wwPDB EM Validation Summary Report

Nov 4, 2024 – 03:11 PM JST

PDB ID	:	7YSV
EMDB ID	:	EMD-34083
Title	:	GluK1-1a extracellular domain captured in SYM2081 bound desensitized state
Authors	:	Dhingra, S.; Kumar, J.
Deposited on	:	2022-08-13
Resolution	:	8.01 Å(reported)
Based on initial models	:	3C32, ?

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:

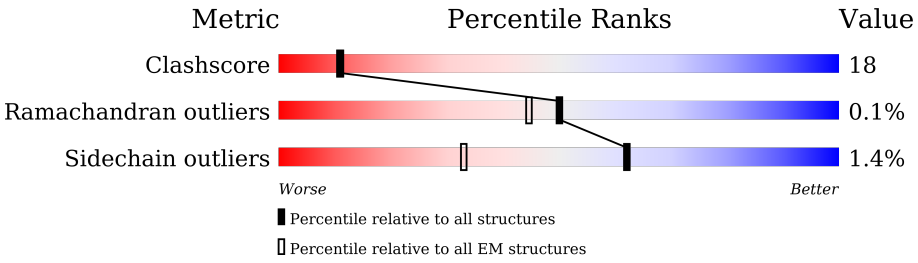
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.01 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	841	46% 31% · 23%
1	B	841	13% 47% 30% 23%
1	C	841	9% 47% 29% 23%
1	D	841	14% 49% 28% · 23%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 20868 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	649	Total	C	N	O	S	0	0
			5217	3329	888	971	29		
1	B	649	Total	C	N	O	S	0	0
			5217	3329	888	971	29		
1	C	649	Total	C	N	O	S	0	0
			5217	3329	888	971	29		
1	D	649	Total	C	N	O	S	0	0
			5217	3329	888	971	29		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	TYR	CYS	engineered mutation	UNP A0A0G2K830
A	557	VAL	CYS	engineered mutation	UNP A0A0G2K830
A	838	LEU	-	expression tag	UNP A0A0G2K830
A	839	VAL	-	expression tag	UNP A0A0G2K830
A	840	PRO	-	expression tag	UNP A0A0G2K830
A	841	ARG	-	expression tag	UNP A0A0G2K830
B	552	TYR	CYS	engineered mutation	UNP A0A0G2K830
B	557	VAL	CYS	engineered mutation	UNP A0A0G2K830
B	838	LEU	-	expression tag	UNP A0A0G2K830
B	839	VAL	-	expression tag	UNP A0A0G2K830
B	840	PRO	-	expression tag	UNP A0A0G2K830
B	841	ARG	-	expression tag	UNP A0A0G2K830
C	552	TYR	CYS	engineered mutation	UNP A0A0G2K830
C	557	VAL	CYS	engineered mutation	UNP A0A0G2K830
C	838	LEU	-	expression tag	UNP A0A0G2K830
C	839	VAL	-	expression tag	UNP A0A0G2K830
C	840	PRO	-	expression tag	UNP A0A0G2K830
C	841	ARG	-	expression tag	UNP A0A0G2K830
D	552	TYR	CYS	engineered mutation	UNP A0A0G2K830
D	557	VAL	CYS	engineered mutation	UNP A0A0G2K830
D	838	LEU	-	expression tag	UNP A0A0G2K830
D	839	VAL	-	expression tag	UNP A0A0G2K830

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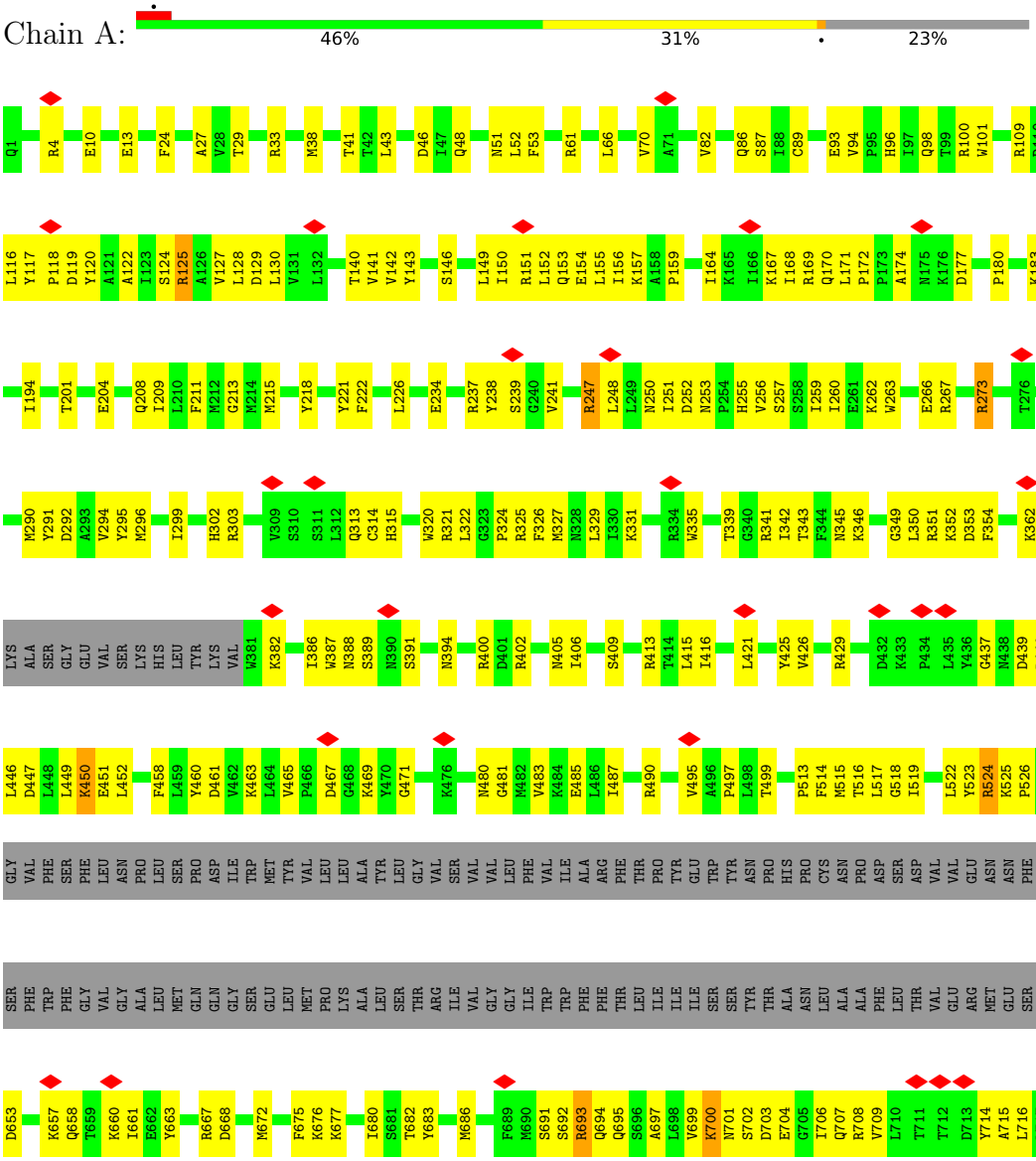
Chain	Residue	Modelled	Actual	Comment	Reference
D	840	PRO	-	expression tag	UNP A0A0G2K830
D	841	ARG	-	expression tag	UNP A0A0G2K830

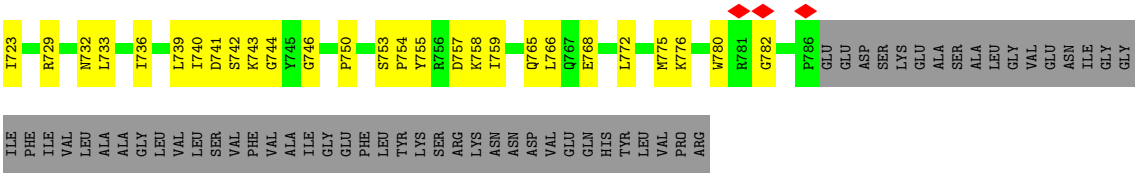
3 Residue-property plots (i)

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

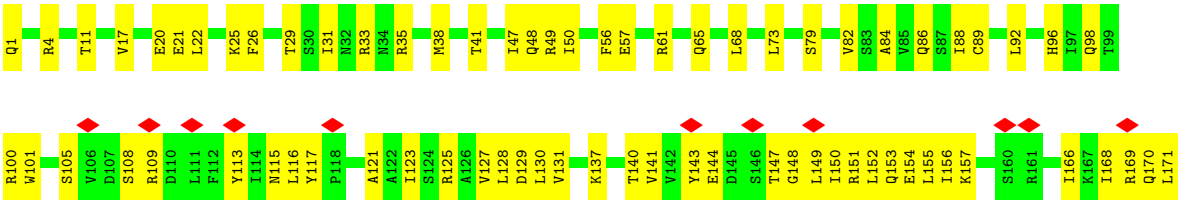
Chain A:

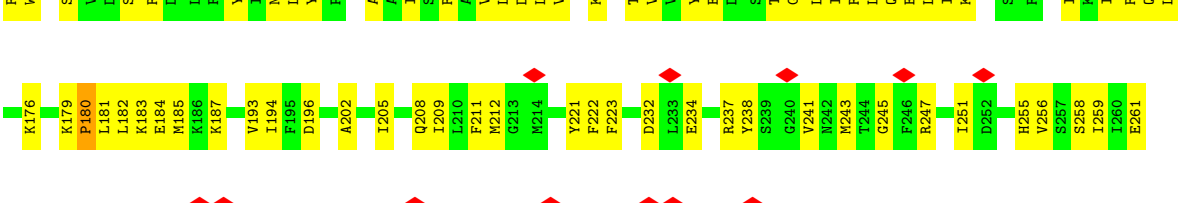


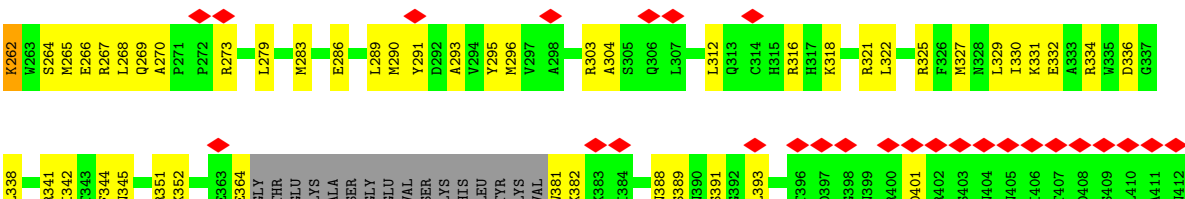


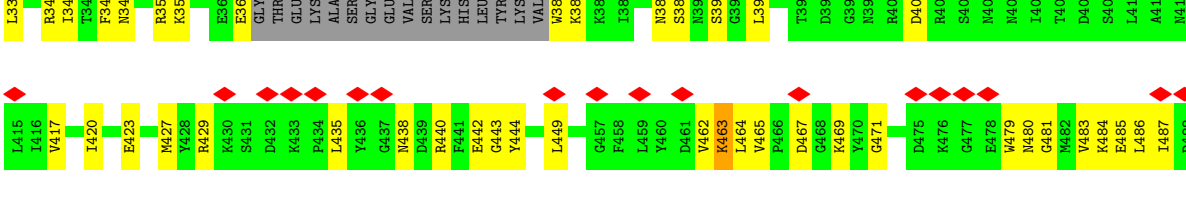
• Molecule 1: Glutamate receptor

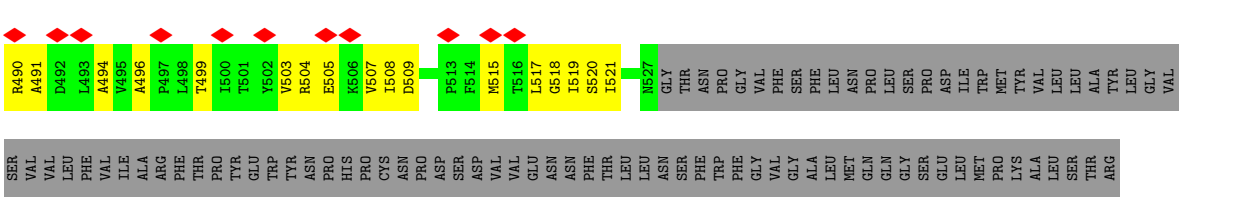
Chain B:

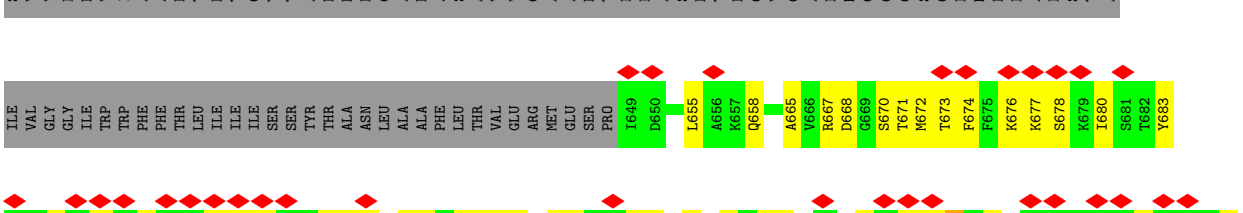


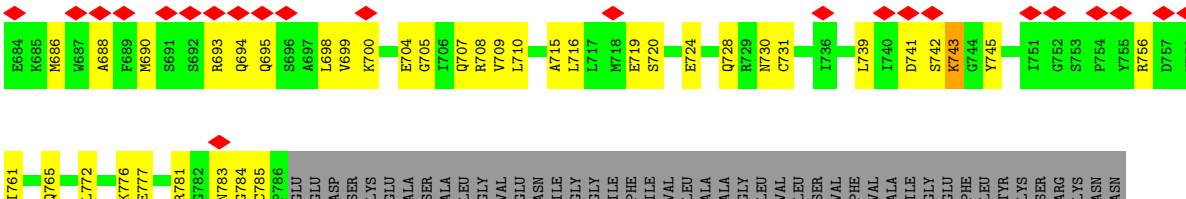






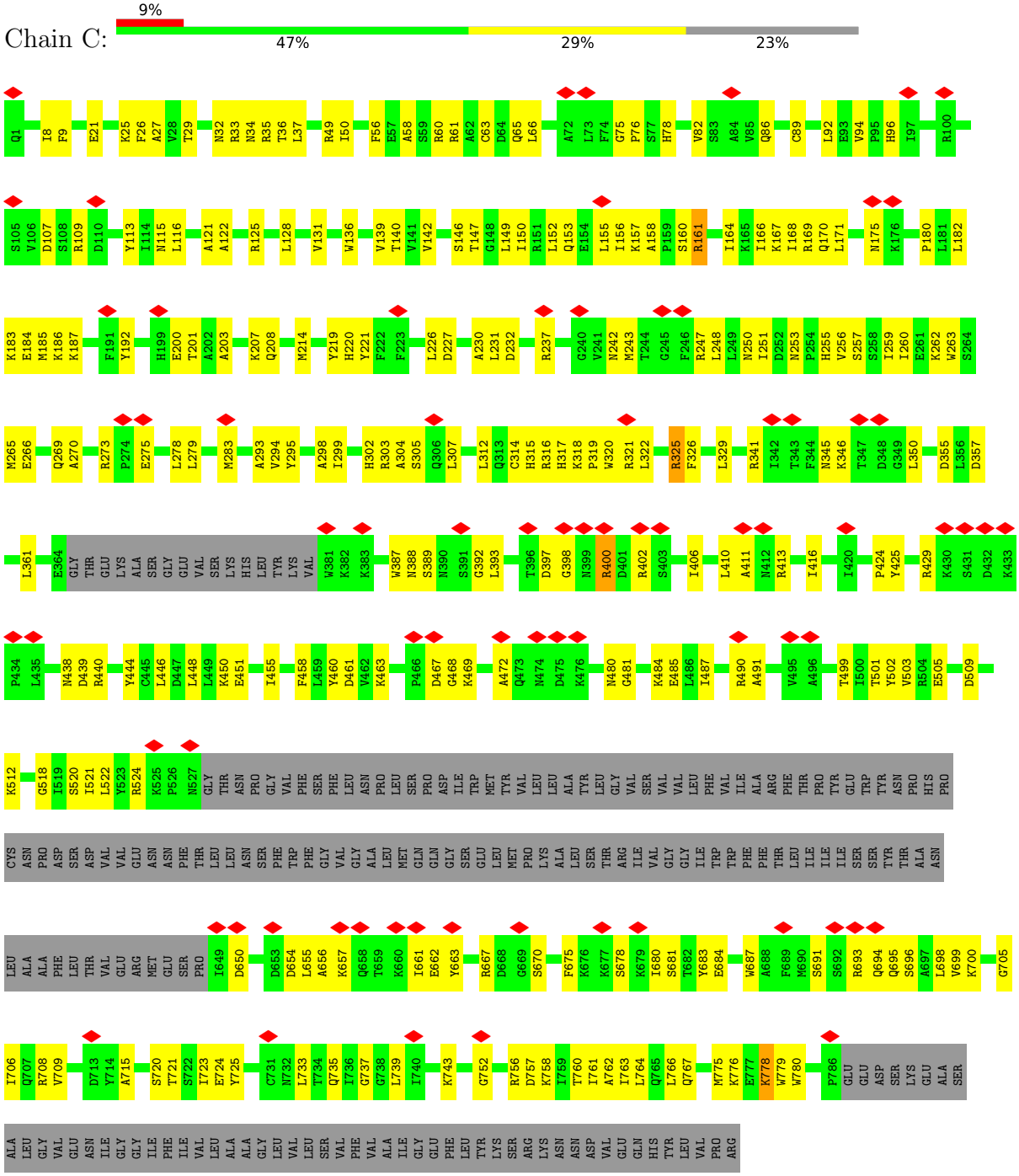






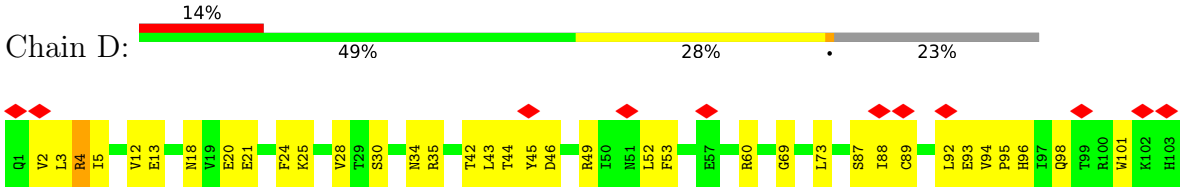
• Molecule 1: Glutamate receptor

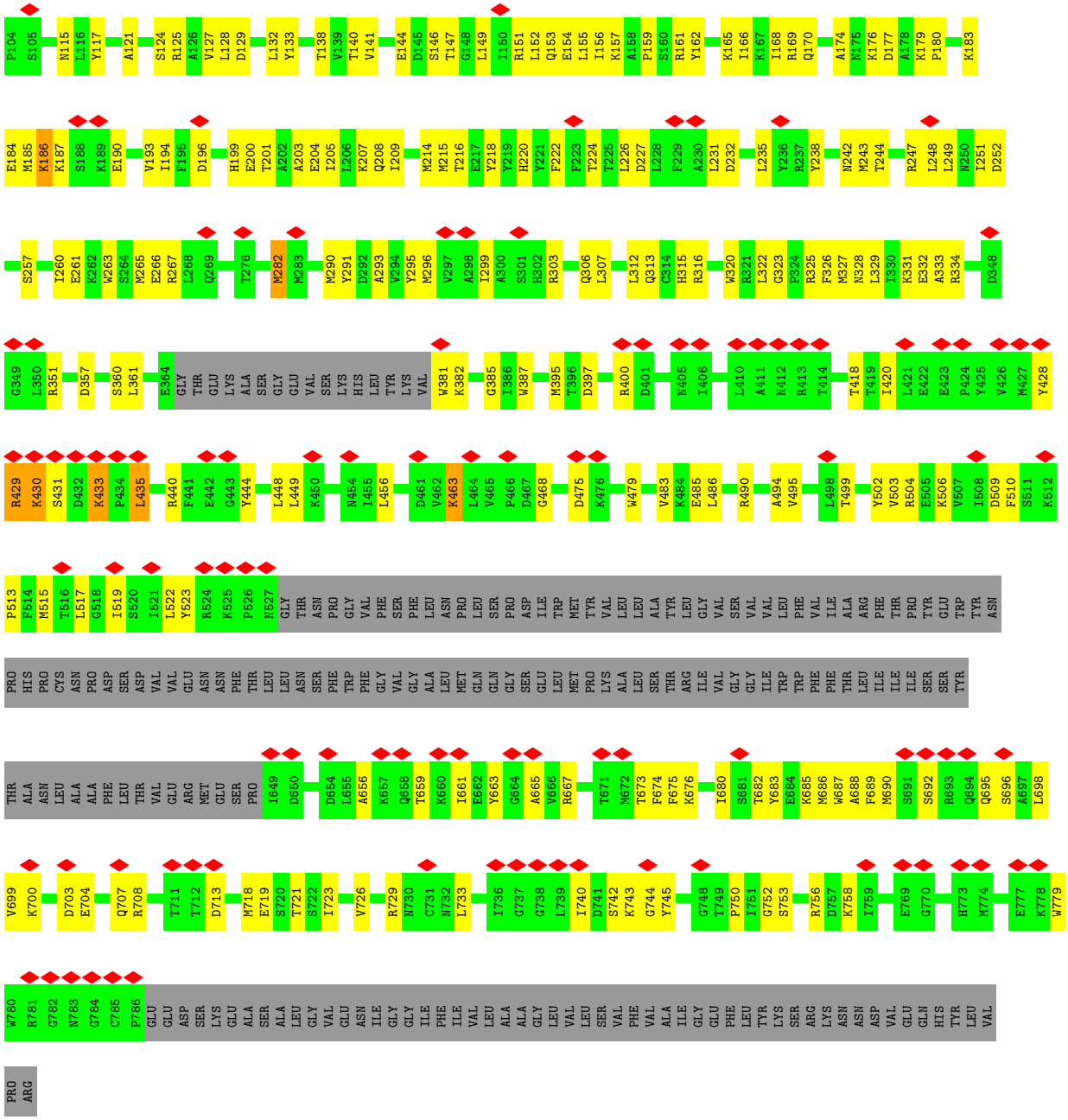
Chain C:



• Molecule 1: Glutamate receptor

Chain D:




P104 S105 N115 L116 Y117 A121 S124 R125 A126 V127 L128 D129 L132 Y133 T138 V139 T140 V141 E144 D145 S146 T147 G148 L149 I150 R151 L152 Q153 E154 L155 I156 K157 A158 P159 S160 R161 Y162 K165 I166 K167 I168 R169 Q170 A174 N175 K176 D177 A178 K179 P180 K183
E184 M185 K186 K187 S188 K189 E190 V193 I194 F195 D196 H199 E200 T201 A202 A203 E204 I205 L206 K207 Q208 I209 M214 M215 T216 E217 Y218 Y219 H220 Y221 F222 F223 T224 T225 L226 D227 L228 F229 A230 L231 D232 L235 Y236 R237 Y238 N242 M243 T244 R247 L248 L249 W250 I251 D252
S257 I260 E261 K262 W263 S264 M265 E266 R267 L268 Q269 T276 M282 W283 M290 Y291 D292 A293 V294 Y295 M296 V297 A298 I299 A300 S301 H302 R303 Q306 L307 L312 Q313 C314 H315 R316 W320 R321 L322 G323 P324 R325 F326 M327 N328 L329 I330 K331 E332 A333 R334 D348
G349 L350 R351 D357 S360 L361 E364 GLY THR GLU LYS ALA SER GLY GLU VAL SER LYS HIS LEU TYR LYS VAL W381 K382 G385 I386 W387 M395 T396 D397 R400 D401 N405 I406 L410 A411 N412 R413 T414 T418 T419 I420 L421 E422 E423 P424 Y425 V426 M427 Y428
R429 K430 S431 D432 K433 P434 L435 R440 F441 E442 G443 Y444 L448 L449 K450 N454 I455 L456 D461 V462 K463 L464 V465 P466 D467 G468 D475 K476 W479 V483 K484 E485 L486 R490 A494 V495 L498 T499 Y502 V503 R504 E505 K506 V507 I508 D509 F510 S511 K512
P513 F514 M515 T516 L517 G518 I519 S520 I521 L522 Y523 R524 K525 P526 N527 GLY THR ASN PRO GLY VAL PHE SER PHE LEU ASN PRO LEU SER PRO ASP ILE TRP MET TYR VAL LEU LEU ALA TYR LEU GLY VAL SER VAL VAL LEU PHE VAL ILE ALA ARG PHE THR PRO TYR GLU TRP TYR ASN
PRO HIS PRO CYS ASN PRO ASP SER ASP VAL VAL GLU ASN ASN PHE THR LEU LEU ASN SER PHE TRP PHE GLY VAL GLY ALA LEU MET GLN GLN GLY SER GLU LEU MET PRO LYS ALA LEU SER THR ARG ILE VAL GLY GLY ILE TRP TRP PHE PHE THR LEU ILE ILE ILE SER SER TYR
THR ALA ASN LEU ALA ALA PHE LEU THR VAL GLU ARG MET GLU SER PRO I649 D650 D654 L655 A656 K657 Q658 T659 K660 I661 E662 Y663 G664 A665 V666 R667 T671 M672 T673 F674 F675 K676 I680 S681 T682 Y683 E684 K685 M686 W687 A688 F689 M690 S691 S692 R693 Q694 Q695 S696 A697 L698
V699 K700 D703 E704 Q707 R708 T711 T712 D713 M718 E719 S720 T721 S722 I723 V726 R729 N730 C731 N732 L733 I736 G737 G738 L739 I740 D741 S742 K743 G744 Y745 G748 T749 P750 I751 G752 S753 R756 D757 K758 I759 E769 G770 H773 M774 E777 K778 W779
W780 R781 G782 N783 G784 C785 P786 GLU GLU ASP SER LYS GLU ALA SER ALA LEU GLY VAL GLU ASN ILE GLY GLY ILE PHE ILE VAL LEU ALA ALA GLY LEU VAL LEU SER VAL PHE VAL ALA ILE GLY GLU PHE LEU TYR LYS SER ARG LYS ASN ASN ASP VAL GLU GLN HIS TYR LEU VAL
PRO ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5372	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	19.5	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.626	Depositor
Minimum map value	-1.336	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.109	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	353.28, 353.28, 353.28	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	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	0.27	0/5326	0.56	0/7202
1	B	0.26	0/5326	0.57	0/7202
1	C	0.27	0/5326	0.56	0/7202
1	D	0.27	0/5326	0.57	0/7202
All	All	0.27	0/21304	0.56	0/28808

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	5217	0	5235	204	0
1	B	5217	0	5235	208	0
1	C	5217	0	5235	193	0
1	D	5217	0	5235	177	0
All	All	20868	0	20940	757	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 18.

The worst 5 of 757 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:D:89:CYS:HB3	1:D:96:HIS:CE1	2.06	0.89
1:D:95:PRO:HG2	1:D:326:PHE:HB2	1.60	0.83
1:C:469:LYS:HE2	1:C:481:GLY:H	1.43	0.83
1:C:226:LEU:HD11	1:C:248:LEU:H	1.43	0.83
1:C:317:HIS:HE1	1:D:60:ARG:HD2	1.42	0.83

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	643/841 (76%)	615 (96%)	27 (4%)	1 (0%)	44 78
1	B	643/841 (76%)	613 (95%)	29 (4%)	1 (0%)	44 78
1	C	643/841 (76%)	622 (97%)	21 (3%)	0	100 100
1	D	643/841 (76%)	628 (98%)	15 (2%)	0	100 100
All	All	2572/3364 (76%)	2478 (96%)	92 (4%)	2 (0%)	50 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	ALA
1	B	180	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	574/738 (78%)	566 (99%)	8 (1%)	62	75
1	B	574/738 (78%)	570 (99%)	4 (1%)	81	87
1	C	574/738 (78%)	566 (99%)	8 (1%)	62	75
1	D	574/738 (78%)	562 (98%)	12 (2%)	48	66
All	All	2296/2952 (78%)	2264 (99%)	32 (1%)	62	75

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	431	SER
1	D	433	LYS
1	C	157	LYS
1	B	743	LYS
1	D	435	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	315	HIS
1	D	707	GLN
1	D	695	GLN
1	B	765	GLN
1	D	98	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 oligosaccharides 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.

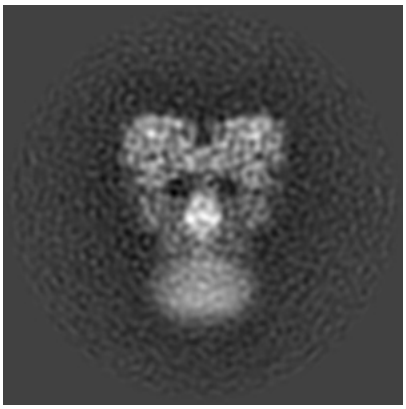
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34083. These allow visual inspection of the internal detail of the map and identification of artifacts.

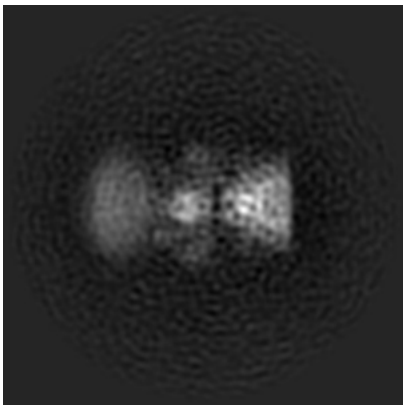
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

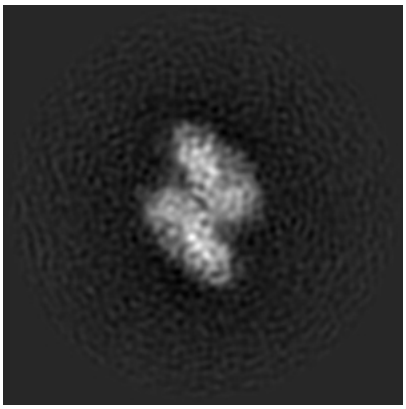
6.1.1 Primary map



X

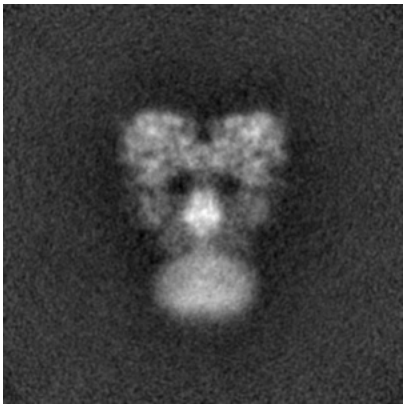


Y



Z

6.1.2 Raw map



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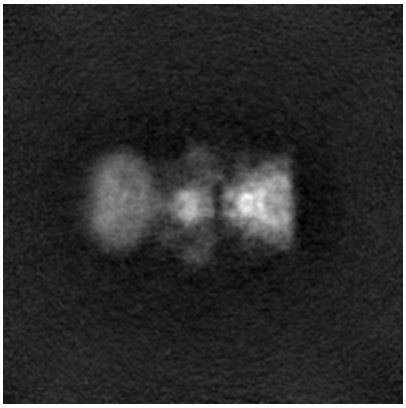
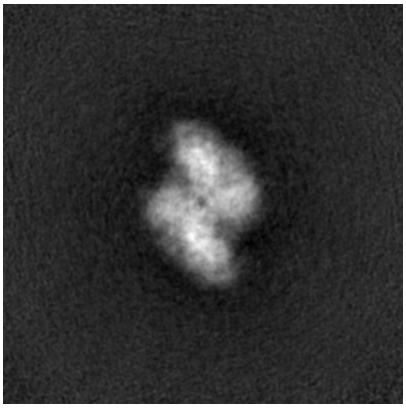


Y

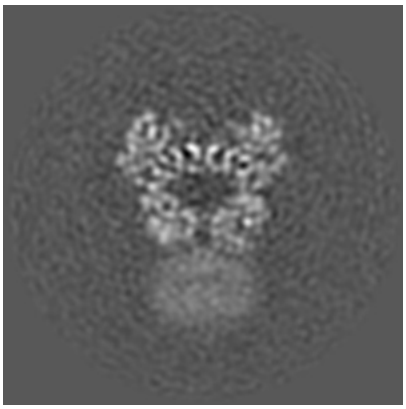


Z

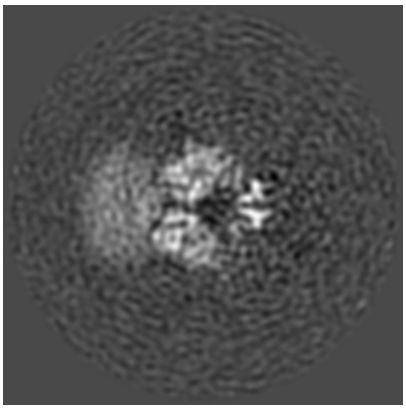
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

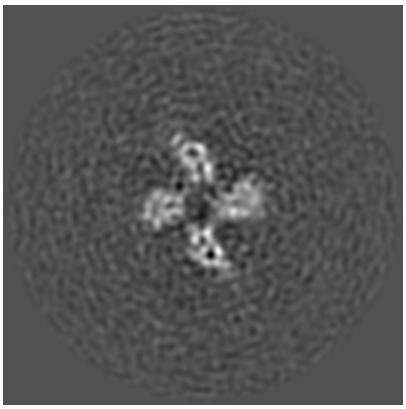
6.2.1 Primary map



X Index: 128

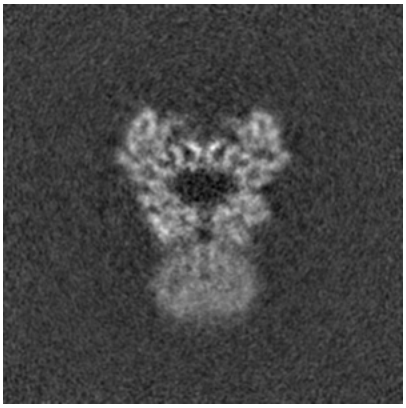


Y Index: 128

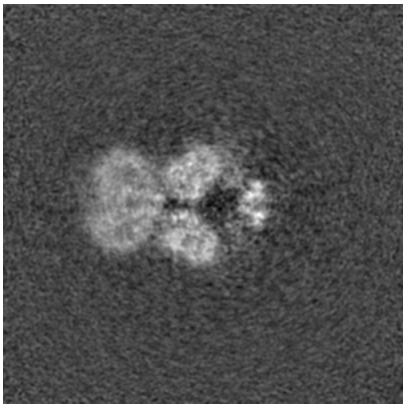


Z Index: 128

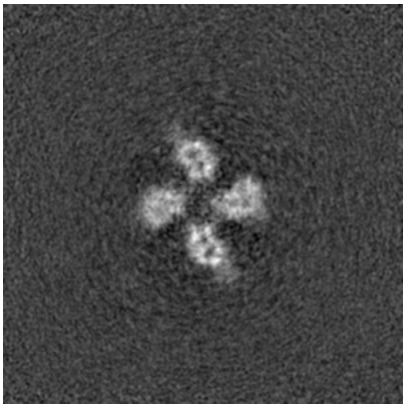
6.2.2 Raw map



X Index: 128



Y Index: 128

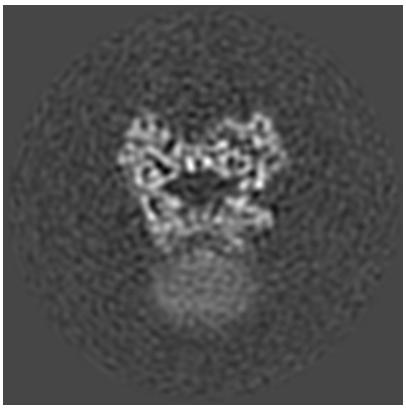


Z Index: 128

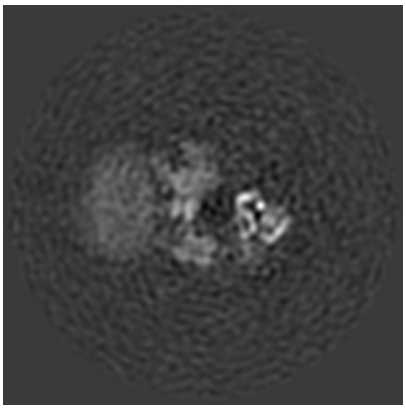
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

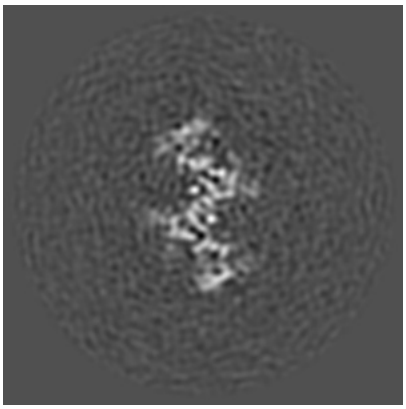
6.3.1 Primary map



X Index: 131

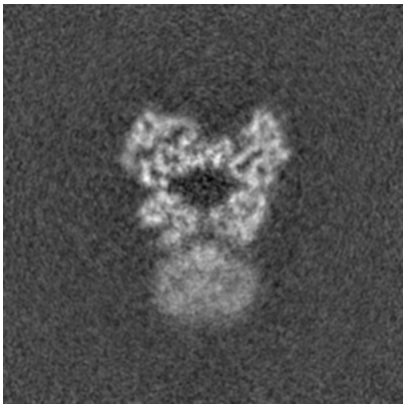


Y Index: 120

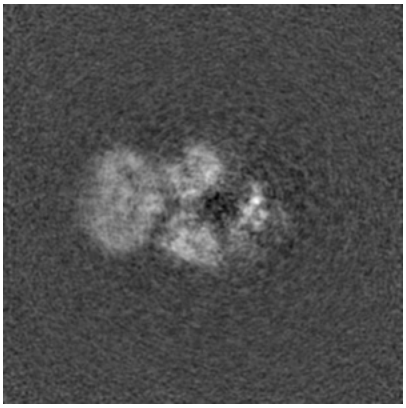


Z Index: 157

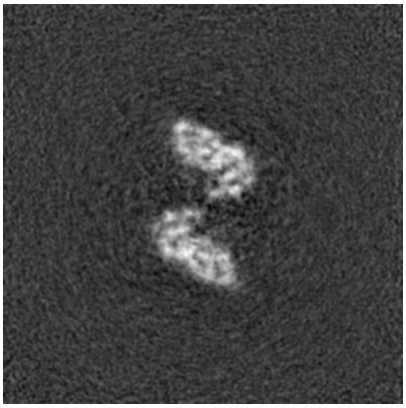
6.3.2 Raw map



X Index: 124



Y Index: 125

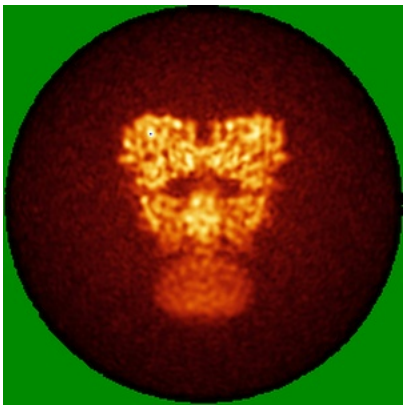


Z Index: 173

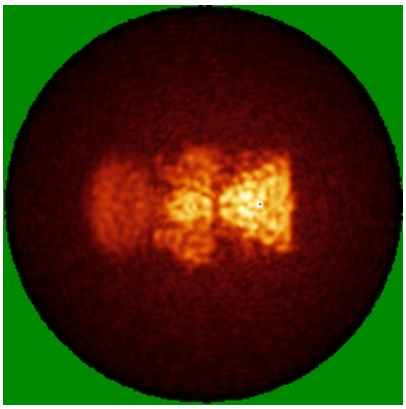
The images above show the largest variance slices of the map in three orthogonal directions.

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

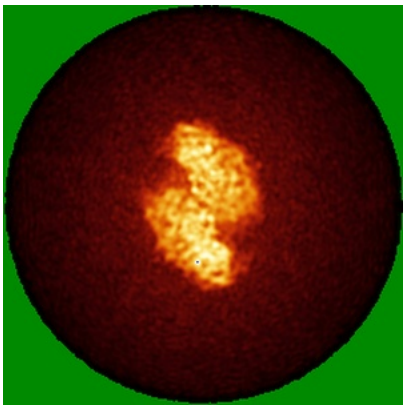
6.4.1 Primary map



X

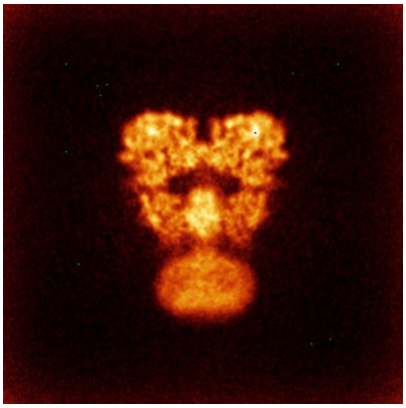


Y

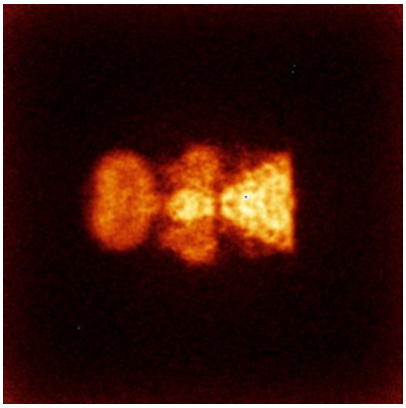


Z

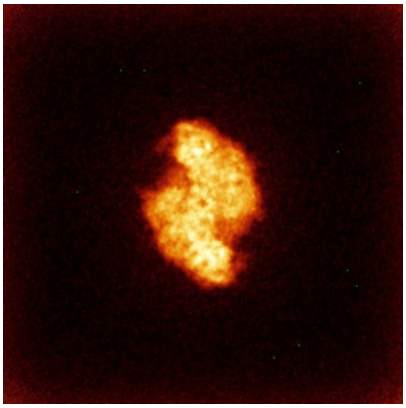
6.4.2 Raw map



X



Y

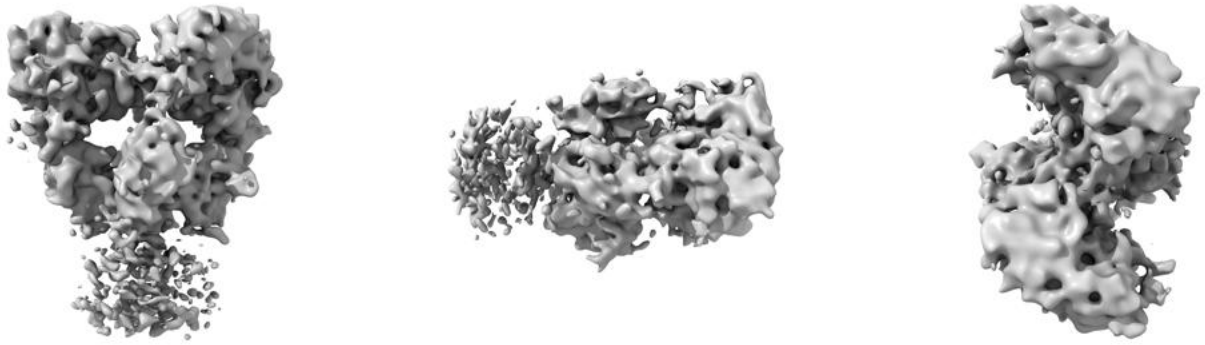


Z

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)

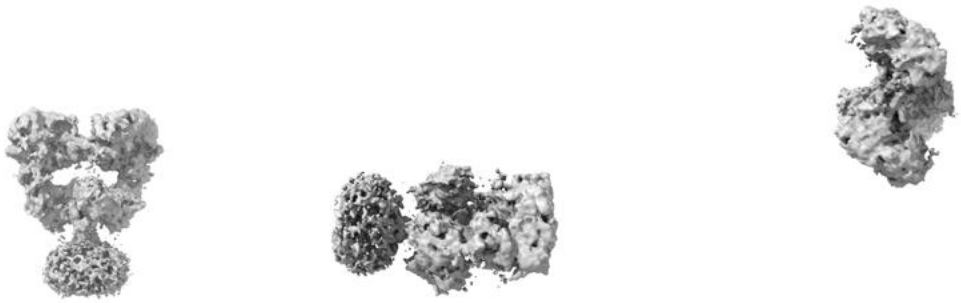
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. 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



X Y Z

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.

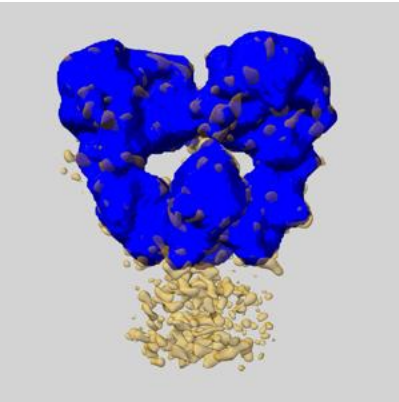
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

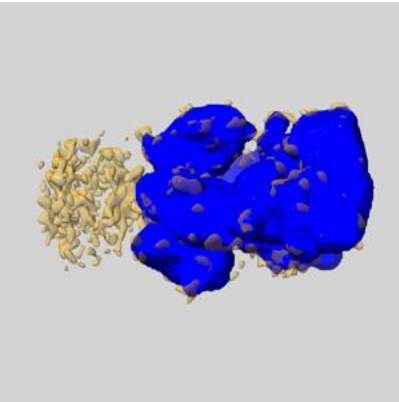
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

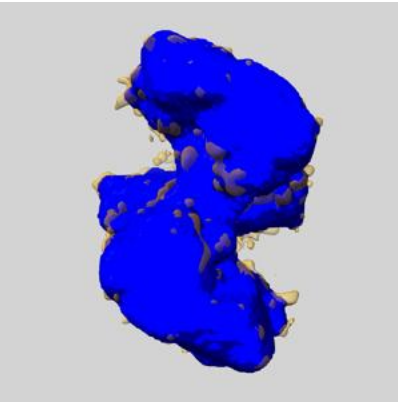
6.6.1 emd_34083_msk_1.map (i)



X



Y

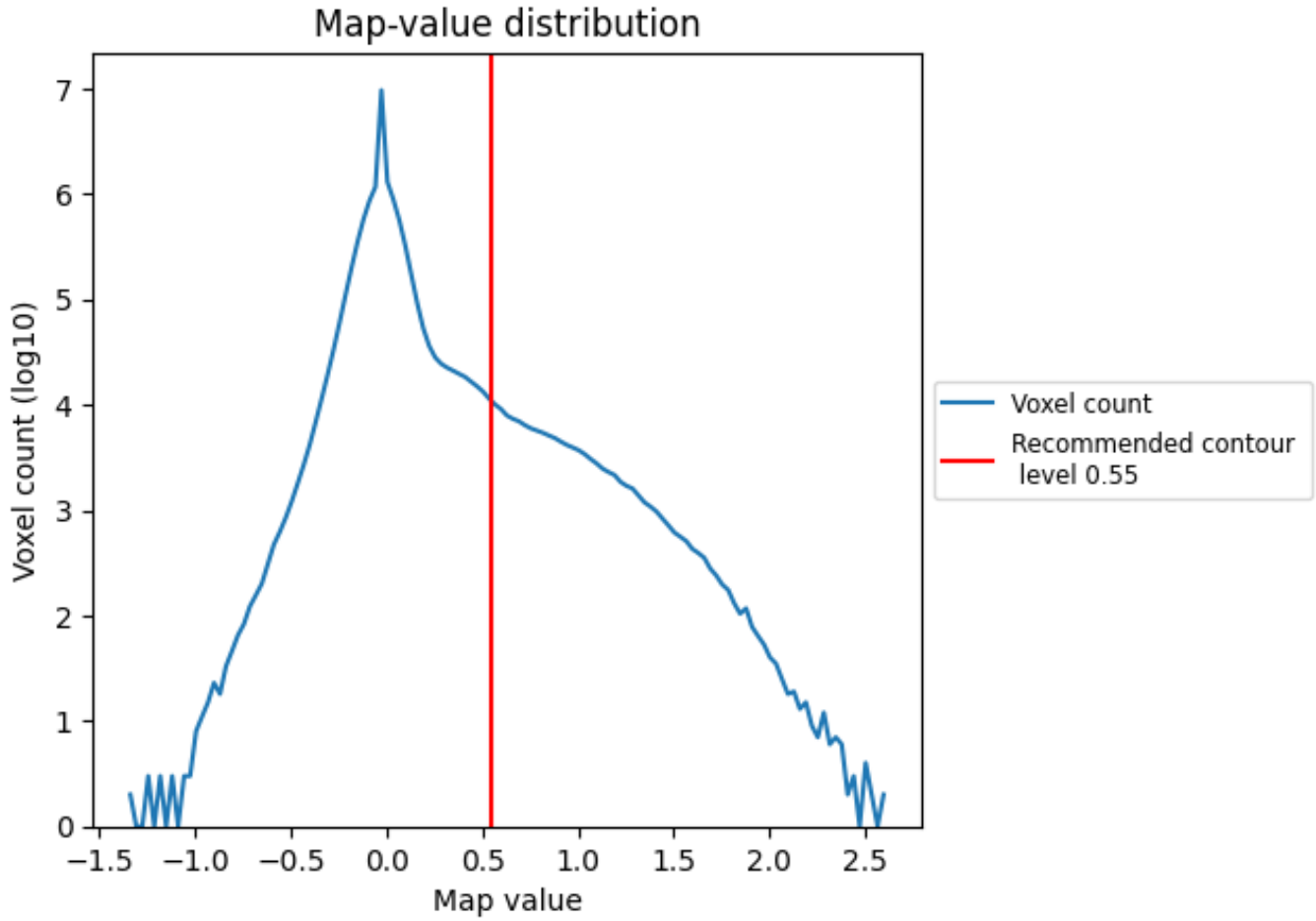


Z

7 Map analysis

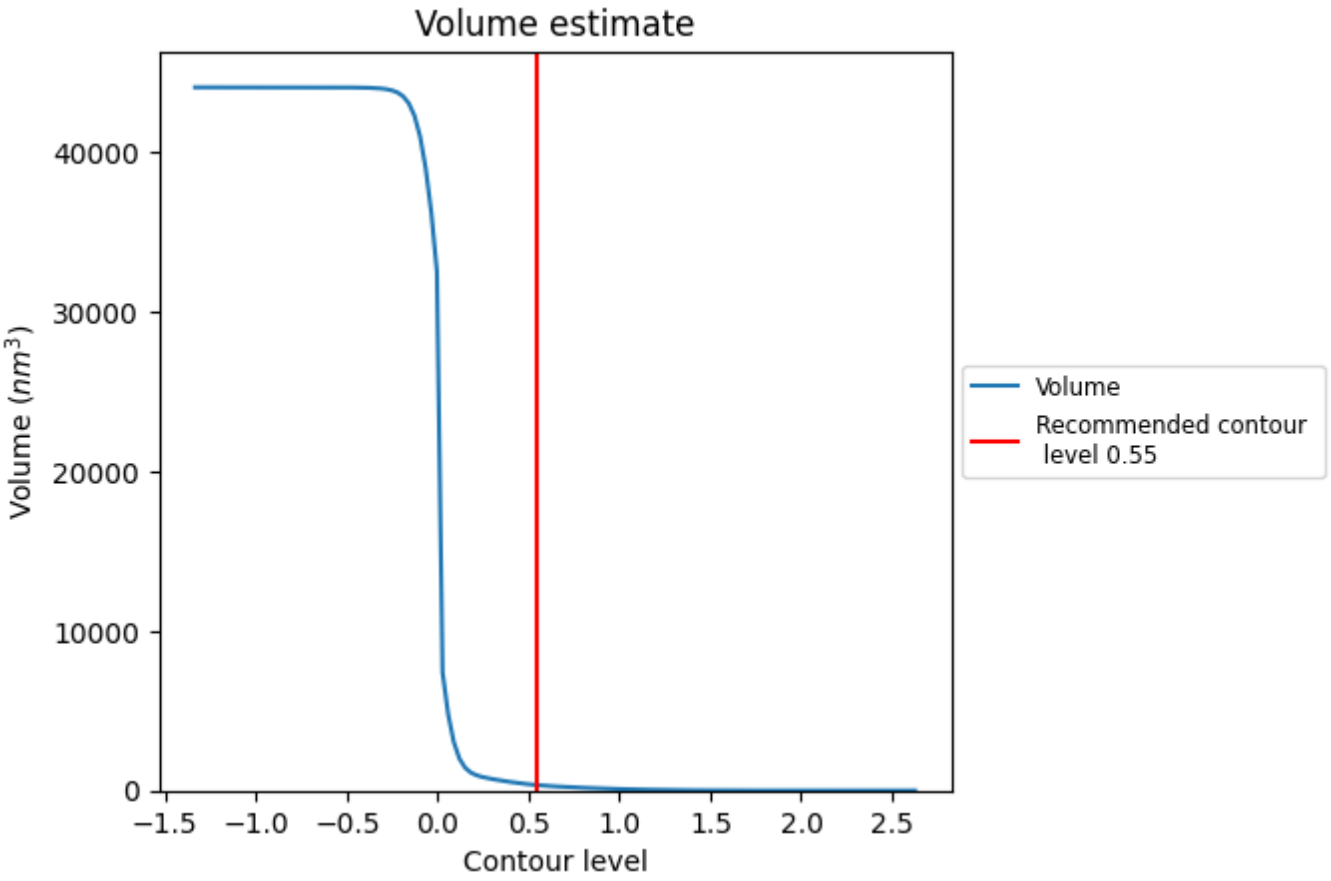
This section contains the results of statistical analysis of the map.

7.1 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.

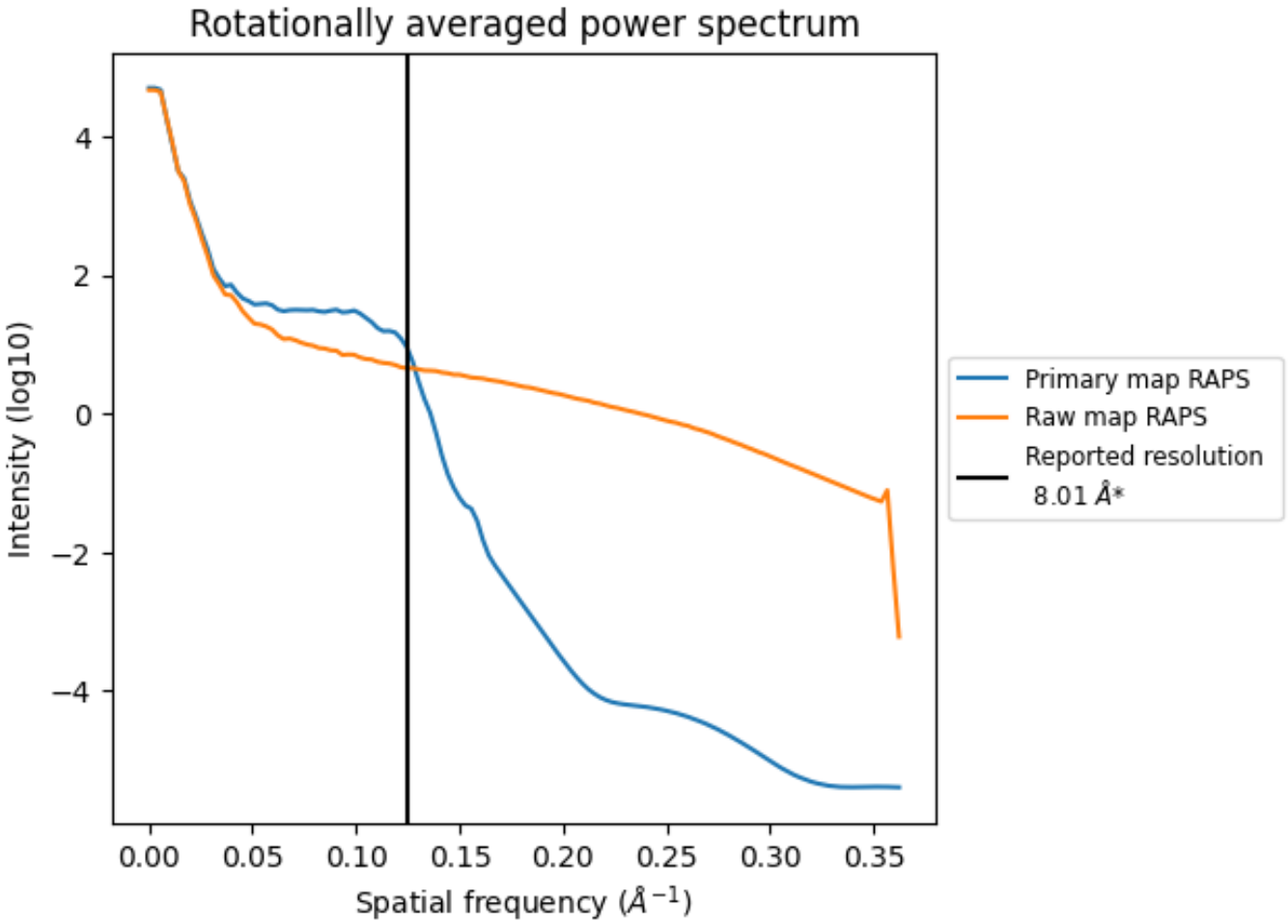
7.2 Volume estimate (i)



The volume at the recommended contour level is 339 nm^3; this corresponds to an approximate mass of 307 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)

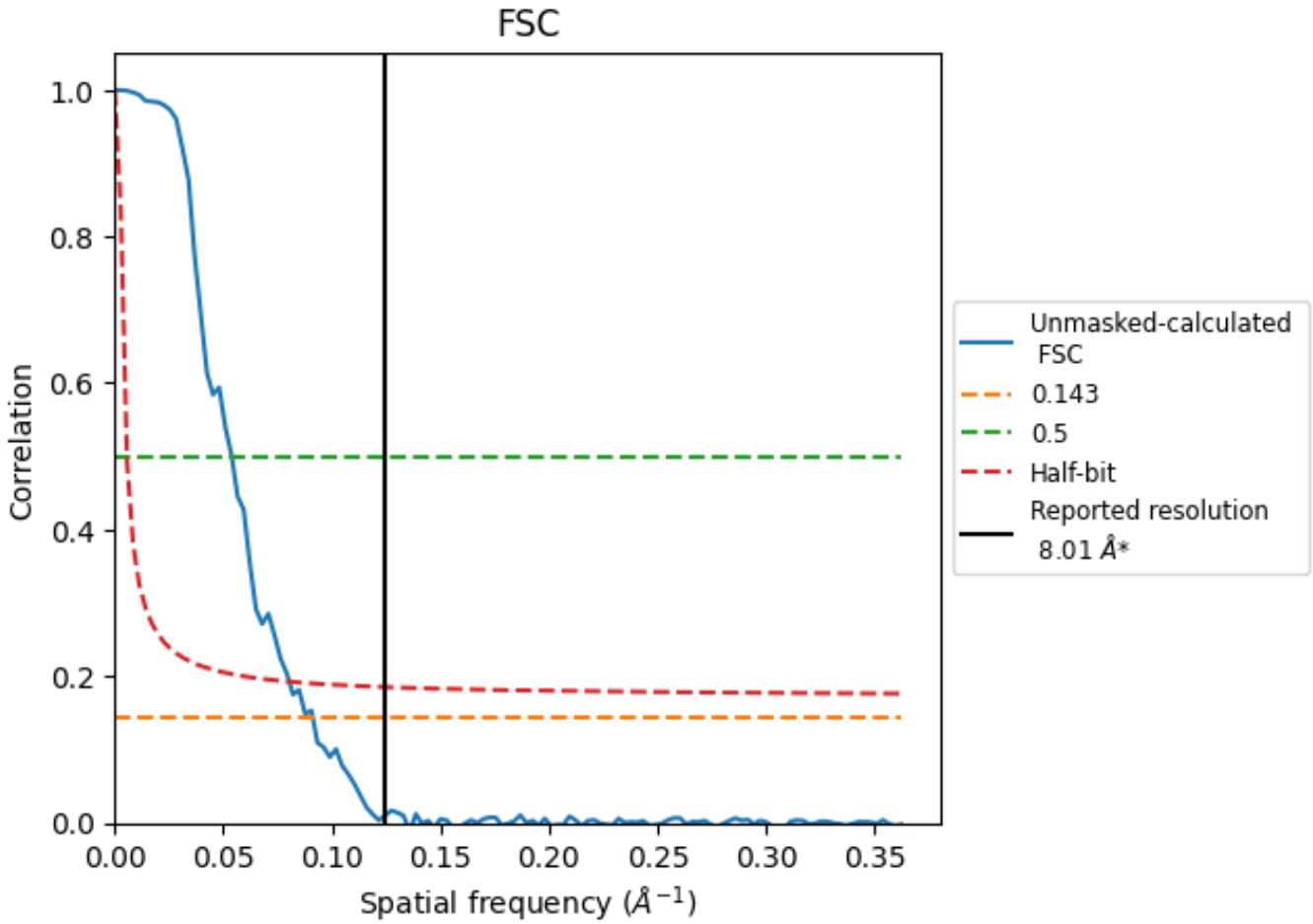


*Reported resolution corresponds to spatial frequency of 0.125 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.125 Å^{-1}

8.2 Resolution estimates (i)

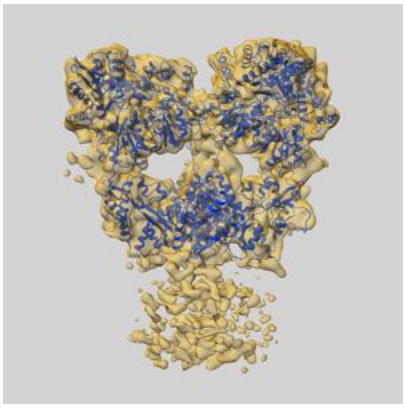
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.01	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.96	18.55	12.45

*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 10.96 differs from the reported value 8.01 by more than 10 %

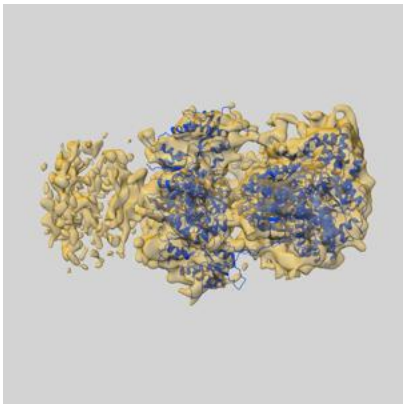
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34083 and PDB model 7YSV. Per-residue inclusion information can be found in section 3 on page 5.

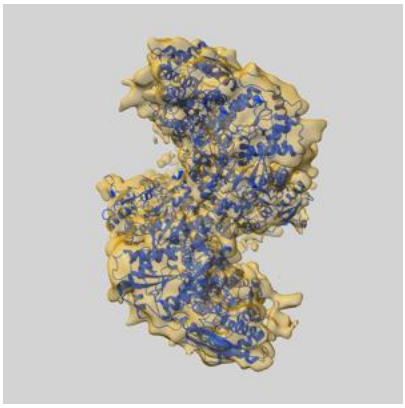
9.1 Map-model overlay



X



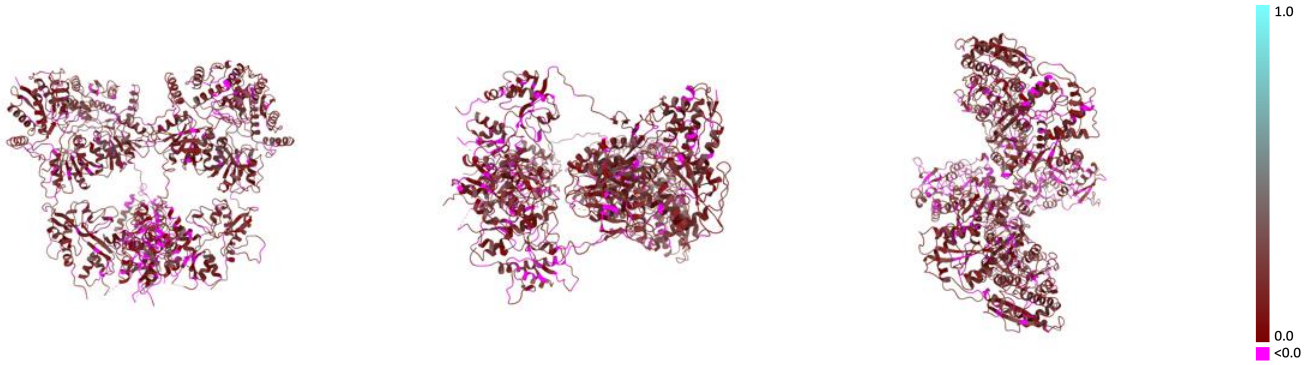
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55 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.

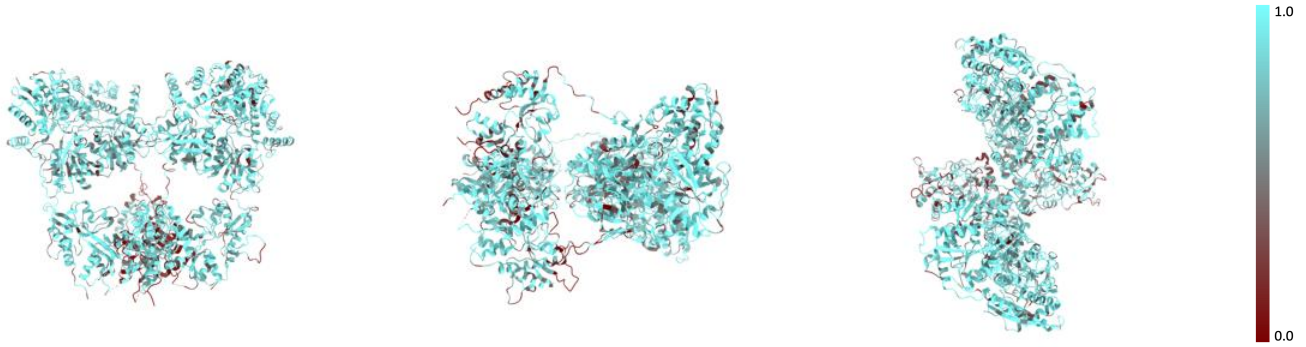
9.2 Q-score mapped to coordinate model (i)



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.

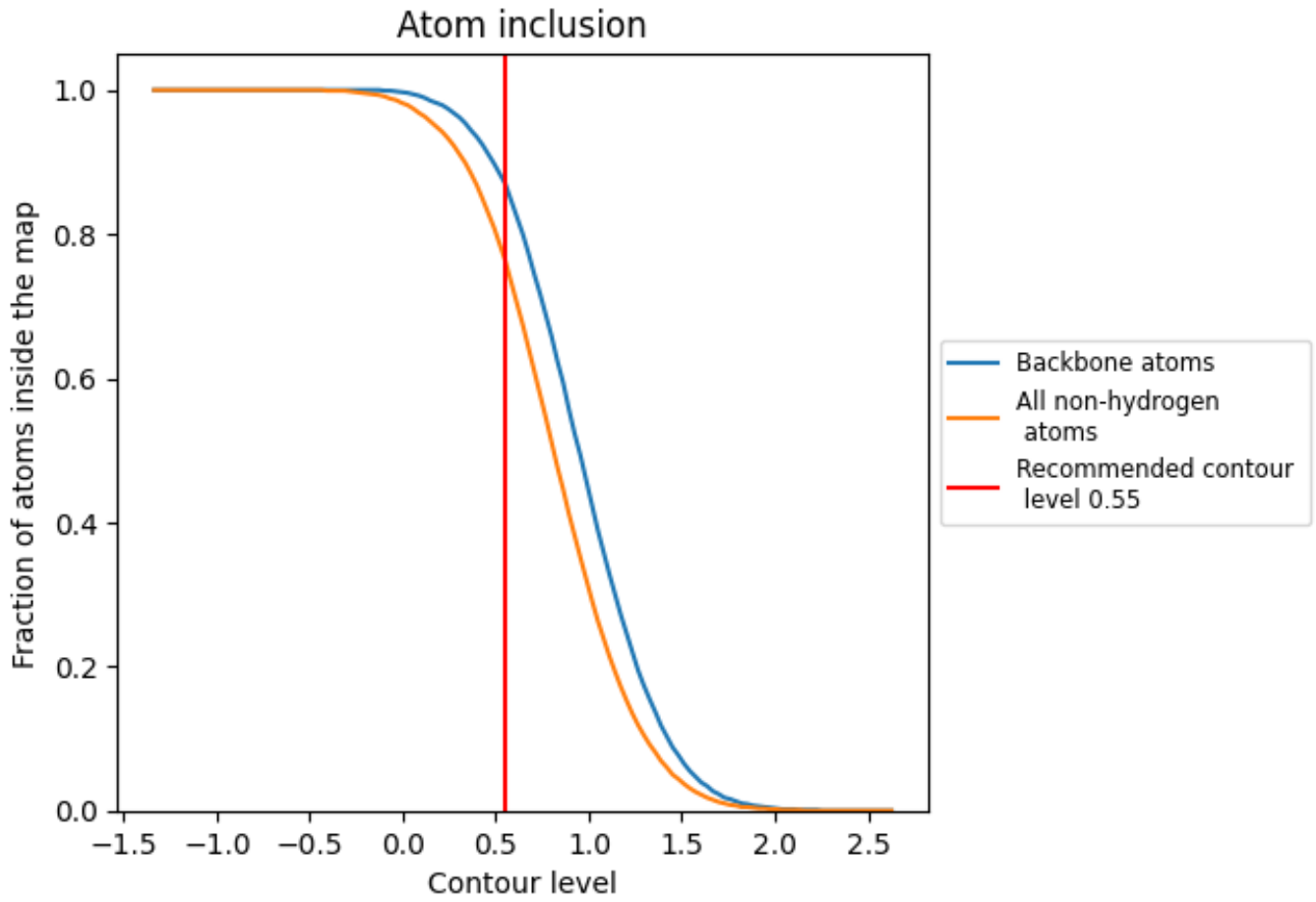
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.55).

9.4 Atom inclusion (i)



At the recommended contour level, 87% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7640	0.1320
A	0.8120	0.1510
B	0.7400	0.1250
C	0.7700	0.1400
D	0.7330	0.1140