



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2024 – 10:39 AM JST

PDB ID : 7BQX
EMDB ID : EMD-30157
Title : Epstein-Barr virus, C5 portal vertex
Authors : Li, Z.; Yu, X.
Deposited on : 2020-03-25
Resolution : 4.20 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 ⓘ 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:

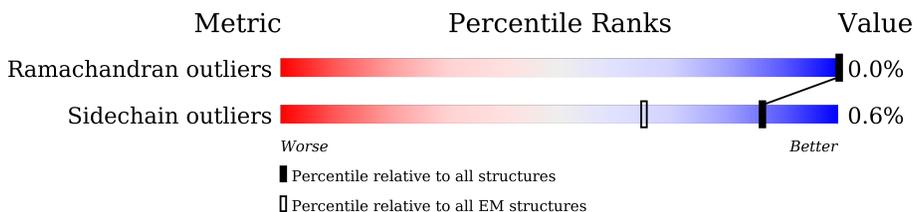
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 4.20 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.



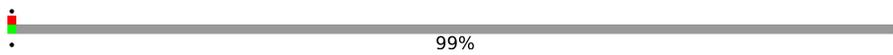
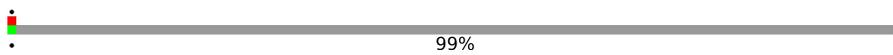
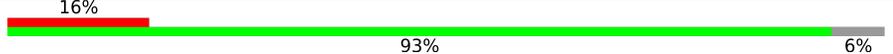
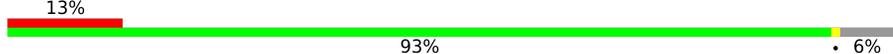
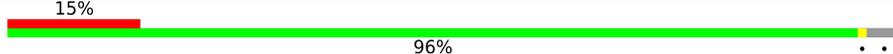
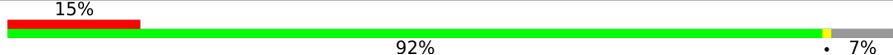
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 ≥ 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	5	364	
1	e	364	
2	6	301	
2	7	301	
2	f	301	
2	g	301	
3	G	570	
3	K	570	
4	C	507	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	B	3149	 99%
5	O	3149	 99%
6	2	176	 38% 40% 58%
6	Y	176	 23% 41% 58%
6	Z	176	 26% 41% 58%
6	y	176	 27% 41% 58%
7	S	1381	 16% 93% 6%
7	T	1381	 13% 93% 6%
7	W	1381	 15% 96% 7%
7	x	1381	 15% 92% 7%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 61847 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 Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	5	284	Total	C	N	O	S	0	0
			2199	1421	374	397	7		
1	e	319	Total	C	N	O	S	0	0
			2505	1608	444	446	7		

- Molecule 2 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	6	297	Total	C	N	O	S	0	0
			2329	1496	385	430	18		
2	7	287	Total	C	N	O	S	0	0
			2262	1452	375	417	18		
2	f	290	Total	C	N	O	S	0	0
			2279	1466	378	419	16		
2	g	290	Total	C	N	O	S	0	0
			2272	1464	376	414	18		

- Molecule 3 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	K	68	Total	C	N	O	S	0	0
			563	343	113	104	3		
3	G	84	Total	C	N	O	S	0	0
			675	412	135	125	3		

- Molecule 4 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	346	Total	C	N	O	S	0	0
			2705	1733	482	478	12		

- Molecule 5 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	B	35	Total	C	N	O	0	0
			301	192	61	48		
5	O	29	Total	C	N	O	0	0
			252	163	49	40		

- Molecule 6 is a protein called Small capsomere-interacting protein.

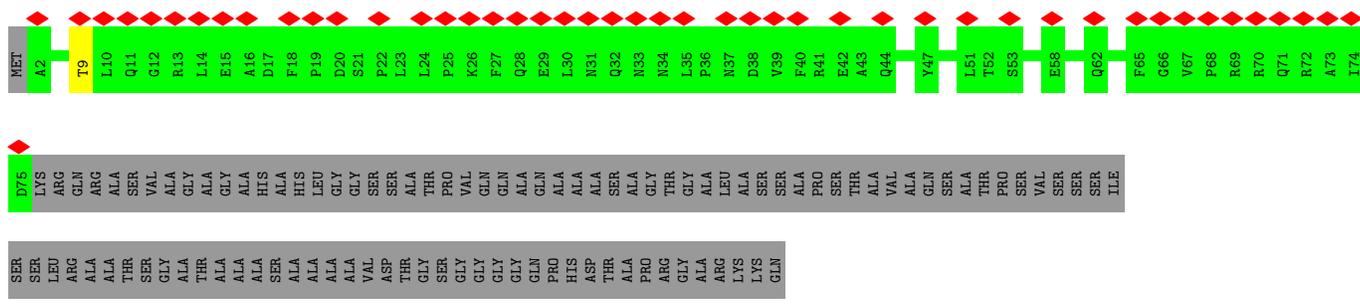
Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
6	Z	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
6	2	74	Total	C	N	O	S	0	0
			621	394	114	112	1		
6	y	74	Total	C	N	O	S	0	0
			621	394	114	112	1		

- Molecule 7 is a protein called Major capsid protein.

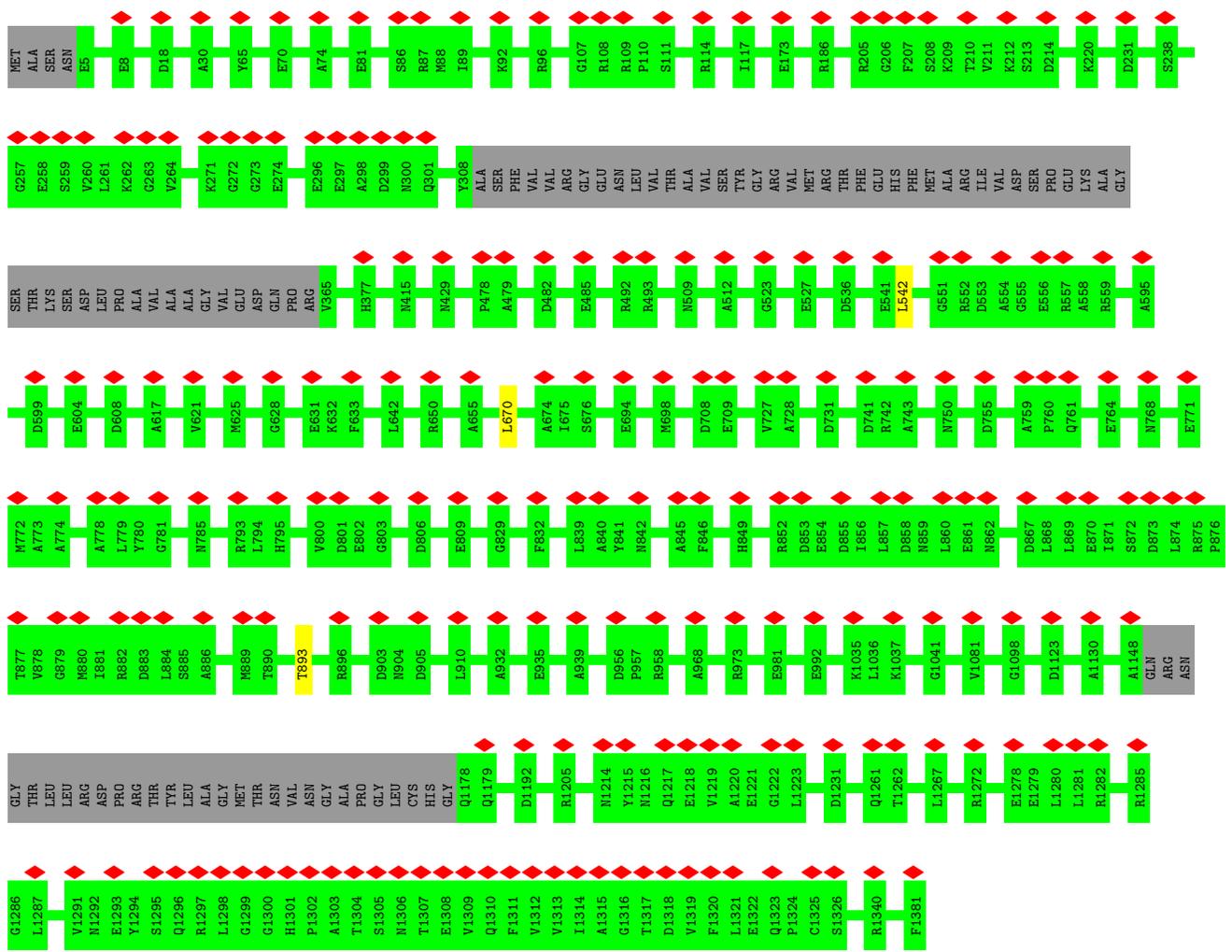
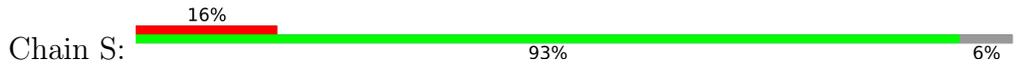
Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	1292	Total	C	N	O	S	0	0
			10166	6462	1758	1889	57		
7	T	1305	Total	C	N	O	S	0	0
			10258	6515	1780	1904	59		
7	W	1330	Total	C	N	O	S	0	0
			10456	6648	1808	1941	59		
7	x	1290	Total	C	N	O	S	0	0
			10141	6438	1760	1884	59		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	89	ILE	THR	conflict	UNP P03226
T	89	ILE	THR	conflict	UNP P03226
W	89	ILE	THR	conflict	UNP P03226
x	89	ILE	THR	conflict	UNP P03226

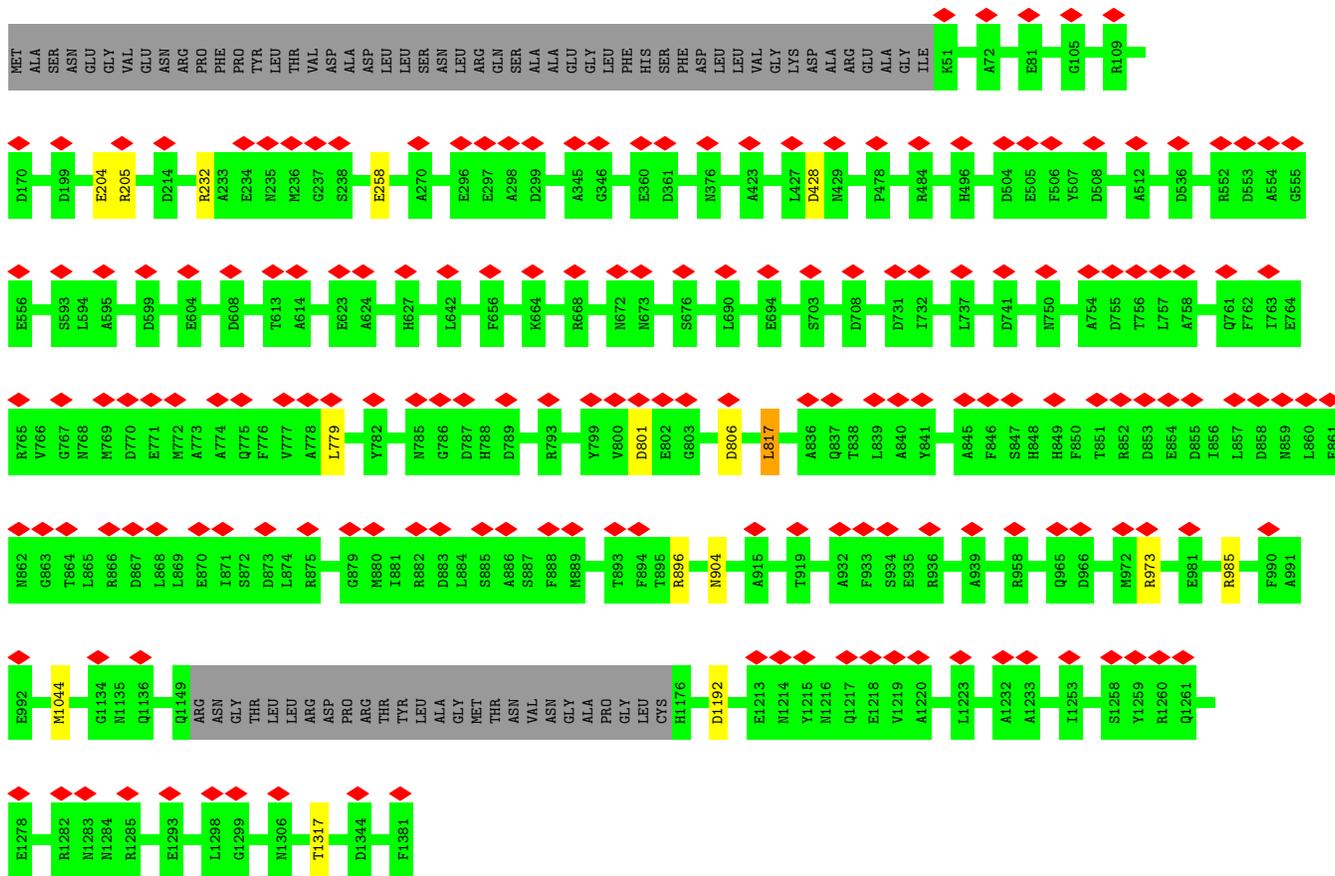


• Molecule 7: Major capsid protein

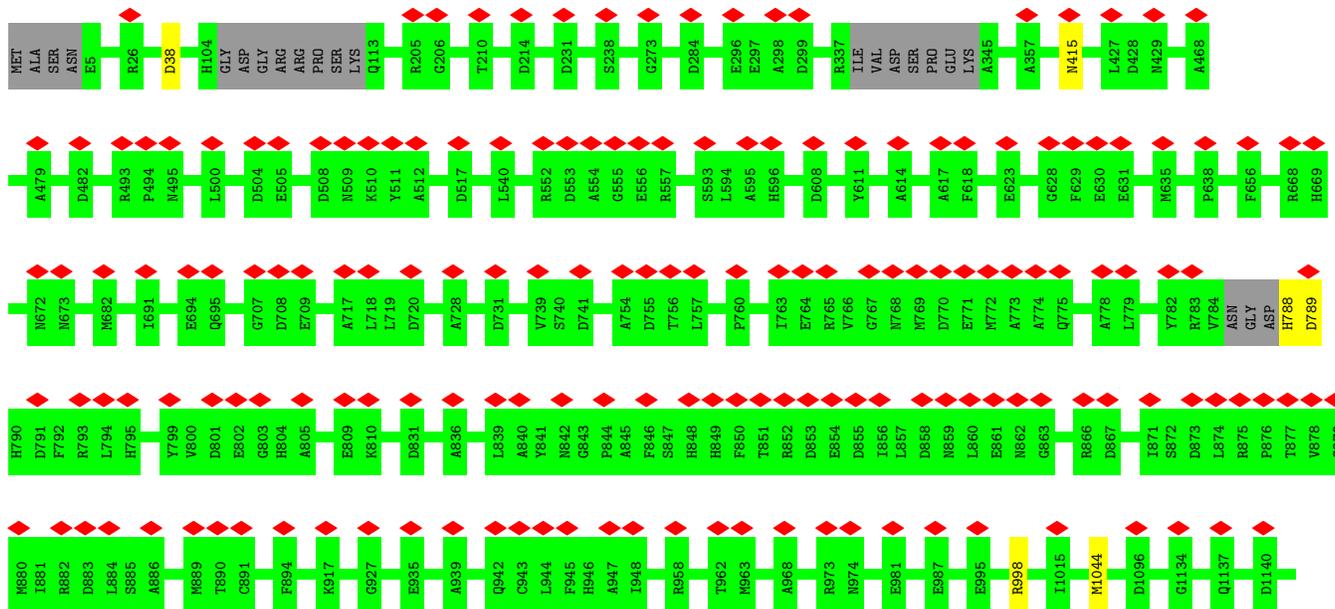


• Molecule 7: Major capsid protein





• Molecule 7: Major capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	28639	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	392.99997, 392.99997, 392.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality i

5.1 Standard geometry i

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	5	0.34	0/2263	0.56	1/3088 (0.0%)
1	e	0.42	0/2572	0.58	1/3503 (0.0%)
2	6	0.35	0/2377	0.62	1/3236 (0.0%)
2	7	0.36	0/2306	0.65	2/3135 (0.1%)
2	f	0.36	0/2327	0.57	1/3169 (0.0%)
2	g	0.38	0/2319	0.61	2/3155 (0.1%)
3	G	0.32	0/684	0.66	1/924 (0.1%)
3	K	0.30	0/570	0.56	0/765
4	C	0.35	0/2770	0.62	2/3763 (0.1%)
5	B	0.27	0/304	0.51	0/404
5	O	0.30	0/255	0.69	0/339
6	2	0.34	0/636	0.69	2/861 (0.2%)
6	Y	0.38	0/636	0.59	1/861 (0.1%)
6	Z	0.33	0/636	0.52	0/861
6	y	0.33	0/636	0.56	0/861
7	S	0.43	0/10405	0.58	1/14142 (0.0%)
7	T	0.43	0/10500	0.59	6/14271 (0.0%)
7	W	0.40	0/10699	0.57	1/14539 (0.0%)
7	x	0.43	1/10380 (0.0%)	0.59	0/14109
All	All	0.40	1/63275 (0.0%)	0.59	22/85986 (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
1	5	0	1
1	e	0	1
2	g	0	1
6	2	0	1
7	T	0	1
7	x	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	x	362	GLN	C-N	8.95	1.51	1.34

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	817	LEU	CA-CB-CG	8.12	133.97	115.30
6	2	23	LEU	CA-CB-CG	6.79	130.92	115.30
4	C	487	LEU	CA-CB-CG	6.74	130.81	115.30
2	g	199	LEU	CA-CB-CG	6.58	130.43	115.30
6	Y	23	LEU	CA-CB-CG	6.50	130.25	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	2	66	GLY	Peptide
1	5	312	HIS	Peptide
7	T	817	LEU	Peptide
7	x	361	ASP	Mainchain
7	x	669	HIS	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 [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	278/364 (76%)	260 (94%)	18 (6%)	0	100	100
1	e	311/364 (85%)	291 (94%)	20 (6%)	0	100	100
2	6	293/301 (97%)	276 (94%)	17 (6%)	0	100	100
2	7	281/301 (93%)	260 (92%)	21 (8%)	0	100	100
2	f	286/301 (95%)	270 (94%)	16 (6%)	0	100	100
2	g	282/301 (94%)	258 (92%)	24 (8%)	0	100	100
3	G	82/570 (14%)	76 (93%)	5 (6%)	1 (1%)	13	50
3	K	66/570 (12%)	65 (98%)	1 (2%)	0	100	100
4	C	334/507 (66%)	301 (90%)	33 (10%)	0	100	100
5	B	33/3149 (1%)	32 (97%)	1 (3%)	0	100	100
5	O	27/3149 (1%)	27 (100%)	0	0	100	100
6	2	72/176 (41%)	60 (83%)	12 (17%)	0	100	100
6	Y	72/176 (41%)	66 (92%)	6 (8%)	0	100	100
6	Z	72/176 (41%)	66 (92%)	6 (8%)	0	100	100
6	y	72/176 (41%)	64 (89%)	8 (11%)	0	100	100
7	S	1286/1381 (93%)	1205 (94%)	81 (6%)	0	100	100
7	T	1301/1381 (94%)	1196 (92%)	105 (8%)	0	100	100
7	W	1320/1381 (96%)	1224 (93%)	95 (7%)	1 (0%)	51	85
7	x	1286/1381 (93%)	1196 (93%)	89 (7%)	1 (0%)	51	85
All	All	7754/16105 (48%)	7193 (93%)	558 (7%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	W	789	ASP
7	x	509	ASN
3	G	15	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5	234/289 (81%)	232 (99%)	2 (1%)	78	87
1	e	268/289 (93%)	266 (99%)	2 (1%)	84	90
2	6	264/267 (99%)	264 (100%)	0	100	100
2	7	256/267 (96%)	255 (100%)	1 (0%)	91	94
2	f	259/267 (97%)	258 (100%)	1 (0%)	91	94
2	g	256/267 (96%)	255 (100%)	1 (0%)	91	94
3	G	70/465 (15%)	68 (97%)	2 (3%)	42	64
3	K	59/465 (13%)	59 (100%)	0	100	100
4	C	288/400 (72%)	283 (98%)	5 (2%)	60	78
5	B	33/2539 (1%)	33 (100%)	0	100	100
5	O	27/2539 (1%)	27 (100%)	0	100	100
6	2	68/128 (53%)	67 (98%)	1 (2%)	65	80
6	Y	68/128 (53%)	68 (100%)	0	100	100
6	Z	68/128 (53%)	67 (98%)	1 (2%)	65	80
6	y	68/128 (53%)	67 (98%)	1 (2%)	65	80
7	S	1101/1171 (94%)	1099 (100%)	2 (0%)	93	96
7	T	1111/1171 (95%)	1101 (99%)	10 (1%)	78	87
7	W	1131/1171 (97%)	1125 (100%)	6 (0%)	88	93
7	x	1099/1171 (94%)	1091 (99%)	8 (1%)	84	90
All	All	6728/13250 (51%)	6685 (99%)	43 (1%)	86	92

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	W	1304	THR
7	x	1109	ARG
7	W	1345	GLU
7	x	637	VAL
7	x	1297	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
7	W	433	GLN
7	W	1149	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	e	137	HIS
7	W	534	ASN
7	W	942	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

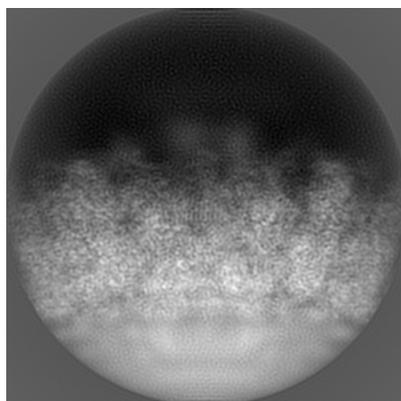
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30157. These allow visual inspection of the internal detail of the map and identification of artifacts.

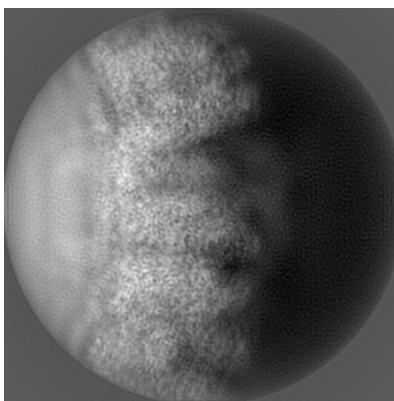
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

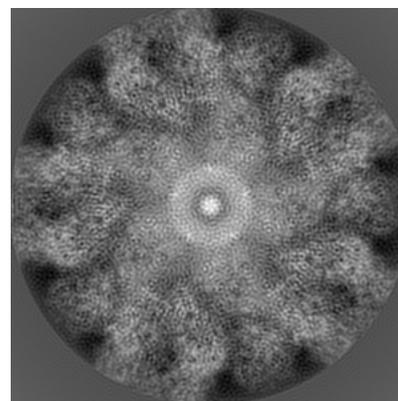
6.1.1 Primary map



X



Y

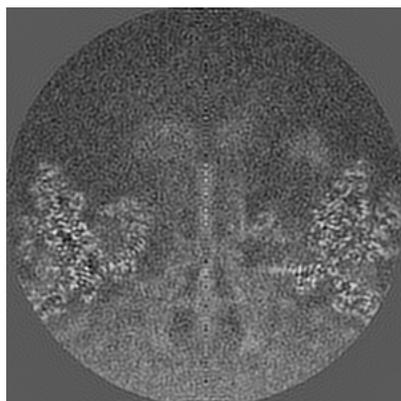


Z

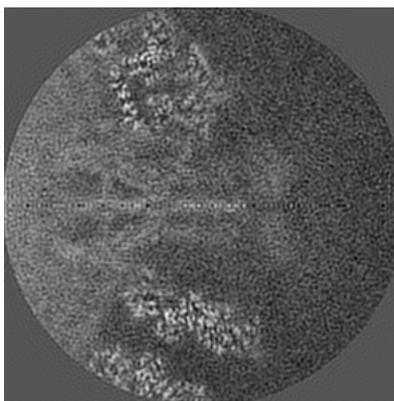
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

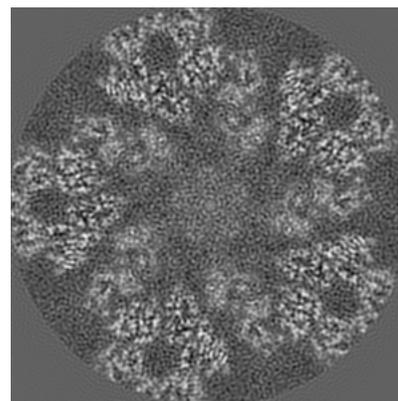
6.2.1 Primary map



X Index: 150



Y Index: 150

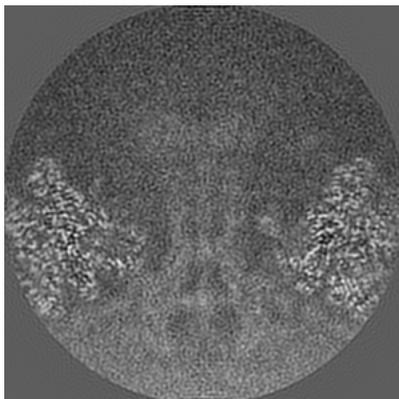


Z Index: 150

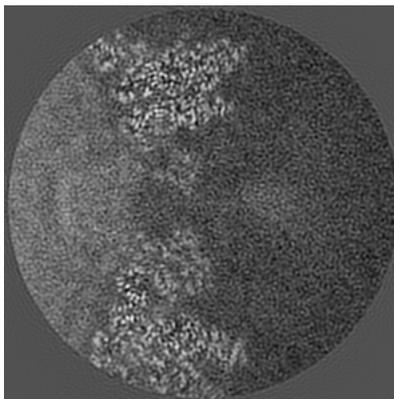
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

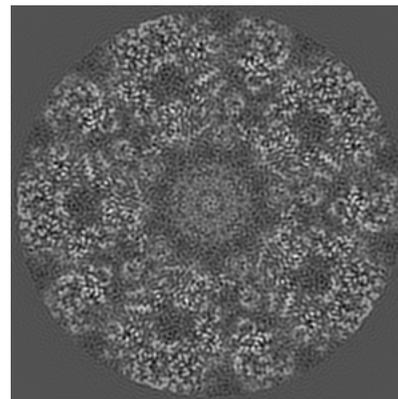
6.3.1 Primary map



X Index: 144



Y Index: 114

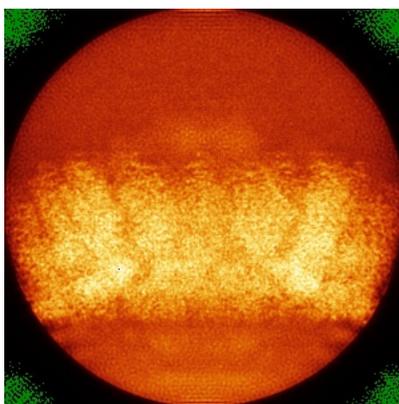


Z Index: 109

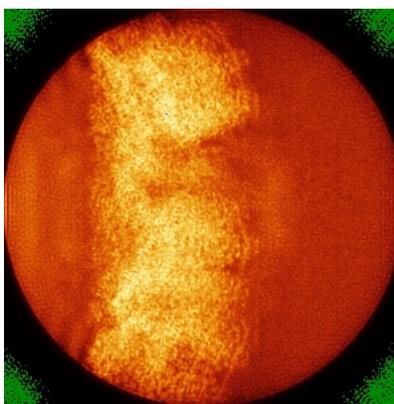
The images above show the largest variance slices of the map in three orthogonal directions.

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

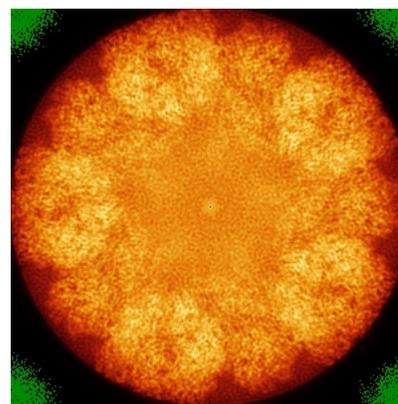
6.4.1 Primary map



X



Y

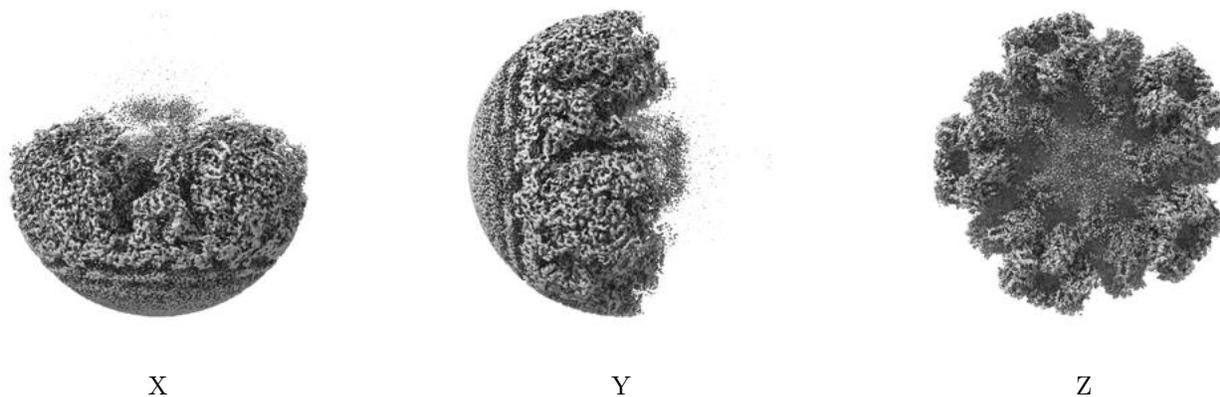


Z

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.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

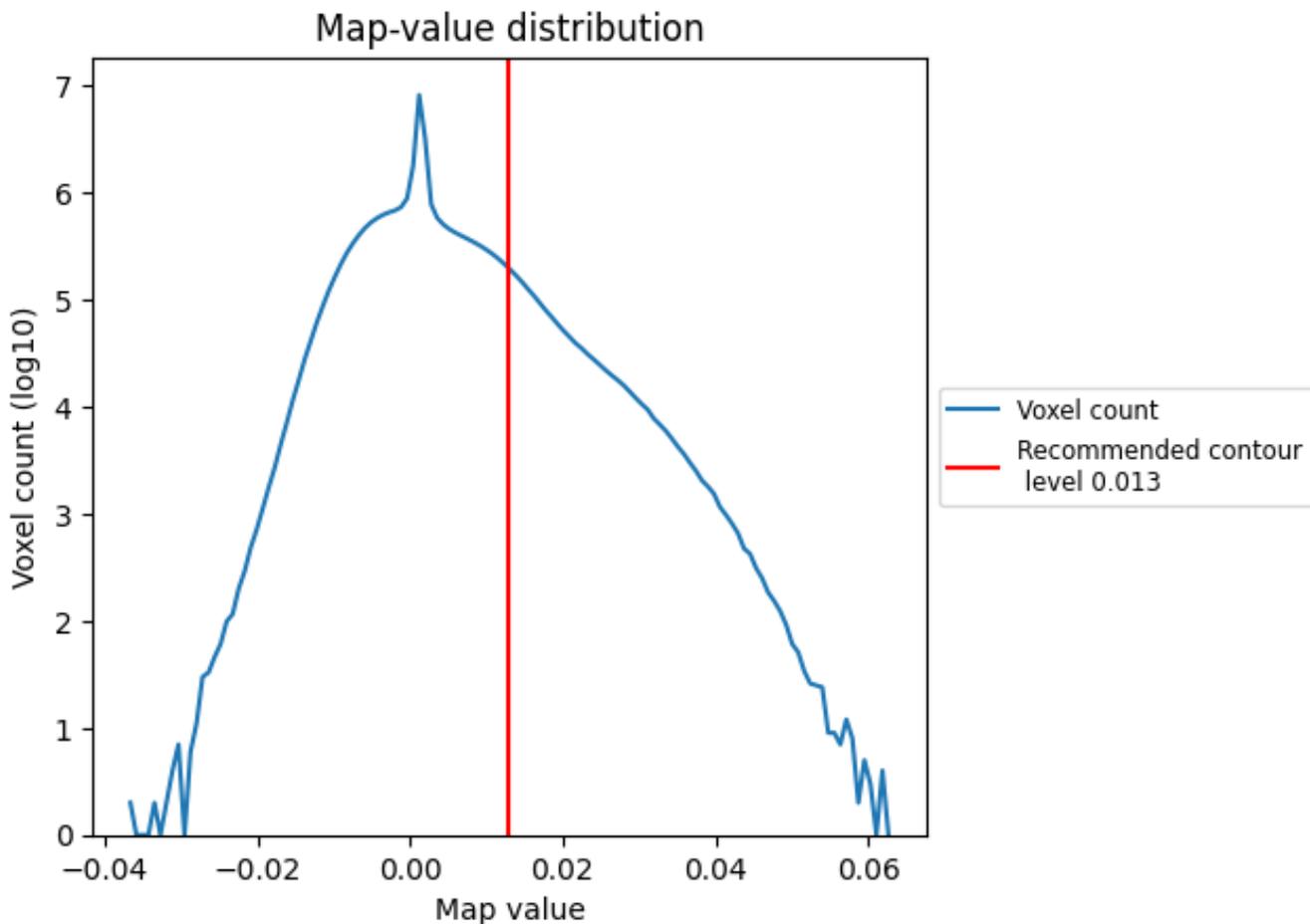
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

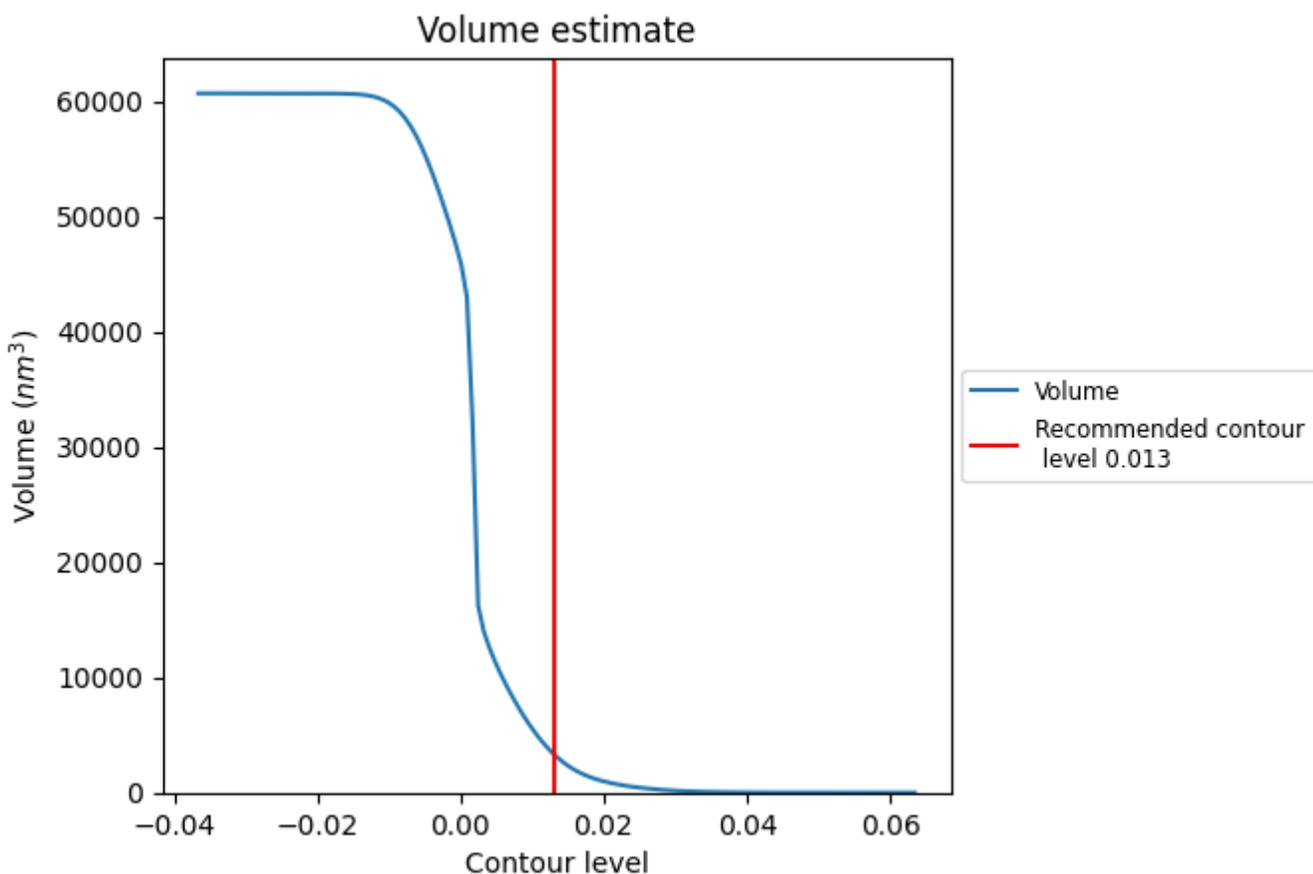
This section contains the results of statistical analysis of the map.

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.

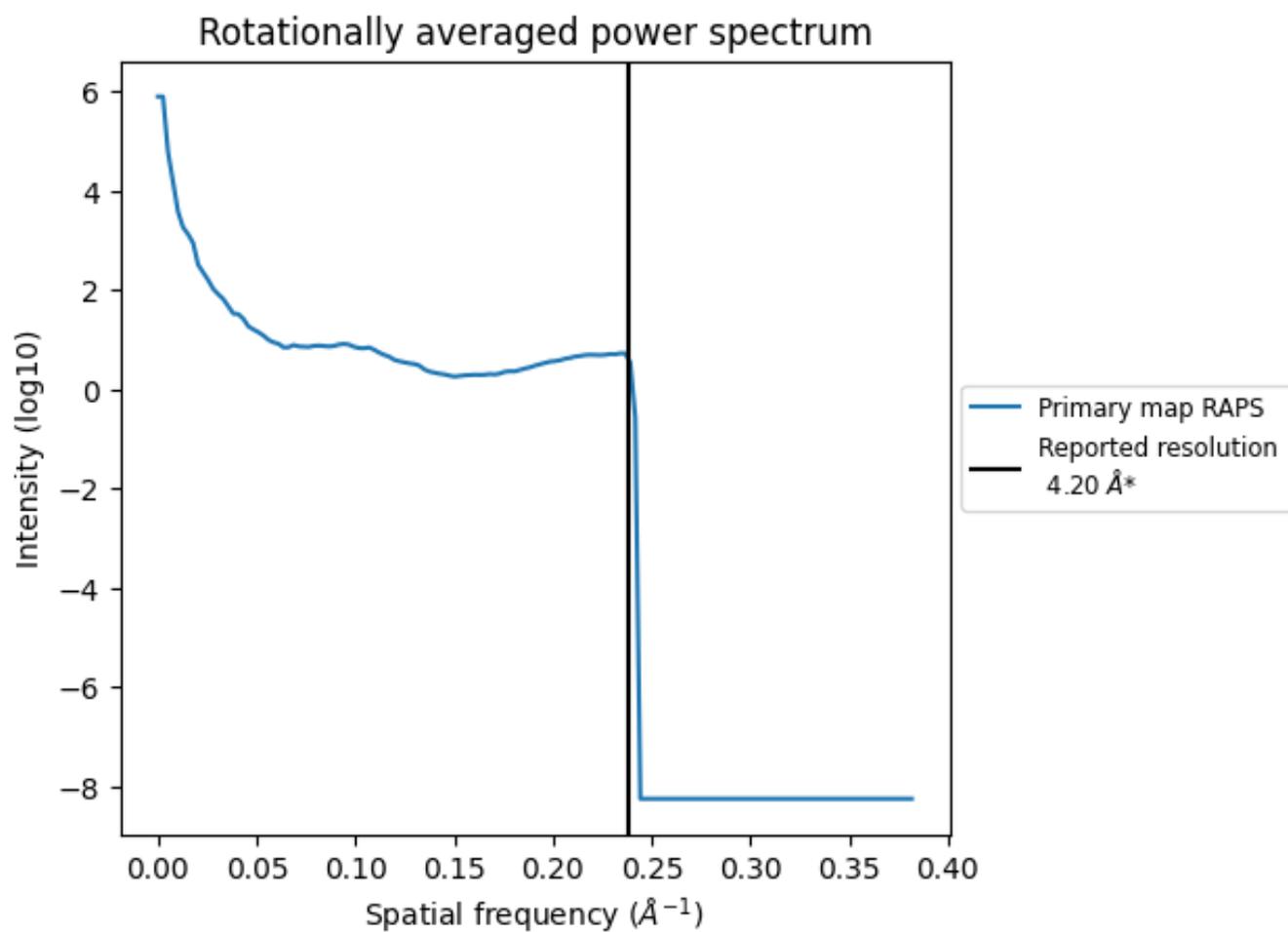
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3365 nm³; this corresponds to an approximate mass of 3040 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation

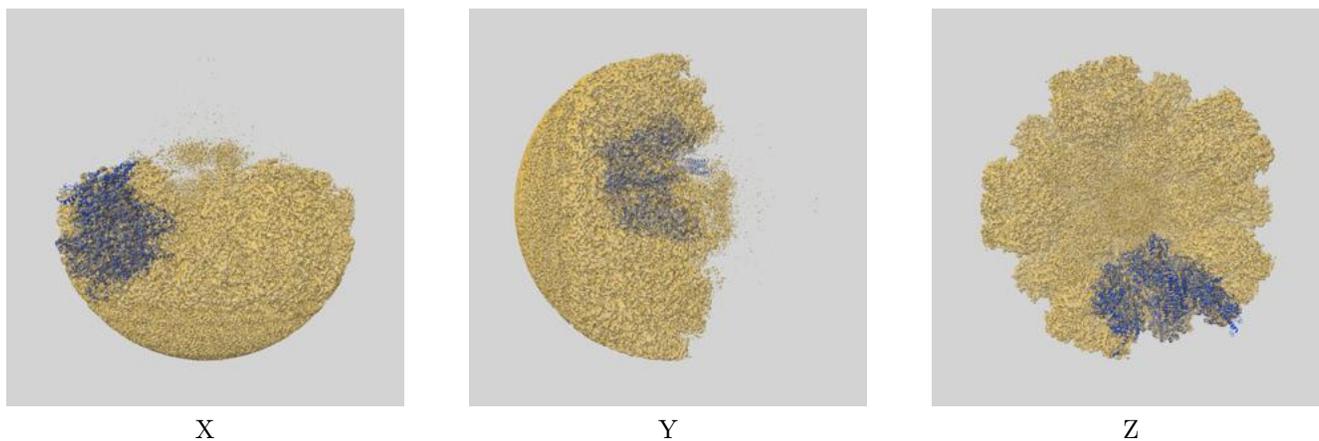
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

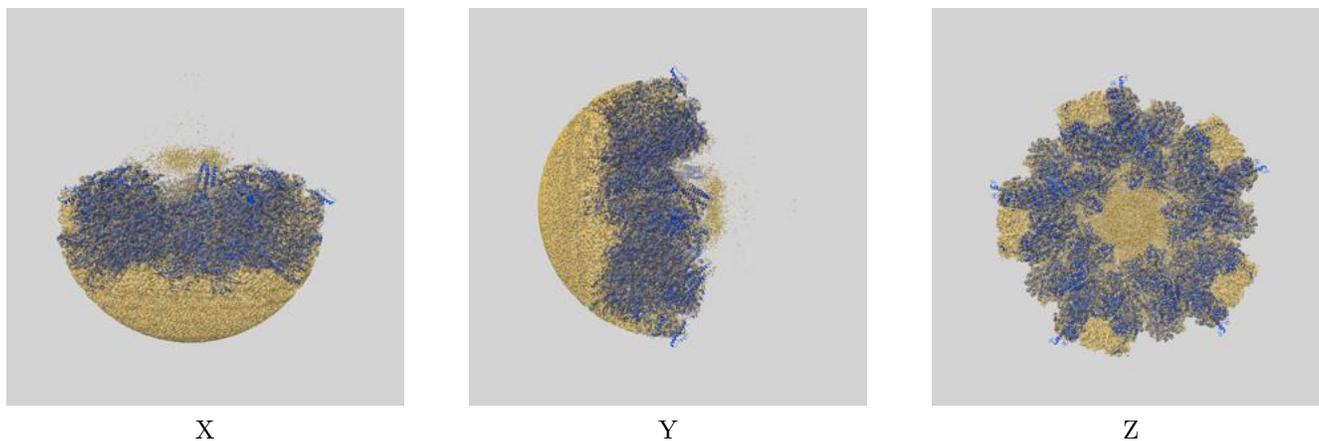
This section contains information regarding the fit between EMDB map EMD-30157 and PDB model 7BQX. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

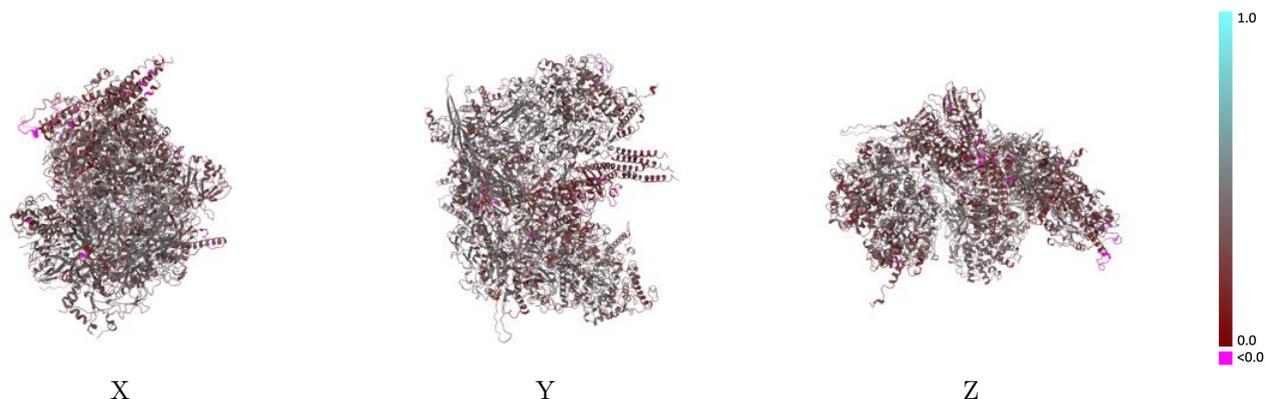


9.1.2 Map-model assembly overlay [i](#)



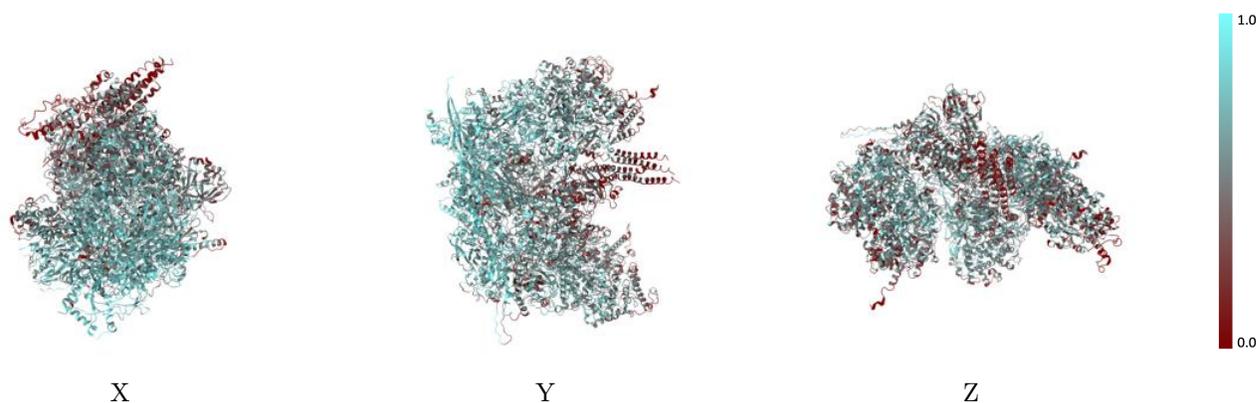
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



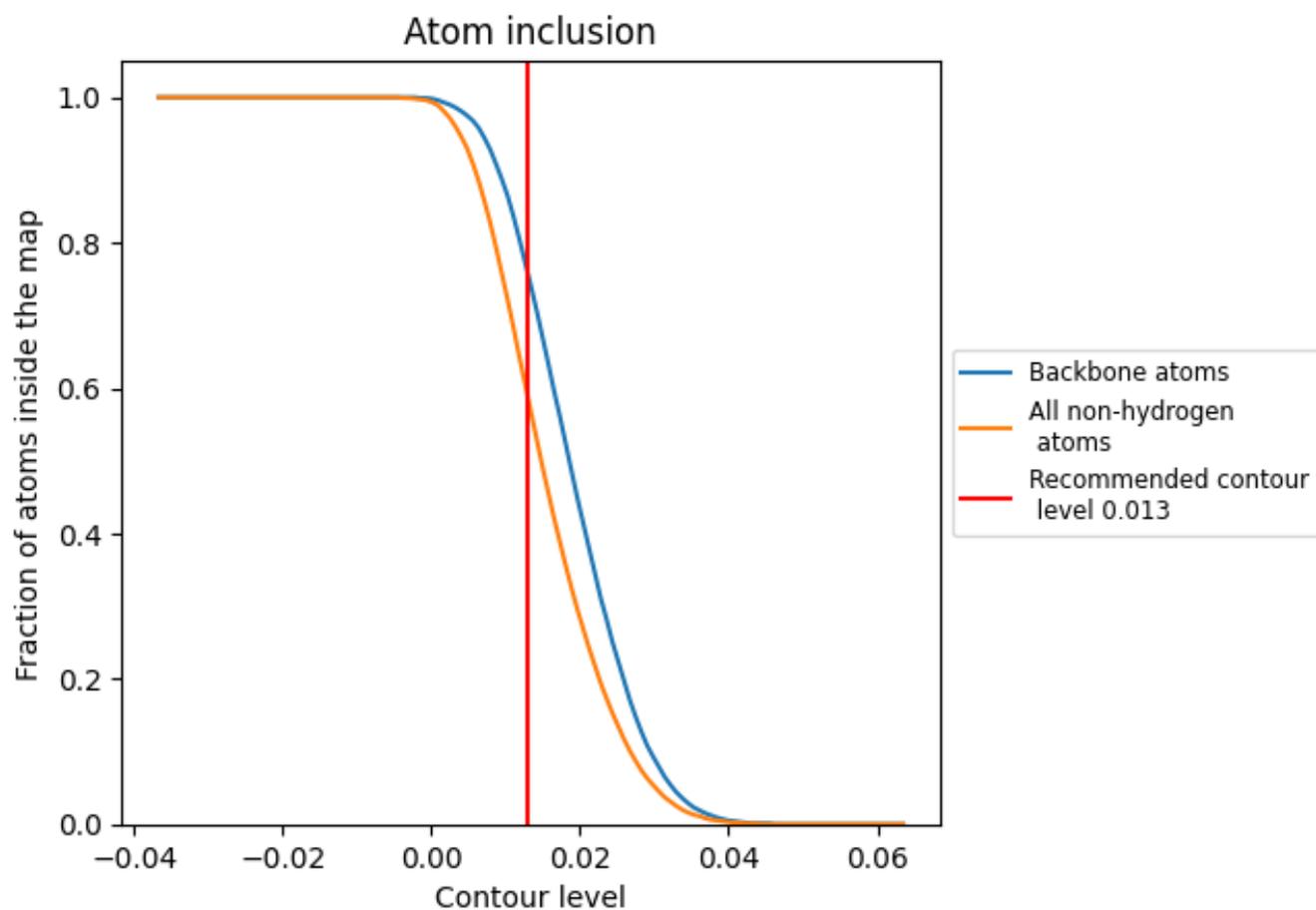
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5870	 0.3650
2	 0.1330	 0.1500
5	 0.4500	 0.3030
6	 0.4870	 0.3080
7	 0.4880	 0.3280
B	 0.1820	 0.2560
C	 0.4060	 0.2870
G	 0.3640	 0.2950
K	 0.3990	 0.3100
O	 0.1370	 0.2440
S	 0.6200	 0.3830
T	 0.6580	 0.3980
W	 0.6290	 0.3780
Y	 0.3750	 0.3180
Z	 0.3150	 0.2840
e	 0.7130	 0.4020
f	 0.6290	 0.3720
g	 0.6380	 0.3760
x	 0.6270	 0.3830
y	 0.3170	 0.2980

