



wwPDB EM Validation Summary Report ⓘ

Nov 16, 2022 – 06:21 AM EST

PDB ID : 7KS0
EMDB ID : EMD-23014
Title : GluK2/K5 with 6-Cyano-7-nitroquinoxaline-2,3-dione (CNQX)
Authors : Khanra, N.; Brown, P.M.G.E.; Perozzo, A.M.; Bowie, D.; Meyerson, J.R.
Deposited on : 2020-11-20
Resolution : 5.30 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.dev43
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) : 2.31.2

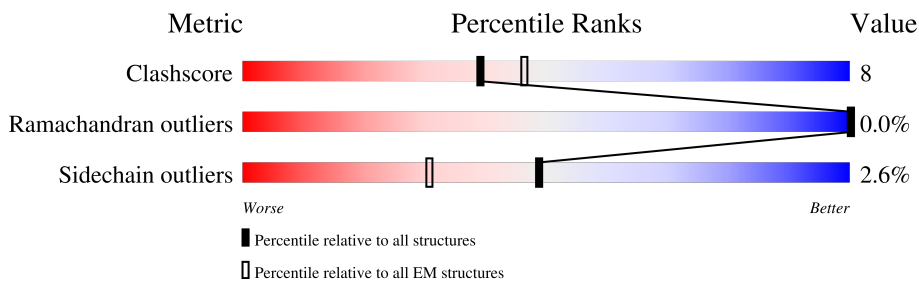
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.30 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	1101	 6% 58% 9% 33%
1	C	1101	 6% 56% 11% 33%
2	B	942	 6% 68% 9% 22%
2	D	942	 6% 67% 11% 22%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 19440 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, kainate 5, Green fluorescent protein chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	741	4844	3005	881	940	18	0	0
1	C	741	4844	3005	881	940	18	0	0

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	VAL	CYS	conflict	UNP Q63273
A	578	SER	CYS	conflict	UNP Q63273
A	619	ILE	CYS	conflict	UNP Q63273
A	813	ALA	CYS	conflict	UNP Q63273
A	828	TYR	-	linker	UNP Q63273
A	829	LYS	-	linker	UNP Q63273
A	830	SER	-	linker	UNP Q63273
A	831	ARG	-	linker	UNP Q63273
A	832	ALA	-	linker	UNP Q63273
A	833	GLU	-	linker	UNP Q63273
A	834	ALA	-	linker	UNP Q63273
A	835	LYS	-	linker	UNP Q63273
A	836	ARG	-	linker	UNP Q63273
A	837	MET	-	linker	UNP Q63273
A	838	LYS	-	linker	UNP Q63273
A	839	GLY	-	linker	UNP Q63273
A	840	LEU	-	linker	UNP Q63273
A	841	VAL	-	linker	UNP Q63273
A	842	PRO	-	linker	UNP Q63273
A	843	ARG	-	linker	UNP Q63273
A	844	GLY	-	linker	UNP Q63273
A	845	SER	-	linker	UNP Q63273
A	846	ALA	-	linker	UNP Q63273
A	847	ALA	-	linker	UNP Q63273
A	848	ALA	-	linker	UNP Q63273

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Chain	Residue	Modelled	Actual	Comment	Reference
A	849	ALA	-	linker	UNP Q63273
A	850	MET	-	linker	UNP Q63273
A	851	VAL	-	linker	UNP Q63273
A	914	LEU	PHE	conflict	UNP P42212
A	915	THR	SER	conflict	UNP P42212
A	1056	LYS	ALA	conflict	UNP P42212
A	1081	LEU	HIS	conflict	UNP P42212
A	1089	SER	-	expression tag	UNP P42212
A	1090	GLY	-	expression tag	UNP P42212
A	1091	LEU	-	expression tag	UNP P42212
A	1092	ARG	-	expression tag	UNP P42212
A	1093	THR	-	expression tag	UNP P42212
A	1094	GLU	-	expression tag	UNP P42212
A	1095	THR	-	expression tag	UNP P42212
A	1096	SER	-	expression tag	UNP P42212
A	1097	GLN	-	expression tag	UNP P42212
A	1098	VAL	-	expression tag	UNP P42212
A	1099	ALA	-	expression tag	UNP P42212
A	1100	PRO	-	expression tag	UNP P42212
A	1101	ALA	-	expression tag	UNP P42212
C	559	VAL	CYS	conflict	UNP Q63273
C	578	SER	CYS	conflict	UNP Q63273
C	619	ILE	CYS	conflict	UNP Q63273
C	813	ALA	CYS	conflict	UNP Q63273
C	828	TYR	-	linker	UNP Q63273
C	829	LYS	-	linker	UNP Q63273
C	830	SER	-	linker	UNP Q63273
C	831	ARG	-	linker	UNP Q63273
C	832	ALA	-	linker	UNP Q63273
C	833	GLU	-	linker	UNP Q63273
C	834	ALA	-	linker	UNP Q63273
C	835	LYS	-	linker	UNP Q63273
C	836	ARG	-	linker	UNP Q63273
C	837	MET	-	linker	UNP Q63273
C	838	LYS	-	linker	UNP Q63273
C	839	GLY	-	linker	UNP Q63273
C	840	LEU	-	linker	UNP Q63273
C	841	VAL	-	linker	UNP Q63273
C	842	PRO	-	linker	UNP Q63273
C	843	ARG	-	linker	UNP Q63273
C	844	GLY	-	linker	UNP Q63273
C	845	SER	-	linker	UNP Q63273

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Chain	Residue	Modelled	Actual	Comment	Reference
C	846	ALA	-	linker	UNP Q63273
C	847	ALA	-	linker	UNP Q63273
C	848	ALA	-	linker	UNP Q63273
C	849	ALA	-	linker	UNP Q63273
C	850	MET	-	linker	UNP Q63273
C	851	VAL	-	linker	UNP Q63273
C	914	LEU	PHE	conflict	UNP P42212
C	915	THR	SER	conflict	UNP P42212
C	1056	LYS	ALA	conflict	UNP P42212
C	1081	LEU	HIS	conflict	UNP P42212
C	1089	SER	-	expression tag	UNP P42212
C	1090	GLY	-	expression tag	UNP P42212
C	1091	LEU	-	expression tag	UNP P42212
C	1092	ARG	-	expression tag	UNP P42212
C	1093	THR	-	expression tag	UNP P42212
C	1094	GLU	-	expression tag	UNP P42212
C	1095	THR	-	expression tag	UNP P42212
C	1096	SER	-	expression tag	UNP P42212
C	1097	GLN	-	expression tag	UNP P42212
C	1098	VAL	-	expression tag	UNP P42212
C	1099	ALA	-	expression tag	UNP P42212
C	1100	PRO	-	expression tag	UNP P42212
C	1101	ALA	-	expression tag	UNP P42212

- Molecule 2 is a protein called Glutamate receptor ionotropic, kainate 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	737	4876	3051	877	931	17	0	0
2	D	737	4876	3051	877	931	17	0	0

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	567	VAL	ILE	conflict	UNP P42260
B	576	VAL	CYS	conflict	UNP P42260
B	595	SER	CYS	conflict	UNP P42260
B	909	SER	-	expression tag	UNP P42260
B	910	GLY	-	expression tag	UNP P42260
B	911	LEU	-	expression tag	UNP P42260
B	912	ARG	-	expression tag	UNP P42260

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Chain	Residue	Modelled	Actual	Comment	Reference
B	913	SER	-	expression tag	UNP P42260
B	914	ALA	-	expression tag	UNP P42260
B	915	TRP	-	expression tag	UNP P42260
B	916	SER	-	expression tag	UNP P42260
B	917	HIS	-	expression tag	UNP P42260
B	918	PRO	-	expression tag	UNP P42260
B	919	GLN	-	expression tag	UNP P42260
B	920	PHE	-	expression tag	UNP P42260
B	921	GLU	-	expression tag	UNP P42260
B	922	LYS	-	expression tag	UNP P42260
B	923	GLY	-	expression tag	UNP P42260
B	924	GLY	-	expression tag	UNP P42260
B	925	GLY	-	expression tag	UNP P42260
B	926	SER	-	expression tag	UNP P42260
B	927	GLY	-	expression tag	UNP P42260
B	928	GLY	-	expression tag	UNP P42260
B	929	GLY	-	expression tag	UNP P42260
B	930	SER	-	expression tag	UNP P42260
B	931	GLY	-	expression tag	UNP P42260
B	932	GLY	-	expression tag	UNP P42260
B	933	GLY	-	expression tag	UNP P42260
B	934	SER	-	expression tag	UNP P42260
B	935	TRP	-	expression tag	UNP P42260
B	936	SER	-	expression tag	UNP P42260
B	937	HIS	-	expression tag	UNP P42260
B	938	PRO	-	expression tag	UNP P42260
B	939	GLN	-	expression tag	UNP P42260
B	940	PHE	-	expression tag	UNP P42260
B	941	GLU	-	expression tag	UNP P42260
B	942	LYS	-	expression tag	UNP P42260
D	567	VAL	ILE	conflict	UNP P42260
D	576	VAL	CYS	conflict	UNP P42260
D	595	SER	CYS	conflict	UNP P42260
D	909	SER	-	expression tag	UNP P42260
D	910	GLY	-	expression tag	UNP P42260
D	911	LEU	-	expression tag	UNP P42260
D	912	ARG	-	expression tag	UNP P42260
D	913	SER	-	expression tag	UNP P42260
D	914	ALA	-	expression tag	UNP P42260
D	915	TRP	-	expression tag	UNP P42260
D	916	SER	-	expression tag	UNP P42260
D	917	HIS	-	expression tag	UNP P42260

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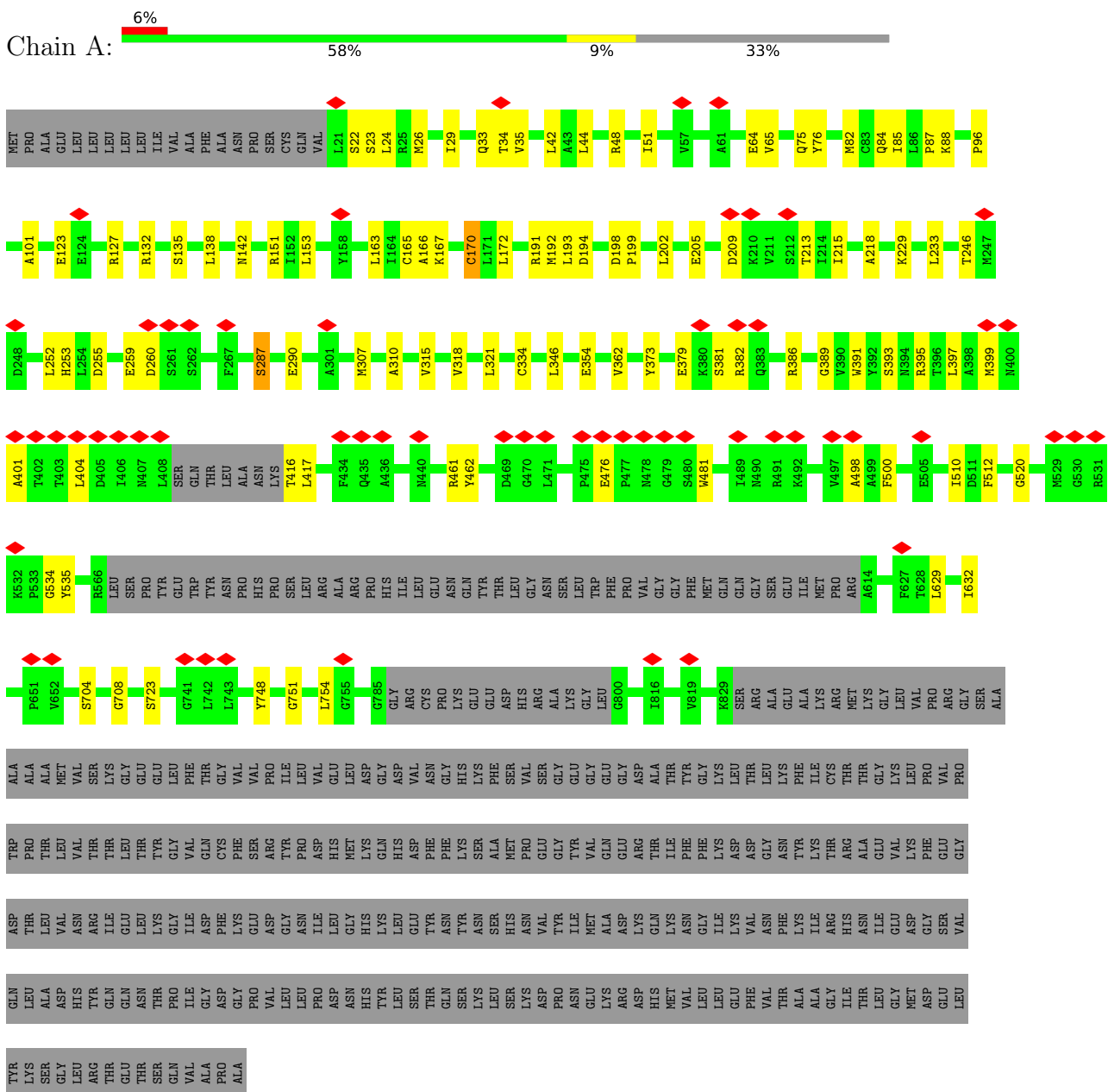
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Chain	Residue	Modelled	Actual	Comment	Reference
D	918	PRO	-	expression tag	UNP P42260
D	919	GLN	-	expression tag	UNP P42260
D	920	PHE	-	expression tag	UNP P42260
D	921	GLU	-	expression tag	UNP P42260
D	922	LYS	-	expression tag	UNP P42260
D	923	GLY	-	expression tag	UNP P42260
D	924	GLY	-	expression tag	UNP P42260
D	925	GLY	-	expression tag	UNP P42260
D	926	SER	-	expression tag	UNP P42260
D	927	GLY	-	expression tag	UNP P42260
D	928	GLY	-	expression tag	UNP P42260
D	929	GLY	-	expression tag	UNP P42260
D	930	SER	-	expression tag	UNP P42260
D	931	GLY	-	expression tag	UNP P42260
D	932	GLY	-	expression tag	UNP P42260
D	933	GLY	-	expression tag	UNP P42260
D	934	SER	-	expression tag	UNP P42260
D	935	TRP	-	expression tag	UNP P42260
D	936	SER	-	expression tag	UNP P42260
D	937	HIS	-	expression tag	UNP P42260
D	938	PRO	-	expression tag	UNP P42260
D	939	GLN	-	expression tag	UNP P42260
D	940	PHE	-	expression tag	UNP P42260
D	941	GLU	-	expression tag	UNP P42260
D	942	LYS	-	expression tag	UNP P42260

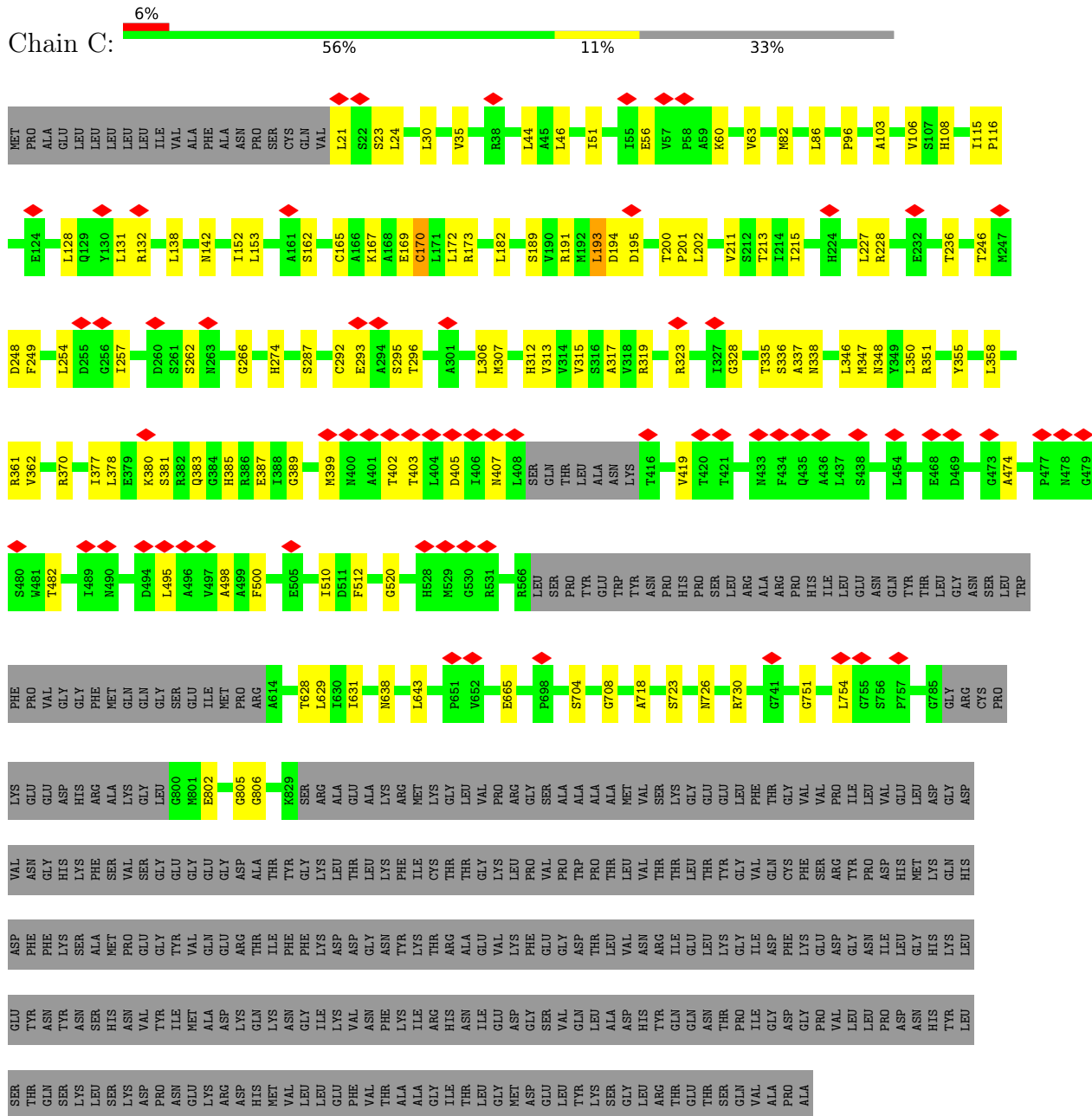
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

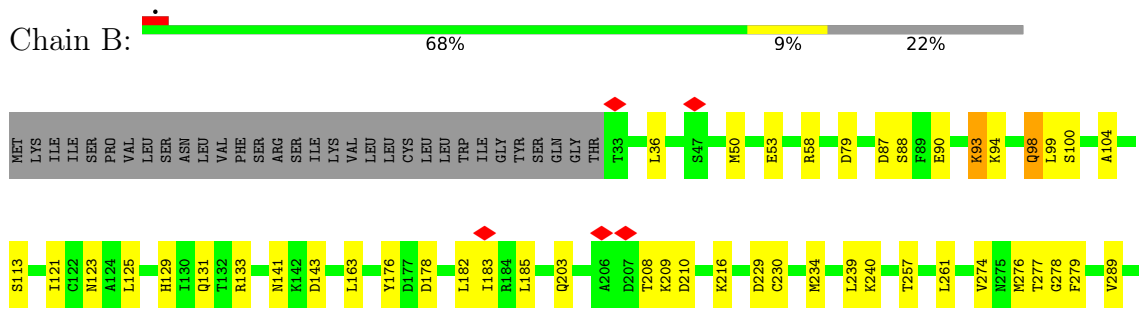
- Molecule 1: Glutamate receptor ionotropic, kainate 5,Green fluorescent protein chimera

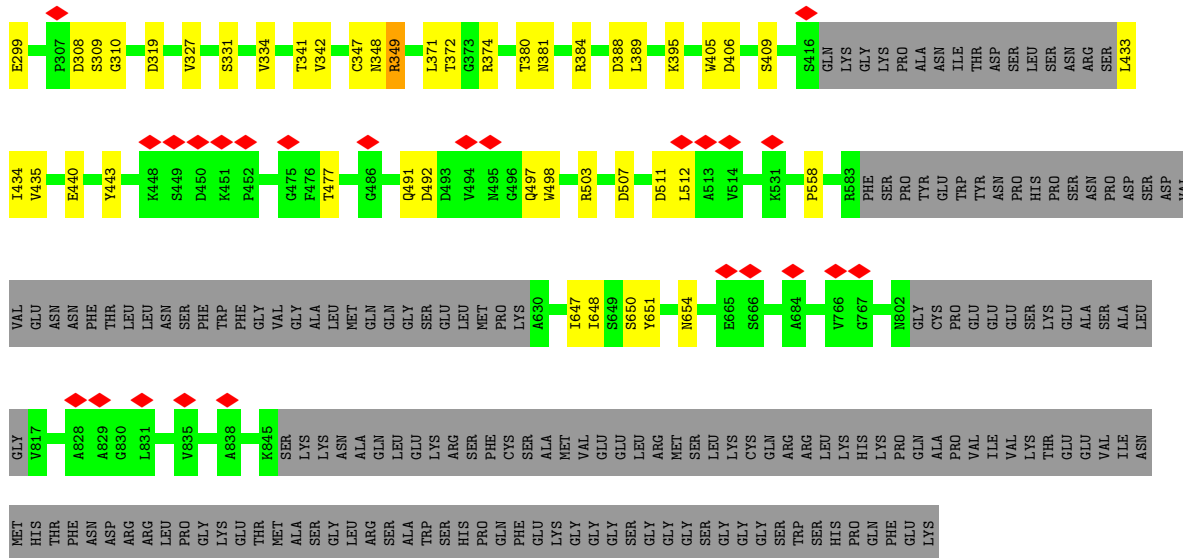


- Molecule 1: Glutamate receptor ionotropic, kainate 5, Green fluorescent protein chimera

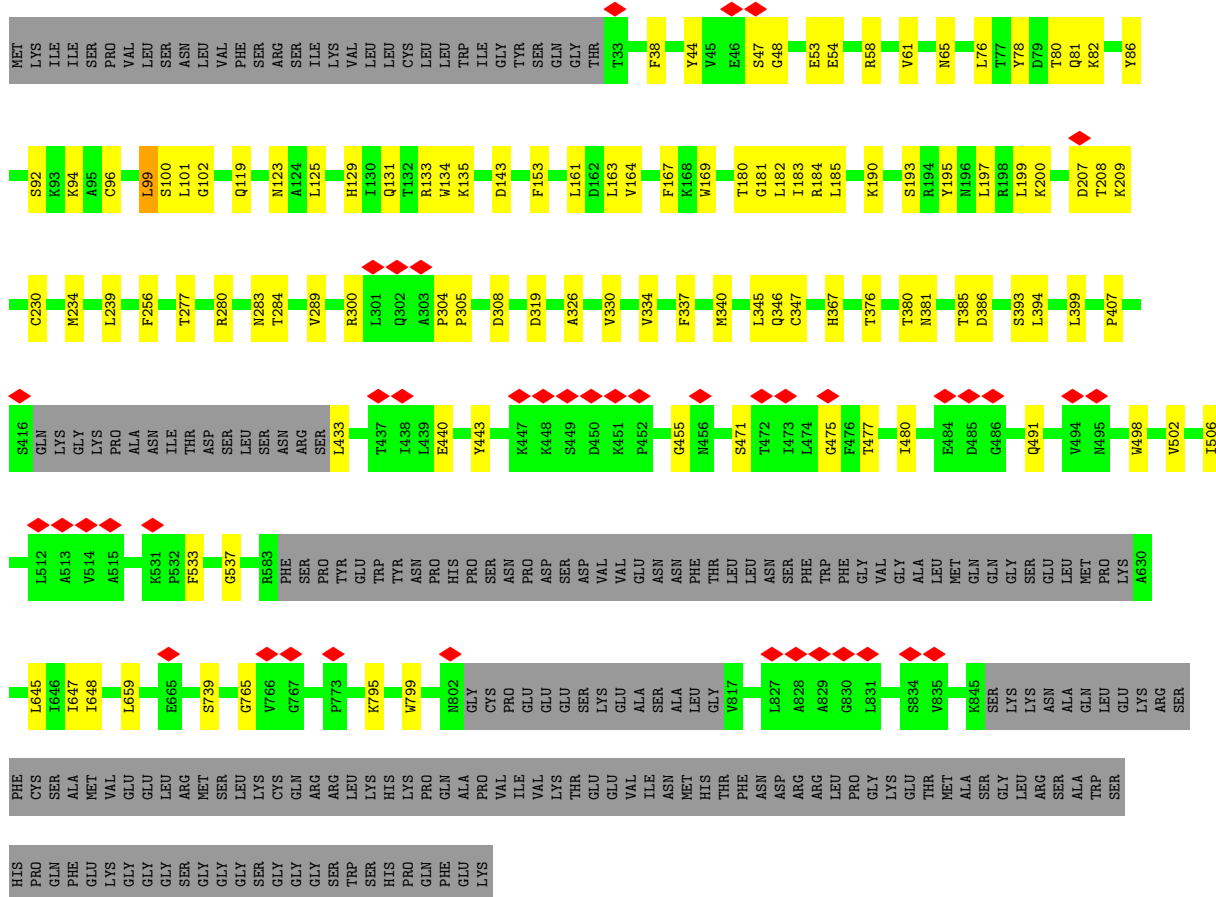


- Molecule 2: Glutamate receptor ionotropic, kainate 2





• Molecule 2: Glutamate receptor ionotropic, kainate 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1021916	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.176	Depositor
Minimum map value	-0.629	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.367	Depositor
Map size (Å)	350.71997, 350.71997, 350.71997	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.096, 1.096, 1.096	Depositor

5 Model quality

5.1 Standard geometry

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	0.58	0/4903	0.64	0/6706
1	C	0.60	0/4903	0.75	0/6706
2	B	0.61	0/4951	0.62	0/6763
2	D	0.62	0/4951	0.62	0/6763
All	All	0.60	0/19708	0.66	0/26938

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

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	4844	0	3989	61	0
1	C	4844	0	3989	84	0
2	B	4876	0	3963	59	0
2	D	4876	0	3963	82	0
All	All	19440	0	15904	275	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 275 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)
2:D:337:PHE:CE2	2:D:340:MET:HB2	1.36	1.57
2:D:337:PHE:HE2	2:D:340:MET:CB	1.47	1.28
2:D:337:PHE:CD2	2:D:340:MET:HB2	1.78	1.18
1:C:313:VAL:CG1	1:C:350:LEU:HD11	1.72	1.18
2:D:337:PHE:CE2	2:D:340:MET:CB	2.22	1.14

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	733/1101 (67%)	641 (87%)	92 (13%)	0	100	100
1	C	733/1101 (67%)	659 (90%)	74 (10%)	0	100	100
2	B	729/942 (77%)	663 (91%)	65 (9%)	1 (0%)	51	85
2	D	729/942 (77%)	675 (93%)	54 (7%)	0	100	100
All	All	2924/4086 (72%)	2638 (90%)	285 (10%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	349	ARG

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	363/950 (38%)	351 (97%)	12 (3%)	38	61
1	C	363/950 (38%)	351 (97%)	12 (3%)	38	61
2	B	358/817 (44%)	351 (98%)	7 (2%)	55	73
2	D	358/817 (44%)	352 (98%)	6 (2%)	60	78
All	All	1442/3534 (41%)	1405 (97%)	37 (3%)	49	67

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	292	CYS
2	D	346	GLN
1	C	293	GLU
2	D	96	CYS
2	B	93	LYS

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

Mol	Chain	Res	Type
1	C	274	HIS
1	C	385	HIS
2	D	123	ASN

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.

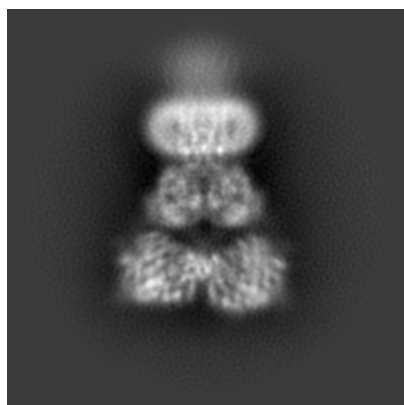
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23014. These allow visual inspection of the internal detail of the map and identification of artifacts.

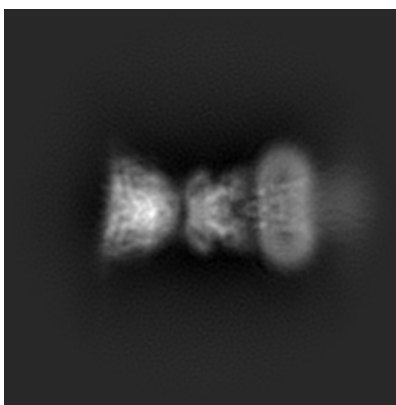
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

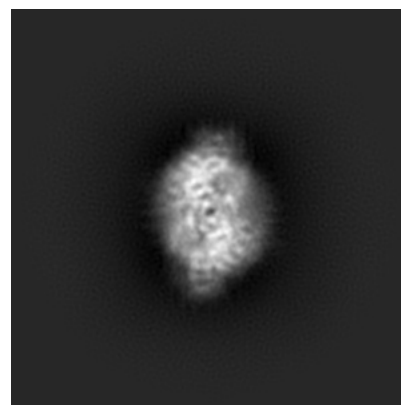
6.1.1 Primary map



X



Y

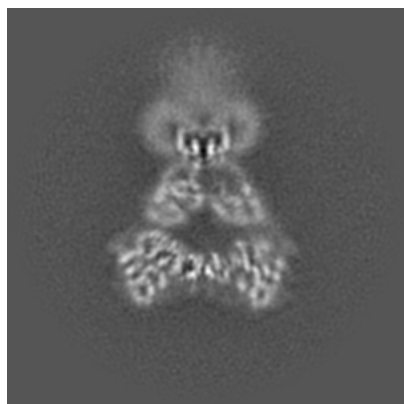


Z

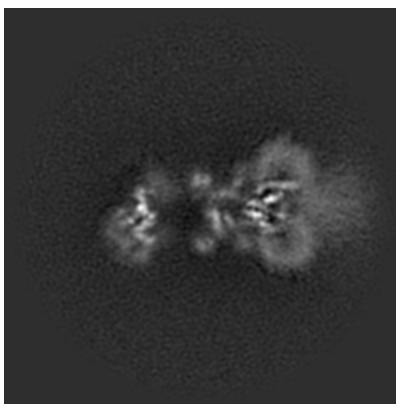
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

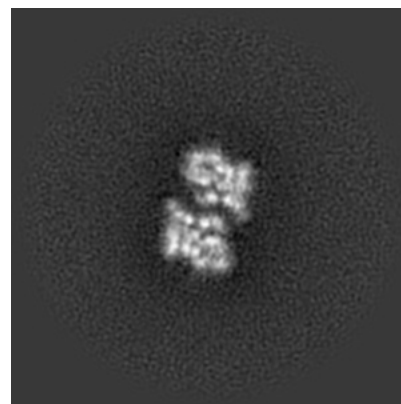
6.2.1 Primary map



X Index: 160



Y Index: 160

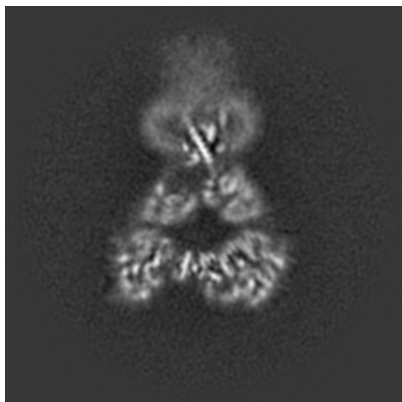


Z Index: 160

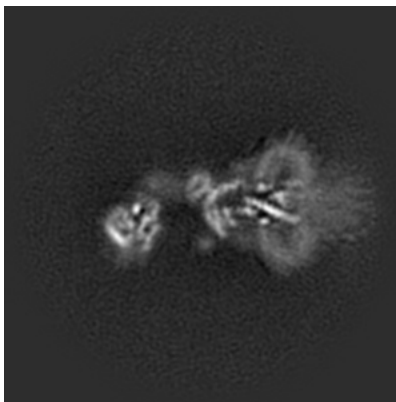
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

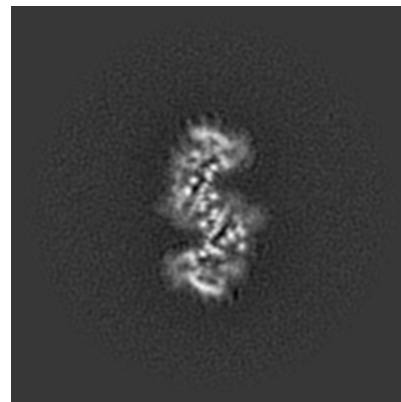
6.3.1 Primary map



X Index: 154



Y Index: 164

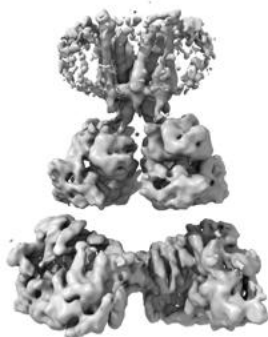


Z Index: 117

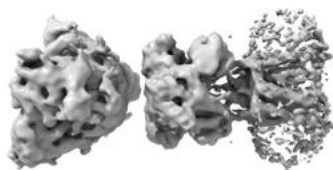
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

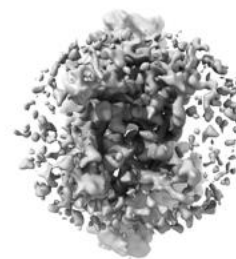
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.367. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

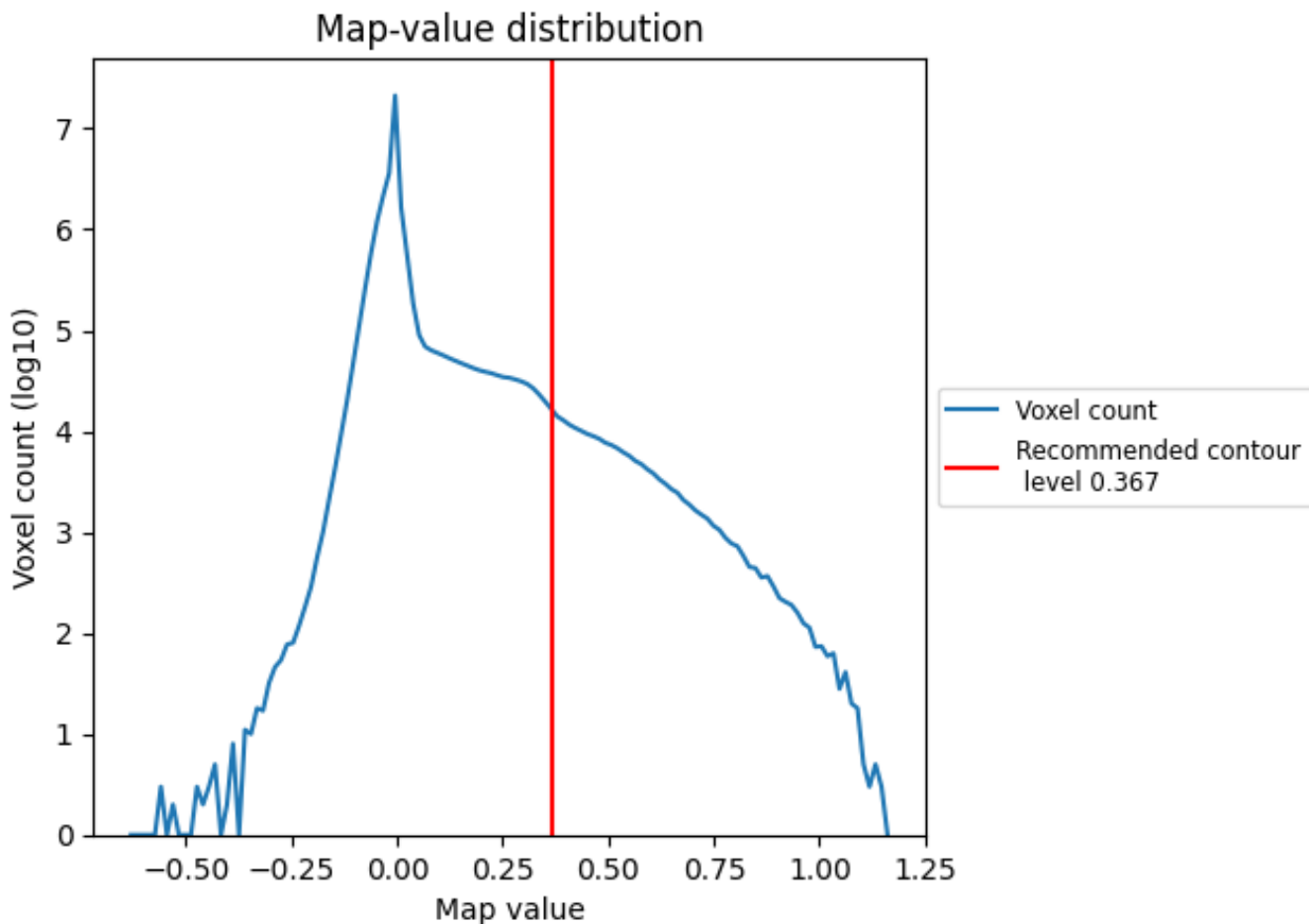
6.5 Mask visualisation

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

7 Map analysis [i](#)

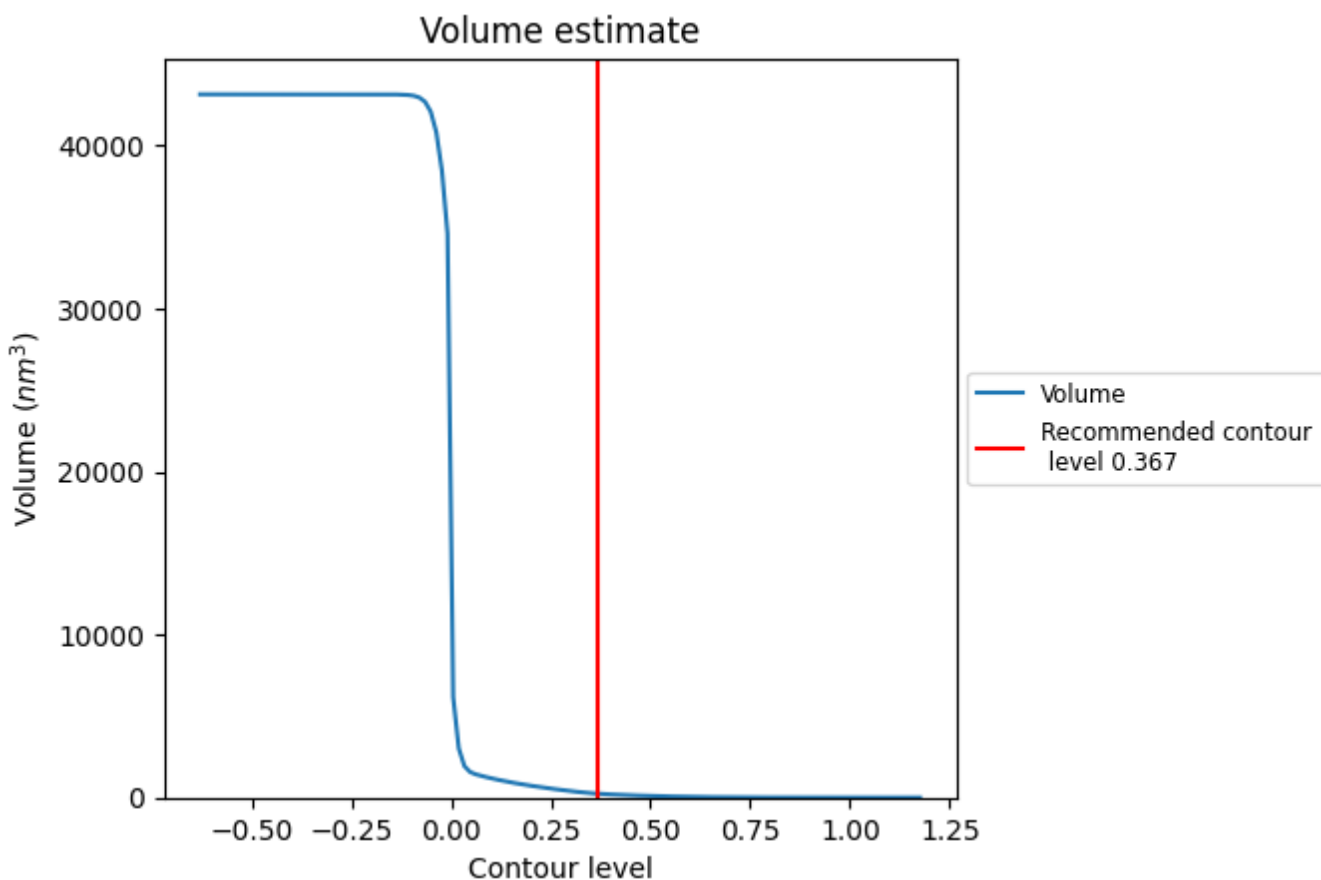
This section contains the results of statistical analysis of the map.

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.

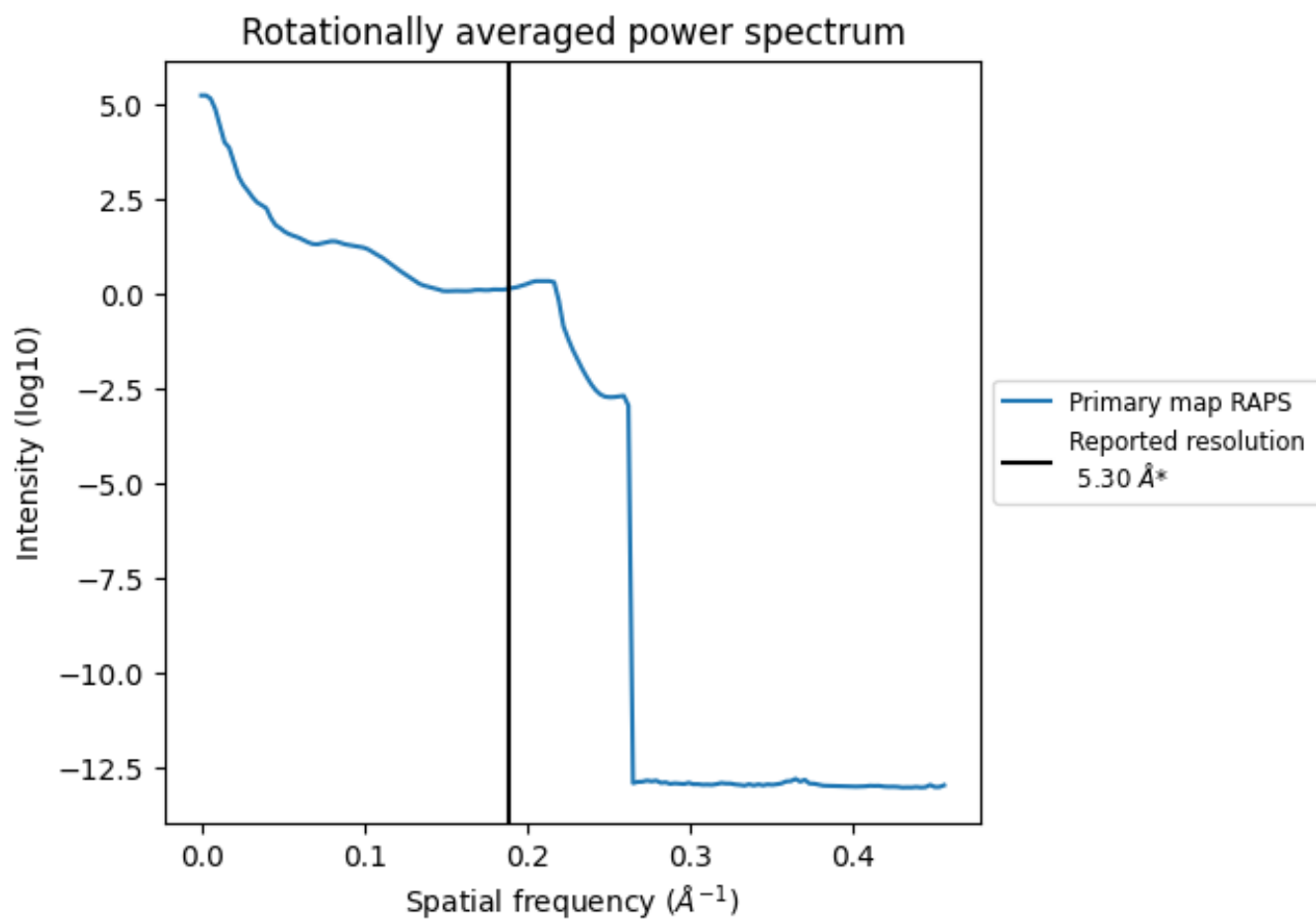
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 239 nm³; this corresponds to an approximate mass of 216 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](#)

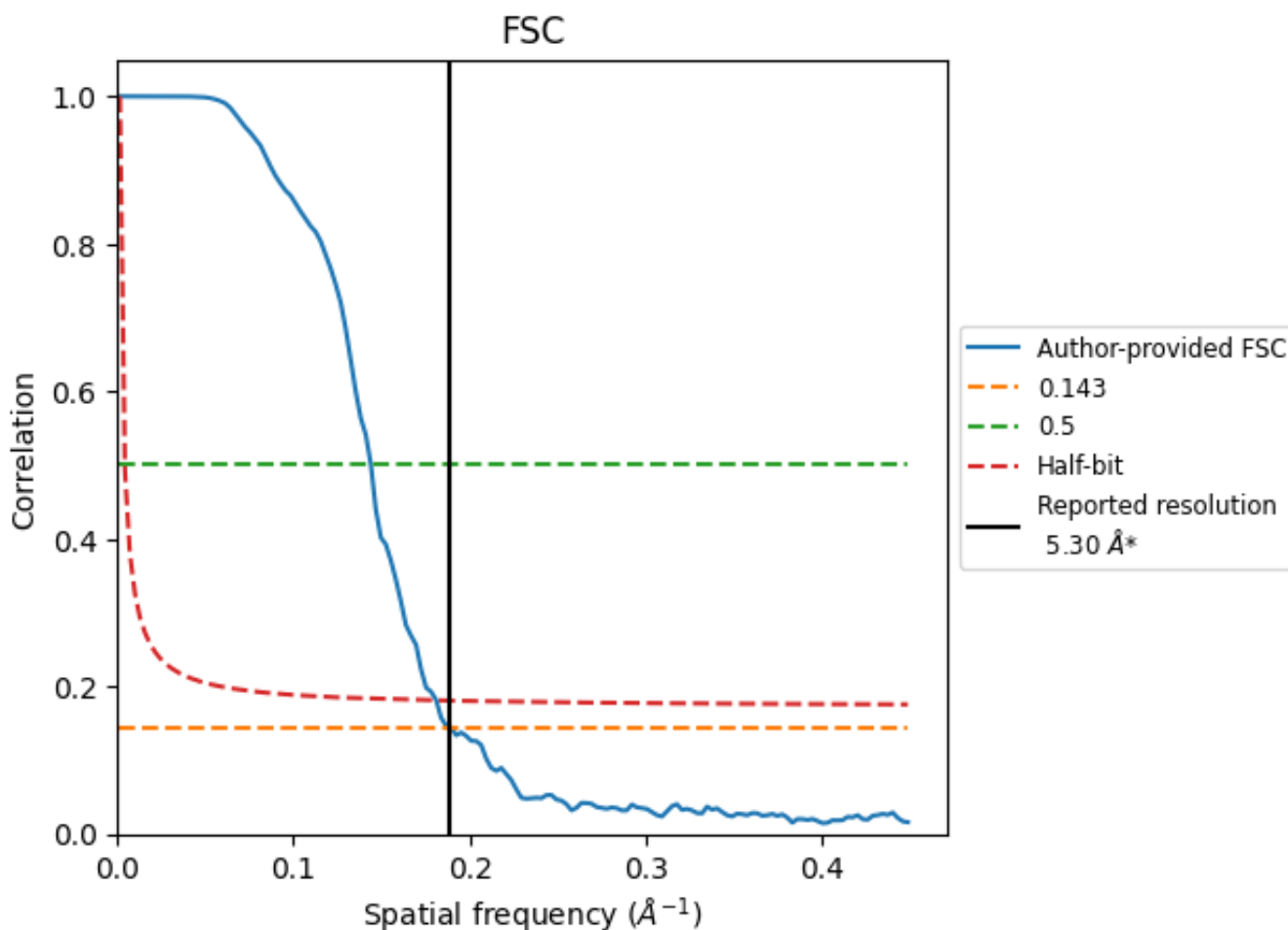


*Reported resolution corresponds to spatial frequency of 0.189 Å⁻¹

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 0.189 Å⁻¹

8.2 Resolution estimates [i](#)

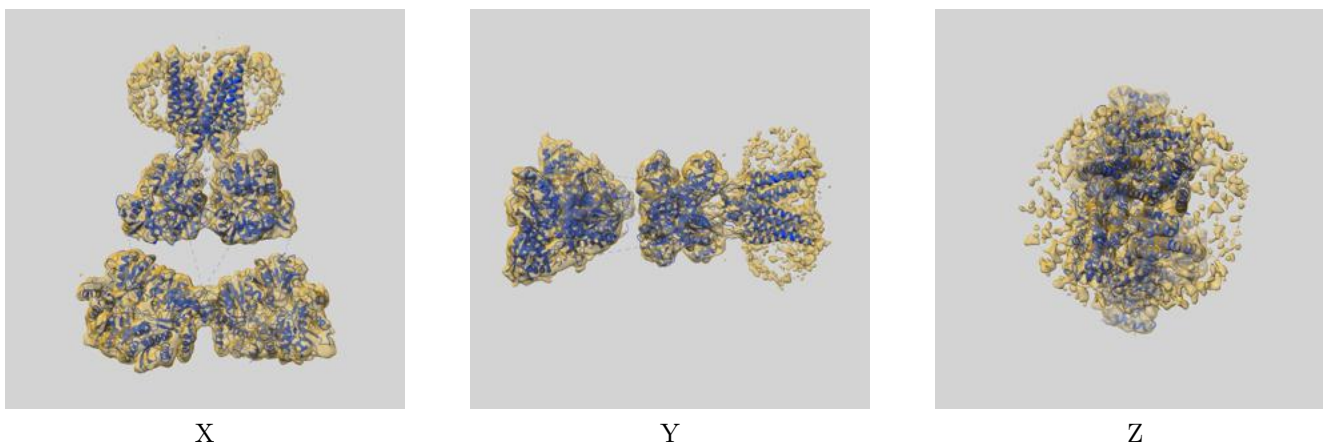
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.30	-	-
Author-provided FSC curve	5.27	6.94	5.52
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

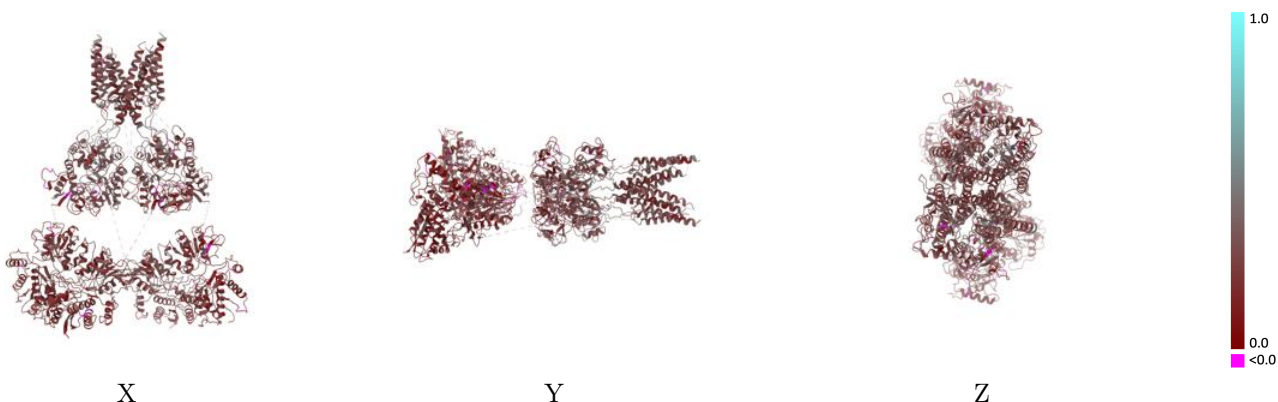
This section contains information regarding the fit between EMDB map EMD-23014 and PDB model 7KS0. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



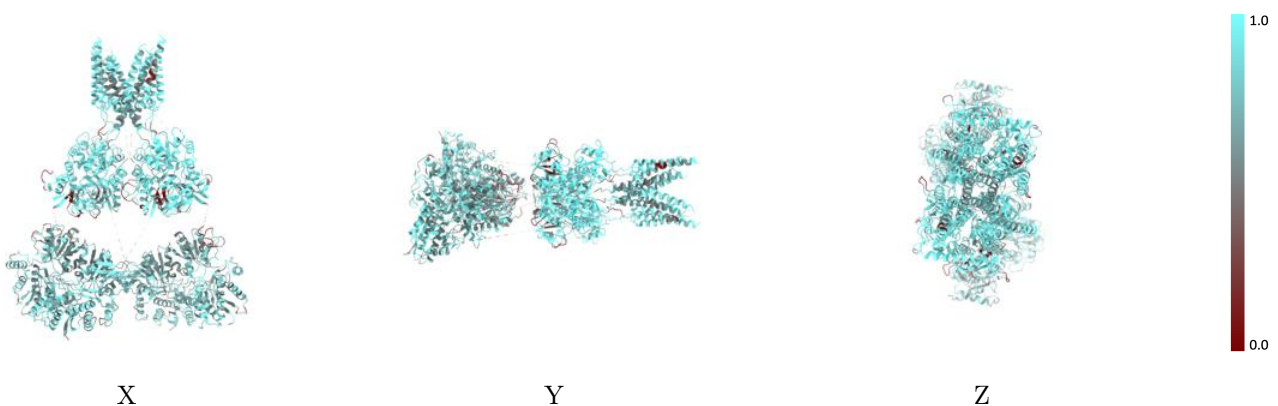
The images above show the 3D surface view of the map at the recommended contour level 0.367 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



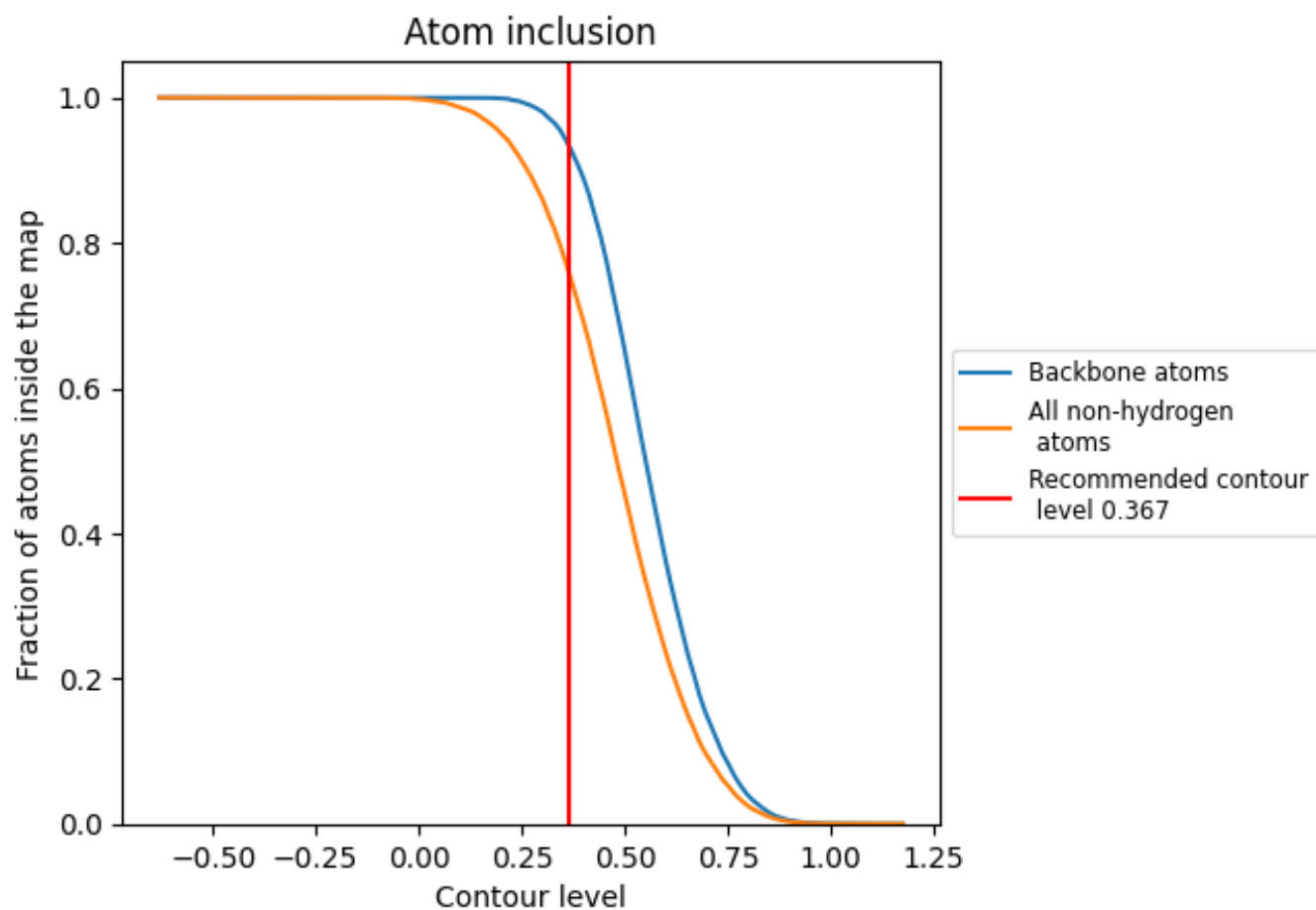
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.367).











9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 76% 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 (0.367) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7560	 0.2460
A	 0.7411	 0.2300
B	 0.7811	 0.2590
C	 0.7390	 0.2360
D	 0.7627	 0.2590

