



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:49 PM UTC

PDB ID : 8U26 / pdb_00008u26
EMDB ID : EMD-41840
Title : Gaussian Mixture Models based single particle refinement - GPCR (Substance P bound to active human neurokinin 1 receptor in complex with miniGs399 from EMPIAR-10786)
Authors : Chen, M.; Pintilie, G.
Deposited on : 2023-09-05
Resolution : 2.50 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

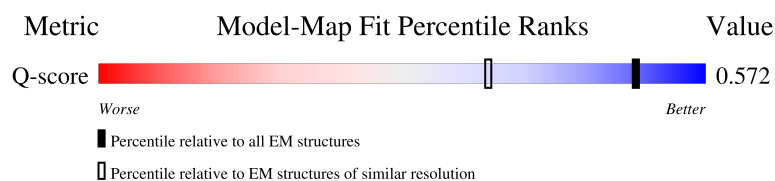
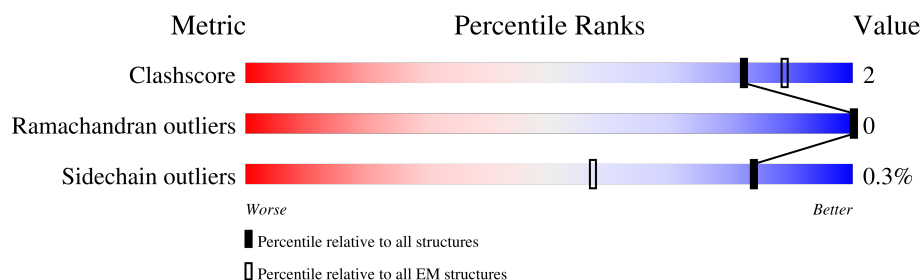
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	248	
2	B	370	
3	G	68	
4	N	142	

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Mol	Chain	Length	Quality of chain
5	R	418	 61% 7% 32%
6	S	11	 91% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14468 atoms, of which 7032 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 Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	216	3217	1071	1552	305	282	7	0	0

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ASN	-	expression tag	UNP P63092
A	7	SER	-	expression tag	UNP P63092
A	8	LYS	-	expression tag	UNP P63092
A	9	THR	-	expression tag	UNP P63092
A	10	GLU	-	expression tag	UNP P63092
A	11	ASP	-	expression tag	UNP P63092
A	12	GLN	-	expression tag	UNP P63092
A	13	ARG	-	expression tag	UNP P63092
A	14	ASN	-	expression tag	UNP P63092
A	15	GLU	-	expression tag	UNP P63092
A	16	GLU	-	expression tag	UNP P63092
A	17	LYS	-	expression tag	UNP P63092
A	18	ALA	-	expression tag	UNP P63092
A	19	GLN	-	expression tag	UNP P63092
A	20	ARG	-	expression tag	UNP P63092
A	21	GLU	-	expression tag	UNP P63092
A	22	ALA	-	expression tag	UNP P63092
A	23	ASN	-	expression tag	UNP P63092
A	24	LYS	-	expression tag	UNP P63092
A	25	LYS	-	expression tag	UNP P63092
A	26	ILE	-	expression tag	UNP P63092
A	27	GLU	-	expression tag	UNP P63092
A	28	LYS	-	expression tag	UNP P63092
A	29	GLN	-	expression tag	UNP P63092
A	30	LEU	-	expression tag	UNP P63092
A	31	GLN	-	expression tag	UNP P63092
A	32	LYS	-	expression tag	UNP P63092

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Chain	Residue	Modelled	Actual	Comment	Reference
A	33	ASP	-	expression tag	UNP P63092
A	34	LYS	-	expression tag	UNP P63092
A	35	GLN	-	expression tag	UNP P63092
A	36	VAL	-	expression tag	UNP P63092
A	37	TYR	-	expression tag	UNP P63092
A	38	ARG	-	expression tag	UNP P63092
A	39	ALA	-	expression tag	UNP P63092
A	40	THR	-	expression tag	UNP P63092
A	41	HIS	-	expression tag	UNP P63092
A	42	ARG	-	expression tag	UNP P63092
A	43	LEU	-	expression tag	UNP P63092
A	44	LEU	-	expression tag	UNP P63092
A	45	LEU	-	expression tag	UNP P63092
A	46	LEU	-	expression tag	UNP P63092
A	47	GLY	-	expression tag	UNP P63092
A	48	ALA	-	expression tag	UNP P63092
A	49	ASP	-	expression tag	UNP P63092
A	50	ASN	-	expression tag	UNP P63092
A	51	SER	-	expression tag	UNP P63092
A	52	GLY	-	expression tag	UNP P63092
A	53	LYS	-	expression tag	UNP P63092
A	54	SER	-	expression tag	UNP P63092
A	55	THR	-	expression tag	UNP P63092
A	56	ILE	-	expression tag	UNP P63092
A	57	VAL	-	expression tag	UNP P63092
A	58	LYS	-	expression tag	UNP P63092
A	59	GLN	-	expression tag	UNP P63092
A	60	MET	-	expression tag	UNP P63092
A	61	ARG	-	expression tag	UNP P63092
A	193	ILE	-	expression tag	UNP P63092
A	194	LEU	-	expression tag	UNP P63092
A	195	HIS	-	expression tag	UNP P63092
A	196	GLY	-	expression tag	UNP P63092
A	197	GLY	-	expression tag	UNP P63092
A	198	SER	-	expression tag	UNP P63092
A	199	GLY	-	expression tag	UNP P63092
A	200	GLY	-	expression tag	UNP P63092
A	201	SER	-	expression tag	UNP P63092
A	202	GLY	-	expression tag	UNP P63092
A	203	GLY	-	expression tag	UNP P63092
A	249	ASP	ALA	conflict	UNP P63092
A	252	ASP	SER	conflict	UNP P63092

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP P63092
A	?	-	MET	deletion	UNP P63092
A	?	-	VAL	deletion	UNP P63092
A	?	-	ILE	deletion	UNP P63092
A	?	-	ARG	deletion	UNP P63092
A	?	-	GLU	deletion	UNP P63092
A	?	-	ASP	deletion	UNP P63092
A	?	-	ASN	deletion	UNP P63092
A	?	-	GLN	deletion	UNP P63092
A	?	-	THR	deletion	UNP P63092
A	372	ALA	ILE	conflict	UNP P63092
A	375	ILE	VAL	conflict	UNP P63092

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	322	Total	C	H	N	O	S	0	0
			4476	1459	2154	409	436	18		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-29	MET	-	initiating methionine	UNP P62873
B	-28	HIS	-	expression tag	UNP P62873
B	-27	HIS	-	expression tag	UNP P62873
B	-26	HIS	-	expression tag	UNP P62873
B	-25	HIS	-	expression tag	UNP P62873
B	-24	HIS	-	expression tag	UNP P62873
B	-23	HIS	-	expression tag	UNP P62873
B	-22	LEU	-	expression tag	UNP P62873
B	-21	GLU	-	expression tag	UNP P62873
B	-20	VAL	-	expression tag	UNP P62873
B	-19	LEU	-	expression tag	UNP P62873
B	-18	PHE	-	expression tag	UNP P62873
B	-17	GLN	-	expression tag	UNP P62873
B	-16	GLY	-	expression tag	UNP P62873
B	-15	PRO	-	expression tag	UNP P62873
B	-14	GLU	-	expression tag	UNP P62873
B	-13	ASP	-	expression tag	UNP P62873
B	-12	GLN	-	expression tag	UNP P62873
B	-11	VAL	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	ASP	-	expression tag	UNP P62873
B	-9	PRO	-	expression tag	UNP P62873
B	-8	ARG	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873
B	-6	ILE	-	expression tag	UNP P62873
B	-5	ASP	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	LYS	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	38	Total	C	H	N	O	S	0	0
			452	154	207	41	47	3		

- Molecule 4 is a protein called Nanobody 35.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	N	115	Total	C	H	N	O	S	0	0
			1640	537	789	147	161	6		

- Molecule 5 is a protein called Substance-P receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	R	284	Total	C	H	N	O	S	0	0
			4522	1534	2253	351	364	20		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-10	ASP	-	expression tag	UNP P25103
R	-9	TYR	-	expression tag	UNP P25103
R	-8	LYS	-	expression tag	UNP P25103
R	-7	ASP	-	expression tag	UNP P25103
R	-6	ASP	-	expression tag	UNP P25103
R	-5	ASP	-	expression tag	UNP P25103
R	-4	ASP	-	expression tag	UNP P25103

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-3	ALA	-	expression tag	UNP P25103
R	-2	SER	-	expression tag	UNP P25103
R	-1	ILE	-	expression tag	UNP P25103
R	0	ASP	-	expression tag	UNP P25103

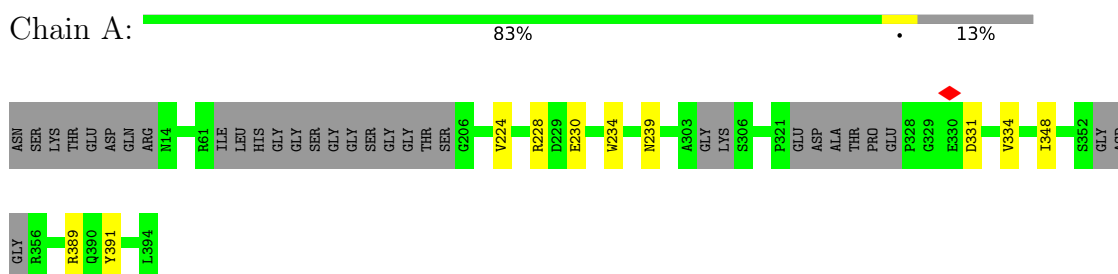
- Molecule 6 is a protein called Protachykinin-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	S	11	Total	C	H	N	O	S	0	0
			161	57	77	13	13	1		

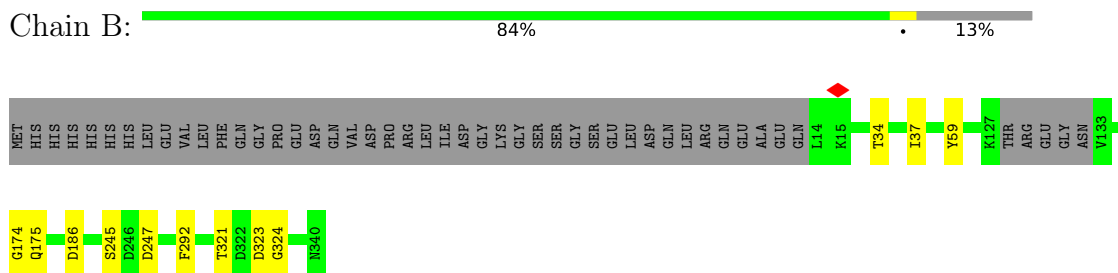
3 Residue-property plots [i](#)

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.

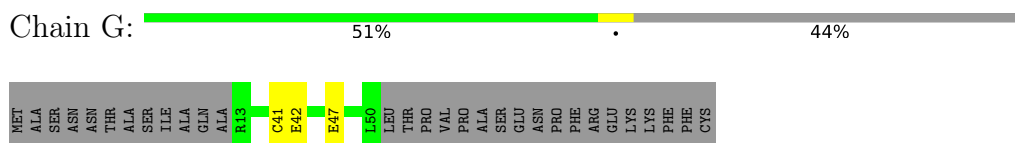
- Molecule 1: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



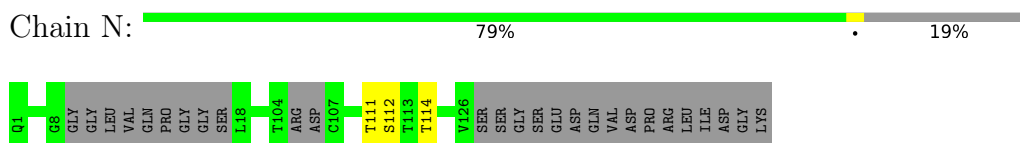
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 4: Nanobody 35



- Molecule 5: Substance-P receptor

THR	LEU	P112	ASP
MET	GLU	V116	TVR
THR	MET		LYS
GLU	LYS		ASP
SER	SER	R141	ASP
PHE	THR	L142	ASP
SER	ARG		ALA
PHE	ARG	T145	SER
SER	LEU		ILE
SER	LEU	V149	ASP
ASN	GLN		ASP
VAL	THR	S169	MET
GLN	GLY		ASN
GLY	GLY	E172	ASP
SER	SER		VAL
VAL	VAL		LEU
THR	TVR	P175	PRO
LYS	LYS	S176	VAL
VAL	VAL		ASP
SER	SER	Y216	SER
ARG	ARG		ASP
LEU	LEU	W224	ASP
GLU	GLU	ALA	LEU
THR	THR	SER	SER
THR	THR	GLU	PRO
ILE	ILE	ILE	ASN
SER	SER	PRO	ILE
THR	THR	GLY	SER
VAL	VAL	ASP	THR
VAL	VAL	SER	ASN
GLY	GLY	SER	THR
ALA	ALA	ASP	SER
HIS	HIS	ARG	GLU
GLU	GLU	THR	PRO
GLU	GLU	HIS	N23
PRO	PRO	GLU	
GLU	GLU	Q239	V41
ASP	ASP		T45
GLY	GLY	M249	
PRO	PRO	M250	V48
LYS	LYS	K280	
ALA	ALA		V52
THR	THR	T283	
PRO	PRO		I57
SER	SER	T298	
SER	SER		M63
LEU	LEU	F320	
ASP	ASP	ARG	N68
LEU	LEU	CYS	
THR	THR	CYS	V72
SER	SER	PRO	
ASN	ASN	PHE	E78
ILE	ILE	ILE	
SER	SER	SER	M61
ALA	ALA	ALA	
ARG	ARG	GLY	N96
SER	SER	ASP	
ASP	ASP	THR	C105
THR	THR	GLU	
LYS	LYS	GLY	F111

Chain S: 91% 9%

A diagram showing three vertical bars labeled R1, F7, and M11. R1 and M11 are green, and F7 is yellow. They are connected by horizontal lines, suggesting a sequence or relationship between the three components.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	288659	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	31.966	Depositor
Minimum map value	-17.381	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3	Depositor
Map size ($\text{\AA}$)	275.04, 275.04, 275.04	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.146, 1.146, 1.146	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	0.12	0/1698	0.27	0/2299
2	B	0.11	0/2368	0.29	0/3229
3	G	0.15	0/247	0.26	0/339
4	N	0.11	0/868	0.30	0/1178
5	R	0.15	0/2345	0.35	0/3219
6	S	0.19	0/87	0.48	0/117
All	All	0.13	0/7613	0.31	0/10381

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	1665	1552	1548	7	0
2	B	2322	2154	2152	9	0
3	G	245	207	206	2	0
4	N	851	789	787	2	0
5	R	2269	2253	2251	18	0
6	S	84	77	77	1	0
All	All	7436	7032	7021	36	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 2.

The worst 5 of 36 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)
5:R:175:PRO:O	5:R:176:SER:OG	2.03	0.75
1:A:228:ARG:NH2	1:A:230:GLU:OE2	2.21	0.73
2:B:321:THR:HG23	2:B:324:GLY:H	1.61	0.65
5:R:96:ASN:ND2	6:S:7:PHE:O	2.33	0.61
2:B:245:SER:OG	2:B:247:ASP:OD1	2.19	0.60

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	206/248 (83%)	199 (97%)	7 (3%)	0	100	100
2	B	318/370 (86%)	311 (98%)	7 (2%)	0	100	100
3	G	36/68 (53%)	36 (100%)	0	0	100	100
4	N	109/142 (77%)	106 (97%)	3 (3%)	0	100	100
5	R	280/418 (67%)	273 (98%)	7 (2%)	0	100	100
6	S	9/11 (82%)	6 (67%)	3 (33%)	0	100	100
All	All	958/1257 (76%)	931 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	154/219 (70%)	153 (99%)	1 (1%)	78	91
2	B	225/309 (73%)	224 (100%)	1 (0%)	84	93
3	G	18/56 (32%)	18 (100%)	0	100	100
4	N	85/118 (72%)	85 (100%)	0	100	100
5	R	237/374 (63%)	237 (100%)	0	100	100
6	S	8/10 (80%)	8 (100%)	0	100	100
All	All	727/1086 (67%)	725 (100%)	2 (0%)	84	94

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

Mol	Chain	Res	Type
1	A	348	ILE
2	B	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	266	HIS
4	N	123	GLN
5	R	165	GLN
5	R	89	ASN
1	A	387	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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.

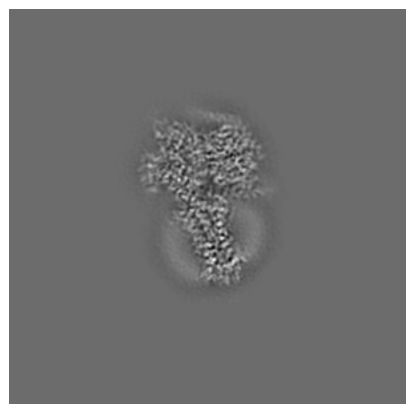
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41840. These allow visual inspection of the internal detail of the map and identification of artifacts.

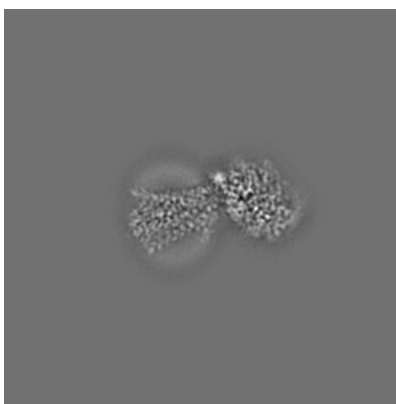
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

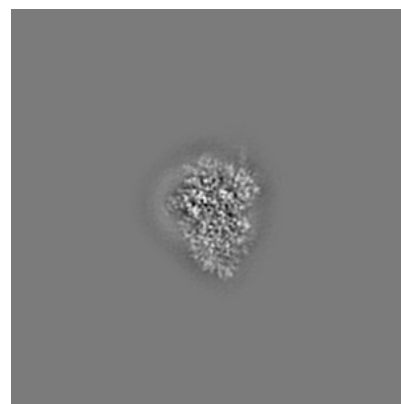
6.1.1 Primary map



X

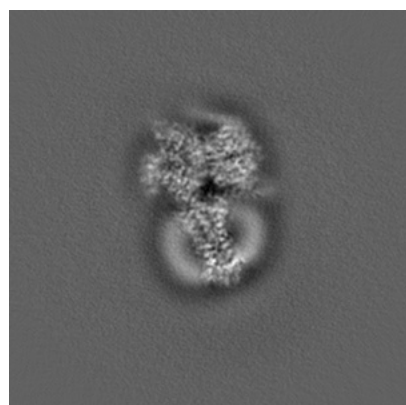


Y

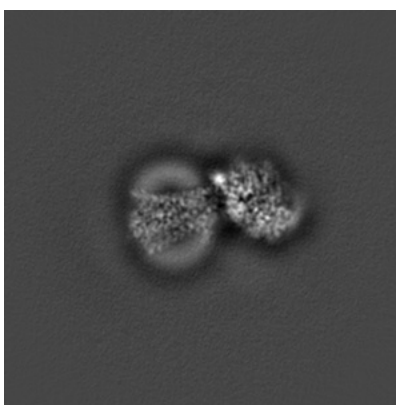


Z

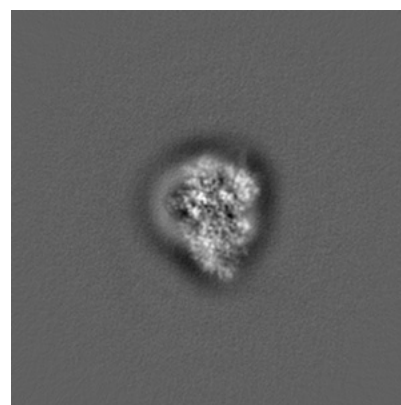
6.1.2 Raw map



X



Y

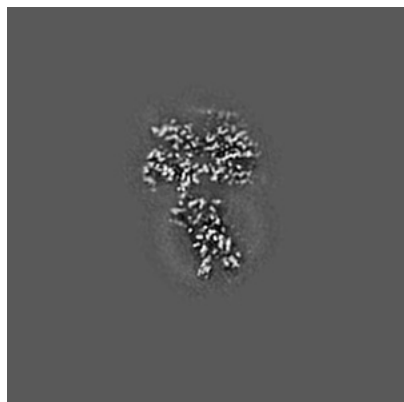


Z

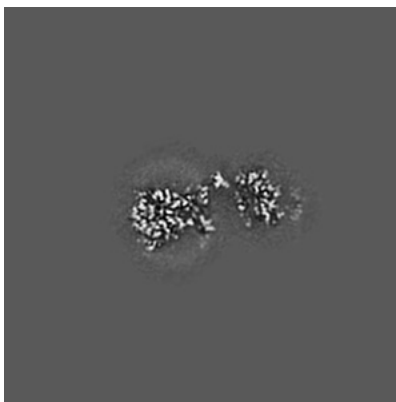
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

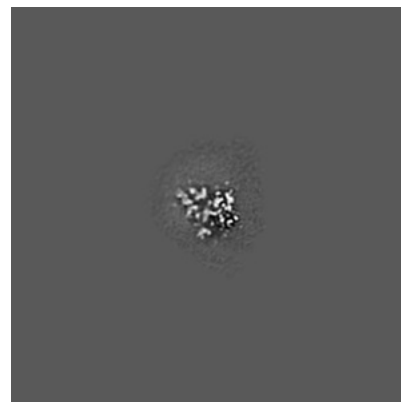
6.2.1 Primary map



X Index: 120

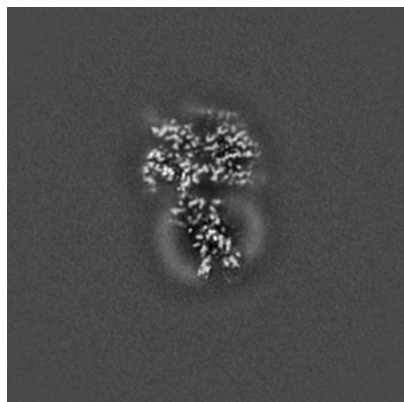


Y Index: 120

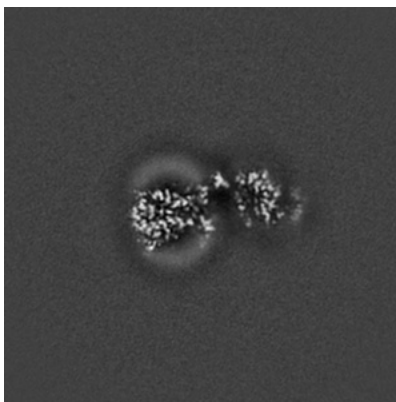


Z Index: 120

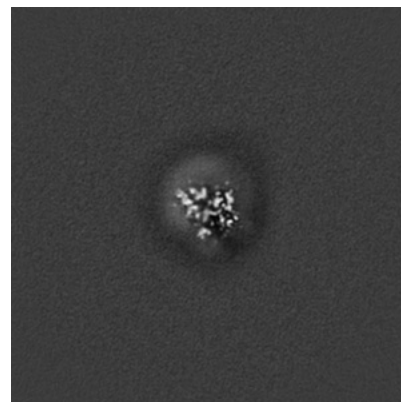
6.2.2 Raw map



X Index: 120



Y Index: 120

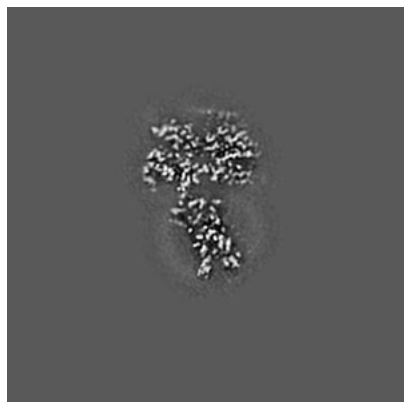


Z Index: 120

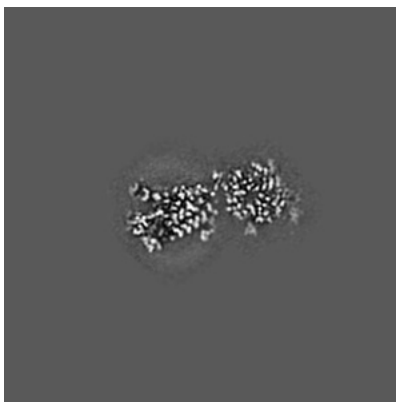
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 120

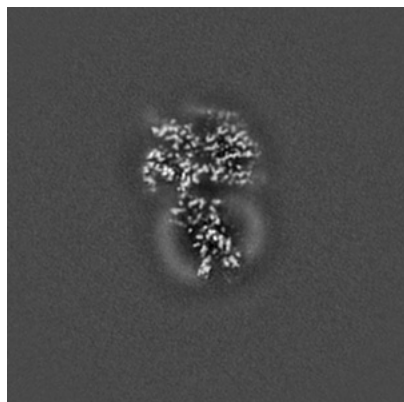


Y Index: 126

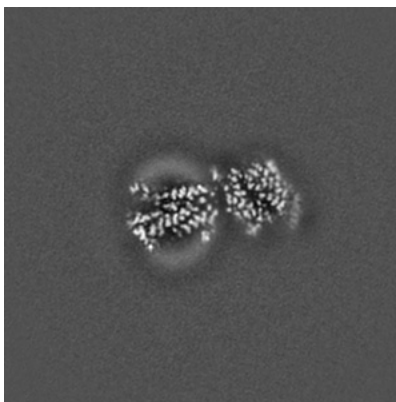


Z Index: 143

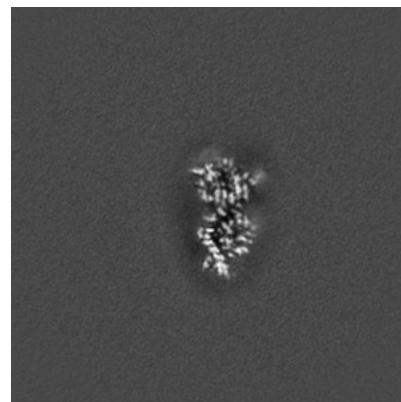
6.3.2 Raw map



X Index: 120



Y Index: 127

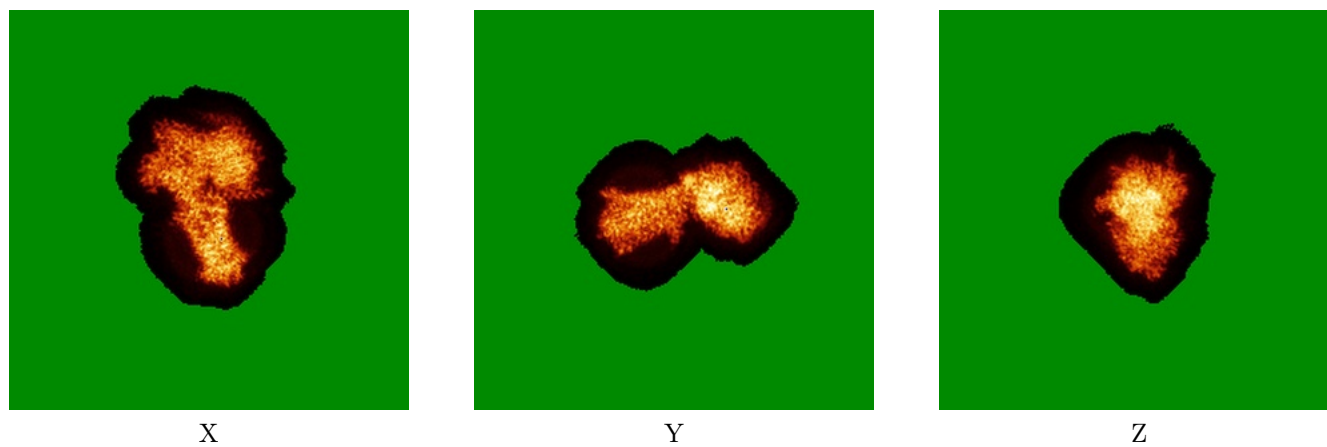


Z Index: 139

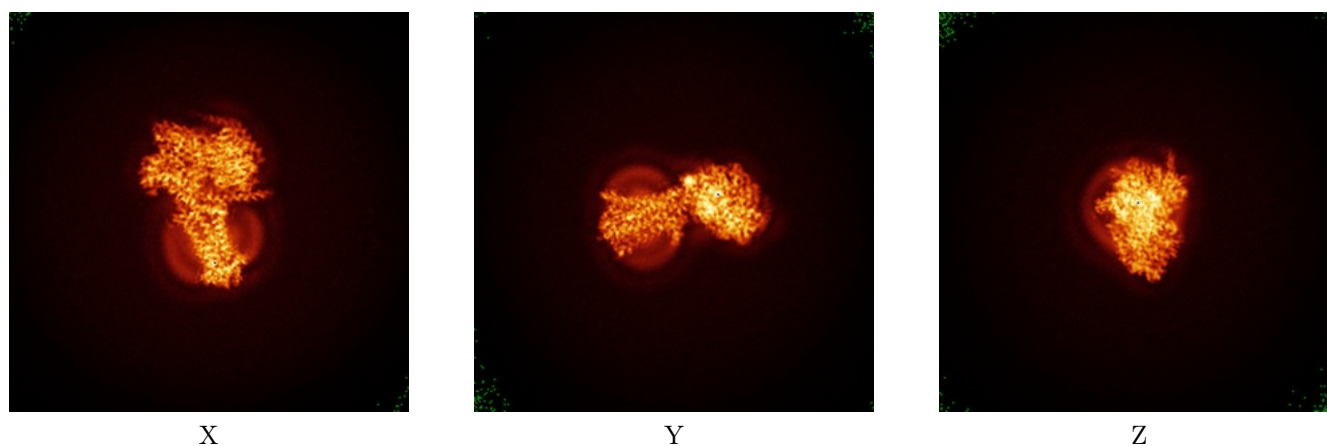
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

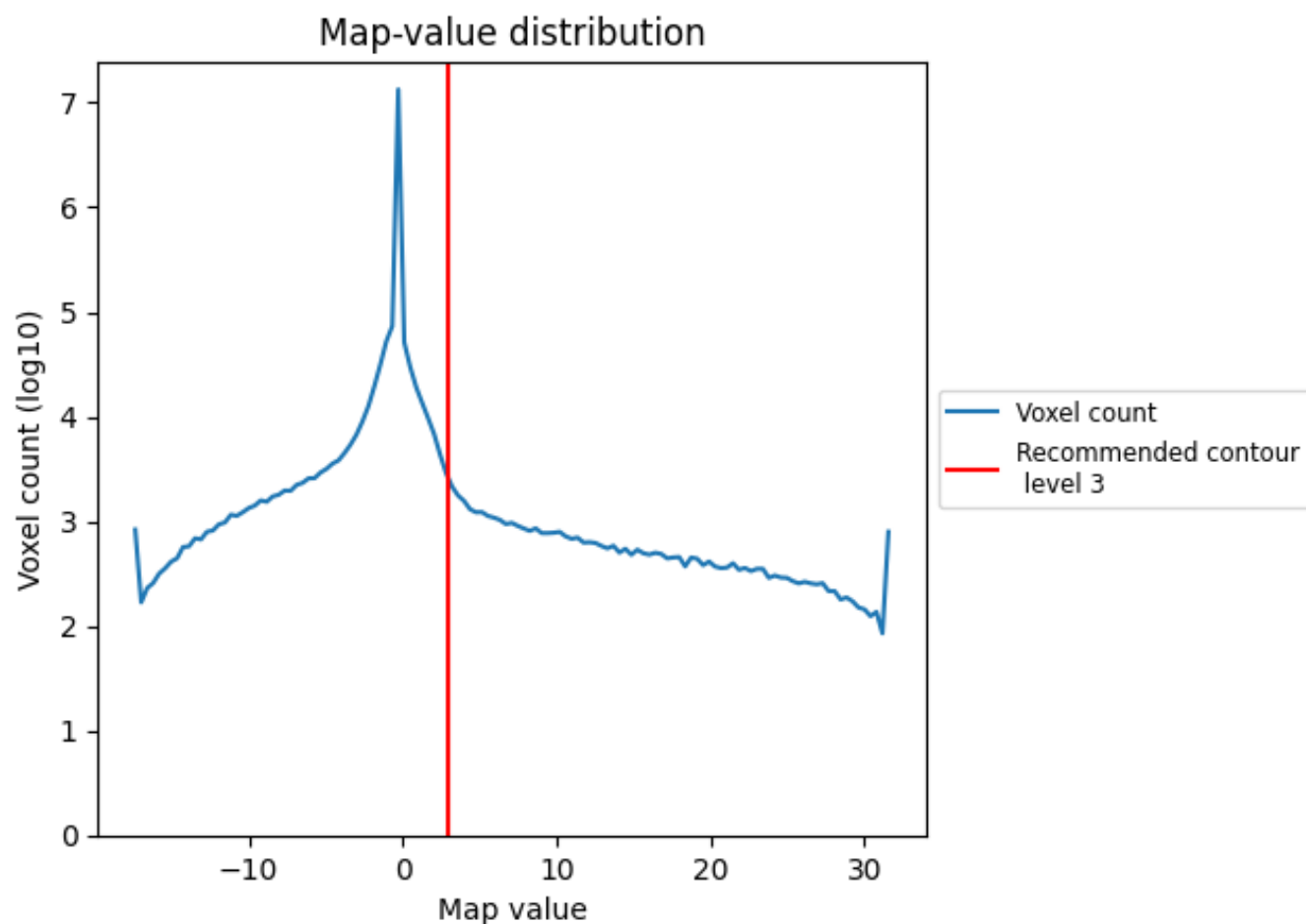
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

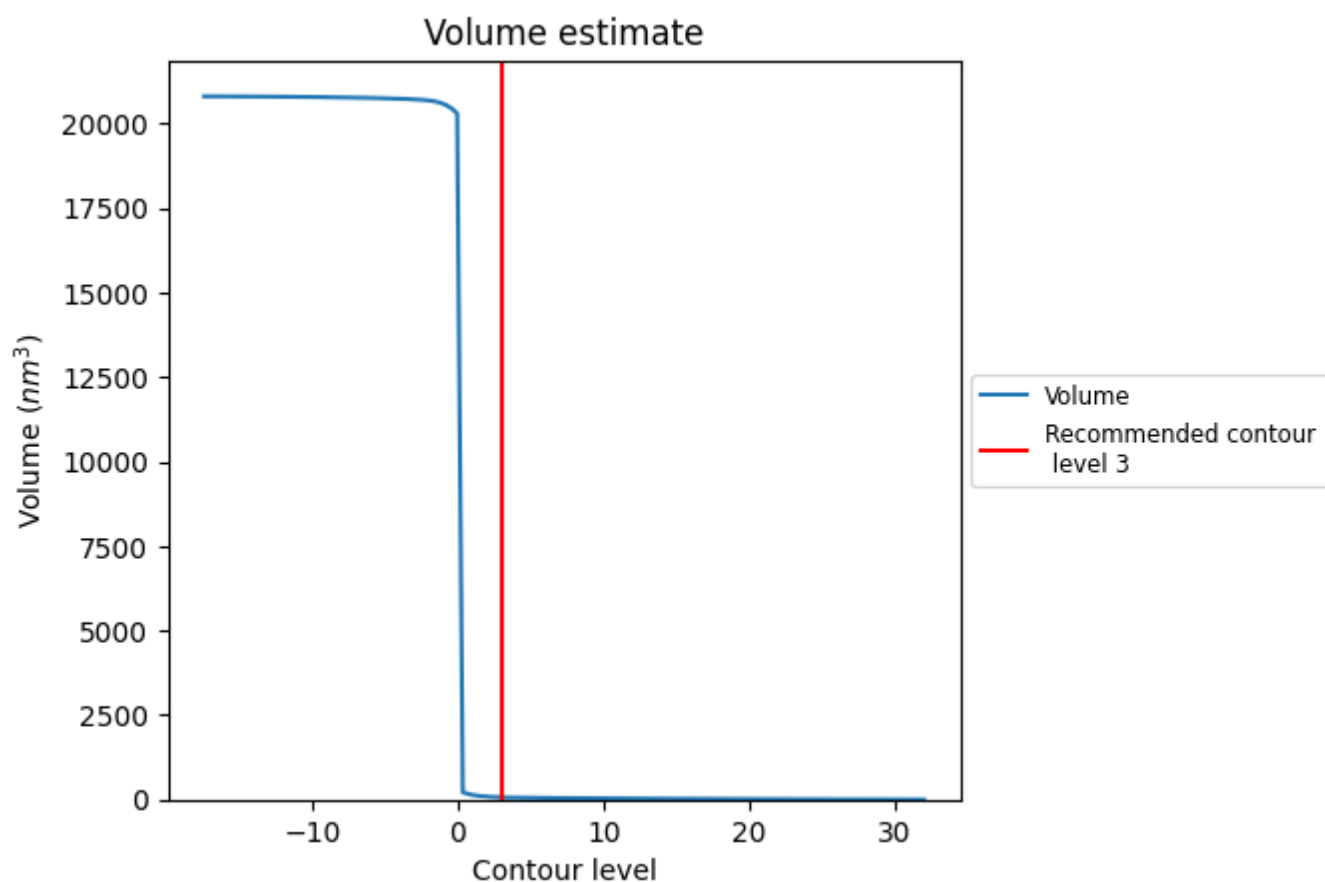
This section contains the results of statistical analysis of the map.

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.

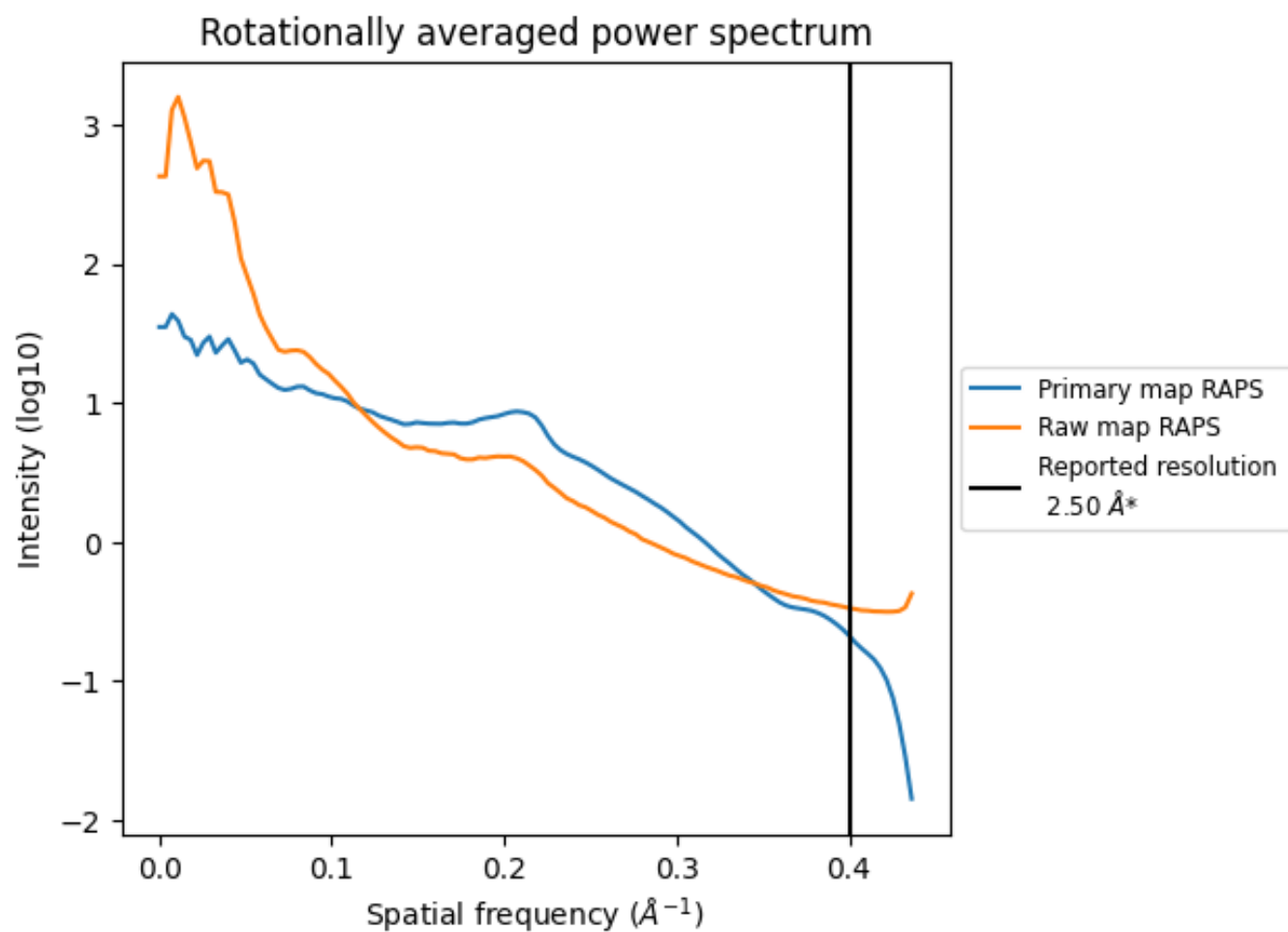
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 66 nm^3 ; this corresponds to an approximate mass of 60 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 ⓘ

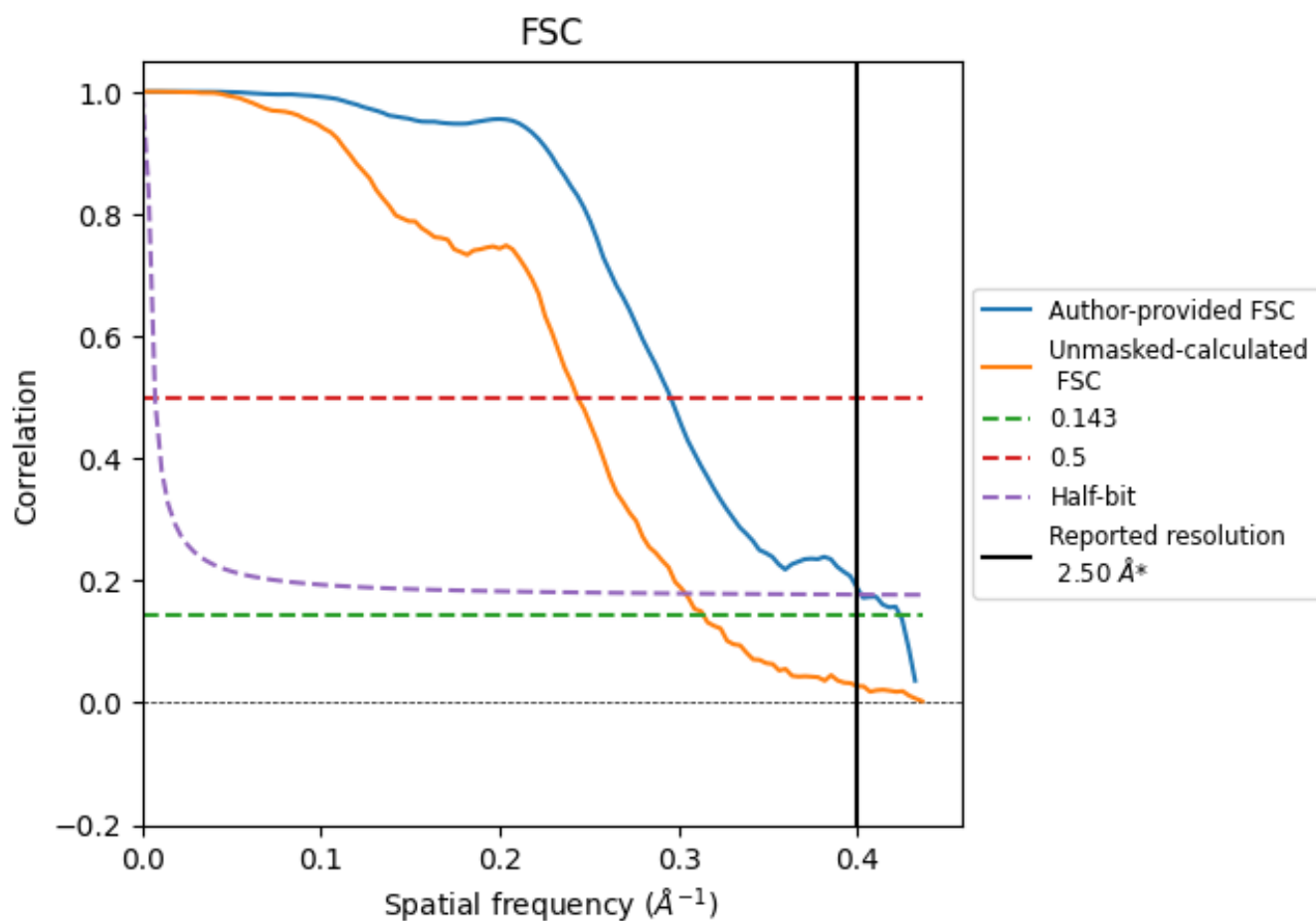


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.36	3.38	2.49
Unmasked-calculated*	3.18	4.11	3.29

*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 3.18 differs from the reported value 2.5 by more than 10 %

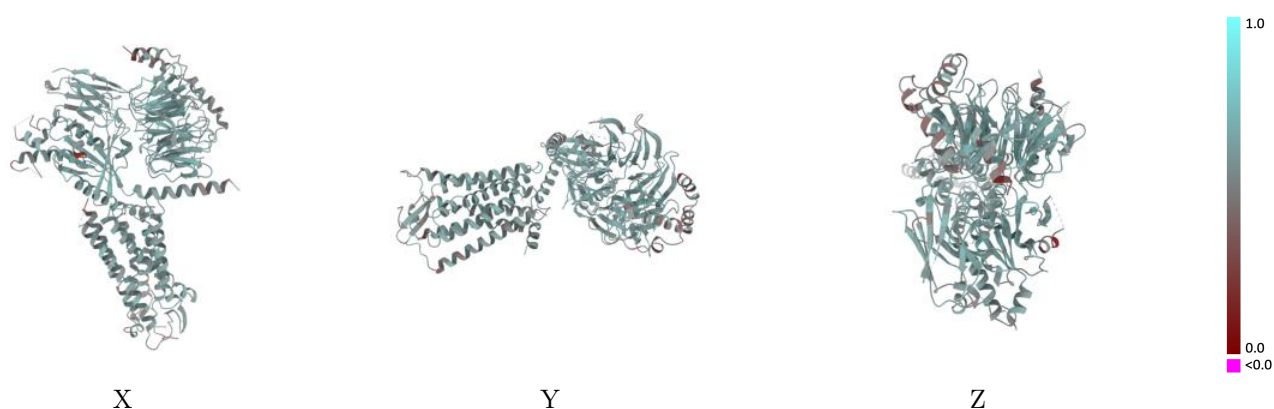
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41840 and PDB model 8U26. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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

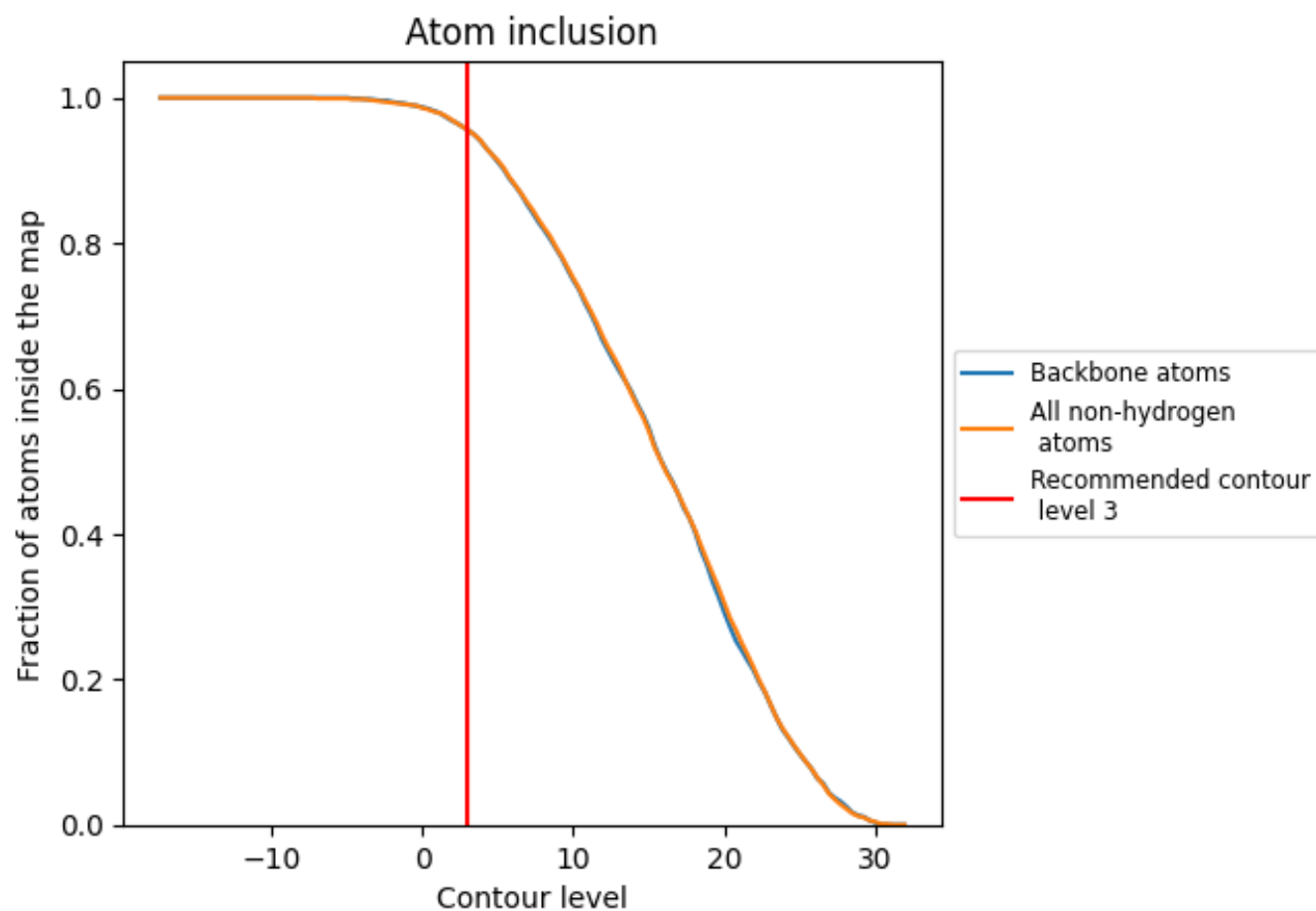


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9560	0.5720
A	0.9680	0.5790
B	0.9610	0.5850
G	0.8360	0.4840
N	0.9660	0.5840
R	0.9520	0.5620
S	0.8930	0.5070

1.0

0.0

<0.0