Full wwPDB EM Validation Report (i)

Oct 9, 2024 – 12:17 PM JST

PDB ID	:	9JR3
EMDB ID	:	EMD-61747
Title	:	Cryo-EM structure of PTH-PTH1R-Gq (tilted state)
Authors	:	Sano, F.K.; Hirano, H.; Itoh, Y.; Nureki, O.
Deposited on	:	2024-09-29
Resolution	:	2.80 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	FAILED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.80 Å.

There are no overall percentile quality scores available for this entry.

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

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 9455 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 Parathyroid hormone/parathyroid hormone-related peptide receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	355	Total 2865	C 1904	N 468	O 473	S 20	0	0

- Molecule 2 is a protein called Parathyroid hormone.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	35	Total 289	C 181	N 56	O 50	S 2	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	35	NH2	-	amidation	UNP P01270

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1 (miniGq).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	220	Total 1722	C 1094	N 304	O 317	S 7	0	0

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	337	Total 2473	C 1541	N 439	O 473	S 20	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P54311

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP P54311
B	-1	GLN	-	expression tag	UNP P54311
B	0	LEU	-	expression tag	UNP P54311
B	1	GLN	-	expression tag	UNP P54311

- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	51	350	221	60	67	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	68	SER	-	expression tag	UNP P63212

- Molecule 6 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	S	231	1727	1099	289	330	9	0	0

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	C	2	28	16	2	10	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
8	R	1	1	1	0

MolProbity 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	259479	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/Å^2)$	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	57.052	Depositor
Minimum map value	-39.422	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.572	Depositor
Recommended contour level	4.7	Depositor
Map size (Å)	193.848, 193.848, 193.848	wwPDB
Map dimensions	394, 394, 394	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.492, 0.492, 0.492	Depositor

4   Model quality ⓘ

4.1   Standard geometry ⓘ

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

4.2   Too-close contacts ⓘ

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

4.3   Torsion angles ⓘ

4.3.1   Protein backbone ⓘ

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

4.3.2   Protein sidechains ⓘ

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

4.3.3   RNA ⓘ

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

4.4   Non-standard residues in protein, DNA, RNA chains ⓘ

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

4.5   Carbohydrates ⓘ

2 monosaccharides 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	$\#\lvert Z\rvert>2$	Counts	RMSZ	$\#\lvert Z\rvert>2$
7	NAG	C	1	1,7	14,14,15	0.24	0	17,19,21	0.39	0
7	NAG	C	2	7	14,14,15	0.21	0	17,19,21	0.41	0

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
7	NAG	C	1	1,7	-	<mark>2/6/23/26</mark>	0/1/1/1
7	NAG	C	2	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1	NAG	O5-C5-C6-O6
7	C	1	NAG	C4-C5-C6-O6

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 oligosaccharide.

Oligosaccharide Chain C
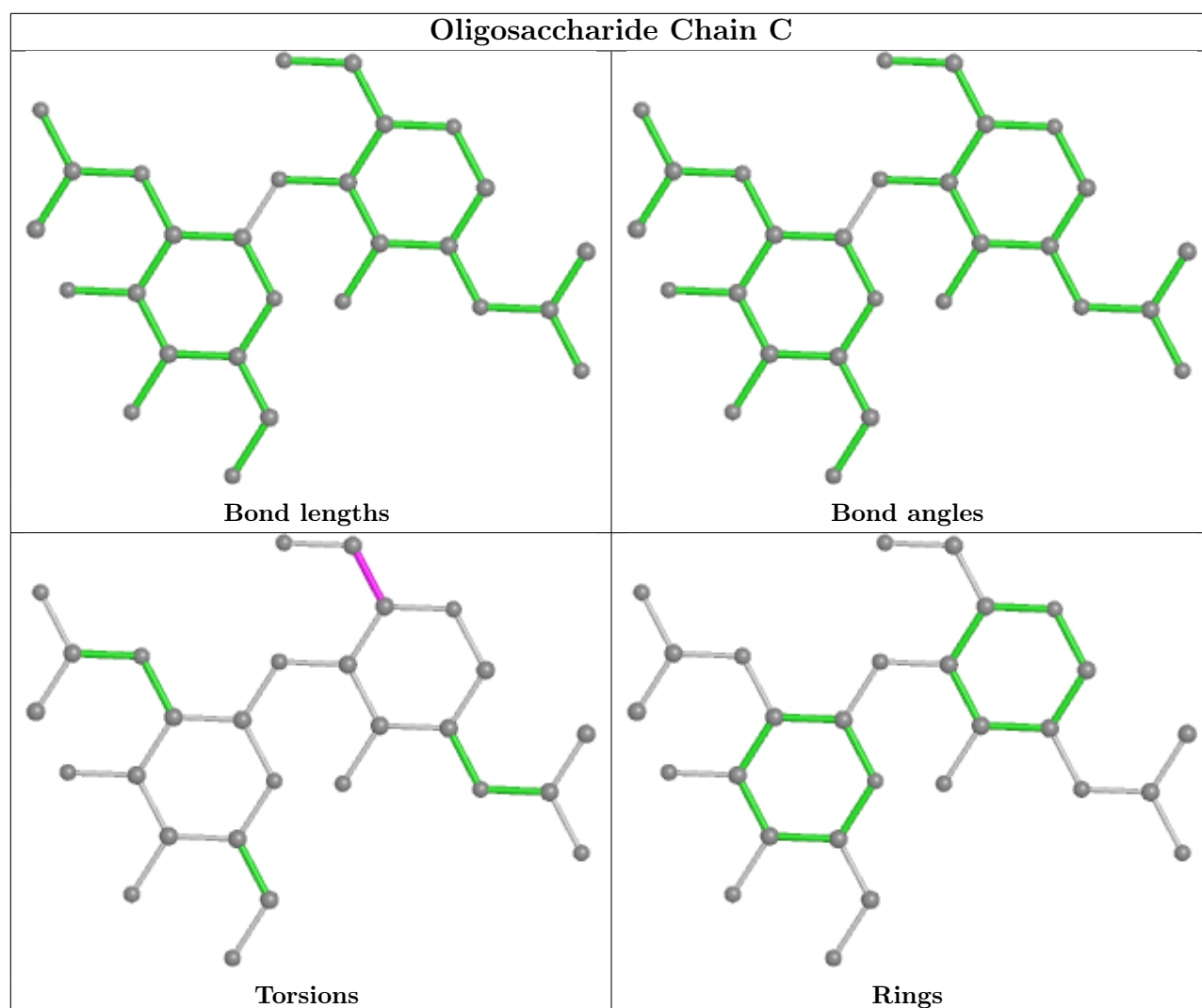
4.6 Ligand geometry ⓘ

There are no ligands in this entry.

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-61747. 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 ⓘ

5.1.1 Primary map

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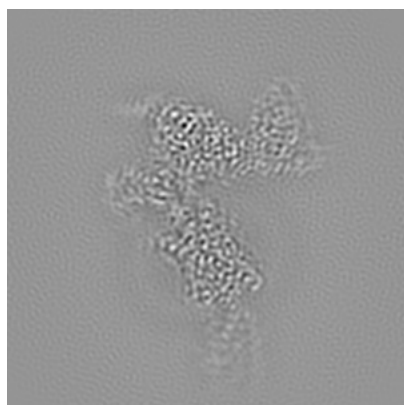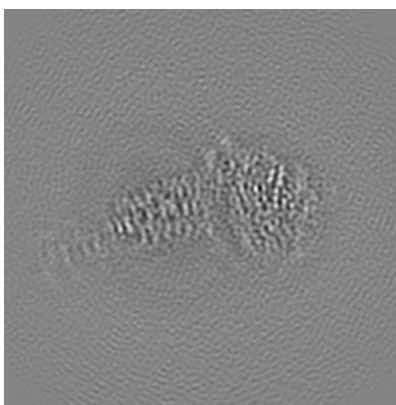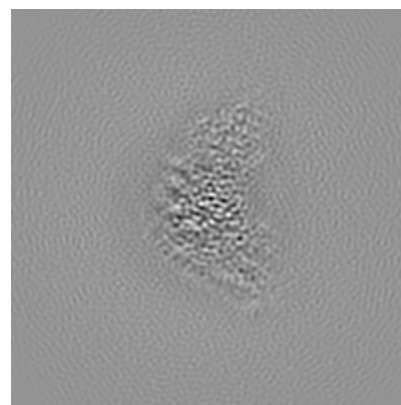
The images above show the map projected in three orthogonal directions.

5.2 Central slices ⓘ
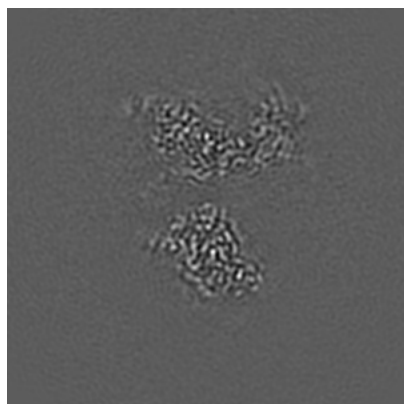
5.2.1 Primary map
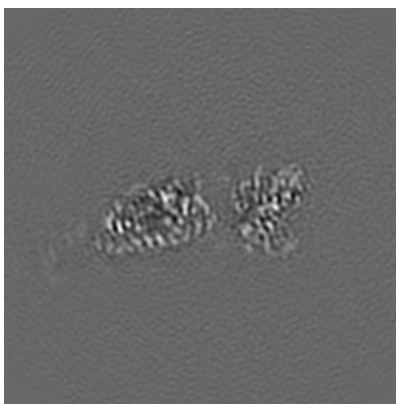
| X Index: 197 | Y Index: 197 | Z Index: 197 |
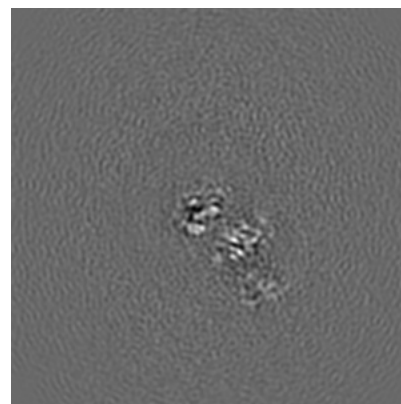
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices ⓘ
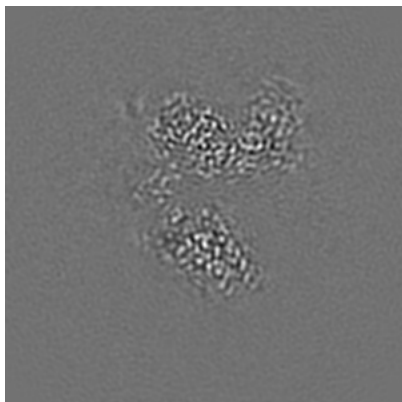
5.3.1 Primary map
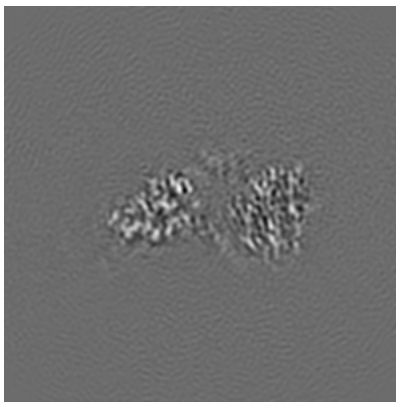
| X Index: 207 | Y Index: 183 | Z Index: 261 |
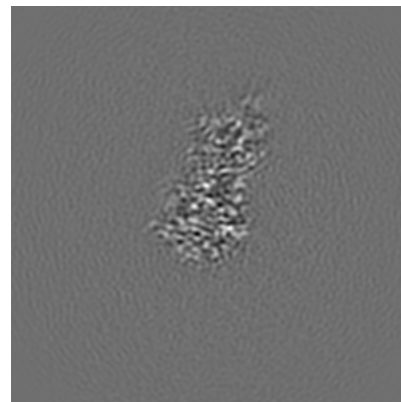
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal standard-deviation projections (False-color) ⓘ

5.4.1 Primary map

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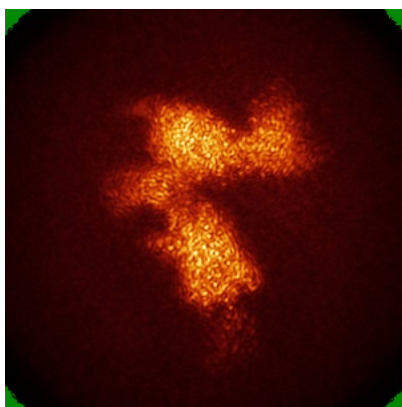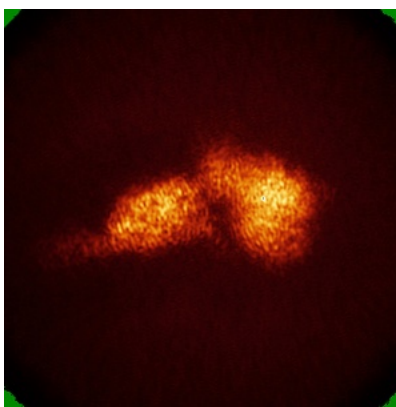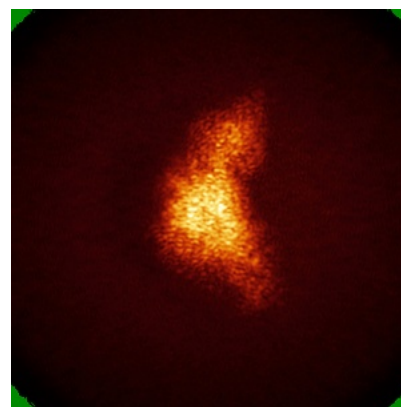
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5   Orthogonal surface views ⓘ

5.5.1   Primary map

X   Y   Z
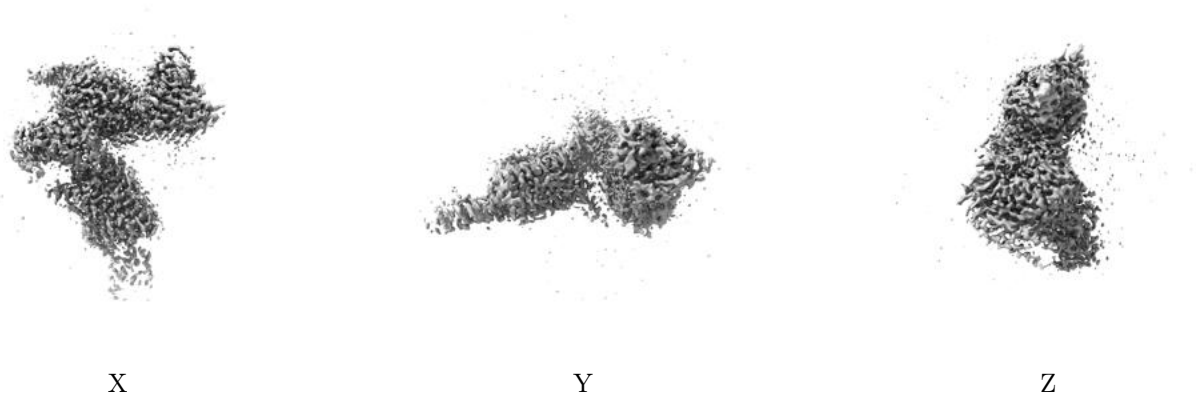
The images above show the 3D surface view of the map at the recommended contour level 4.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.6   Mask visualisation ⓘ

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

6 Map analysis ⓘ

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

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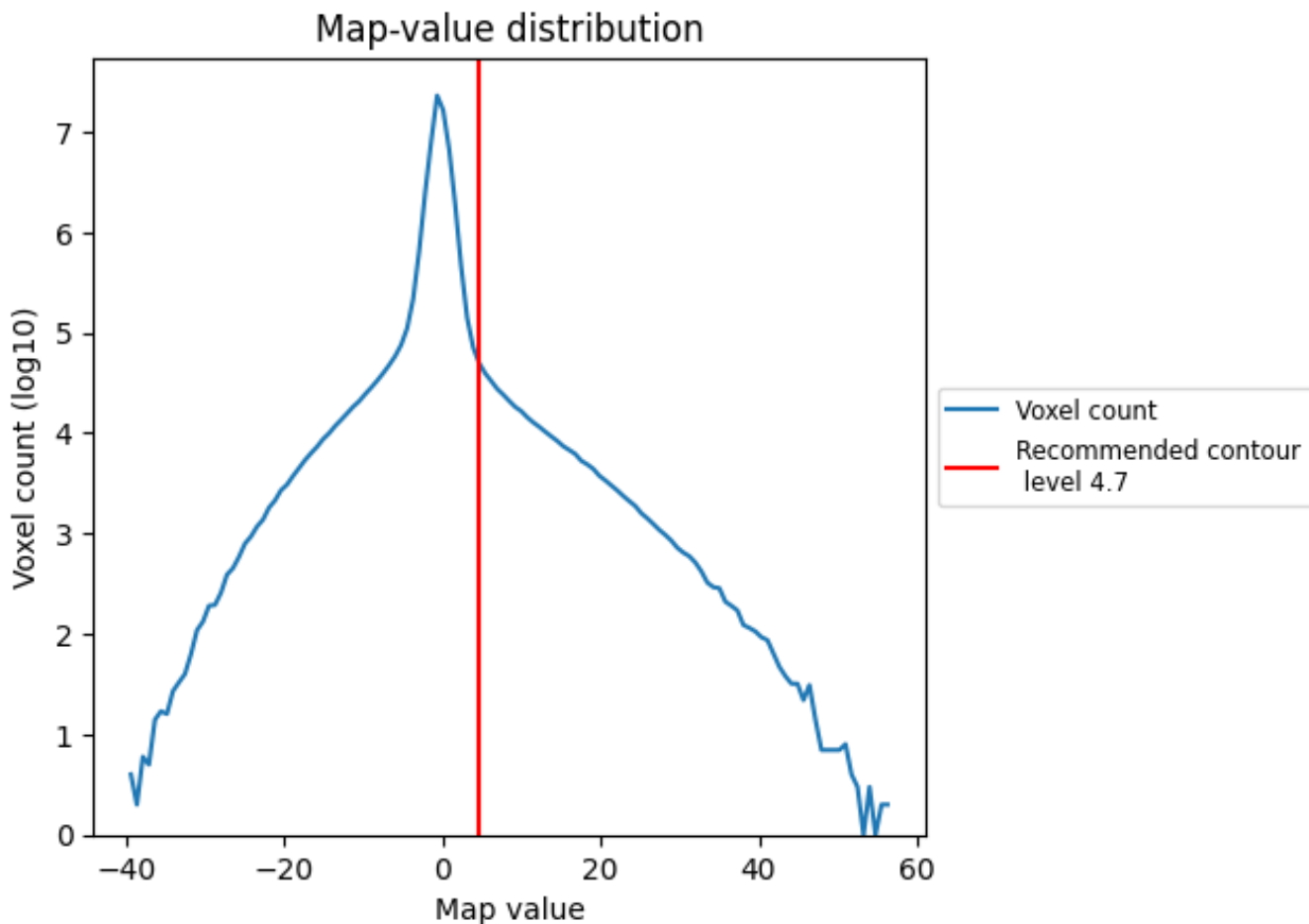
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

6.2   Volume estimate ⓘ
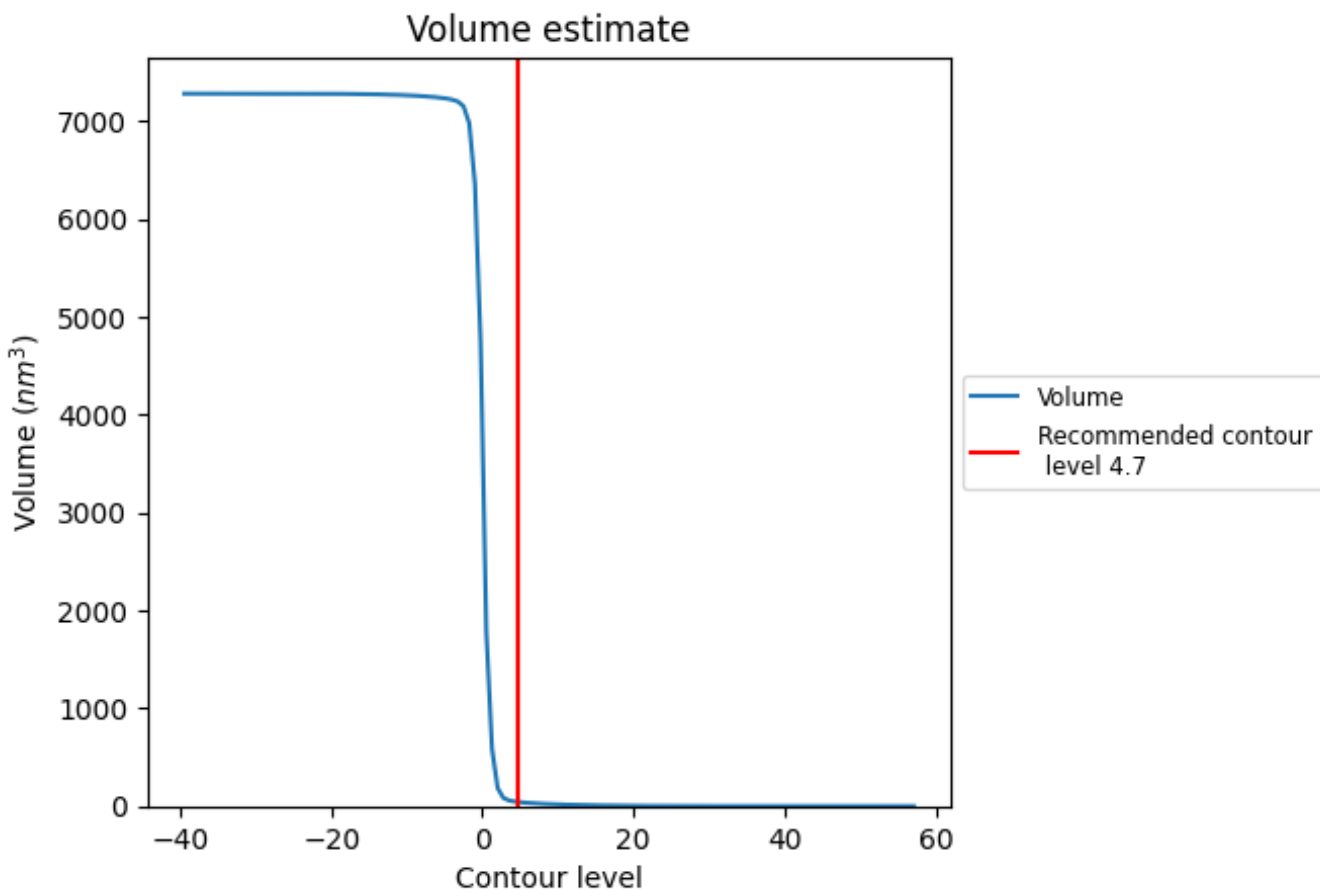
The volume at the recommended contour level is 43 nm^3; this corresponds to an approximate mass of 39 kDa.

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 ⓘ
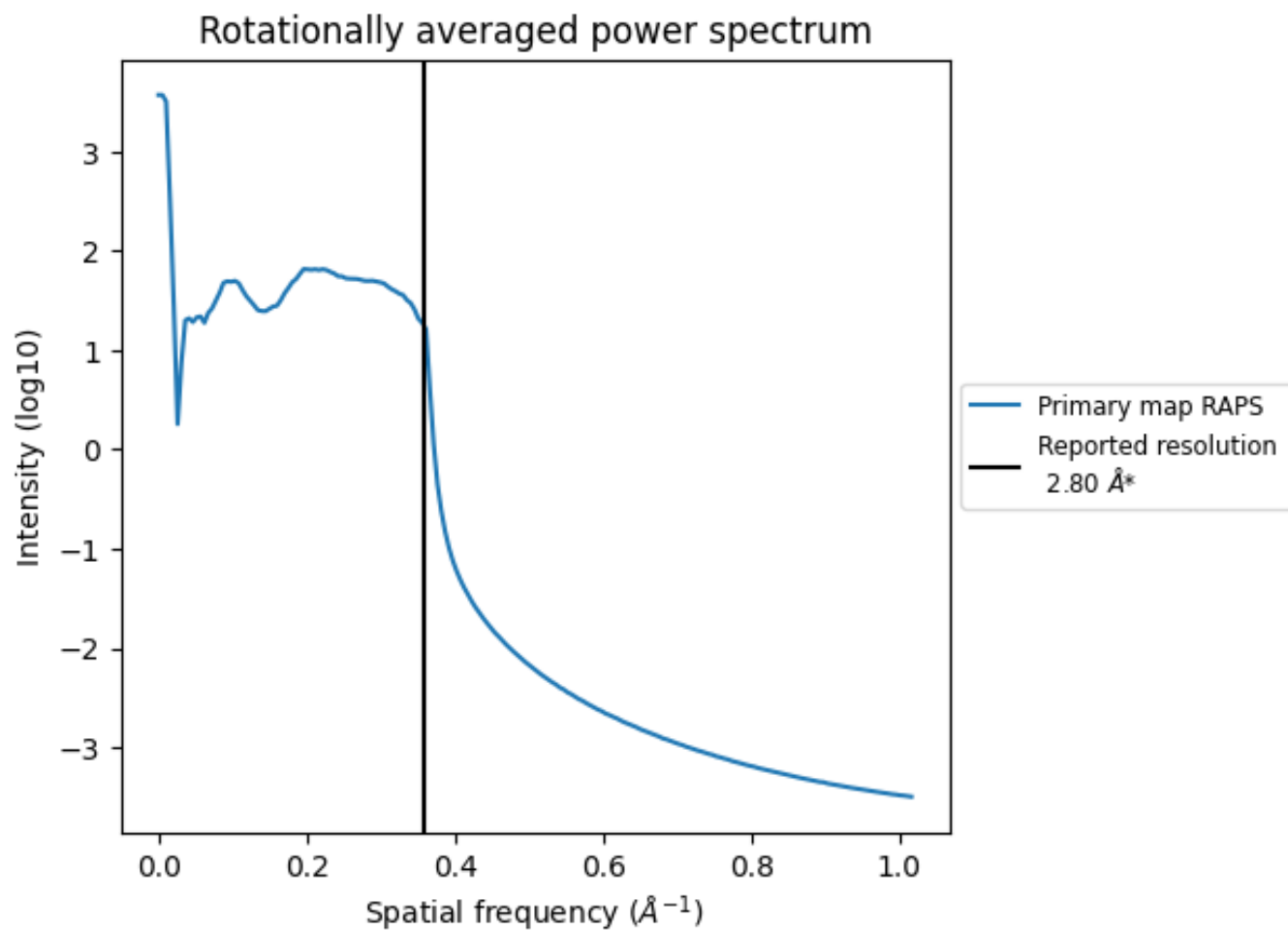
*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

7 Fourier-Shell correlation (i)

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

8   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-61747 and PDB model 9JR3. Per-residue inclusion information can be found in section **??** on page **??**.

8.1   Map-model overlay ⓘ

X	Y	Z
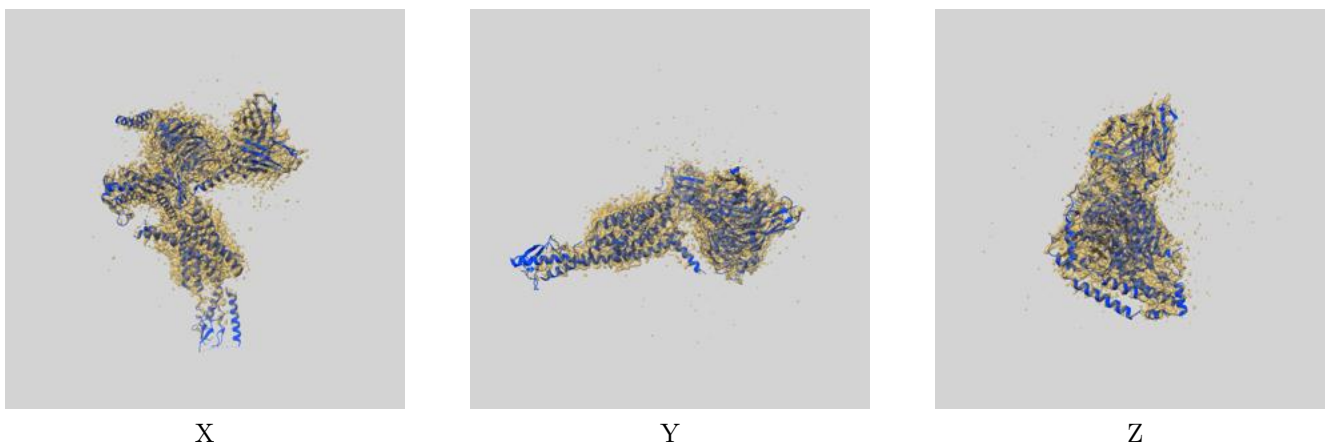
The images above show the 3D surface view of the map at the recommended contour level 4.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

8.2 Q-score mapped to coordinate model ⓘ

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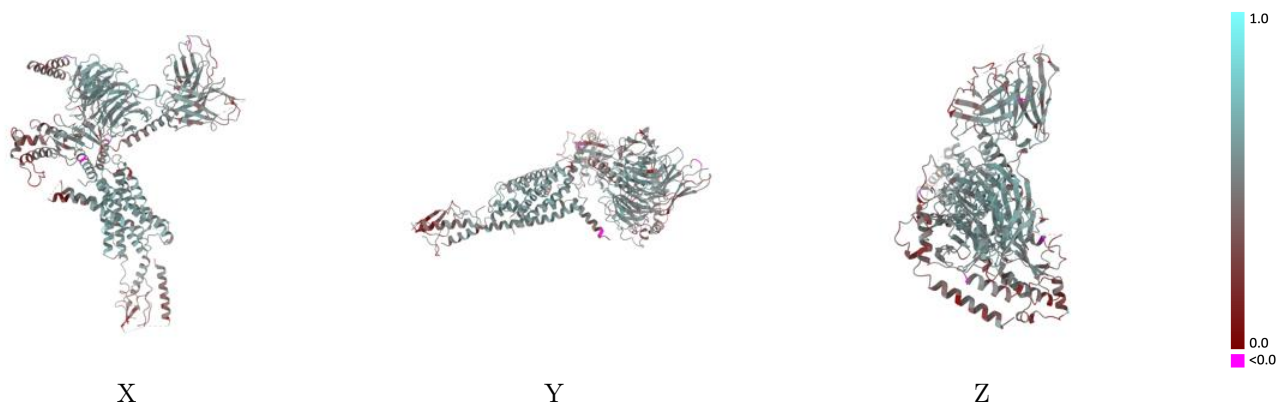
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 Atom inclusion mapped to coordinate model ⓘ

X Y Z
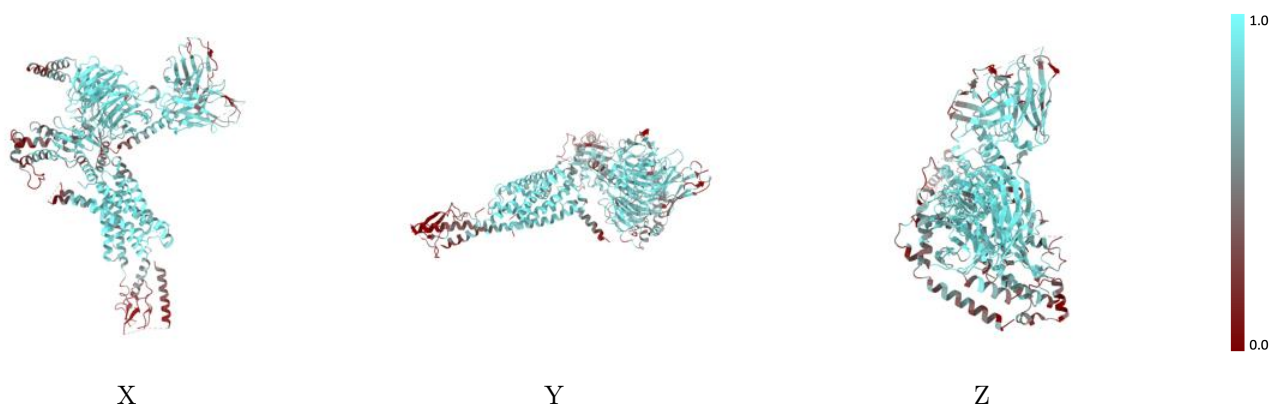
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.7).

8.4　Atom inclusion　ⓘ
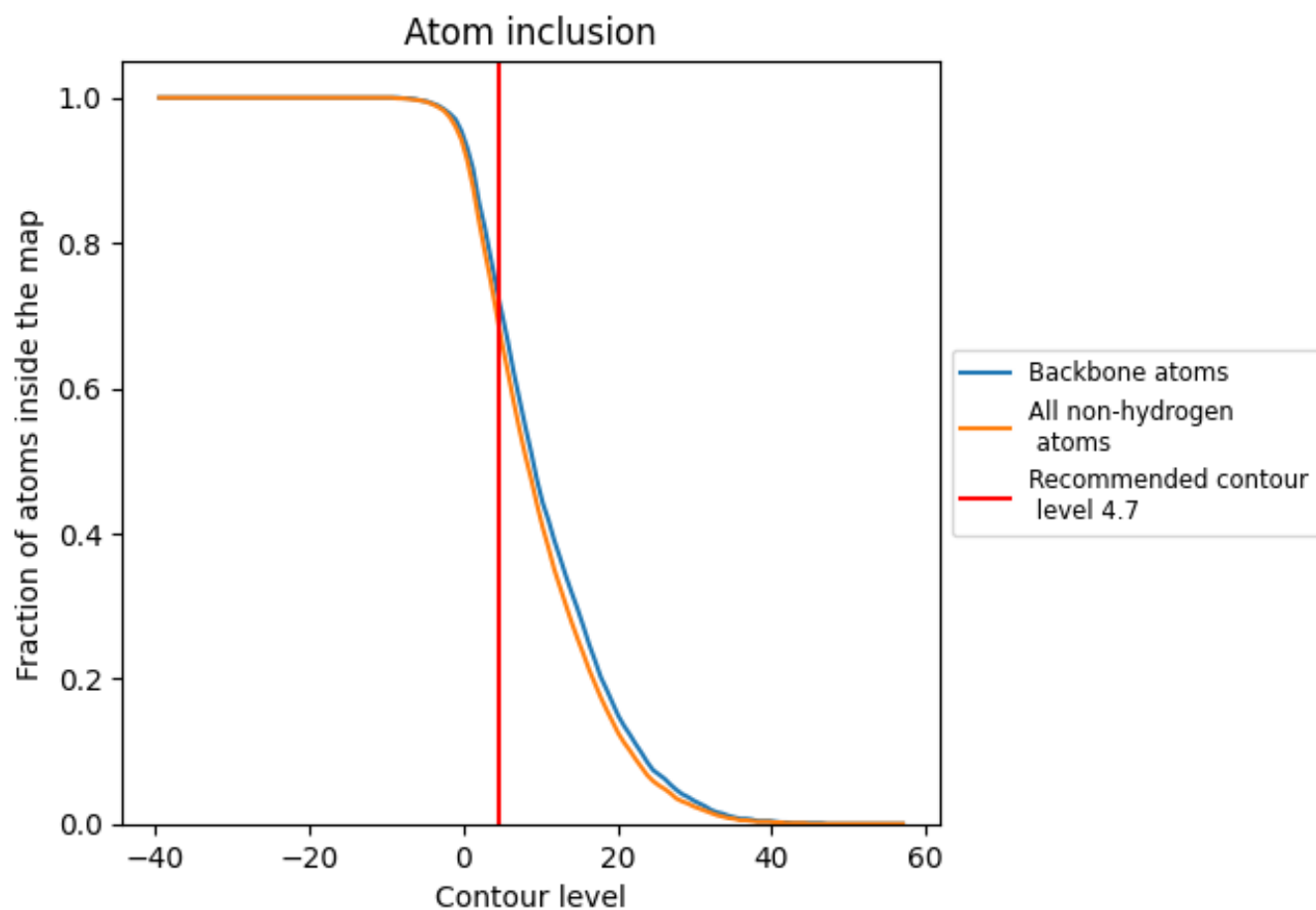
At the recommended contour level, 72% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6810	0.4870
A	0.6030	0.4300
B	0.8020	0.5320
C	0.3210	0.4470
G	0.5070	0.3840
P	0.6230	0.5110
R	0.6550	0.4950
S	0.6920	0.4820

1.0

0.0
<0.0