



wwPDB EM Validation Summary Report ⓘ

May 13, 2024 – 02:31 PM JST

PDB ID : 8JF7
EMDB ID : EMD-36209
Title : Triheteromeric NMDA receptor GluN1-GluN2A-GluN3A in complex with glycine, glutamate, a GluN1-specific Fab, and a GluN2A-specific Fab
Authors : Kou, Z.; Zhu, S.
Deposited on : 2023-05-17
Resolution : 7.73 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.dev92
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) : 2.36.2

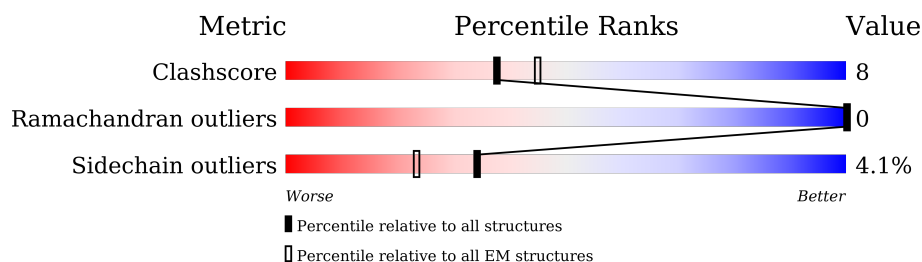
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.73 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)
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	847	 57% 19% 23%
1	C	847	 59% 18% 22%
2	B	1116	 43% 13% 43%
3	D	1228	 30% 45% 12% 13%
4	E	237	 24% 74% 2% 2%
4	G	237	 29% 75% 2% 2%
5	F	217	 15% 81% 2% 2%
5	H	217	 30% 78% 2% 2%

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Mol	Chain	Length	Quality of chain
6	K	212	
7	J	227	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 31416 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 Glutamate receptor ionotropic, NMDA 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	651	Total	C	N	O	S	0	0
			5169	3266	908	967	28		
1	C	657	Total	C	N	O	S	0	0
			5224	3300	919	977	28		

- Molecule 2 is a protein called Glutamate receptor ionotropic, NMDA 2A,Enhanced green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	640	Total	C	N	O	S	0	0
			5063	3235	843	957	28		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	843	LYS	-	linker	UNP Q00959
B	844	SER	-	linker	UNP Q00959
B	845	ARG	-	linker	UNP Q00959
B	846	ALA	-	linker	UNP Q00959
B	847	GLU	-	linker	UNP Q00959
B	848	ALA	-	linker	UNP Q00959
B	849	LYS	-	linker	UNP Q00959
B	850	ARG	-	linker	UNP Q00959
B	851	MET	-	linker	UNP Q00959
B	852	LYS	-	linker	UNP Q00959
B	853	GLY	-	linker	UNP Q00959
B	854	LEU	-	linker	UNP Q00959
B	855	GLU	-	linker	UNP Q00959
B	856	VAL	-	linker	UNP Q00959
B	857	LEU	-	linker	UNP Q00959
B	858	PHE	-	linker	UNP Q00959
B	859	GLN	-	linker	UNP Q00959
B	860	GLY	-	linker	UNP Q00959

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Chain	Residue	Modelled	Actual	Comment	Reference
B	861	PRO	-	linker	UNP Q00959
B	862	ALA	-	linker	UNP Q00959
B	863	ALA	-	linker	UNP Q00959
B	864	ALA	-	linker	UNP Q00959
B	865	ALA	-	linker	UNP Q00959
B	866	VAL	-	linker	UNP Q00959
B	1071	LYS	ALA	conflict	UNP A0A7G8ZY66
B	1109	HIS	-	expression tag	UNP A0A7G8ZY66
B	1110	HIS	-	expression tag	UNP A0A7G8ZY66
B	1111	HIS	-	expression tag	UNP A0A7G8ZY66
B	1112	HIS	-	expression tag	UNP A0A7G8ZY66
B	1113	HIS	-	expression tag	UNP A0A7G8ZY66
B	1114	HIS	-	expression tag	UNP A0A7G8ZY66
B	1115	HIS	-	expression tag	UNP A0A7G8ZY66
B	1116	HIS	-	expression tag	UNP A0A7G8ZY66

- Molecule 3 is a protein called Glutamate receptor ionotropic, NMDA 3A, Enhanced green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	714	Total	C	N	O	S	0	0
			5643	3591	947	1068	37		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	927	GLU	GLY	conflict	UNP Q9R1M7
D	966	LEU	-	linker	UNP Q9R1M7
D	967	GLU	-	linker	UNP Q9R1M7
D	968	VAL	-	linker	UNP Q9R1M7
D	969	LEU	-	linker	UNP Q9R1M7
D	970	PHE	-	linker	UNP Q9R1M7
D	971	GLN	-	linker	UNP Q9R1M7
D	972	GLY	-	linker	UNP Q9R1M7
D	973	PRO	-	linker	UNP Q9R1M7
D	974	ALA	-	linker	UNP Q9R1M7
D	975	ALA	-	linker	UNP Q9R1M7
D	976	ALA	-	linker	UNP Q9R1M7
D	977	ALA	-	linker	UNP Q9R1M7
D	978	VAL	-	linker	UNP Q9R1M7
D	1183	LYS	ALA	conflict	UNP A0A7G8ZY66
D	1221	TRP	-	expression tag	UNP A0A7G8ZY66

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1222	SER	-	expression tag	UNP A0A7G8ZY66
D	1223	HIS	-	expression tag	UNP A0A7G8ZY66
D	1224	PRO	-	expression tag	UNP A0A7G8ZY66
D	1225	GLN	-	expression tag	UNP A0A7G8ZY66
D	1226	PHE	-	expression tag	UNP A0A7G8ZY66
D	1227	GLU	-	expression tag	UNP A0A7G8ZY66
D	1228	LYS	-	expression tag	UNP A0A7G8ZY66

- Molecule 4 is a protein called GluN1-specific antibody fragment light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	237	Total	C	N	O	S	0	0
			1811	1132	303	370	6		
4	G	237	Total	C	N	O	S	0	0
			1811	1132	303	370	6		

- Molecule 5 is a protein called GluN1-specific antibody fragment heavy chain.

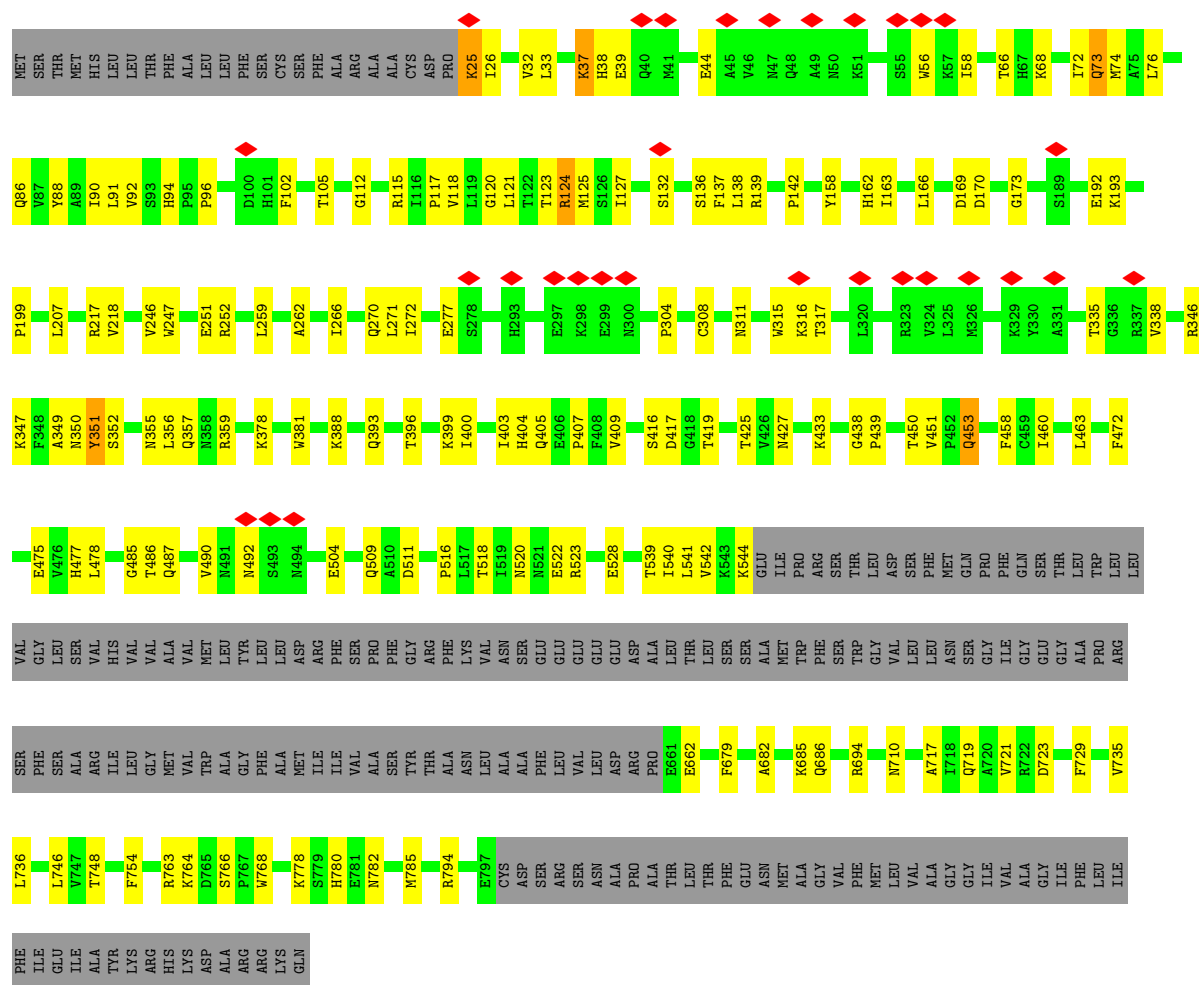
Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	217	Total	C	N	O	S	0	0
			1651	1047	267	331	6		
5	H	217	Total	C	N	O	S	0	0
			1651	1047	267	331	6		

- Molecule 6 is a protein called GluN2A-specific antibody fragment light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	212	Total	C	N	O	S	0	0
			1636	1025	274	332	5		

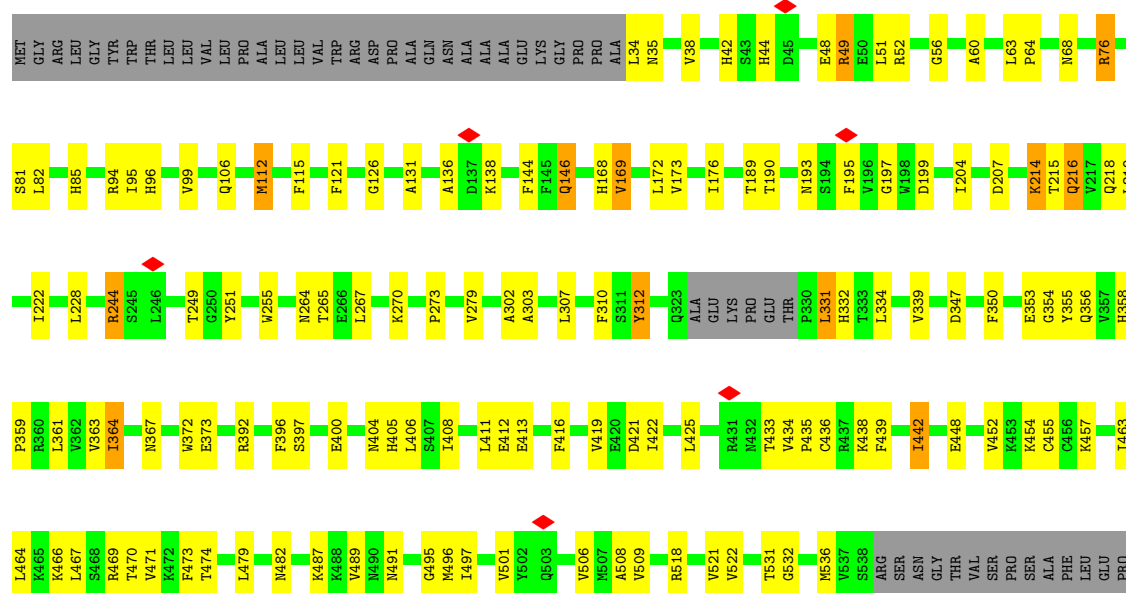
- Molecule 7 is a protein called GluN2A-specific antibody fragment heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	227	Total	C	N	O	S	0	0
			1757	1110	297	345	5		

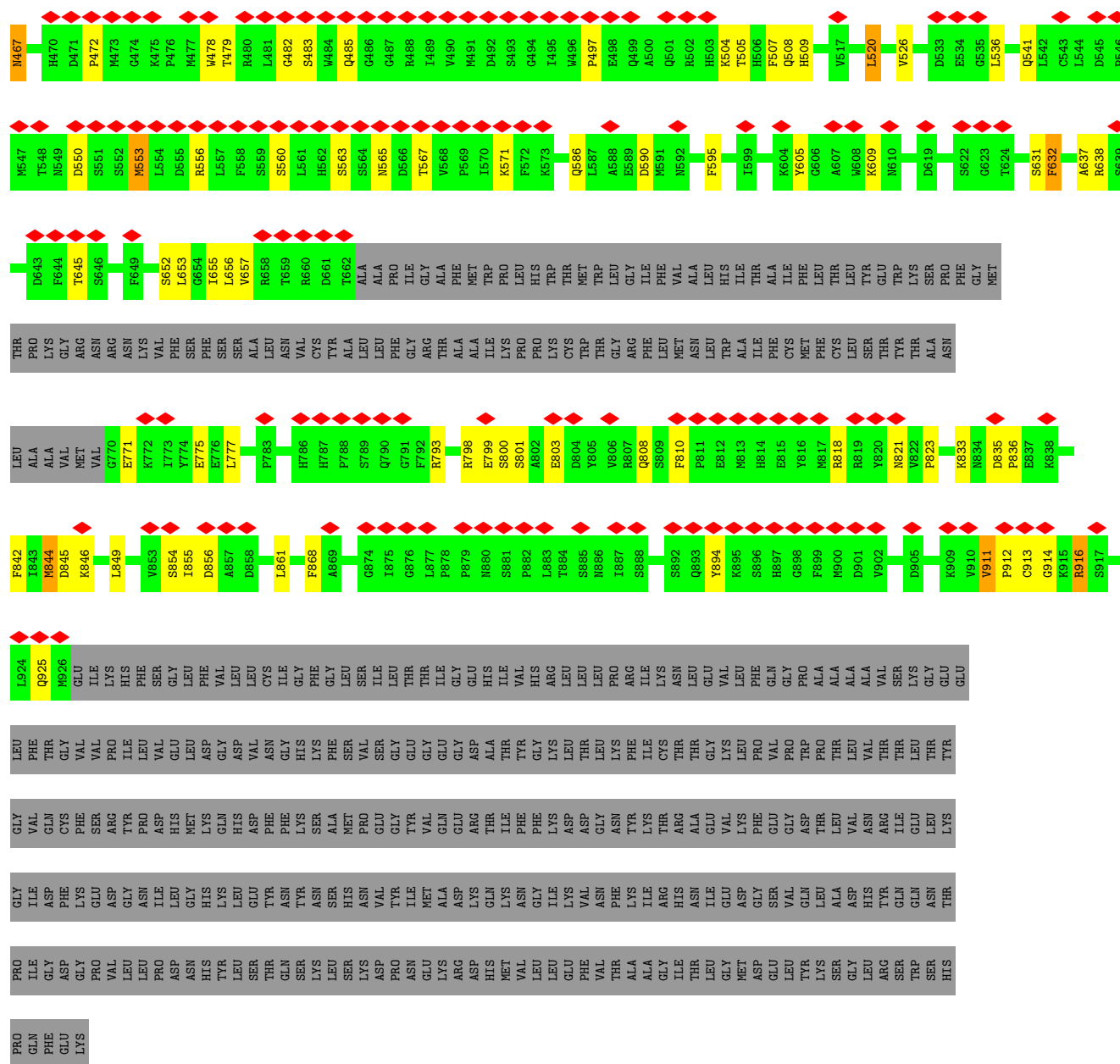


- Molecule 2: Glutamate receptor ionotropic, NMDA 2A,Enhanced green fluorescent protein

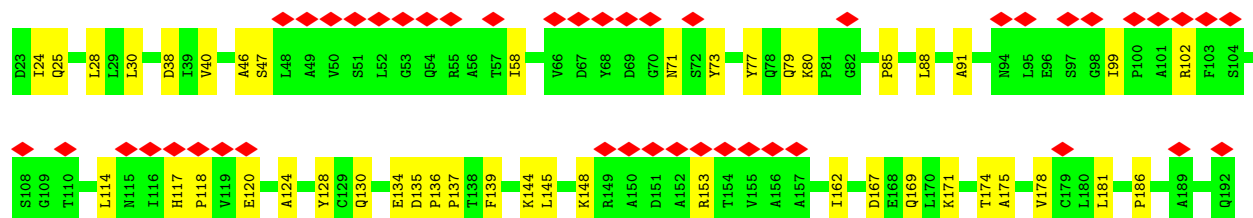
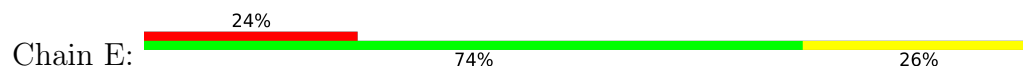
Chain B: 43% 13% 43%

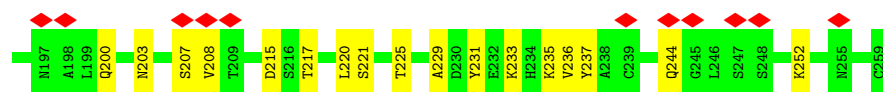




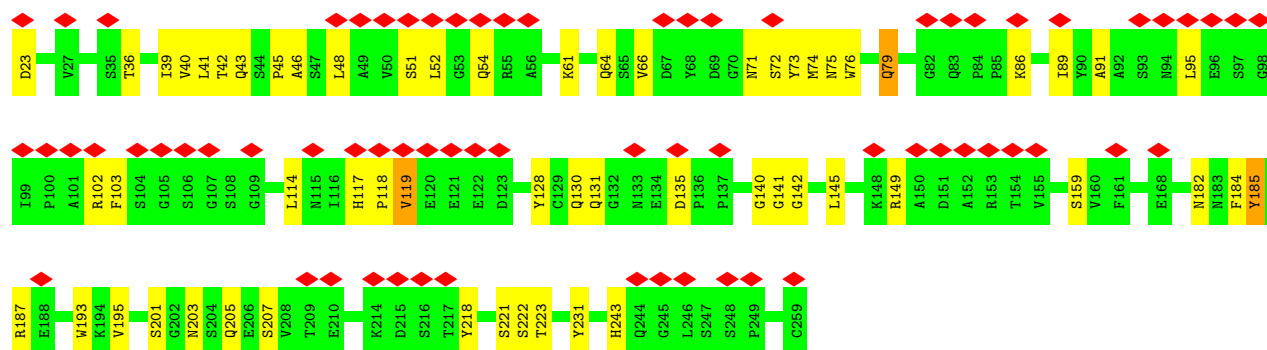
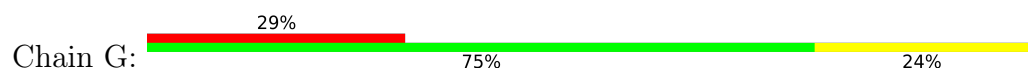


• Molecule 4: GluN1-specific antibody fragment light chain

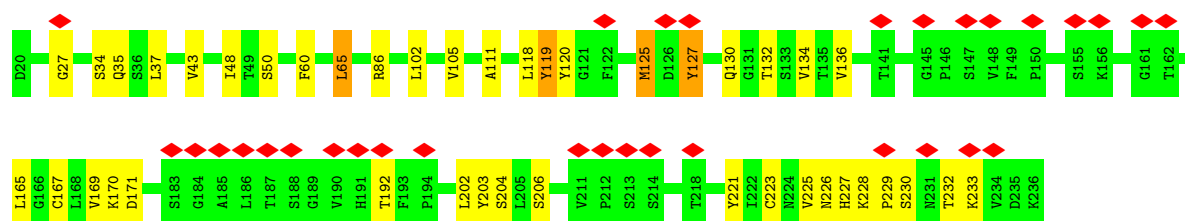
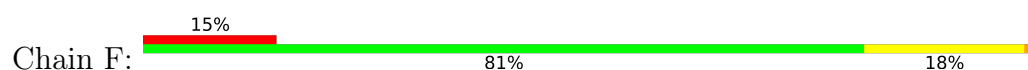




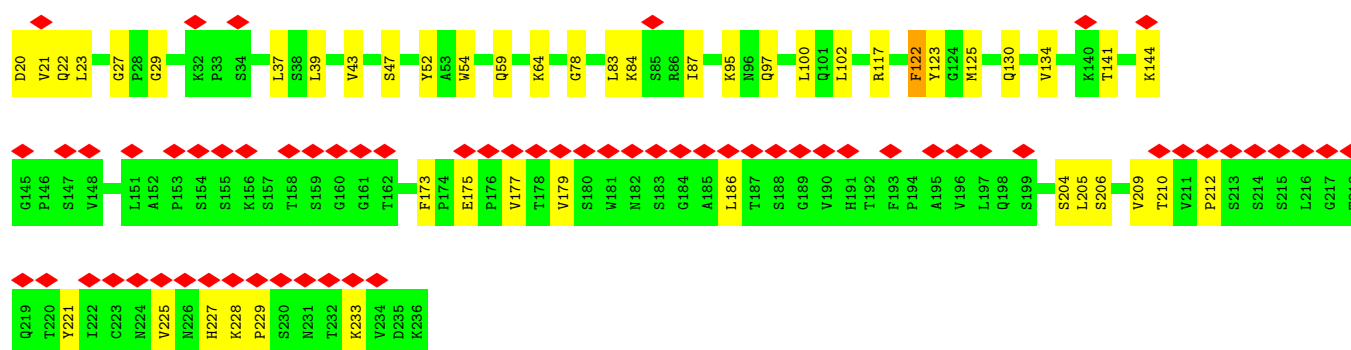
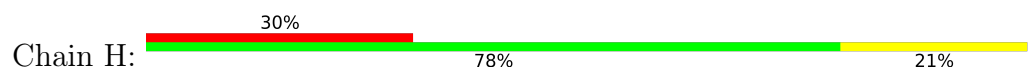
• Molecule 4: GluN1-specific antibody fragment light chain



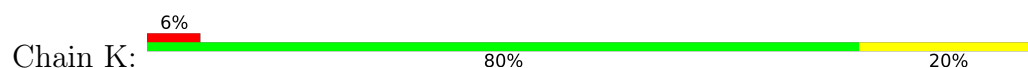
• Molecule 5: GluN1-specific antibody fragment heavy chain

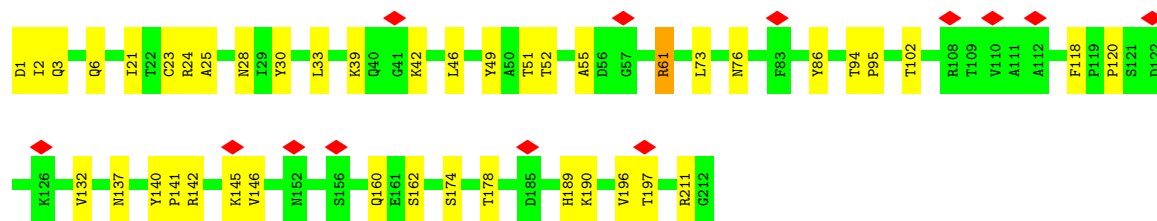


• Molecule 5: GluN1-specific antibody fragment heavy chain

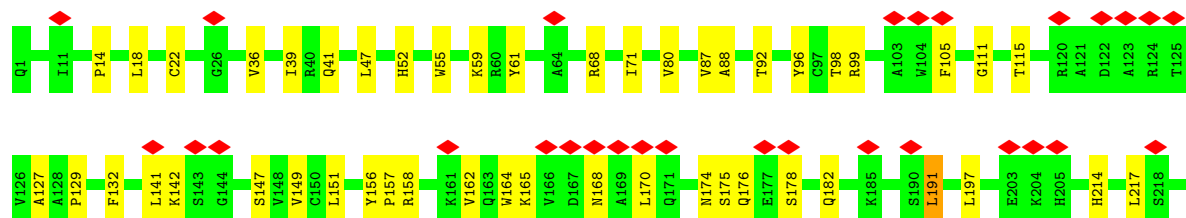
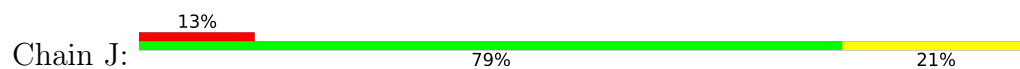


• Molecule 6: GluN2A-specific antibody fragment light chain





• Molecule 7: GluN2A-specific antibody fragment heavy chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	162395	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-16 (4k x 4k)	Depositor
Maximum map value	0.036	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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	A	0.24	0/5282	0.40	0/7152
1	C	0.24	0/5337	0.39	0/7223
2	B	0.24	0/5176	0.40	0/7021
3	D	0.24	0/5779	0.40	0/7853
4	E	0.24	0/1852	0.44	0/2520
4	G	0.24	0/1852	0.43	0/2520
5	F	0.24	0/1695	0.45	0/2314
5	H	0.24	0/1695	0.45	0/2314
6	K	0.24	0/1673	0.42	0/2271
7	J	0.24	0/1799	0.45	0/2446
All	All	0.24	0/32140	0.41	0/43634

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5169	0	5124	89	0
1	C	5224	0	5186	90	0
2	B	5063	0	4995	91	0
3	D	5643	0	5515	85	0
4	E	1811	0	1739	38	0
4	G	1811	0	1737	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1651	0	1596	25	0
5	H	1651	0	1596	29	0
6	K	1636	0	1576	24	0
7	J	1757	0	1725	27	0
All	All	31416	0	30789	502	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 8.

The worst 5 of 502 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:C:490:VAL:HG13	1:C:492:ASN:H	1.59	0.67
2:B:172:LEU:HA	2:B:228:LEU:HB2	1.76	0.66
2:B:364:ILE:HG13	2:B:372:TRP:HB3	1.76	0.66
1:A:459:CYS:HB2	1:A:514:VAL:HB	1.77	0.65
1:A:355:ASN:H	1:A:363:GLN:HA	1.62	0.64

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	647/847 (76%)	618 (96%)	29 (4%)	0	100	100
1	C	653/847 (77%)	637 (98%)	16 (2%)	0	100	100
2	B	634/1116 (57%)	613 (97%)	21 (3%)	0	100	100
3	D	706/1228 (58%)	695 (98%)	11 (2%)	0	100	100
4	E	235/237 (99%)	228 (97%)	7 (3%)	0	100	100
4	G	235/237 (99%)	229 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
5	H	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
6	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
7	J	225/227 (99%)	209 (93%)	16 (7%)	0	100	100
All	All	3975/5385 (74%)	3847 (97%)	128 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	568/730 (78%)	537 (94%)	31 (6%)	21	47
1	C	574/730 (79%)	555 (97%)	19 (3%)	38	61
2	B	565/967 (58%)	539 (95%)	26 (5%)	27	52
3	D	639/1068 (60%)	610 (96%)	29 (4%)	27	52
4	E	202/202 (100%)	197 (98%)	5 (2%)	47	68
4	G	202/202 (100%)	195 (96%)	7 (4%)	36	59
5	F	189/189 (100%)	180 (95%)	9 (5%)	25	51
5	H	189/189 (100%)	181 (96%)	8 (4%)	30	54
6	K	185/185 (100%)	182 (98%)	3 (2%)	62	79
7	J	197/197 (100%)	189 (96%)	8 (4%)	30	55
All	All	3510/4659 (75%)	3365 (96%)	145 (4%)	34	55

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	127	TYR
7	J	191	LEU
4	G	74	MET
5	H	97	GLN

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Mol	Chain	Res	Type
2	B	355	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	897	HIS
4	G	243	HIS
4	E	25	GLN
5	F	226	ASN
6	K	40	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.

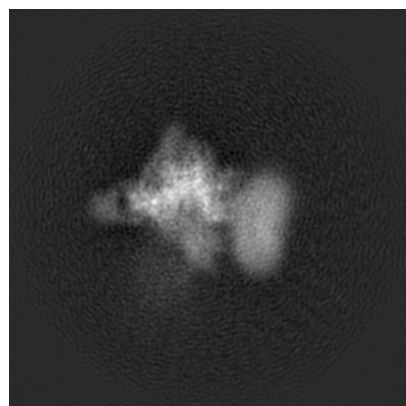
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36209. These allow visual inspection of the internal detail of the map and identification of artifacts.

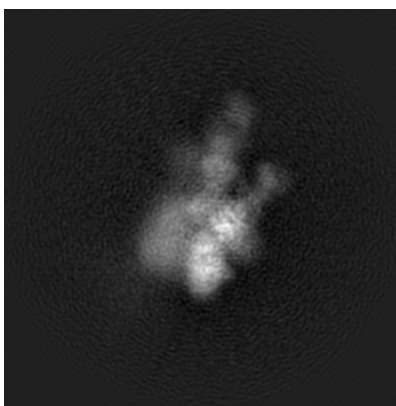
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

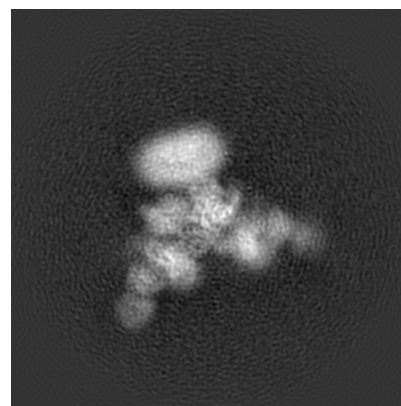
6.1.1 Primary map



X

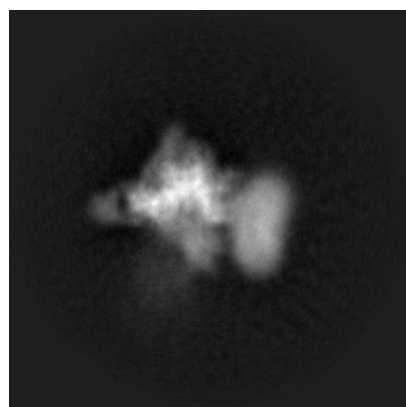


Y

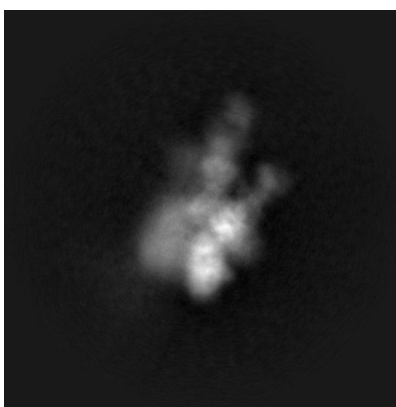


Z

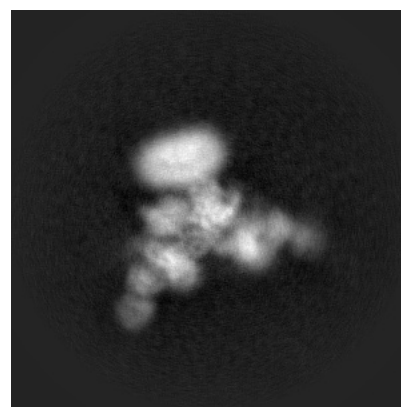
6.1.2 Raw map



X



Y

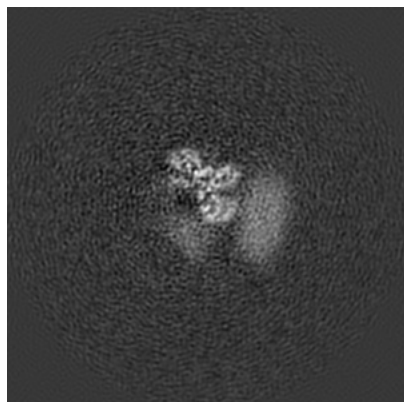


Z

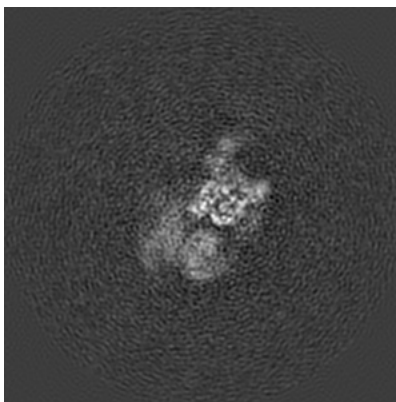
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

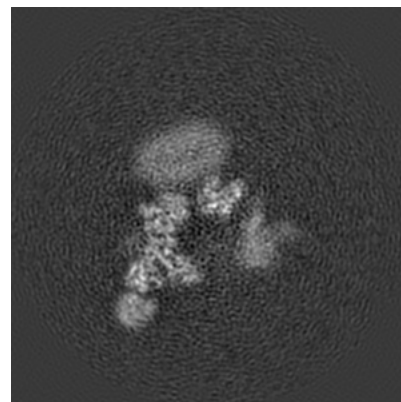
6.2.1 Primary map



X Index: 200

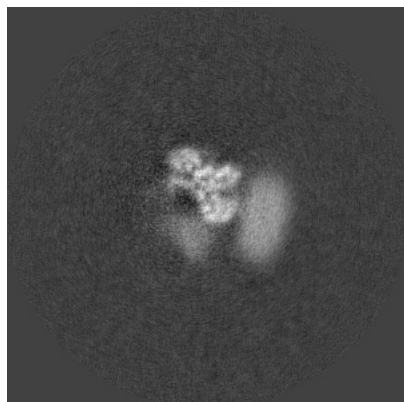


Y Index: 200

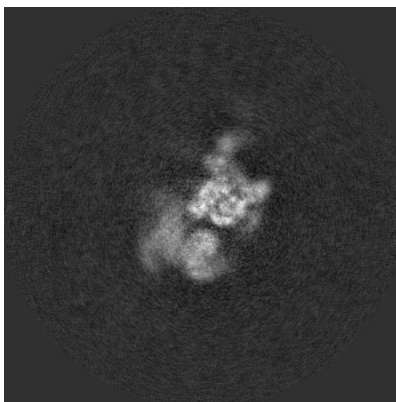


Z Index: 200

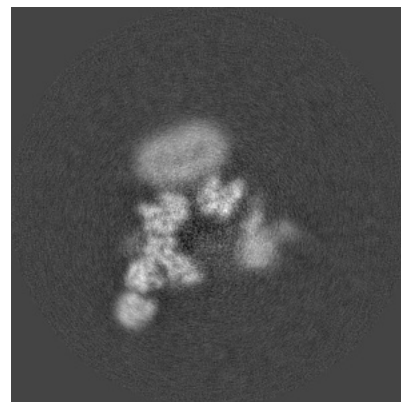
6.2.2 Raw map



X Index: 200



Y Index: 200

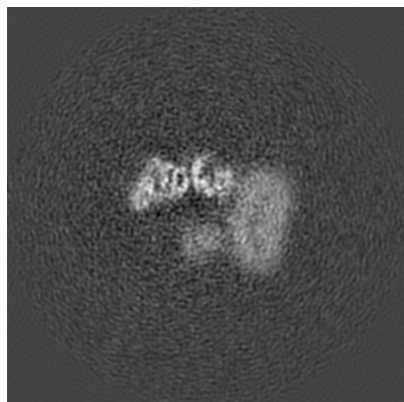


Z Index: 200

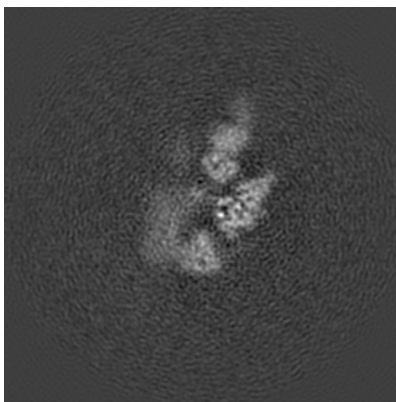
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

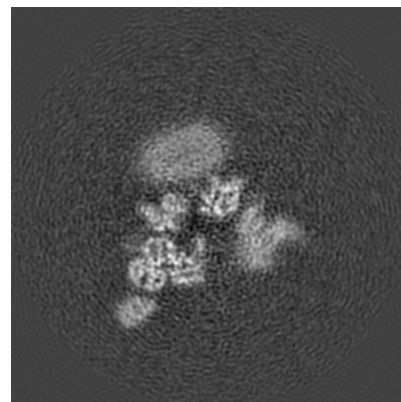
6.3.1 Primary map



X Index: 183

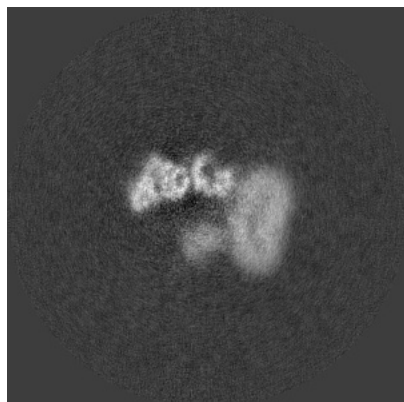


Y Index: 189

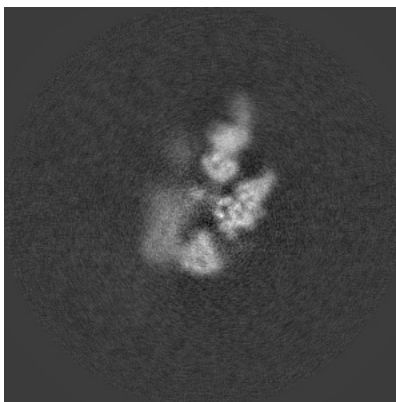


Z Index: 206

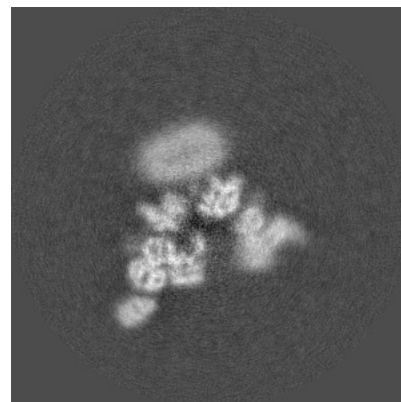
6.3.2 Raw map



X Index: 182



Y Index: 189

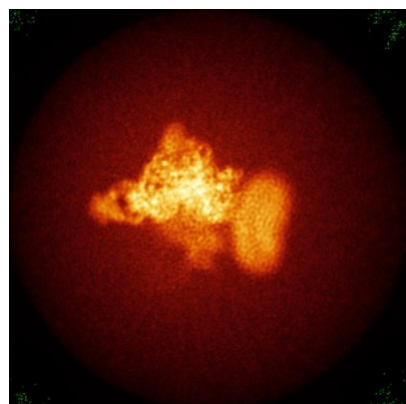


Z Index: 207

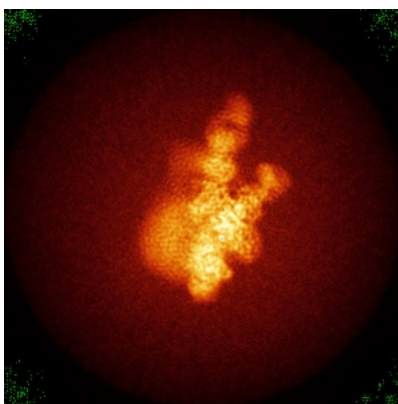
The images above show the largest variance slices of the map in three orthogonal directions.

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

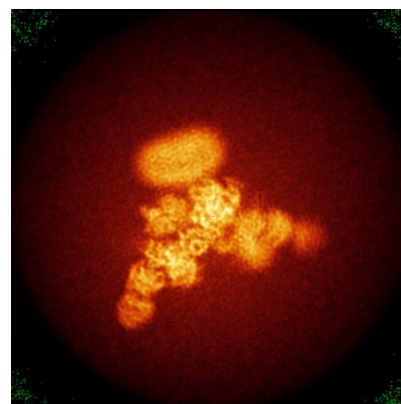
6.4.1 Primary map



X



Y

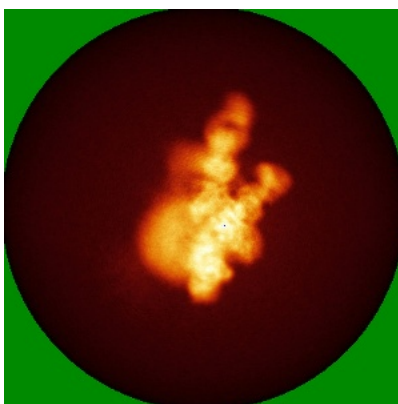


Z

6.4.2 Raw map



X



Y

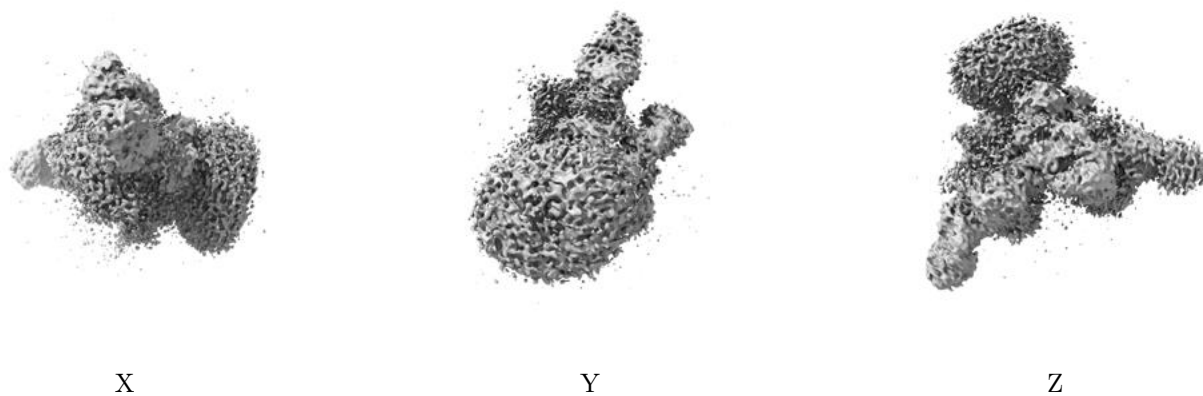


Z

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 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

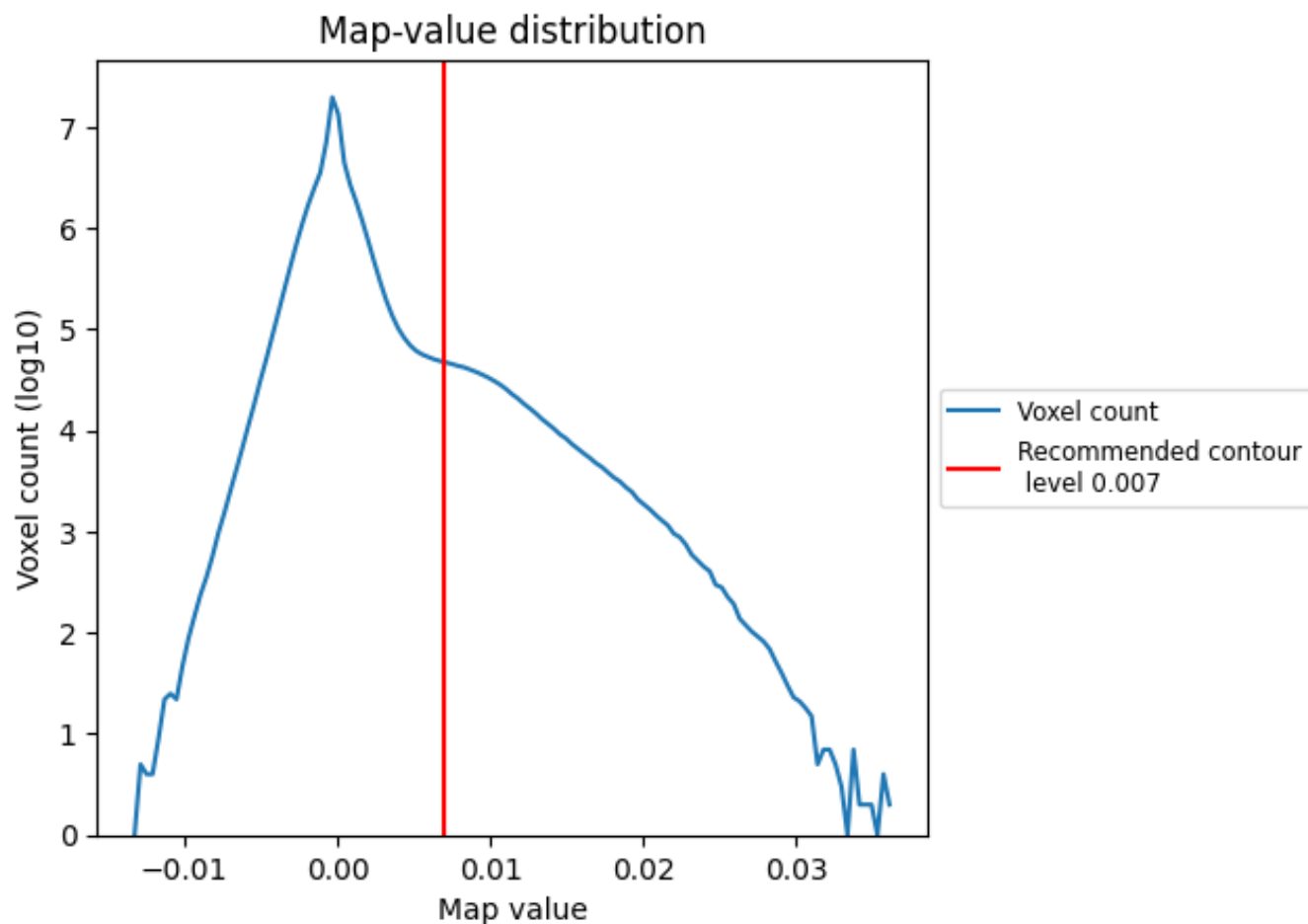
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

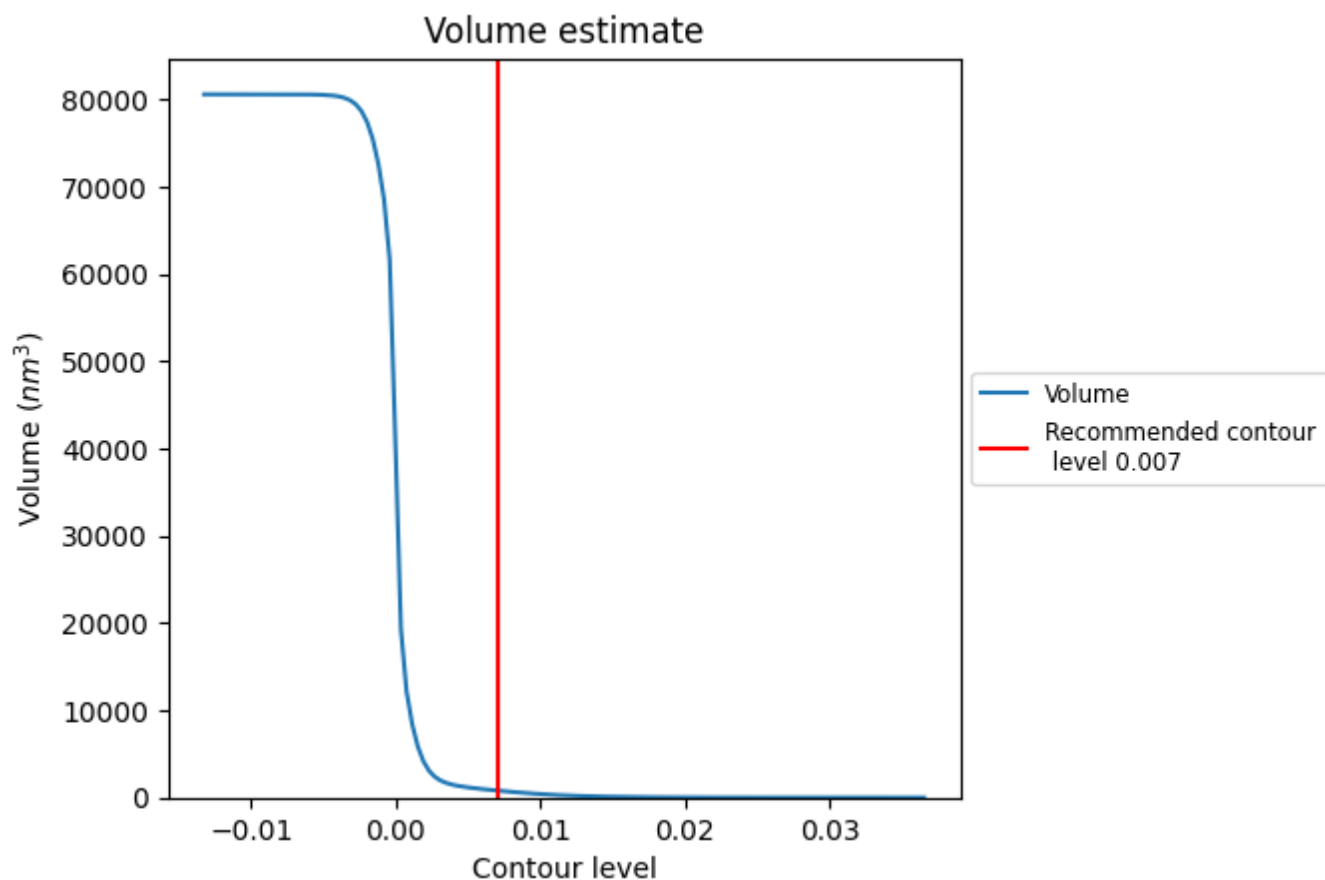
This section contains the results of statistical analysis of the map.

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.

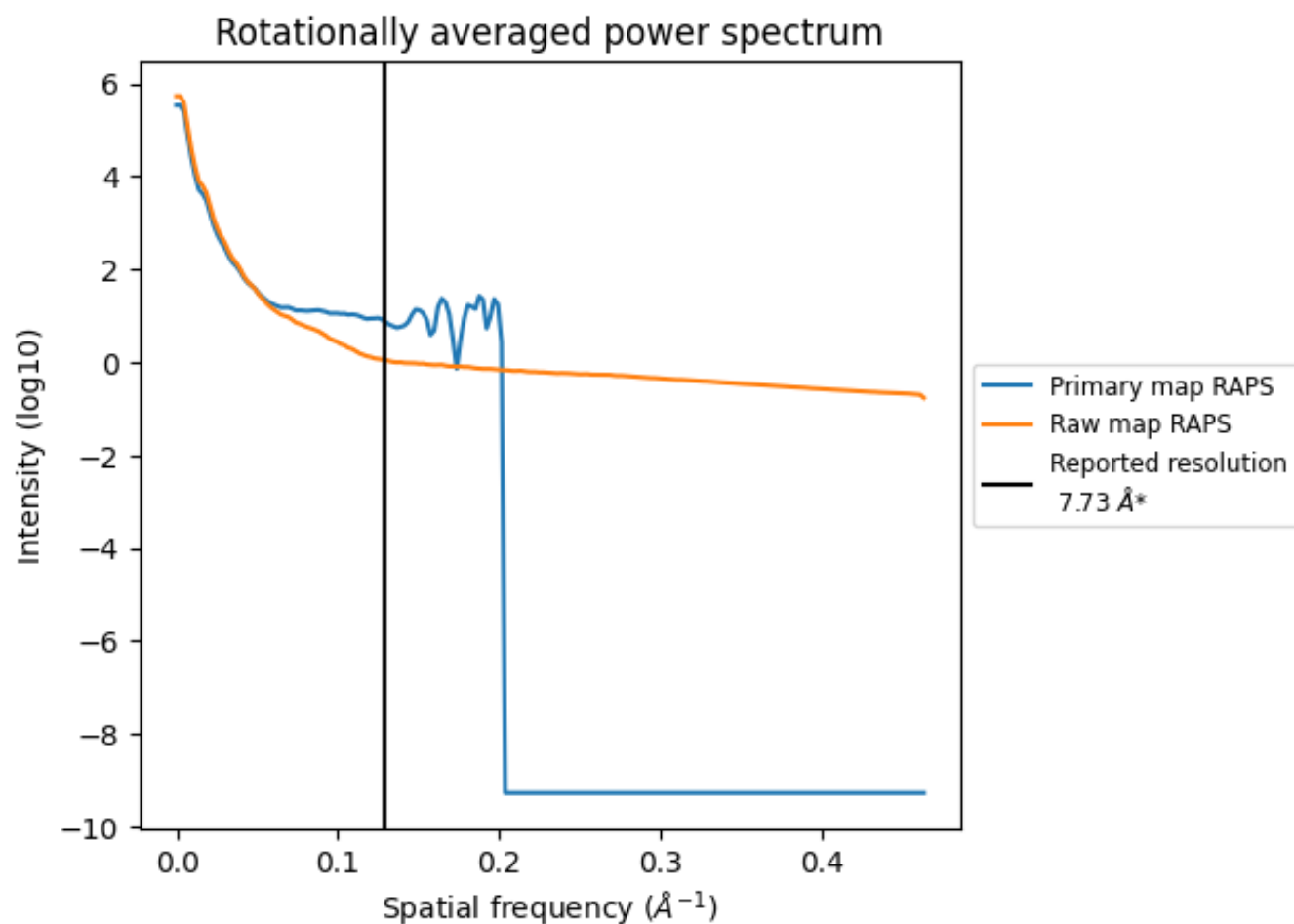
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 802 nm³; this corresponds to an approximate mass of 725 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 ⓘ

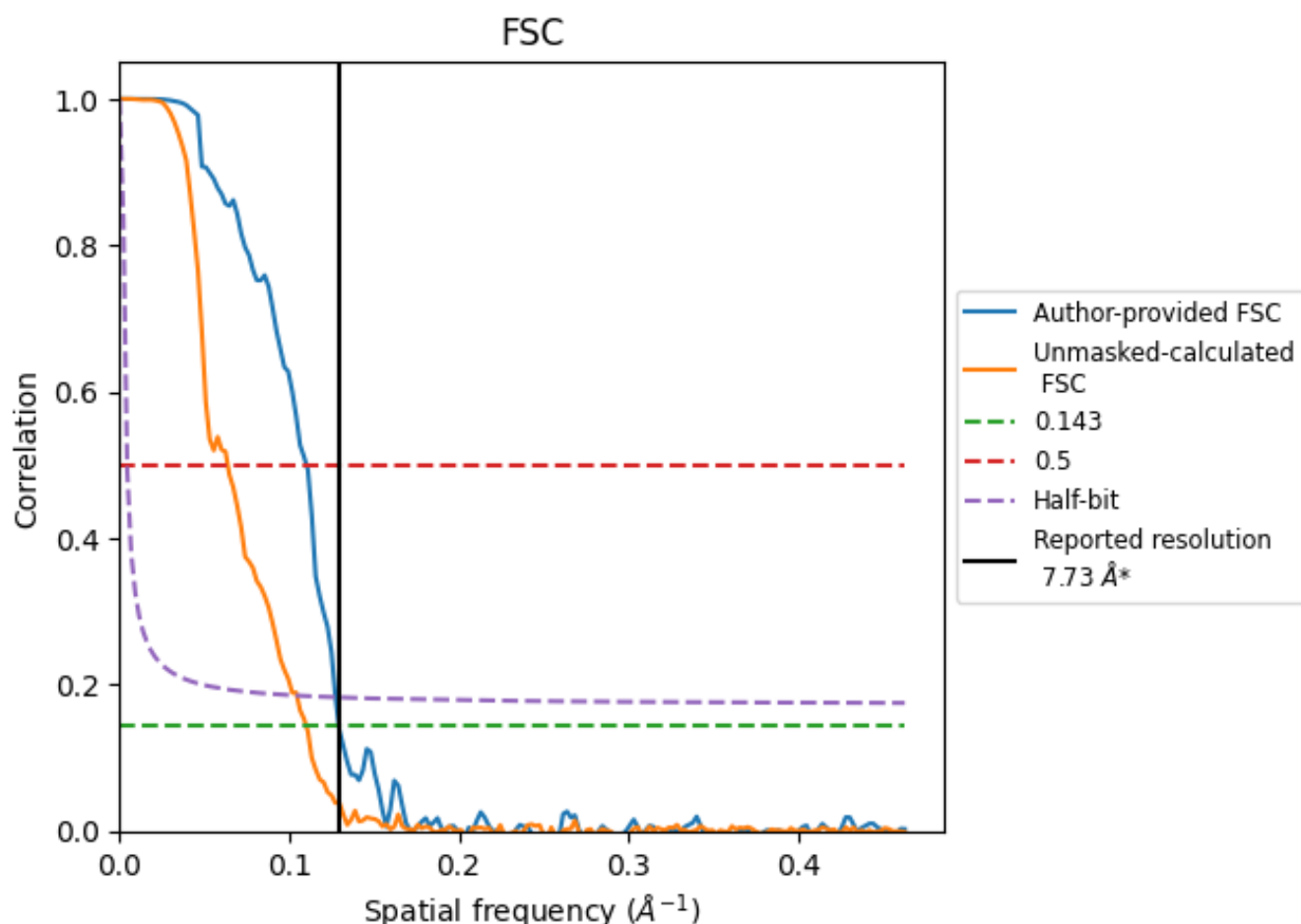


*Reported resolution corresponds to spatial frequency of 0.129 Å⁻¹

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 0.129 Å⁻¹

8.2 Resolution estimates [i](#)

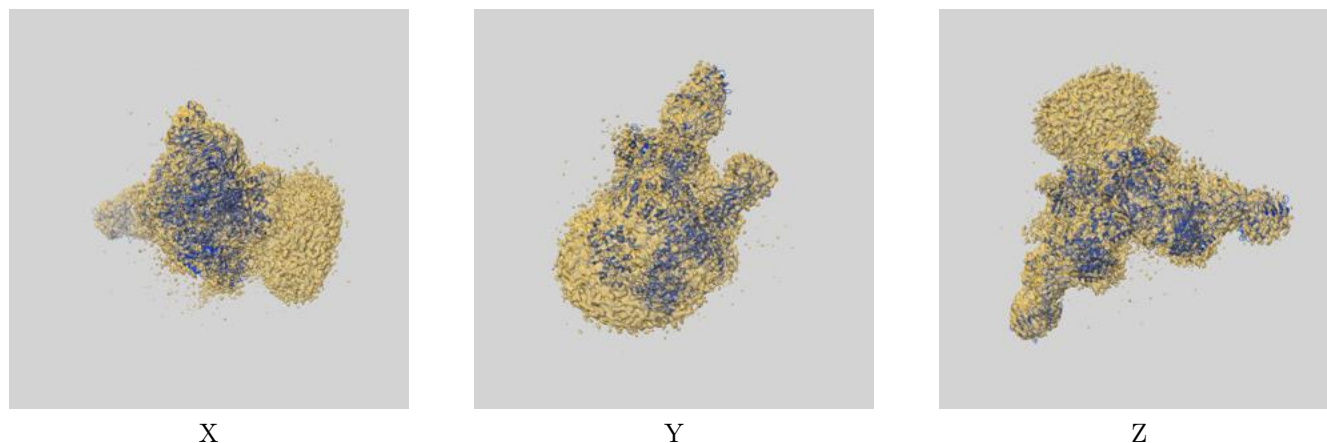
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.73	-	-
Author-provided FSC curve	7.73	9.07	7.85
Unmasked-calculated*	9.08	15.67	9.56

*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 9.08 differs from the reported value 7.73 by more than 10 %

9 Map-model fit [i](#)

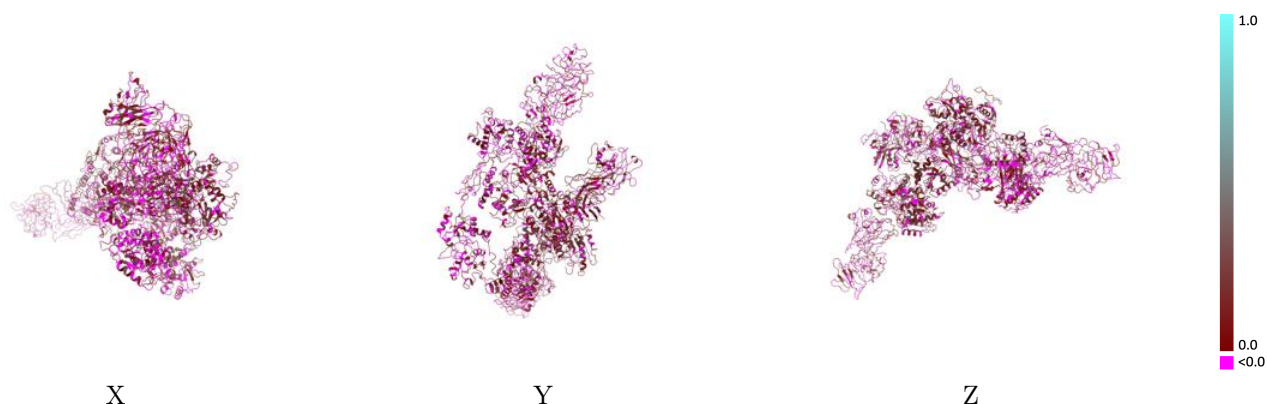
This section contains information regarding the fit between EMDB map EMD-36209 and PDB model 8JF7. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



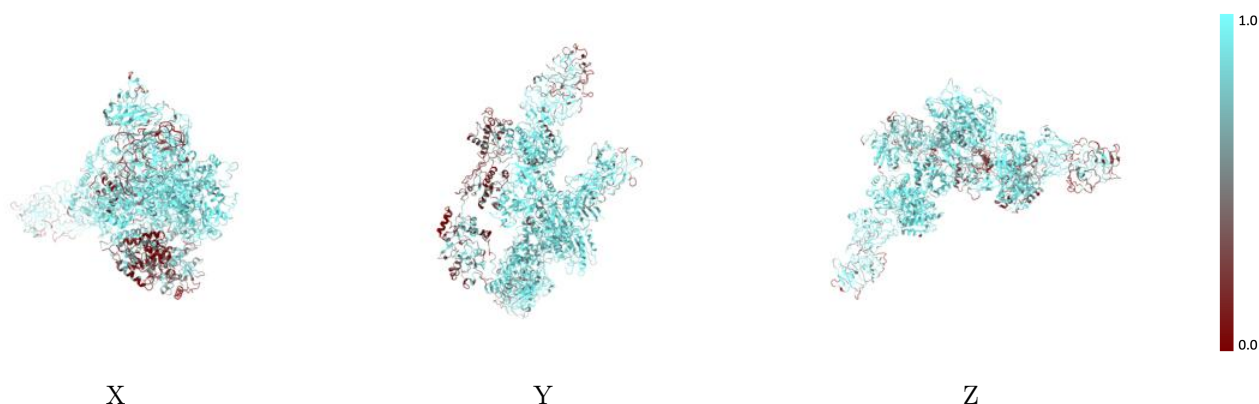
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



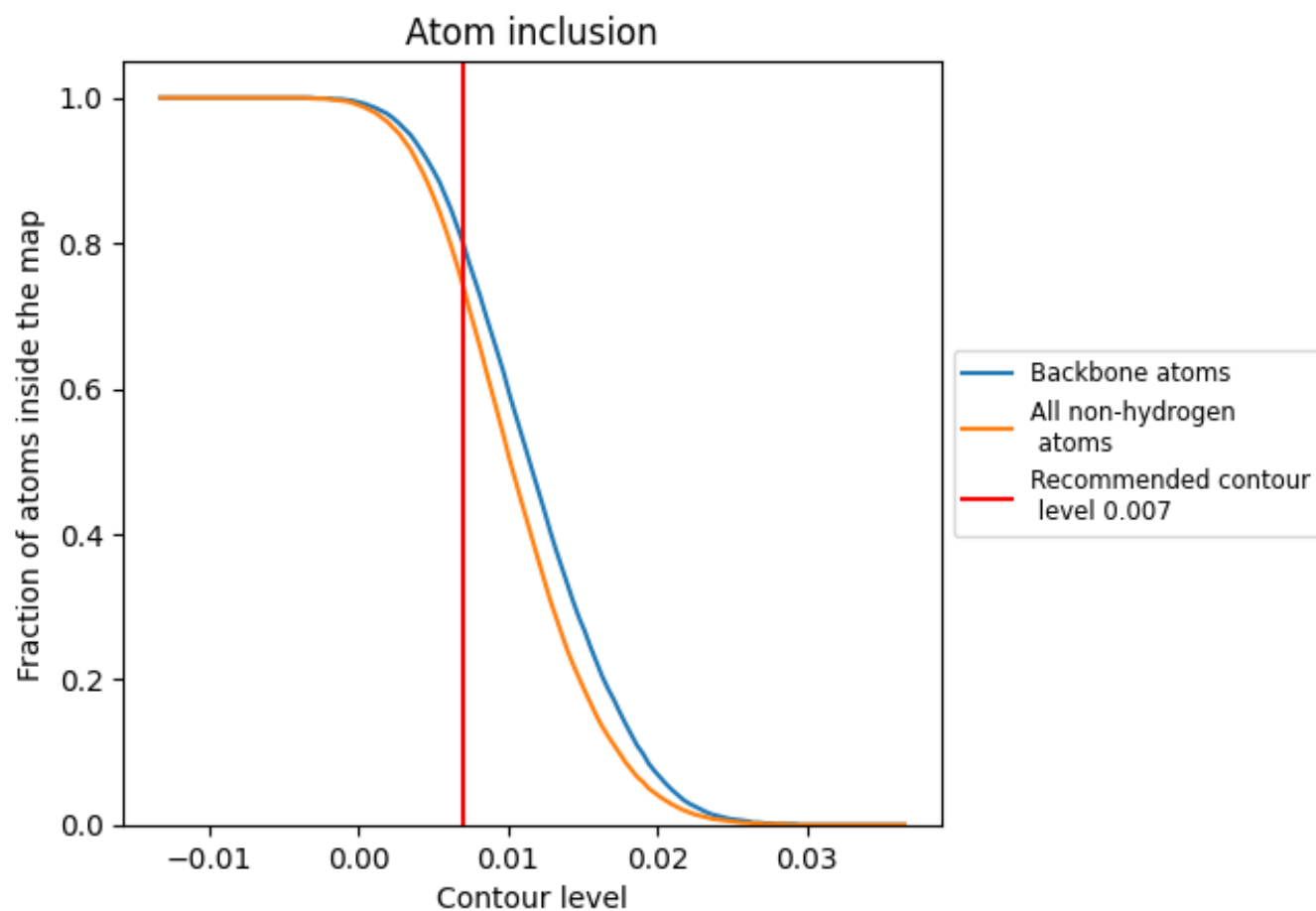
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7400	<div></div> 0.0940
A	<div></div> 0.8470	<div></div> 0.1050
B	<div></div> 0.8680	<div></div> 0.1470
C	<div></div> 0.8630	<div></div> 0.1070
D	<div></div> 0.4290	<div></div> 0.0520
E	<div></div> 0.7190	<div></div> 0.0480
F	<div></div> 0.7640	<div></div> 0.0940
G	<div></div> 0.6500	<div></div> 0.0500
H	<div></div> 0.6690	<div></div> 0.0510
J	<div></div> 0.7570	<div></div> 0.1140
K	<div></div> 0.8340	<div></div> 0.1150

1.0

0.0

<0.0