



Preliminary Full wwPDB EM Validation Report ⓘ

Mar 25, 2023 – 06:30 PM EDT

This wwPDB validation report is NOT for manuscript review

This is a Preliminary Full wwPDB EM Validation Report.

This report is produced by the standalone wwPDB validation server.
The structure in question has not been deposited to the wwPDB.
This report should not be submitted to journals.

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.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
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)	:	2.32.1

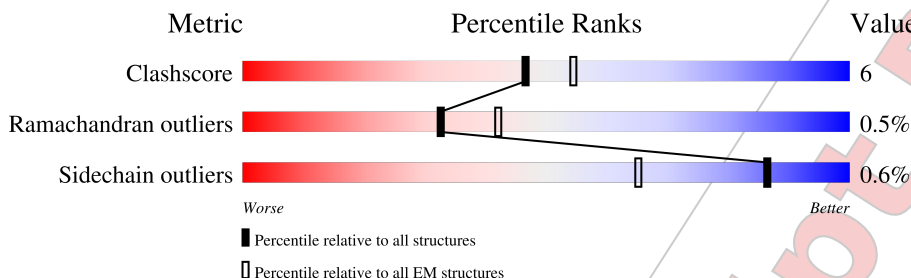
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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)
Clashscore	158937	4297
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	A	203	<div> <div>29%</div> <div>84%</div> <div>16%</div> </div>
2	E	175	<div> <div>29%</div> <div>79%</div> <div>21%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GDP	E	200	X	-	-	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6041 atoms, of which 3014 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.

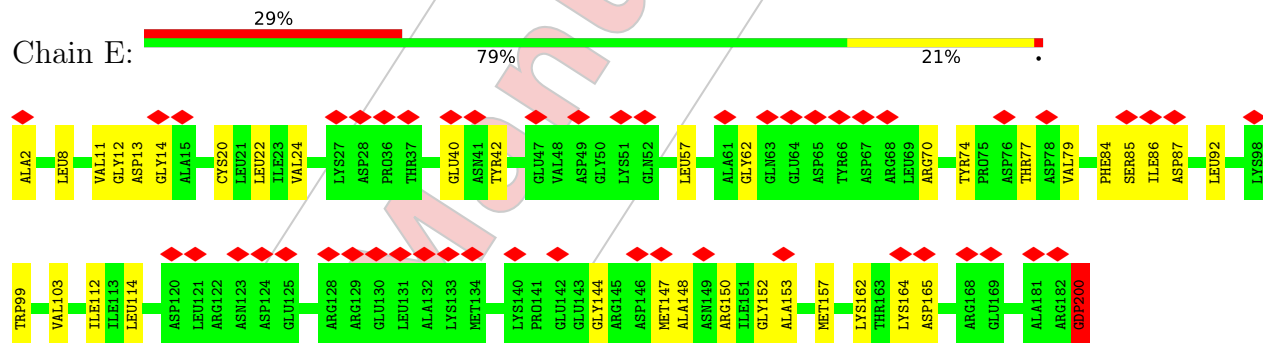
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	203	3263	1031	1633	296	297	6	0	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms							AltConf	Trace
2	E	175	Total	C	H	N	O	P	S	0	0
			2778	868	1381	243	274	2	10		

i

- Molecule 1:



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	Not provided	
Voltage (kV)	Not provided	
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	
Maximum map value	1.311	Depositor
Minimum map value	-0.879	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.247	Depositor
Map size (Å)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP

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	0.40	0/1664	0.64	1/2251 (0.0%)
2	E	0.33	0/1392	0.65	0/1878
All	All	0.37	0/3056	0.64	1/4129 (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
2	E	2	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	329	VAL	CG1-CB-CG2	7.41	122.75	110.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	200	GDP	C3',C1'

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	164	LYS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1630	1633	1630	16	0
2	E	1397	1381	1376	24	0
All	All	3027	3014	3006	39	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ASP:OD2	2:E:2:ALA:N	2.20	0.74
2:E:85:SER:OG	2:E:87:ASP:OD1	2.06	0.72
1:A:160:ARG:NH1	1:A:165:ASP:OD2	2.25	0.69
1:A:256:LEU:O	1:A:260:GLN:NE2	2.28	0.67
2:E:162:LYS:N	2:E:200:GDP:O6	2.27	0.67
1:A:274:GLN:OE1	1:A:320:ARG:NH2	2.29	0.65
2:E:8:LEU:HD23	2:E:57:LEU:HD23	1.78	0.64
1:A:224:ARG:NH1	1:A:261:GLY:O	2.31	0.63
2:E:8:LEU:HD23	2:E:57:LEU:CD2	2.29	0.63
1:A:179:ARG:NH2	1:A:225:GLU:OE1	2.35	0.59
2:E:22:LEU:CD1	2:E:57:LEU:HD22	2.33	0.59
1:A:209:THR:O	1:A:213:LEU:HD23	2.05	0.56
1:A:206:ARG:NH1	1:A:208:ASP:OD1	2.39	0.56
2:E:84:PHE:CE1	2:E:114:LEU:HD23	2.43	0.54
2:E:147:MET:SD	2:E:150:ARG:NH1	2.81	0.54
1:A:169:LEU:O	1:A:173:LEU:N	2.37	0.54
2:E:62:GLY:O	2:E:70:ARG:NH2	2.41	0.53
2:E:112:ILE:HG13	2:E:153:ALA:HB2	1.92	0.51
1:A:331:ILE:HD12	1:A:331:ILE:O	2.10	0.51
2:E:144:GLY:O	2:E:148:ALA:N	2.44	0.49
2:E:148:ALA:O	2:E:152:GLY:N	2.41	0.48
2:E:20:CYS:O	2:E:24:VAL:HG23	2.14	0.48
2:E:40:GLU:O	2:E:42:TYR:N	2.44	0.47
2:E:74:TYR:O	2:E:77:THR:HG22	2.13	0.47
1:A:314:MET:SD	1:A:314:MET:N	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:79:VAL:HG22	2:E:79:VAL:O	2.14	0.46
1:A:305:THR:OG1	1:A:306:GLU:OE1	2.33	0.46
2:E:13:ASP:OD1	2:E:14:GLY:N	2.50	0.45
2:E:92:LEU:HD12	2:E:147:MET:HG3	1.98	0.45
2:E:86:ILE:HG22	2:E:86:ILE:O	2.18	0.43
1:A:193:THR:HG22	1:A:194:CYS:H	1.83	0.43
2:E:157:MET:N	2:E:157:MET:SD	2.90	0.43
1:A:158:VAL:CG2	1:A:198:ALA:HB2	2.50	0.42
2:E:22:LEU:HD11	2:E:57:LEU:HD22	2.00	0.42
1:A:272:PHE:O	1:A:274:GLN:N	2.53	0.41
1:A:190:THR:OG1	1:A:191:GLY:N	2.54	0.41
2:E:99:TRP:O	2:E:103:VAL:HG22	2.21	0.41
2:E:11:VAL:HG12	2:E:12:GLY:N	2.37	0.40
2:E:8:LEU:CD1	2:E:79:VAL:HG13	2.51	0.40

There are no symmetry-related clashes.

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	A	201/203 (99%)	177 (88%)	23 (11%)	1 (0%)	29	29
2	E	170/175 (97%)	128 (75%)	41 (24%)	1 (1%)	25	25
All	All	371/378 (98%)	305 (82%)	64 (17%)	2 (0%)	32	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	165	ASP
1	A	262	ALA

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	A	176/176 (100%)	174 (99%)	2 (1%)	73	73
2	E	150/150 (100%)	150 (100%)	0	100	100
All	All	326/326 (100%)	324 (99%)	2 (1%)	86	86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
1	A	338	ASN

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

Mol	Chain	Res	Type
1	A	201	ASN
1	A	207	ASN
2	E	180	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](#)

1 non-standard protein/DNA/RNA residue is 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
2	GDP	E	200	-	24,30,30	2.55	7 (29%)	30,47,47	2.26	12 (40%)

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
2	GDP	E	200	-	2/2/6/6	1/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	200	GDP	O6-C6	8.31	1.40	1.23
2	E	200	GDP	C2-N2	4.72	1.45	1.34
2	E	200	GDP	O4'-C1'	4.24	1.47	1.41
2	E	200	GDP	C2'-C1'	-3.08	1.49	1.53
2	E	200	GDP	PB-O2B	-2.17	1.46	1.54
2	E	200	GDP	PB-O3B	-2.16	1.46	1.54
2	E	200	GDP	C2'-C3'	-2.02	1.47	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	200	GDP	C2'-C3'-C4'	5.47	113.28	102.64
2	E	200	GDP	O4'-C1'-C2'	4.74	113.86	106.93
2	E	200	GDP	O3'-C3'-C4'	3.98	122.55	111.05
2	E	200	GDP	O3'-C3'-C2'	3.42	122.89	111.82
2	E	200	GDP	C5-C6-N1	3.27	119.73	113.95
2	E	200	GDP	C2-N1-C6	-3.04	119.51	125.10
2	E	200	GDP	PA-O3A-PB	-2.92	122.80	132.83
2	E	200	GDP	O2B-PB-O3A	2.86	114.22	104.64
2	E	200	GDP	O3B-PB-O3A	2.83	114.14	104.64
2	E	200	GDP	O6-C6-C5	-2.75	119.01	124.37
2	E	200	GDP	O2A-PA-O1A	-2.19	101.39	112.24
2	E	200	GDP	C8-N7-C5	2.01	106.81	102.99

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	200	GDP	C3'

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Mol	Chain	Res	Type	Atom
2	E	200	GDP	C1'

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	200	GDP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	200	GDP	1	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	182:ARG	C	200:GDP	O3'	35.29
1	E	28:ASP	C	36:PRO	N	16.60

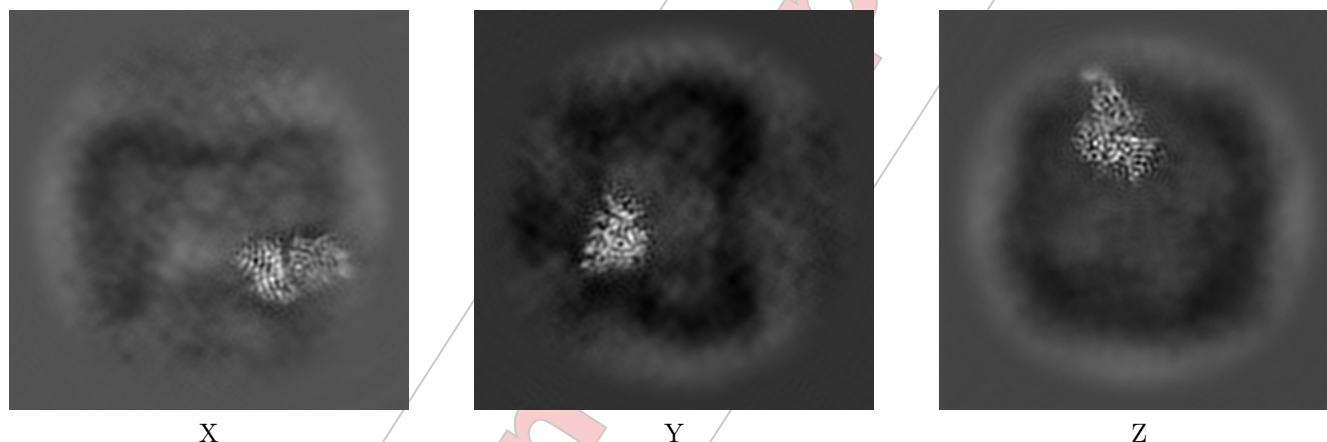
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry D_9100078174. 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](#)

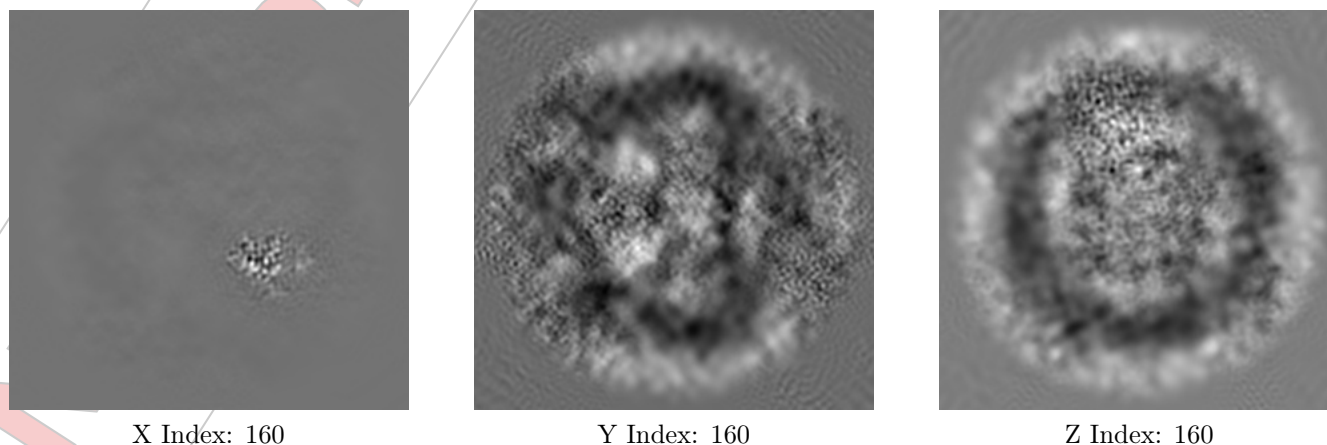
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160

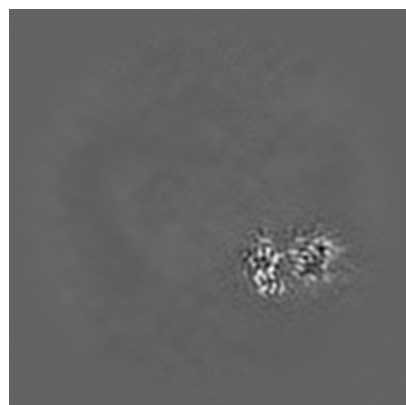
Y Index: 160

Z Index: 160

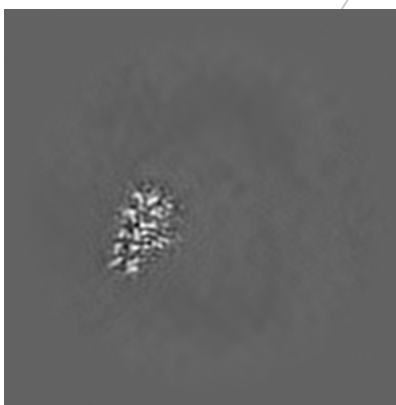
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

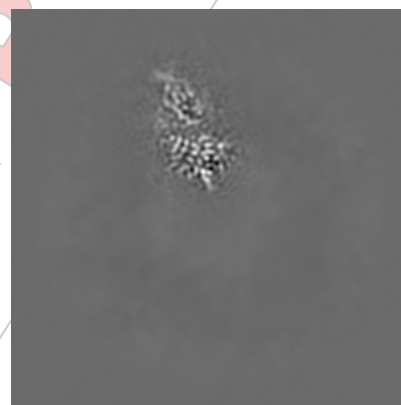
6.3.1 Primary map



X Index: 140



Y Index: 210

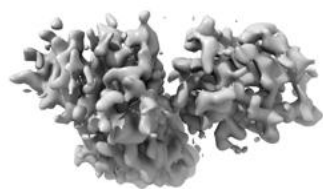


Z Index: 120

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

6.4 Orthogonal surface views [i](#)

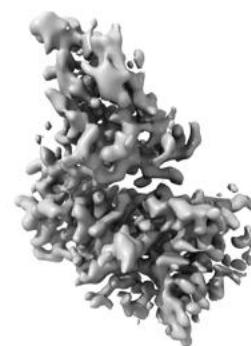
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.247. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 Mask visualisation

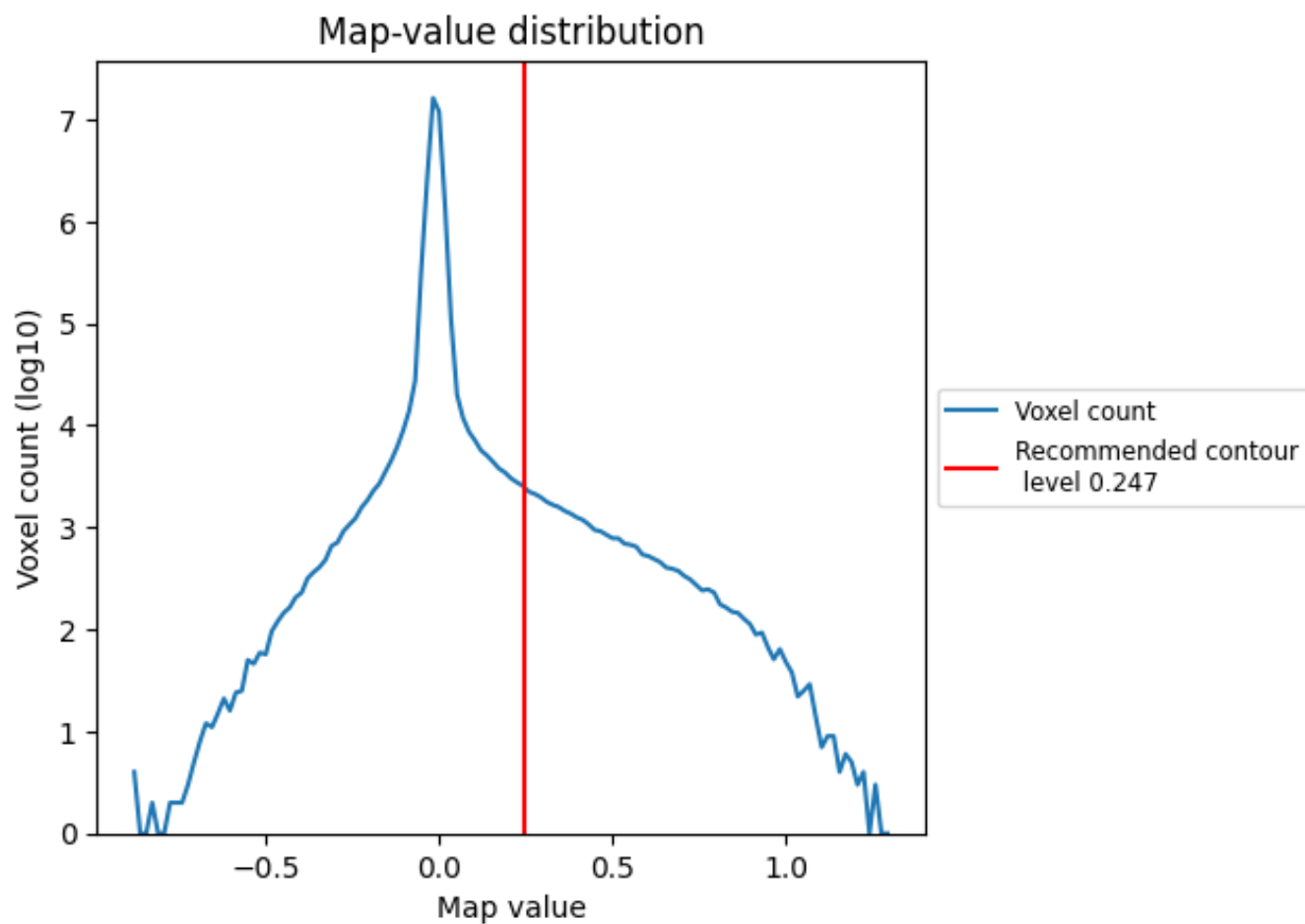
This section was not generated. No masks/segmentation were deposited.

Not For Manuscript Review

7 Map analysis [i](#)

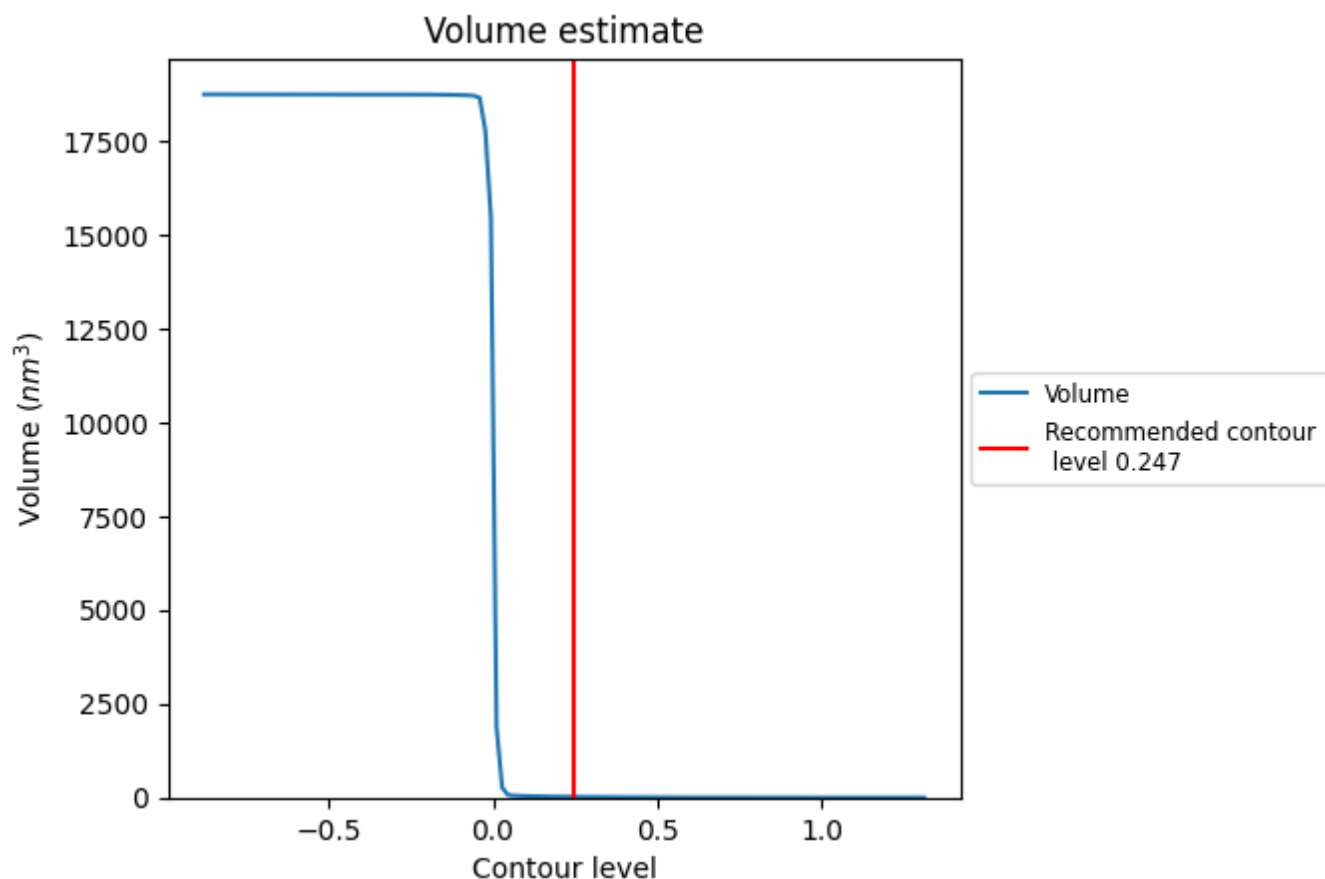
This section contains the results of statistical analysis of the map.

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.

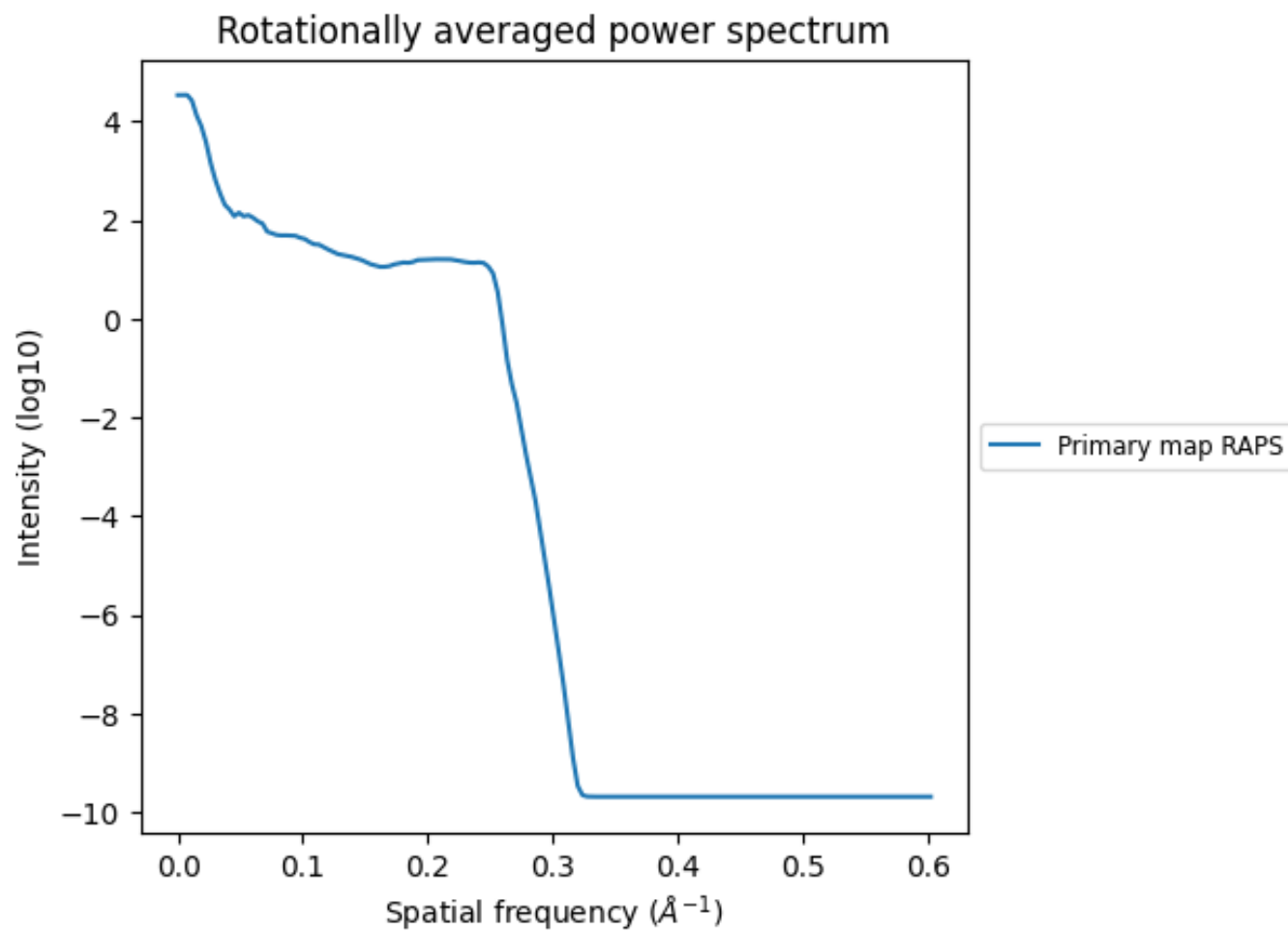
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 18 nm^3 ; this corresponds to an approximate mass of 17 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 ⓘ



8 Fourier-Shell correlation ⓘ

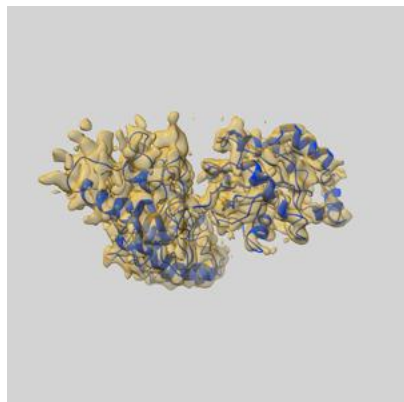
This section was not generated. No FSC curve or half-maps provided.

Not For Manuscript Review

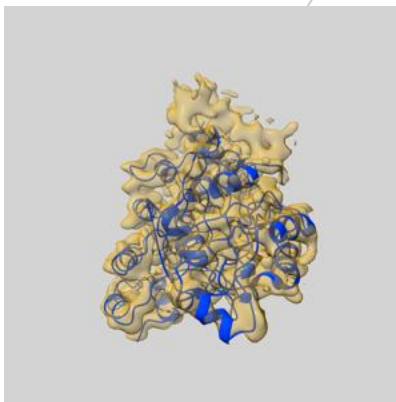
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map D_9100078174 and PDB model D_9100078174. Per-residue inclusion information can be found in section 3 on page 4.

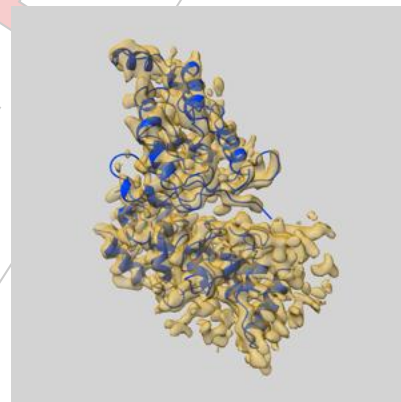
9.1 Map-model overlay ⓘ



X



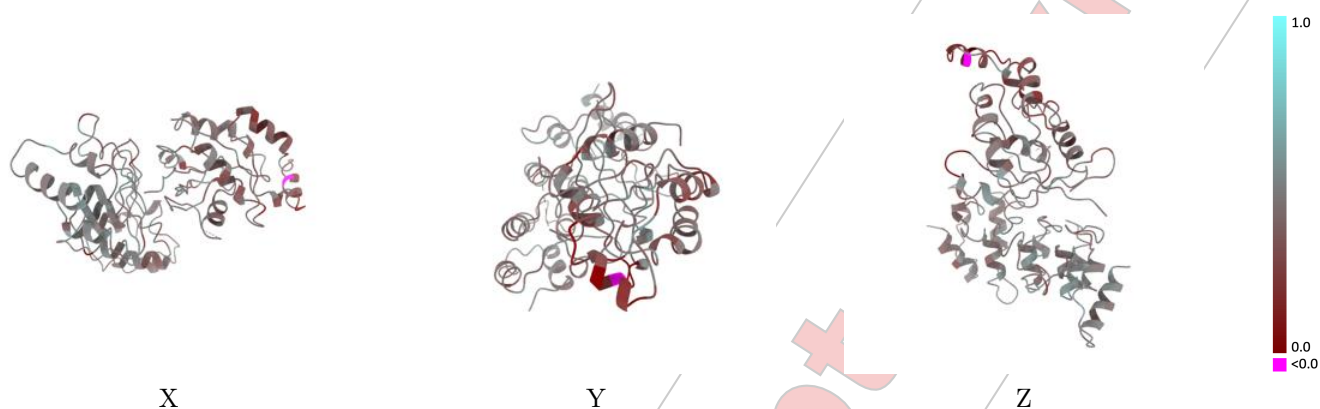
Y



Z

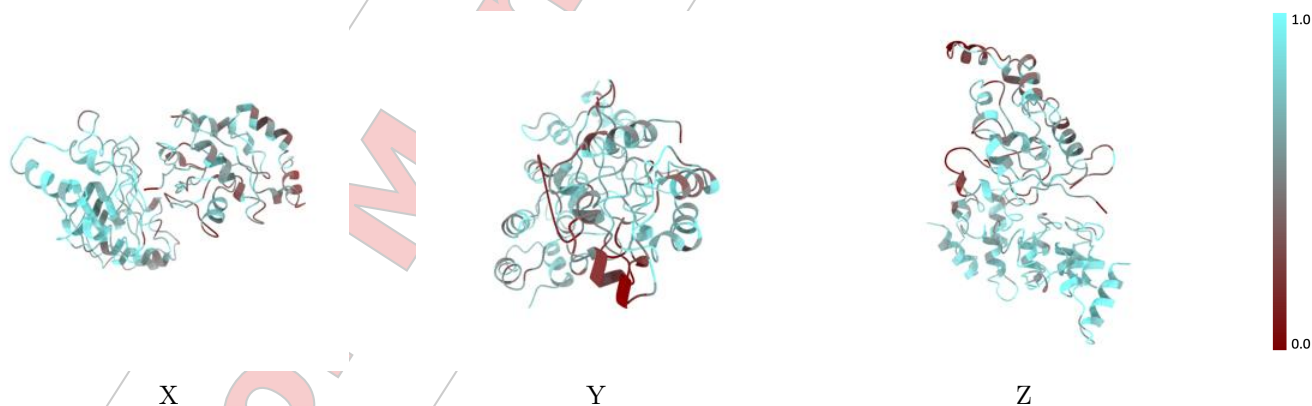
The images above show the 3D surface view of the map at the recommended contour level 0.247 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



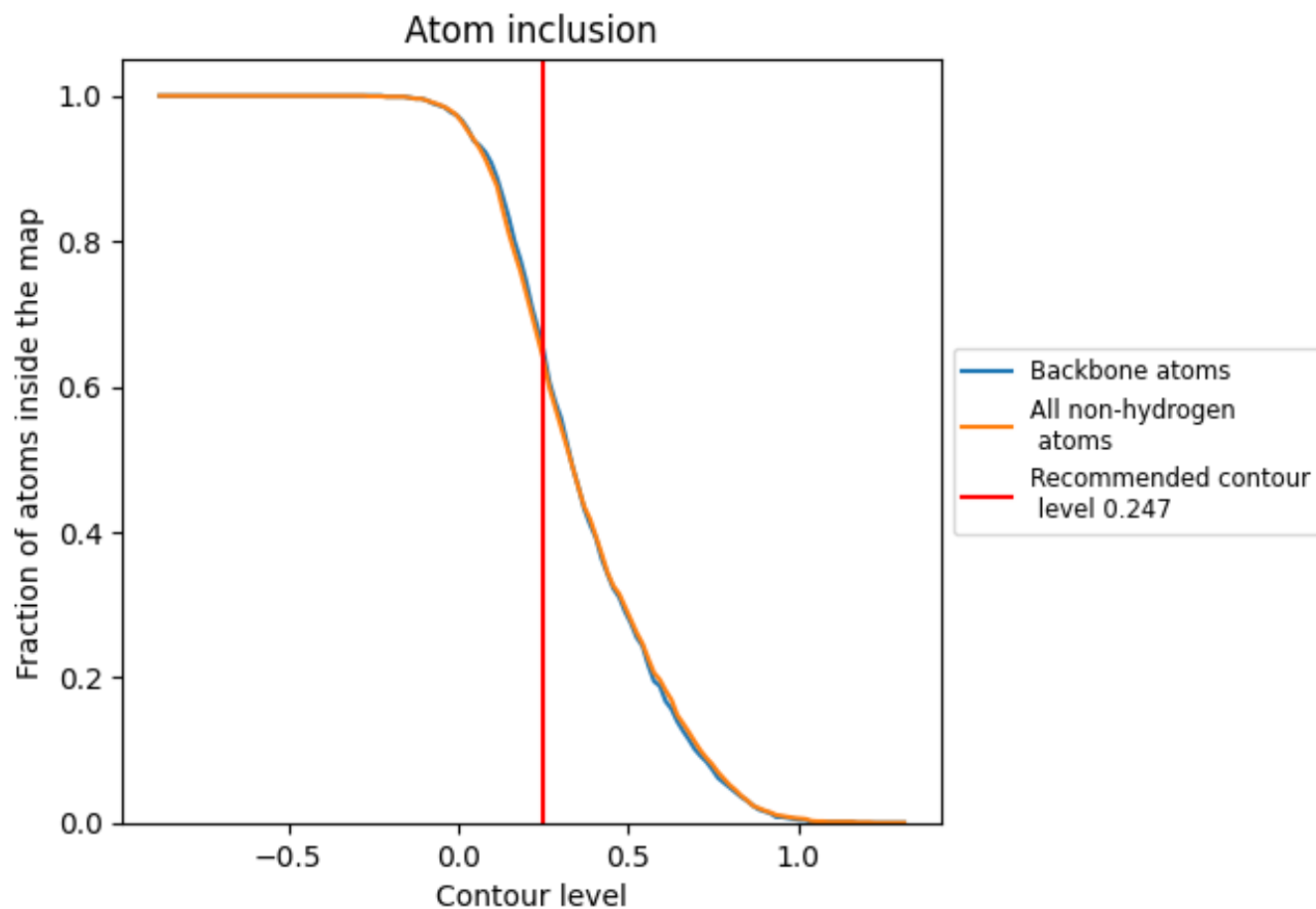
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.247).







9.4 Atom inclusion ⓘ



At the recommended contour level, 66% of all backbone atoms, 64% 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 (0.247) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6423	 0.4130
A	 0.7476	 0.4430
E	 0.5581	 0.3780

