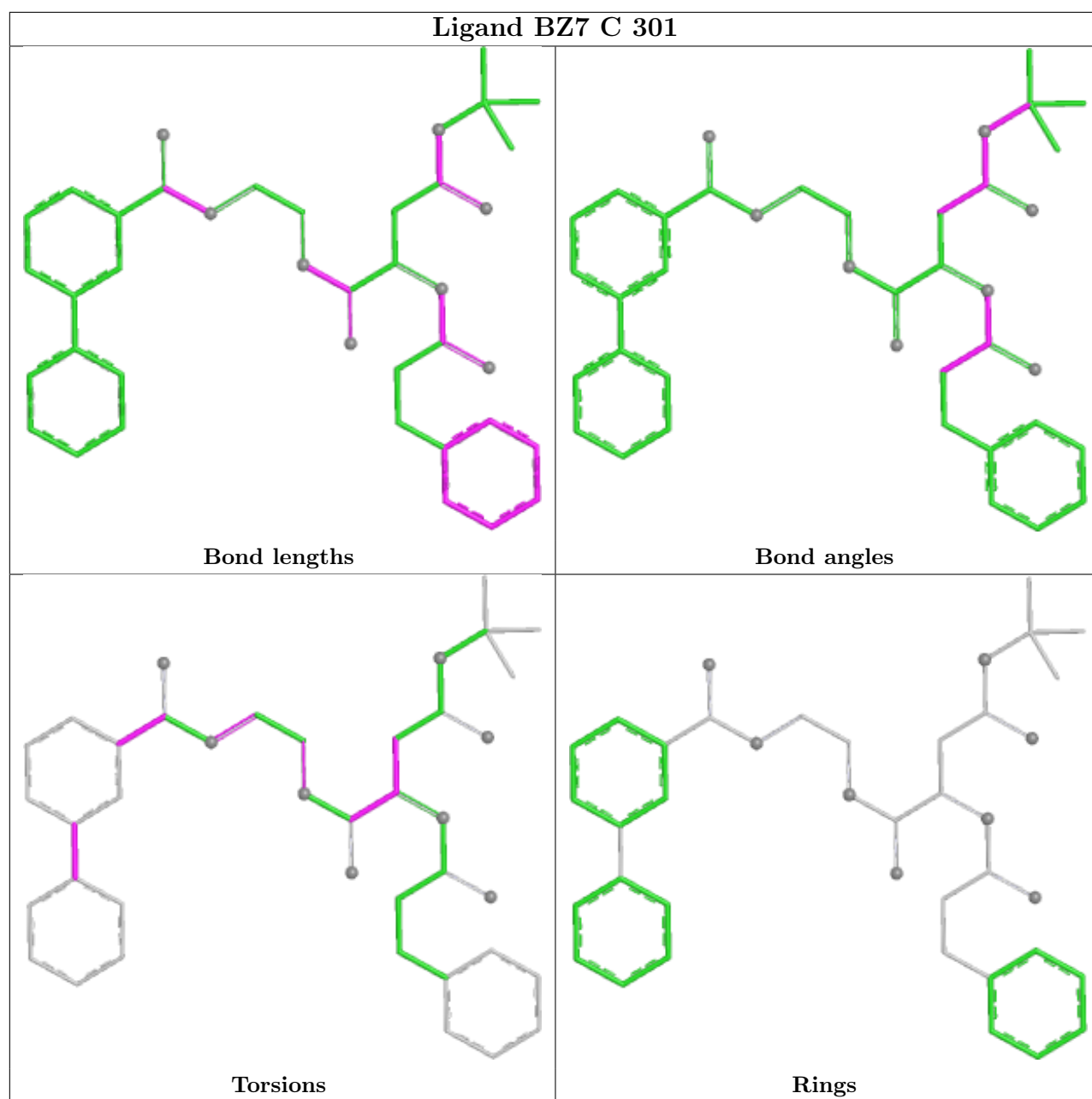
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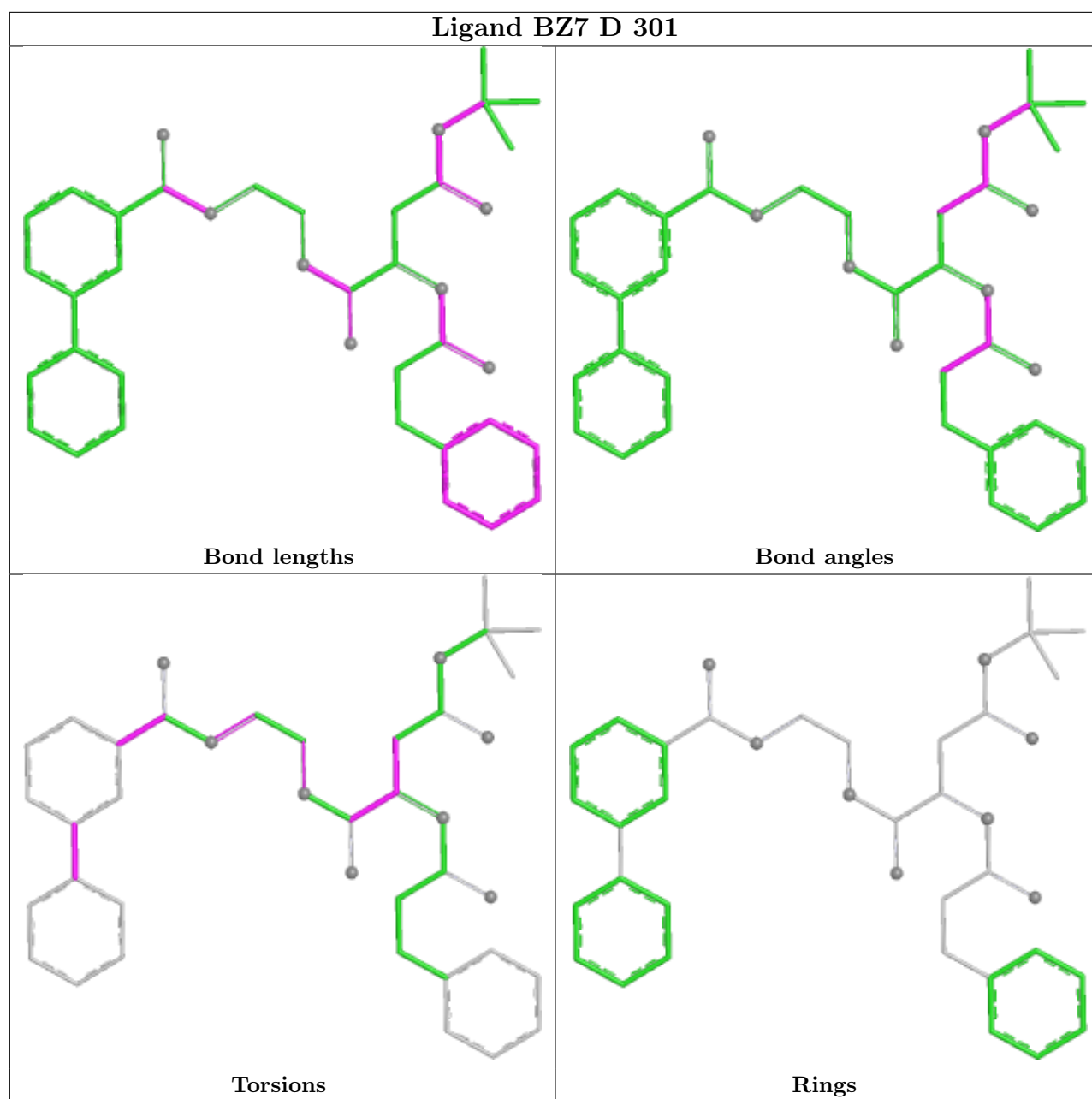
Mol	Chain	Res	Type	Atoms
15	D	301	BZ7	CAX-CAY-NAZ-CBA
15	D	301	BZ7	NAN-C-CA-N
15	C	301	BZ7	NAN-C-CA-N
15	C	301	BZ7	O-C-CA-N
15	D	301	BZ7	O-C-CA-N
15	D	301	BZ7	O-C-CA-CB
15	C	301	BZ7	O-C-CA-CB
15	D	301	BZ7	NAN-C-CA-CB
15	C	301	BZ7	NAN-C-CA-CB

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.





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

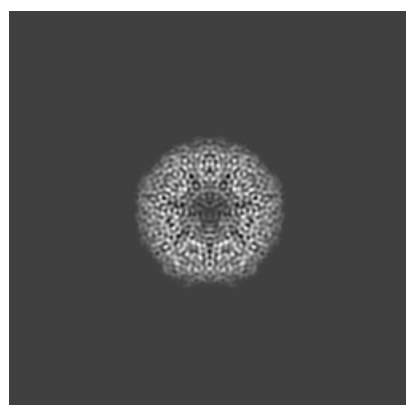
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7010. These allow visual inspection of the internal detail of the map and identification of artifacts.

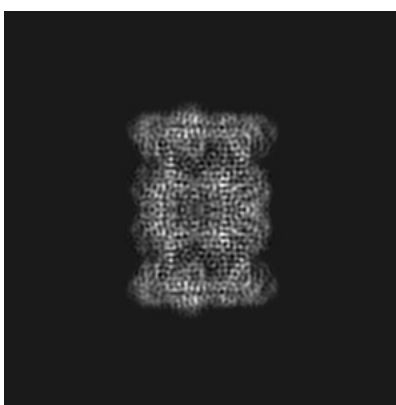
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections [i](#)

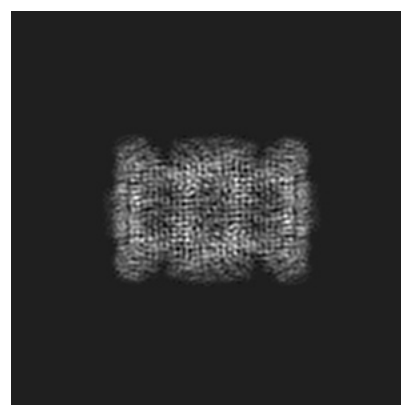
5.1.1 Primary map



X



Y

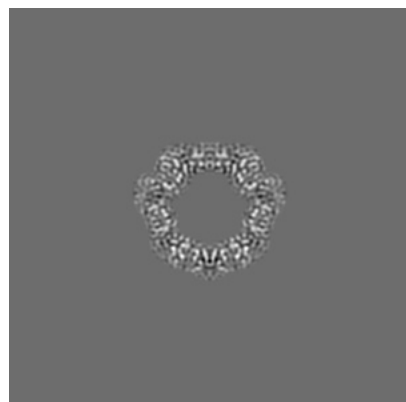


Z

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

5.2 Central slices [i](#)

5.2.1 Primary map



X Index: 128



Y Index: 128

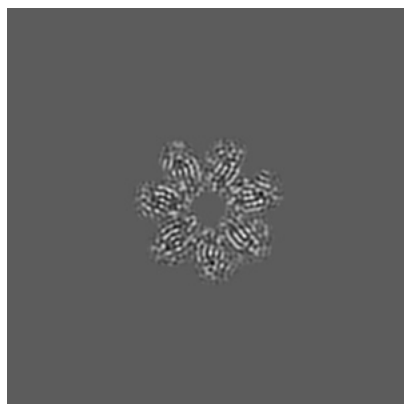


Z Index: 128

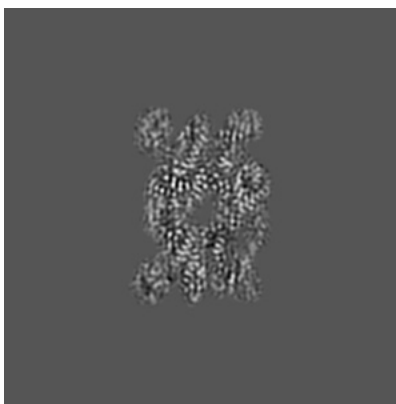
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

5.3.1 Primary map



X Index: 144



Y Index: 106

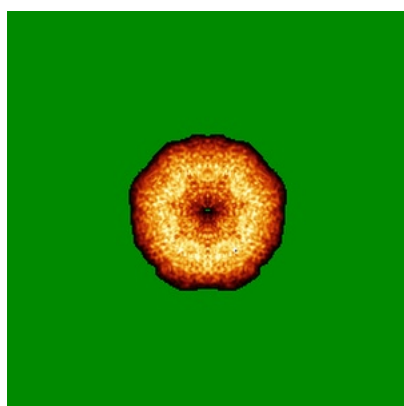


Z Index: 105

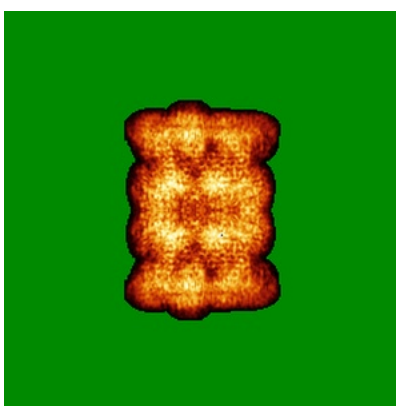
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal standard-deviation projections (False-color) [i](#)

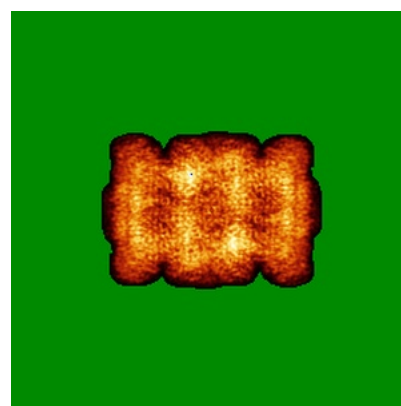
5.4.1 Primary map



X



Y

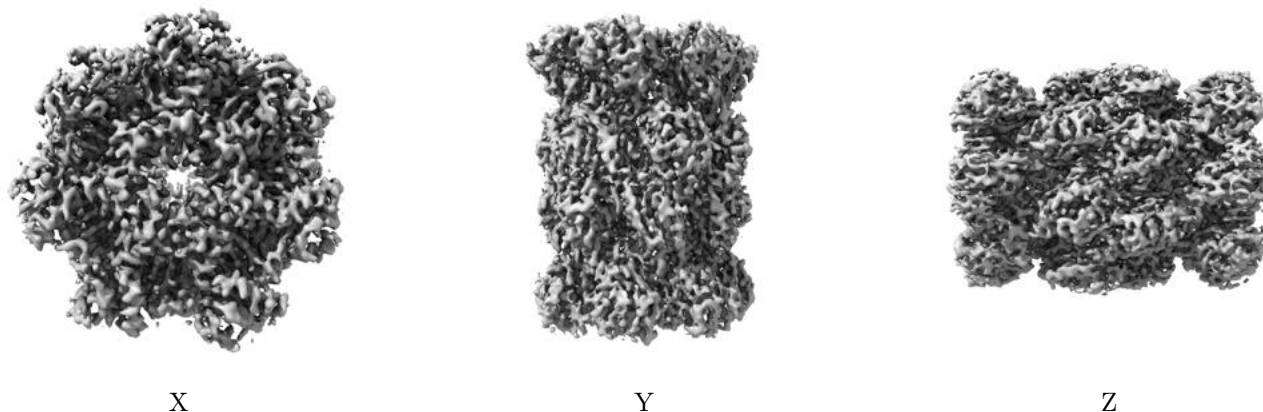


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0383. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

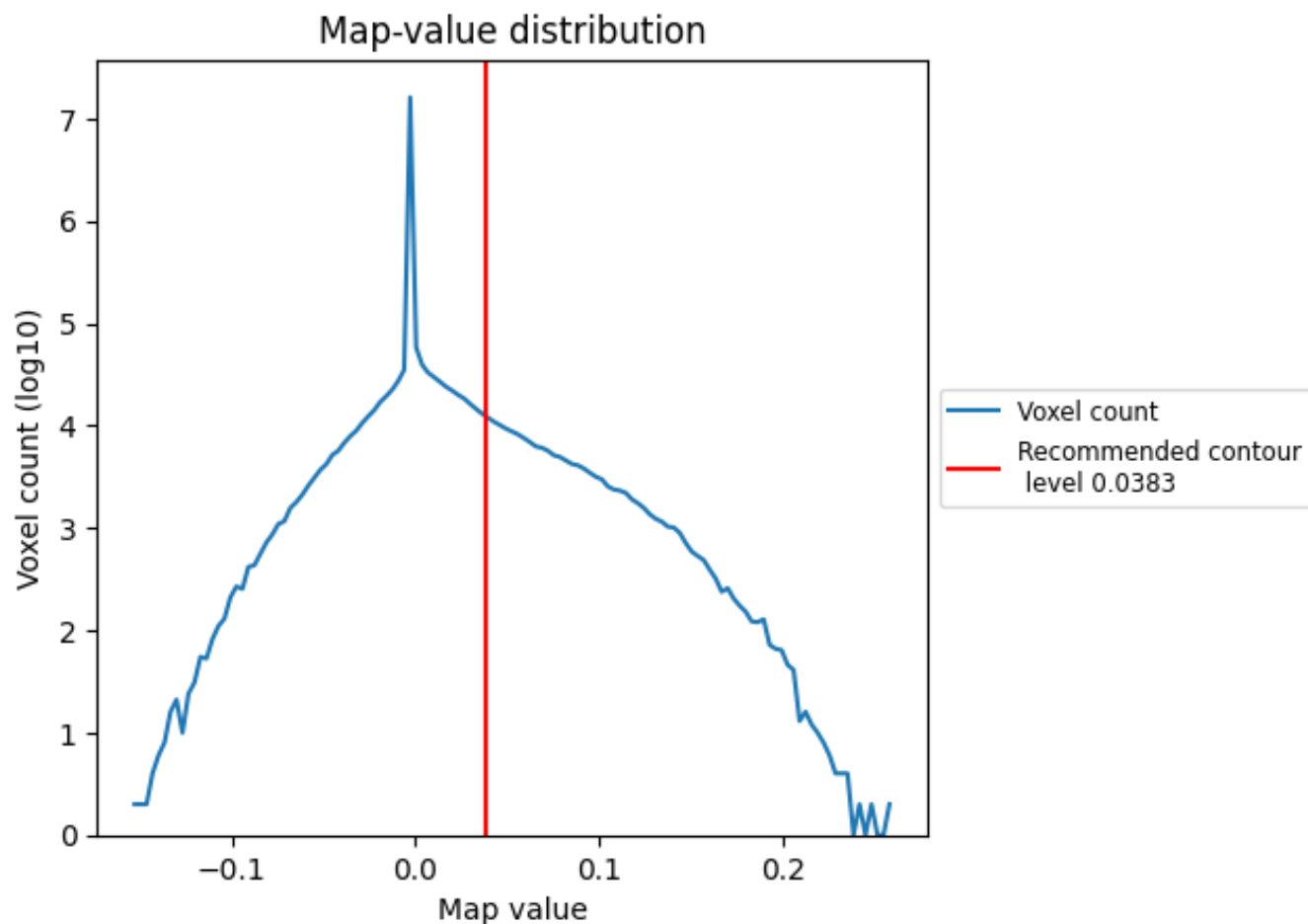
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

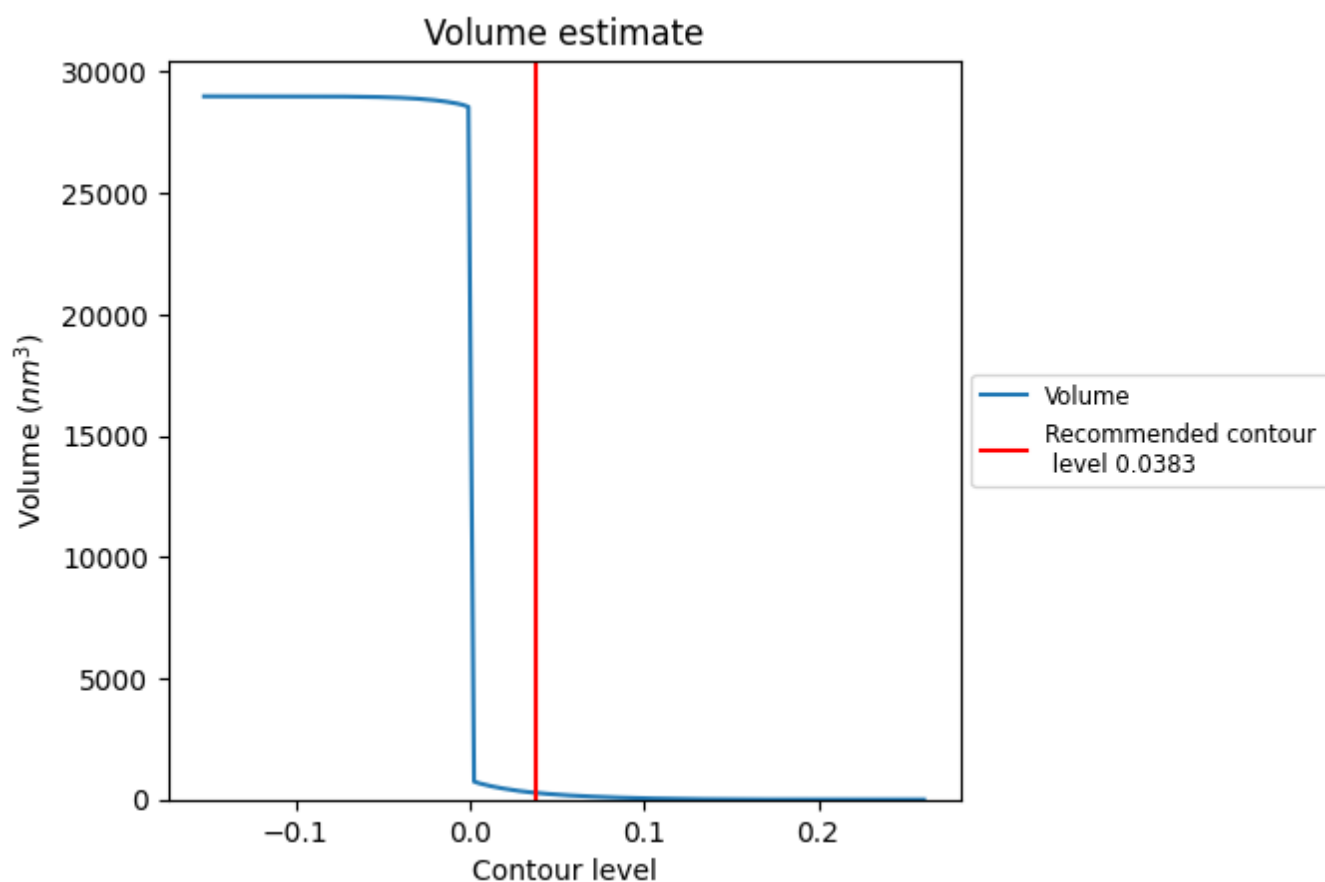
This section contains the results of statistical analysis of the map.

6.1 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.

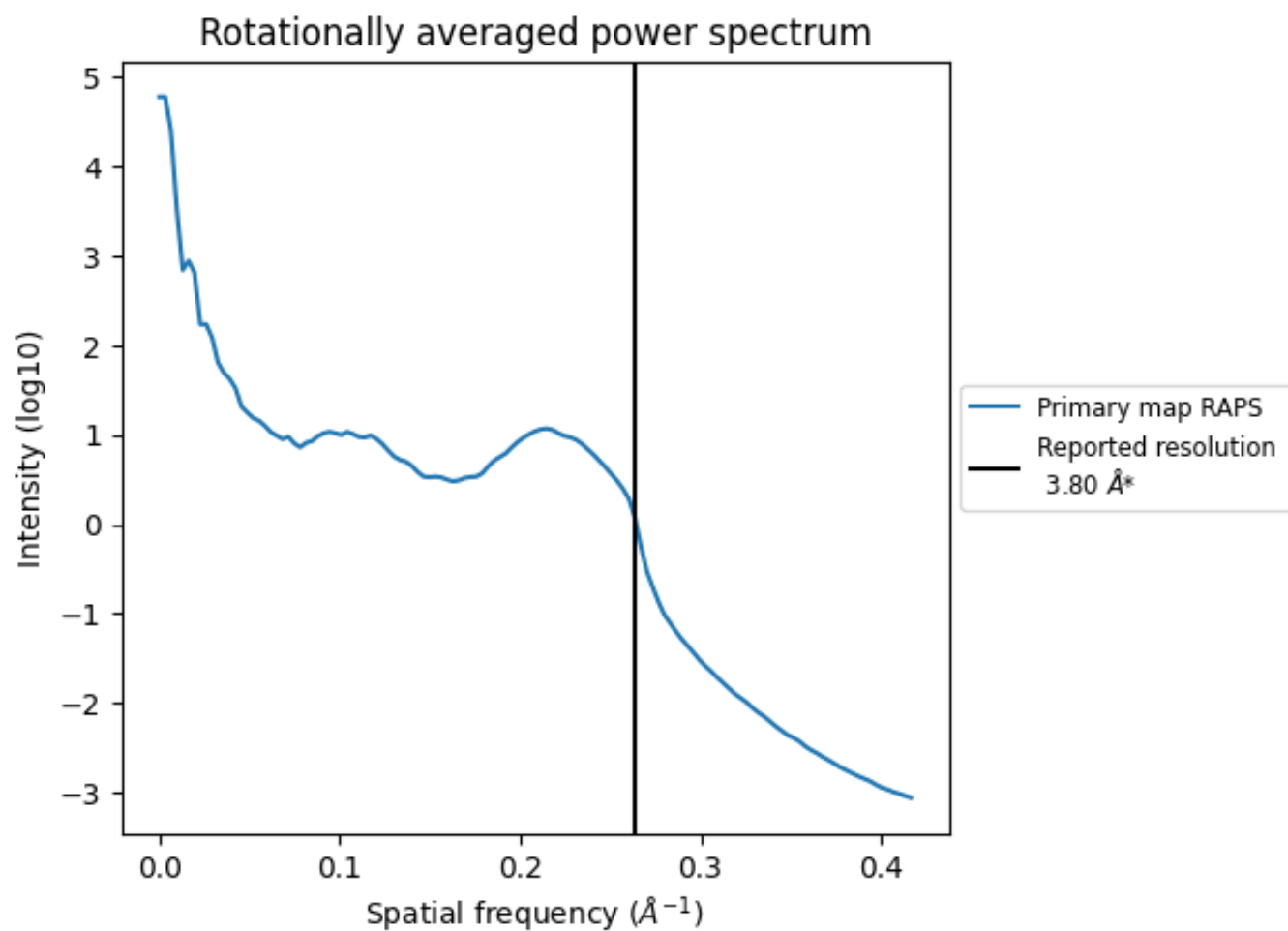
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 273 nm³; this corresponds to an approximate mass of 247 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.

6.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

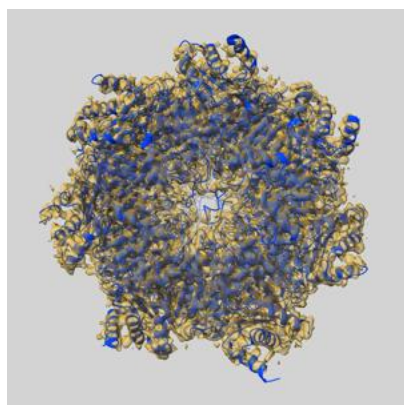
7 Fourier-Shell correlation ⓘ

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

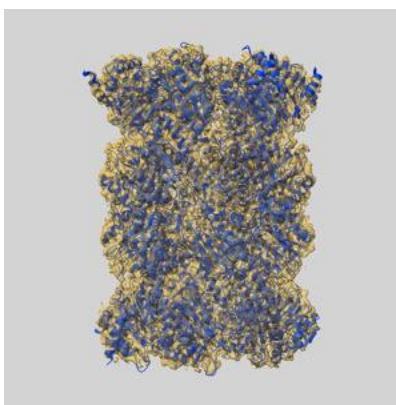
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7010 and PDB model 6AVO. Per-residue inclusion information can be found in section ?? on page ??.

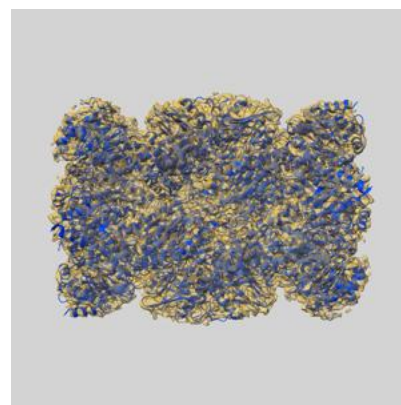
8.1 Map-model overlay [i](#)



X



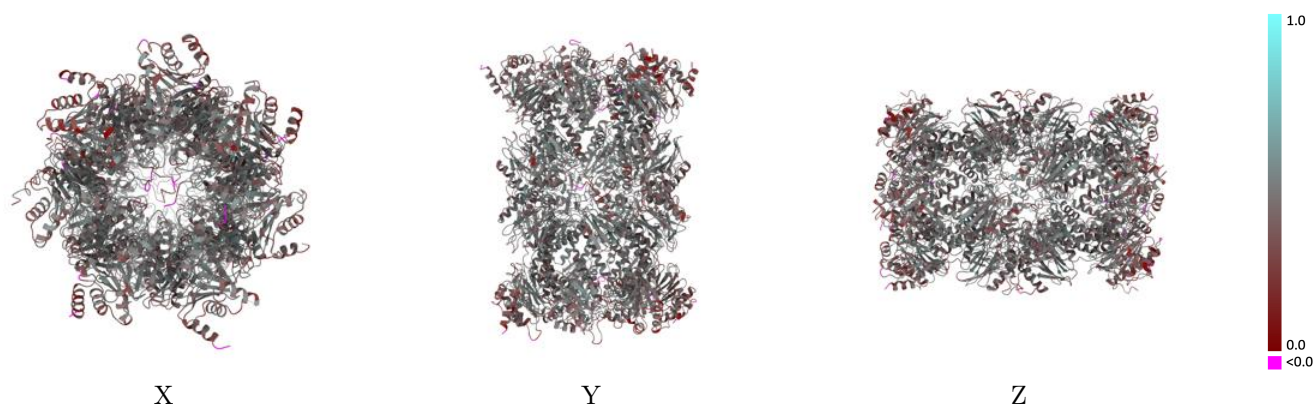
Y



Z

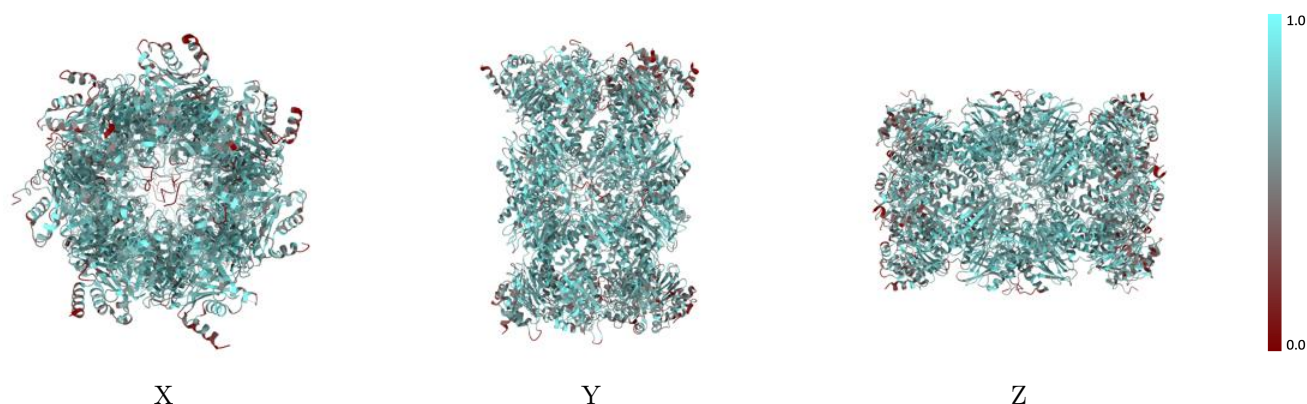
The images above show the 3D surface view of the map at the recommended contour level 0.0383 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



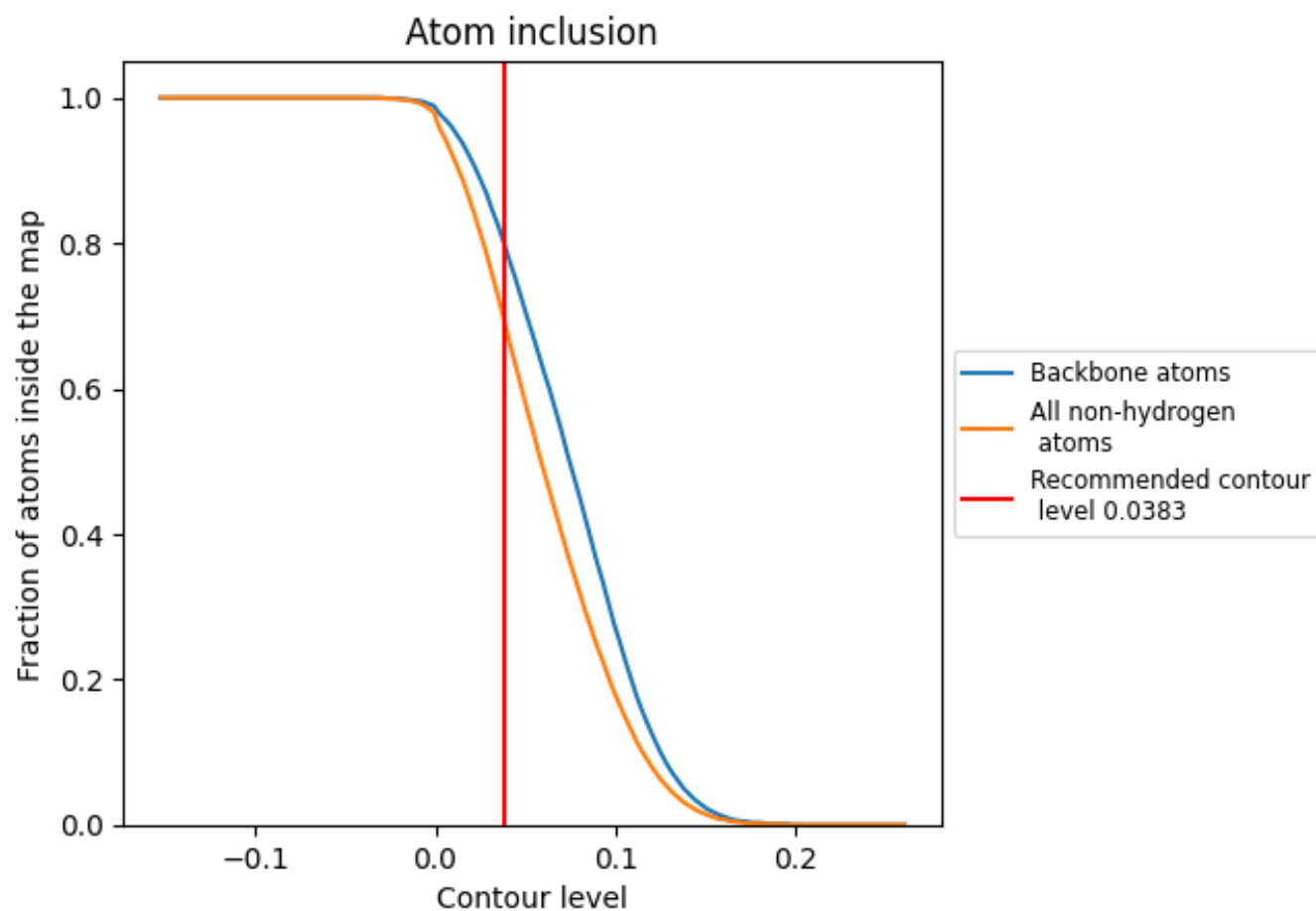
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 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 (0.0383).

8.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0383) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6940	 0.4310
A	 0.7410	 0.4580
B	 0.7110	 0.4360
C	 0.7810	 0.4510
D	 0.7670	 0.4470
E	 0.7030	 0.4390
F	 0.7430	 0.4620
G	 0.6810	 0.4290
H	 0.5670	 0.3760
I	 0.6380	 0.4060
J	 0.6770	 0.4190
K	 0.6810	 0.4260
L	 0.6800	 0.4280
M	 0.5700	 0.3790
N	 0.6330	 0.4050
O	 0.6120	 0.4020
P	 0.6980	 0.4290
Q	 0.6770	 0.4190
R	 0.6960	 0.4290
S	 0.7250	 0.4570
T	 0.7250	 0.4380
U	 0.7600	 0.4650
V	 0.7260	 0.4410
W	 0.7600	 0.4620
X	 0.7270	 0.4590
Y	 0.7450	 0.4630
Z	 0.6110	 0.3960
a	 0.7650	 0.4620
b	 0.6980	 0.4290

