



wwPDB EM Validation Summary Report ⓘ

Oct 19, 2024 – 11:45 PM EDT

PDB ID : 6Q2N
EMDB ID : EMD-20575
Title : Cryo-EM structure of RET/GFRa1/GDNF extracellular complex
Authors : Li, J.; Shang, G.J.; Chen, Y.J.; Brautigam, C.A.; Liou, J.; Zhang, X.W.; Bai, X.C.
Deposited on : 2019-08-08
Resolution : 4.40 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.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

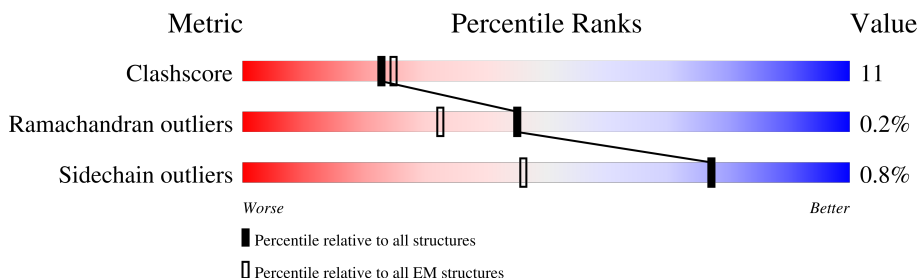
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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 $\leq 5\%$. 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	134	
1	B	134	
2	C	412	
2	D	412	
3	E	617	
3	F	617	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13140 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 Glial cell line-derived neurotrophic factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	86	Total	C	N	O	S	0	0
			659	413	113	126	7		
1	B	86	Total	C	N	O	S	0	0
			659	413	113	126	7		

- Molecule 2 is a protein called GDNF family receptor alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	200	Total	C	N	O	S	0	0
			1554	956	274	302	22		
2	D	200	Total	C	N	O	S	0	0
			1554	956	274	302	22		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	427	GLY	-	expression tag	UNP P56159
C	428	THR	-	expression tag	UNP P56159
C	429	HIS	-	expression tag	UNP P56159
C	430	HIS	-	expression tag	UNP P56159
C	431	HIS	-	expression tag	UNP P56159
C	432	HIS	-	expression tag	UNP P56159
C	433	HIS	-	expression tag	UNP P56159
C	434	HIS	-	expression tag	UNP P56159
C	435	HIS	-	expression tag	UNP P56159
C	436	HIS	-	expression tag	UNP P56159
D	427	GLY	-	expression tag	UNP P56159
D	428	THR	-	expression tag	UNP P56159
D	429	HIS	-	expression tag	UNP P56159
D	430	HIS	-	expression tag	UNP P56159
D	431	HIS	-	expression tag	UNP P56159
D	432	HIS	-	expression tag	UNP P56159
D	433	HIS	-	expression tag	UNP P56159

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Chain	Residue	Modelled	Actual	Comment	Reference
D	434	HIS	-	expression tag	UNP P56159
D	435	HIS	-	expression tag	UNP P56159
D	436	HIS	-	expression tag	UNP P56159

- Molecule 3 is a protein called Proto-oncogene tyrosine-protein kinase receptor Ret.

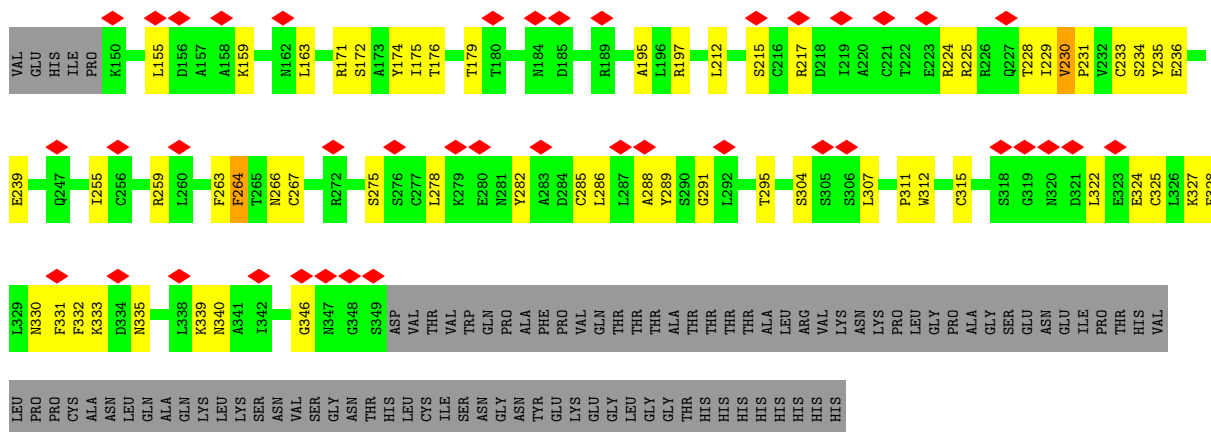
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	553	Total	C	N	O	S	0	0
			4353	2745	764	815	29		
3	F	553	Total	C	N	O	S	0	0
			4353	2745	764	815	29		

There are 22 discrepancies between the modelled and reference sequences:

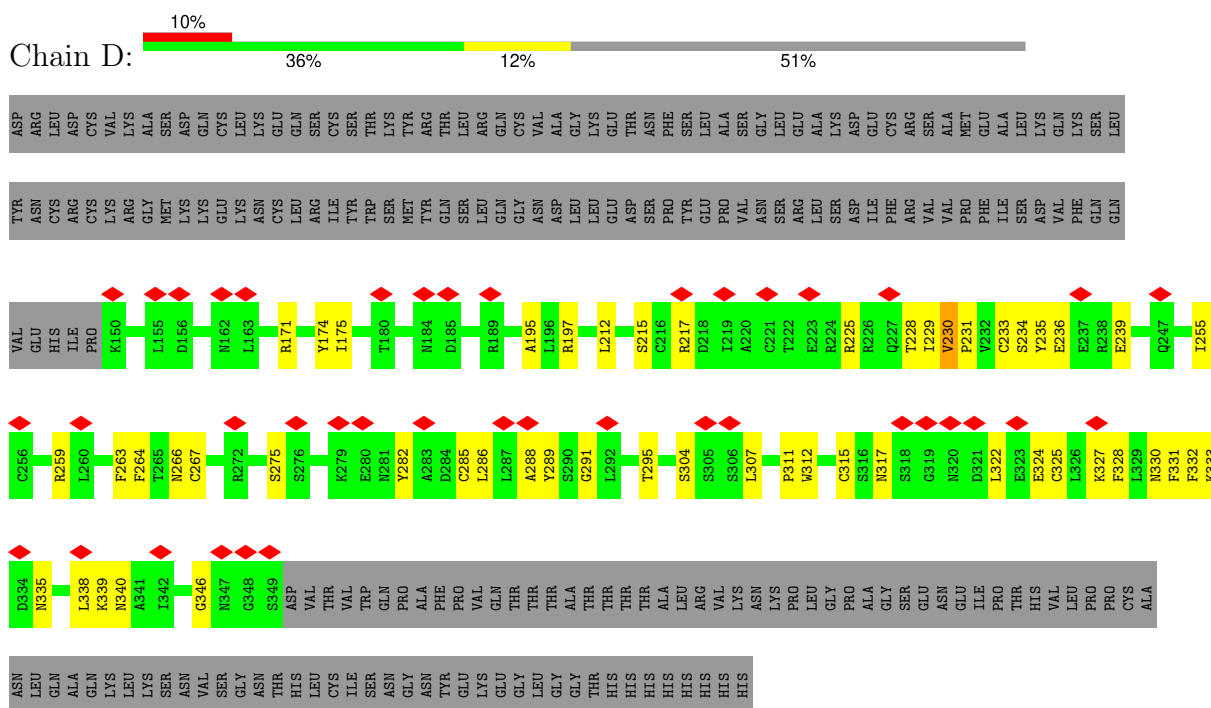
Chain	Residue	Modelled	Actual	Comment	Reference
E	114	HIS	ARG	conflict	UNP P07949
E	636	GLY	-	expression tag	UNP P07949
E	637	THR	-	expression tag	UNP P07949
E	638	HIS	-	expression tag	UNP P07949
E	639	HIS	-	expression tag	UNP P07949
E	640	HIS	-	expression tag	UNP P07949
E	641	HIS	-	expression tag	UNP P07949
E	642	HIS	-	expression tag	UNP P07949
E	643	HIS	-	expression tag	UNP P07949
E	644	HIS	-	expression tag	UNP P07949
E	645	HIS	-	expression tag	UNP P07949
F	114	HIS	ARG	conflict	UNP P07949
F	636	GLY	-	expression tag	UNP P07949
F	637	THR	-	expression tag	UNP P07949
F	638	HIS	-	expression tag	UNP P07949
F	639	HIS	-	expression tag	UNP P07949
F	640	HIS	-	expression tag	UNP P07949
F	641	HIS	-	expression tag	UNP P07949
F	642	HIS	-	expression tag	UNP P07949
F	643	HIS	-	expression tag	UNP P07949
F	644	HIS	-	expression tag	UNP P07949
F	645	HIS	-	expression tag	UNP P07949

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

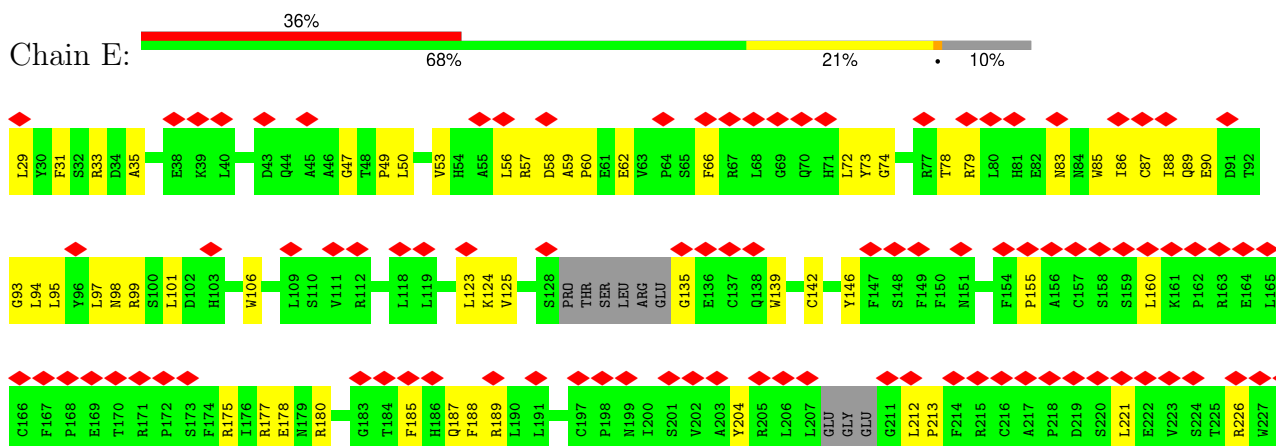
Mol	Chain	Residues	Atoms		AltConf
4	E	4	Total 4	Ca 4	0
4	F	4	Total 4	Ca 4	0

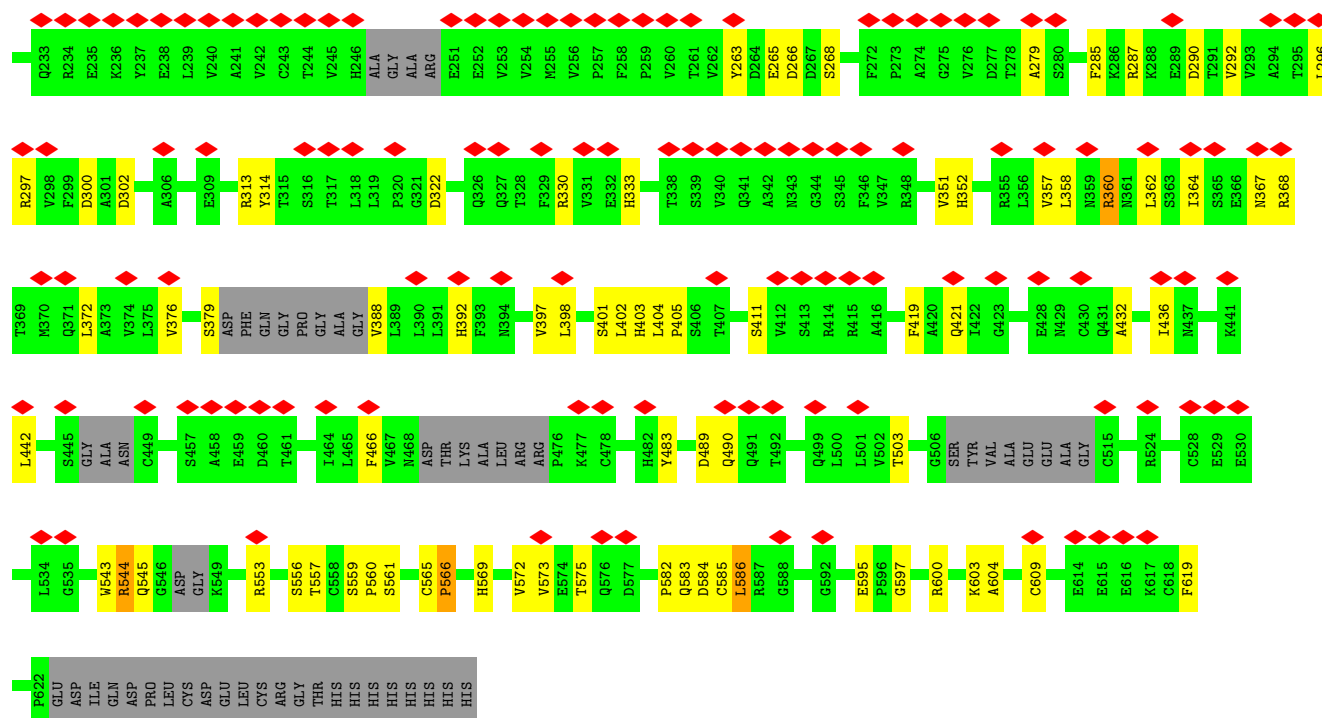


• Molecule 2: GDNF family receptor alpha-1

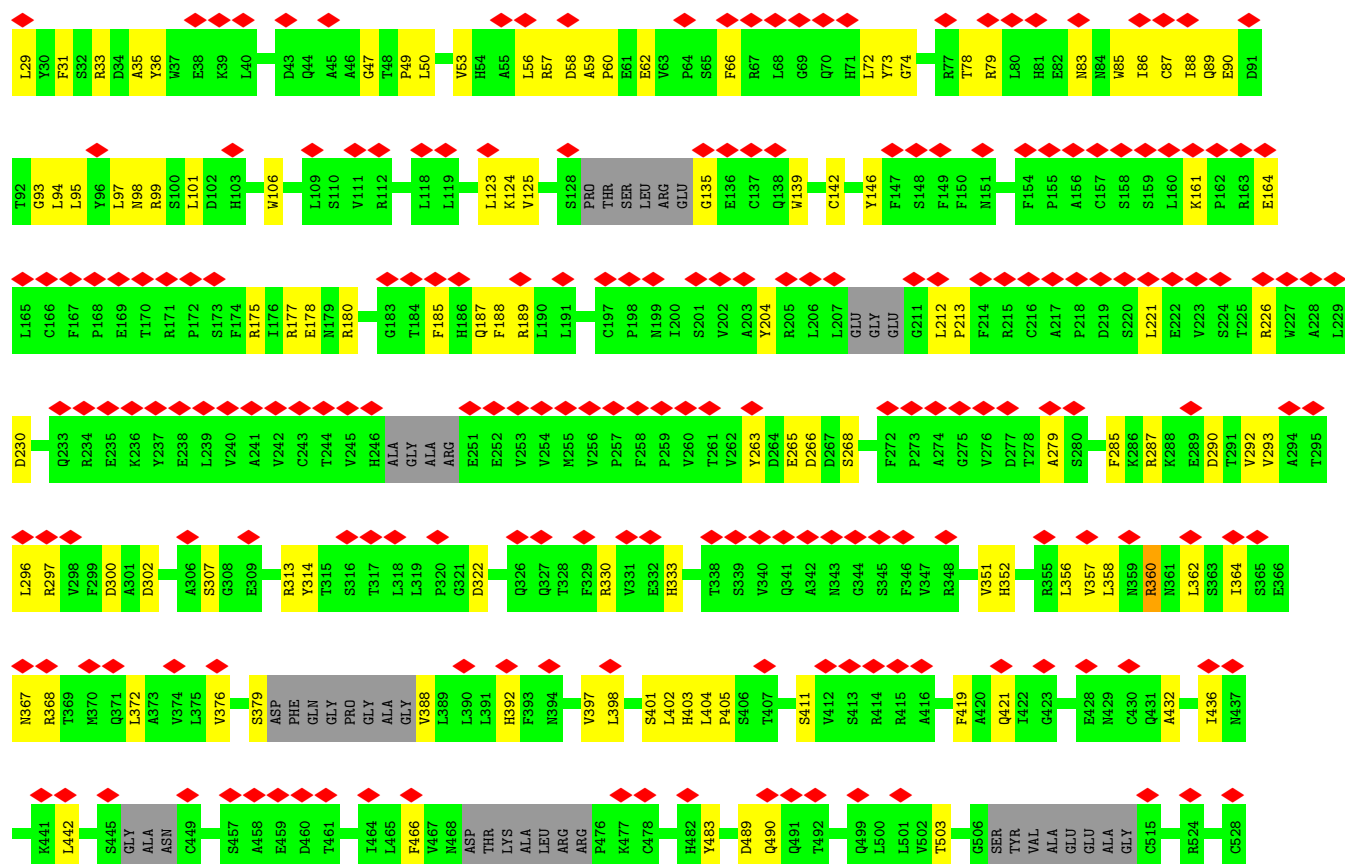


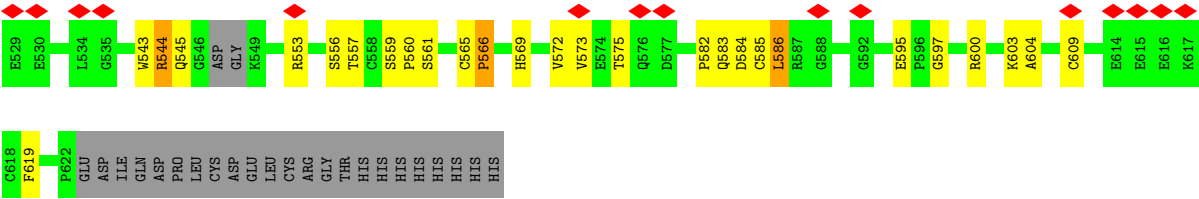
• Molecule 3: Proto-oncogene tyrosine-protein kinase receptor Ret





• Molecule 3: Proto-oncogene tyrosine-protein kinase receptor Ret





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37098	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	46729	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.097	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	235.40001, 235.40001, 235.40001	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.47	0/668	0.82	2/900 (0.2%)
1	B	0.47	0/668	0.82	2/900 (0.2%)
2	C	0.46	0/1581	0.68	0/2133
2	D	0.46	0/1581	0.68	0/2133
3	E	0.38	0/4454	0.63	1/6053 (0.0%)
3	F	0.38	0/4454	0.63	1/6053 (0.0%)
All	All	0.41	0/13406	0.66	6/18172 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	0	1
3	F	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	268	SER	C-N-CA	7.92	141.51	121.70
3	F	268	SER	C-N-CA	7.92	141.49	121.70
1	A	130	LEU	CA-CB-CG	5.98	129.05	115.30
1	B	130	LEU	CA-CB-CG	5.96	129.01	115.30
1	B	192	ASP	CB-CG-OD1	5.46	123.21	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	566	PRO	Peptide
3	F	566	PRO	Peptide

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	659	0	636	29	0
1	B	659	0	636	16	0
2	C	1554	0	1484	46	0
2	D	1554	0	1484	32	0
3	E	4353	0	4202	88	0
3	F	4353	0	4202	91	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
All	All	13140	0	12644	283	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 11.

The worst 5 of 283 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)
3:F:180:ARG:NH1	3:F:265:GLU:OE2	1.99	0.95
3:E:180:ARG:NH1	3:E:265:GLU:OE2	1.99	0.95
3:E:330:ARG:NH1	3:E:358:LEU:O	2.08	0.87
3:F:330:ARG:NH1	3:F:358:LEU:O	2.08	0.87
3:F:544:ARG:HH11	3:F:566:PRO:HB2	1.41	0.85

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	82/134 (61%)	73 (89%)	8 (10%)	1 (1%)	11	43
1	B	82/134 (61%)	73 (89%)	8 (10%)	1 (1%)	11	43
2	C	198/412 (48%)	177 (89%)	20 (10%)	1 (0%)	25	63
2	D	198/412 (48%)	177 (89%)	20 (10%)	1 (0%)	25	63
3	E	535/617 (87%)	485 (91%)	50 (9%)	0	100	100
3	F	535/617 (87%)	485 (91%)	50 (9%)	0	100	100
All	All	1630/2326 (70%)	1470 (90%)	156 (10%)	4 (0%)	45	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	GLU
1	B	153	GLU
2	D	230	VAL
2	C	230	VAL

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	72/113 (64%)	71 (99%)	1 (1%)	62	76
1	B	72/113 (64%)	71 (99%)	1 (1%)	62	76
2	C	179/369 (48%)	177 (99%)	2 (1%)	70	80
2	D	179/369 (48%)	177 (99%)	2 (1%)	70	80
3	E	487/537 (91%)	484 (99%)	3 (1%)	84	88
3	F	487/537 (91%)	484 (99%)	3 (1%)	84	88
All	All	1476/2038 (72%)	1464 (99%)	12 (1%)	77	85

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	217	ARG
2	D	264	PHE
3	F	586	LEU
3	F	360	ARG
3	E	360	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	153	ASN
2	D	340	ASN
3	F	421	GLN
2	D	266	ASN
3	F	83	ASN

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 ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

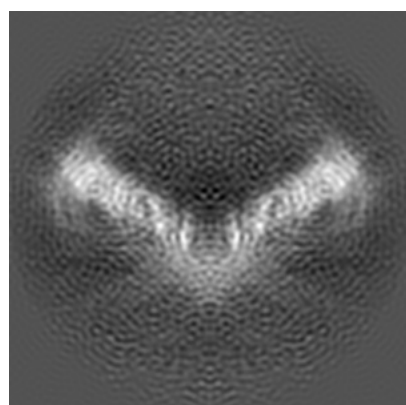
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20575. These allow visual inspection of the internal detail of the map and identification of artifacts.

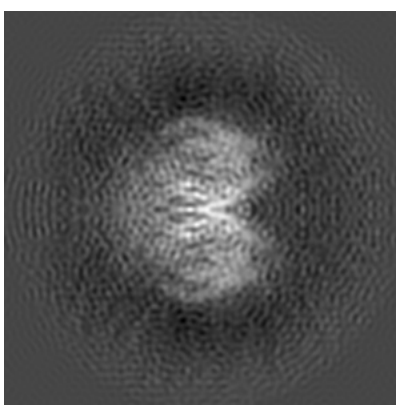
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

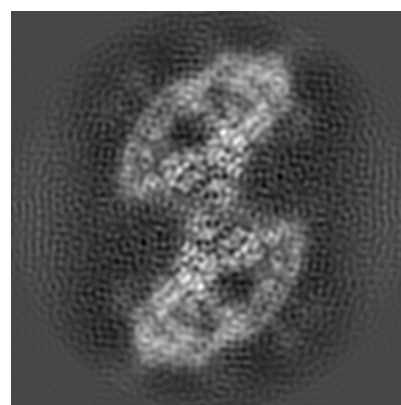
6.1.1 Primary map



X



Y

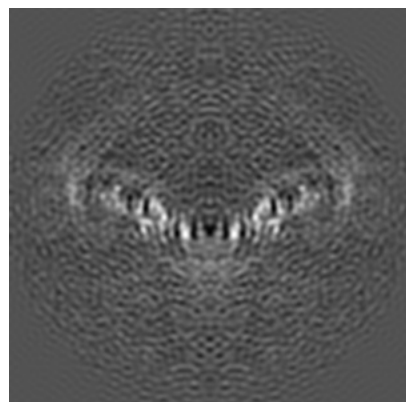


Z

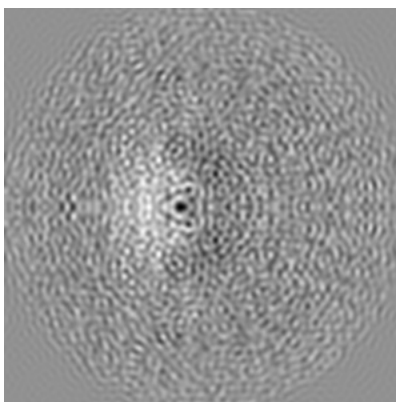
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

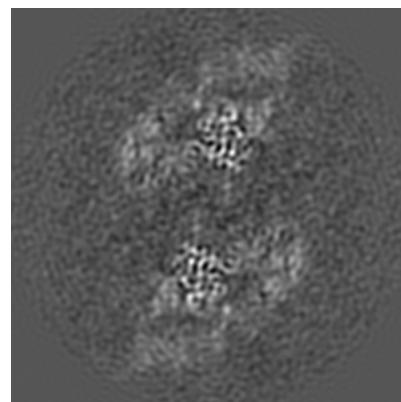
6.2.1 Primary map



X Index: 110



Y Index: 110

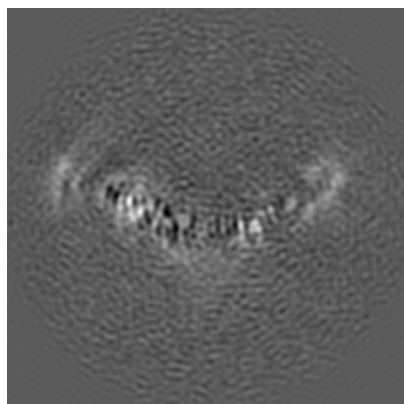


Z Index: 110

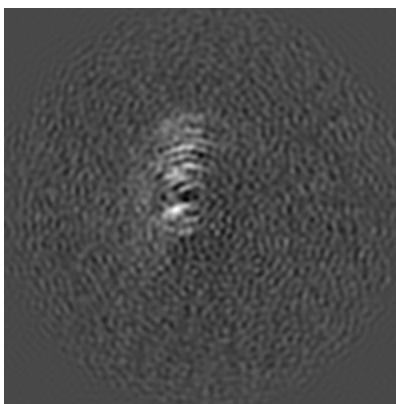
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

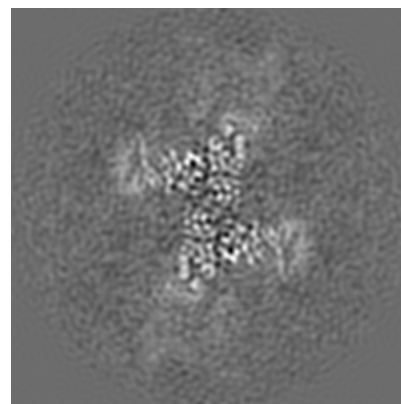
6.3.1 Primary map



X Index: 103



Y Index: 96

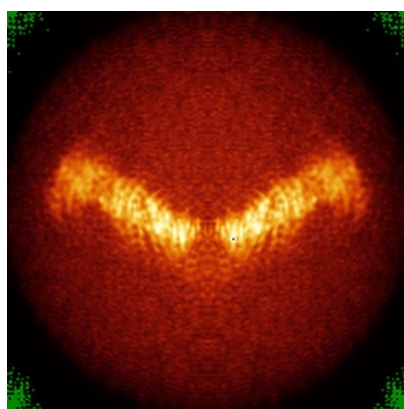


Z Index: 101

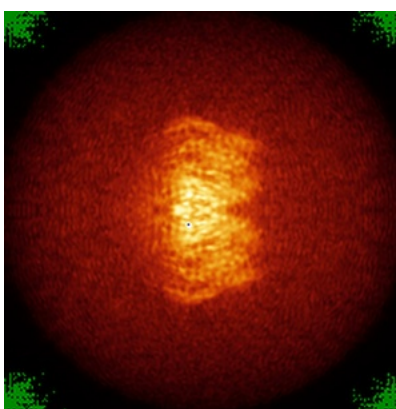
The images above show the largest variance slices of the map in three orthogonal directions.

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

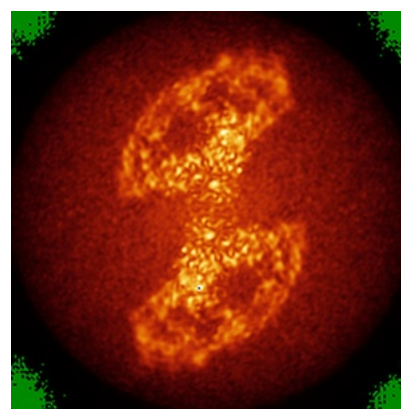
6.4.1 Primary map



X



Y

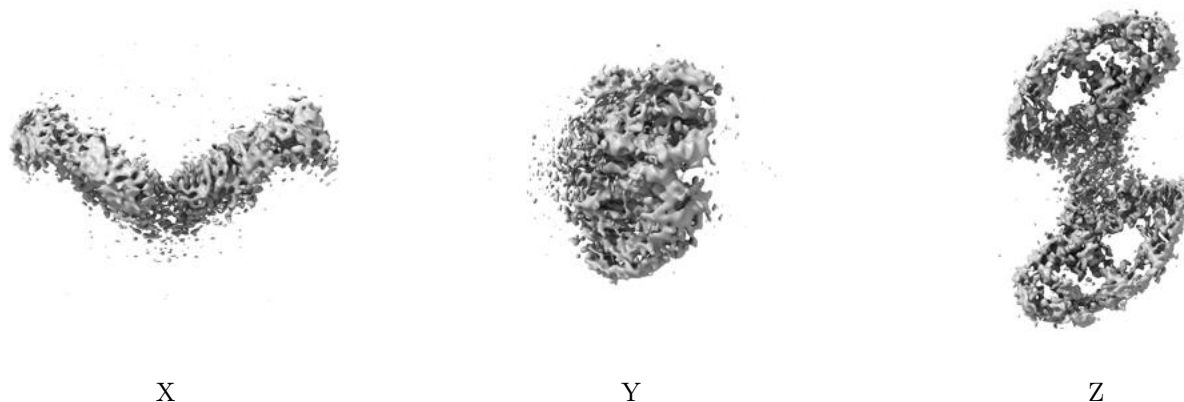


Z

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

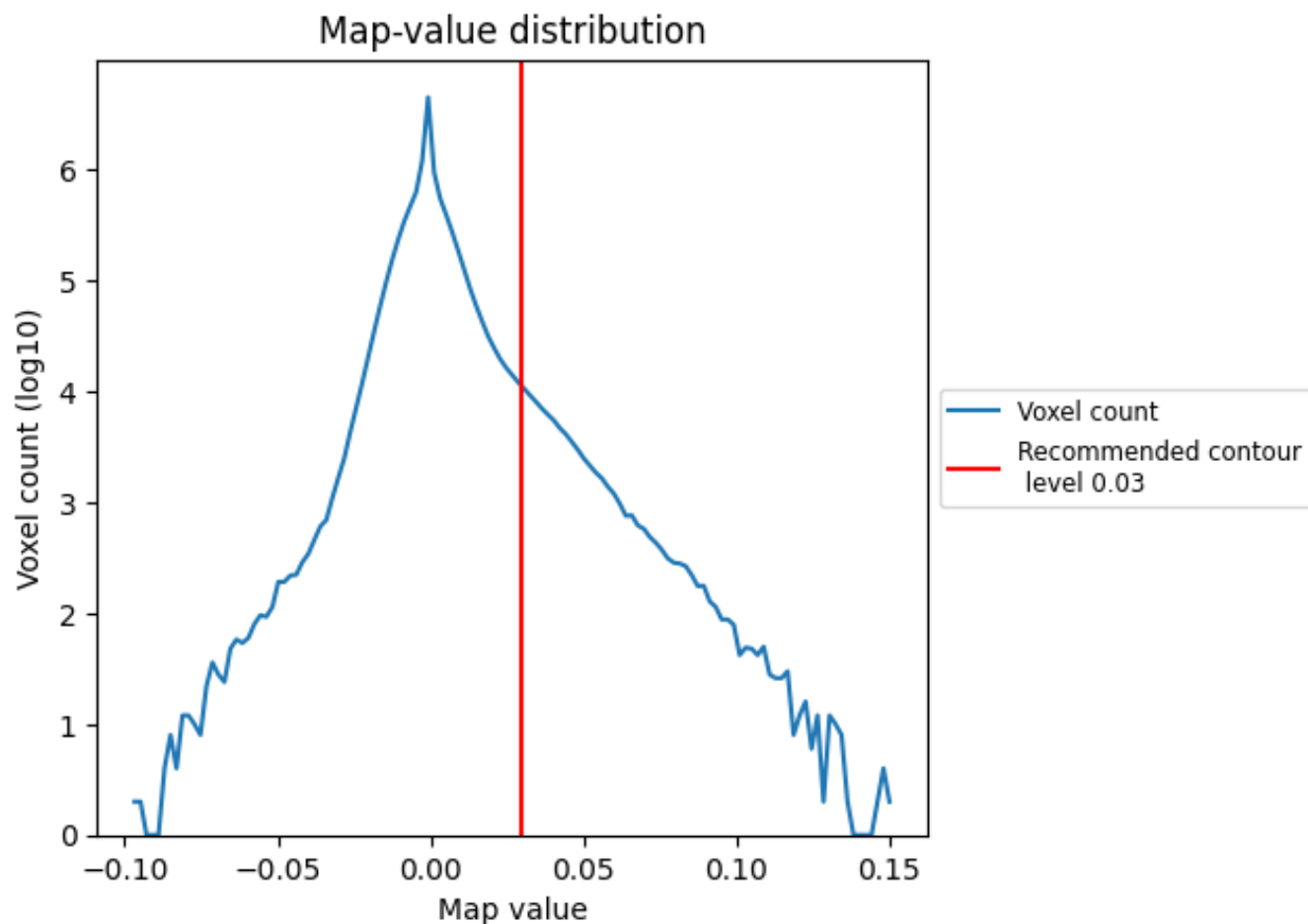
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

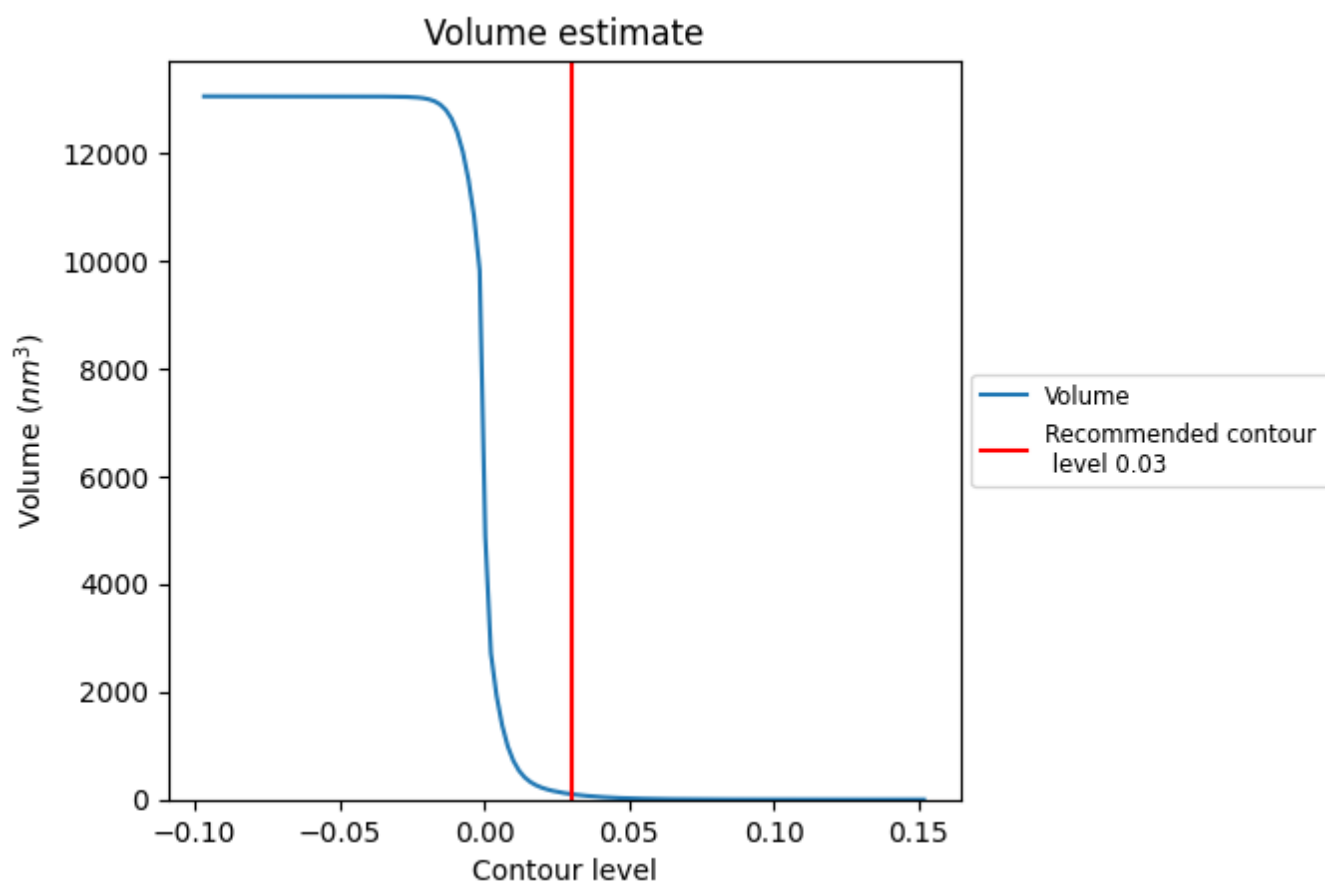
This section contains the results of statistical analysis of the map.

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.

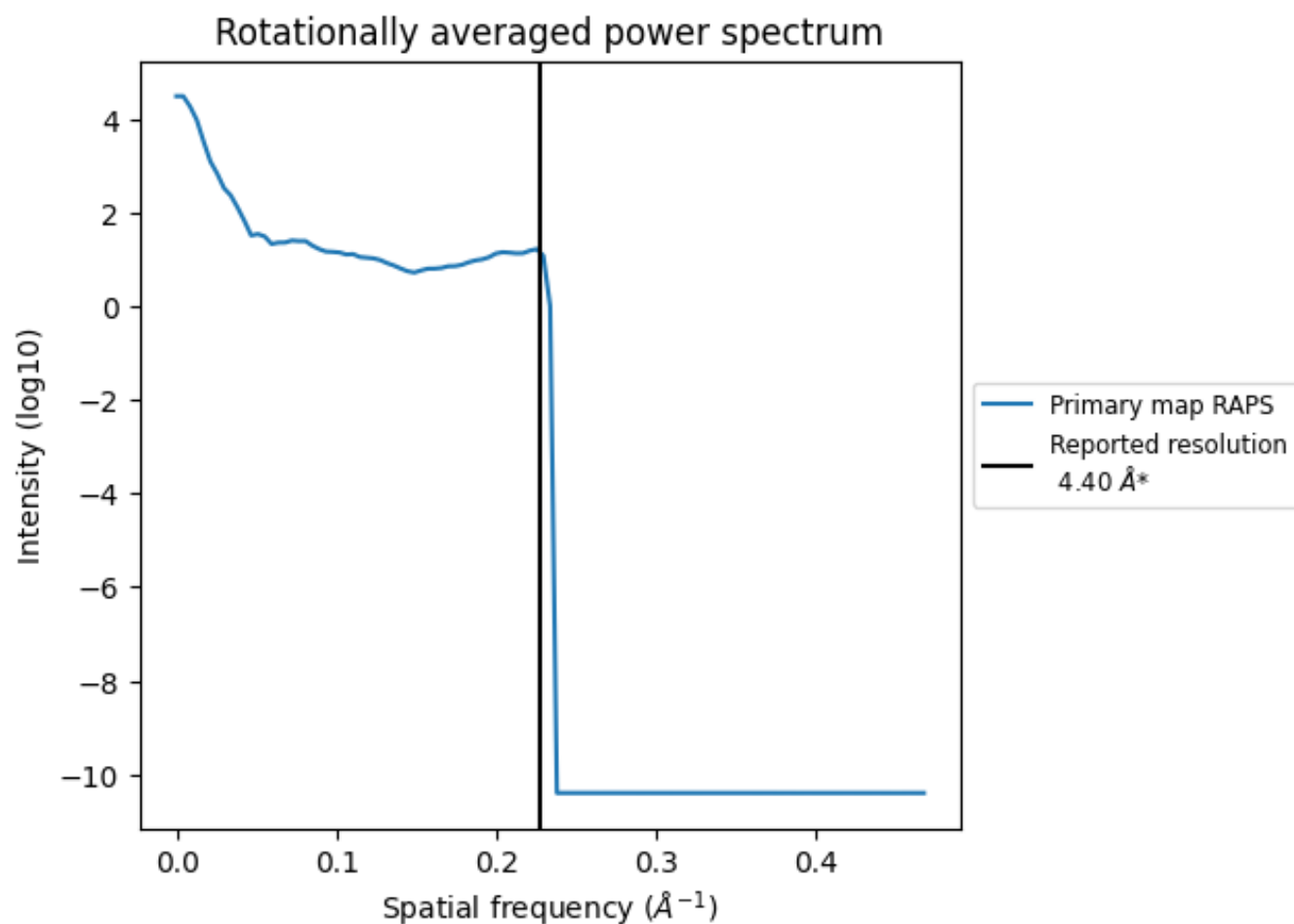
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm³; this corresponds to an approximate mass of 93 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 0.227 Å⁻¹

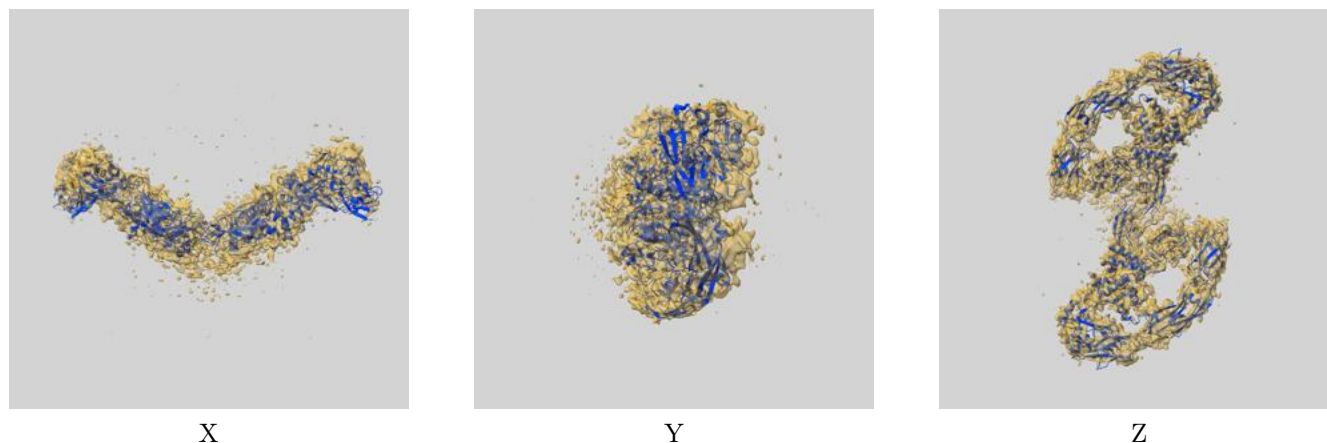
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

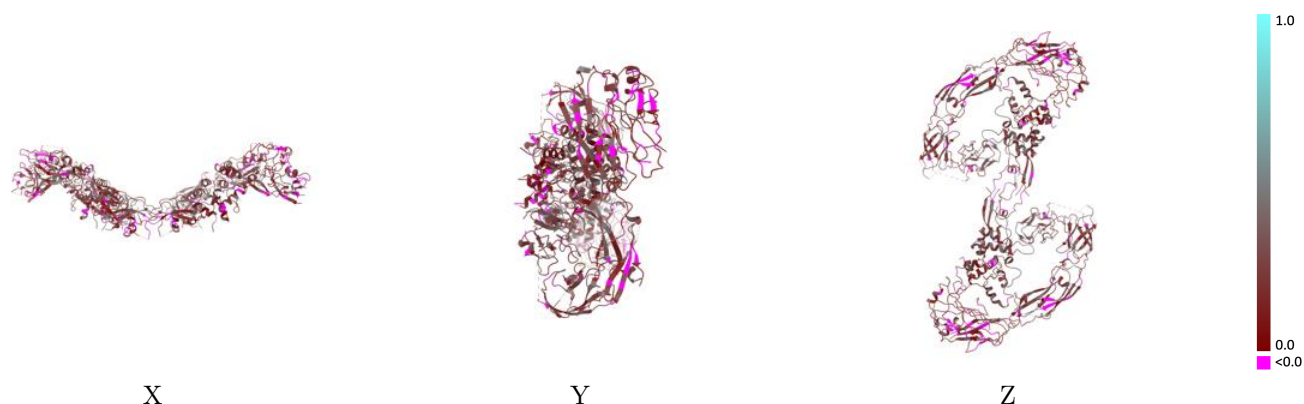
This section contains information regarding the fit between EMDB map EMD-20575 and PDB model 6Q2N. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



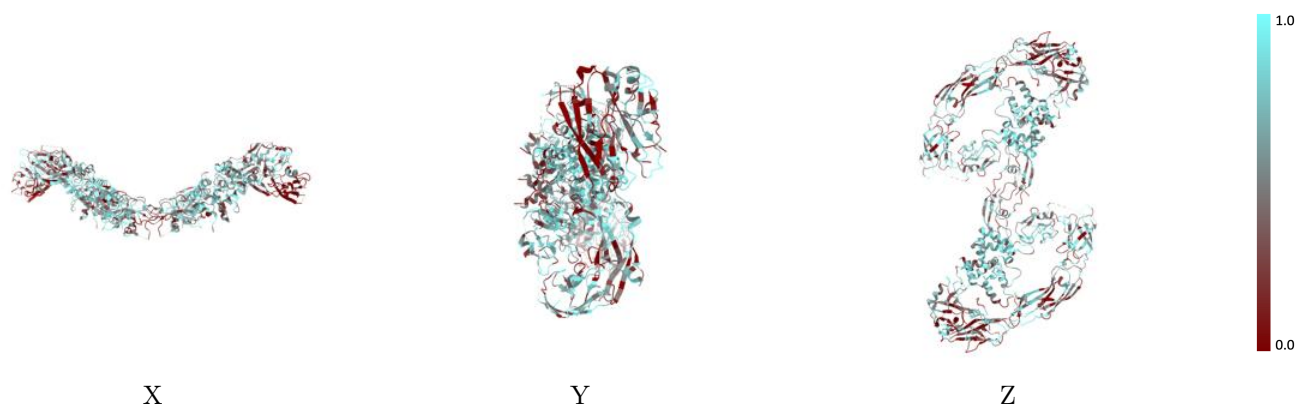
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



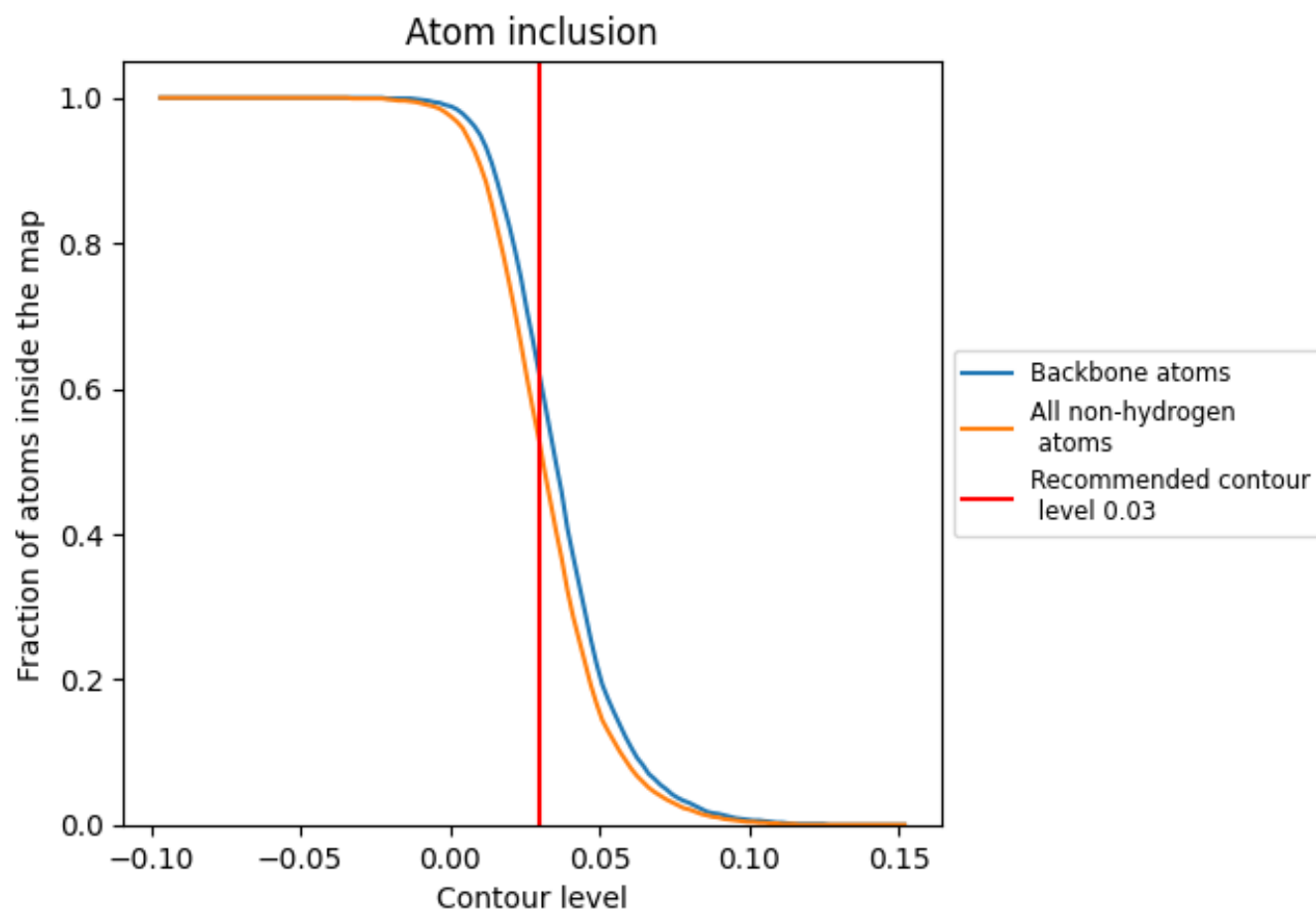
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 53% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5260	<div></div> 0.2230
A	<div></div> 0.4200	<div></div> 0.1830
B	<div></div> 0.4360	<div></div> 0.1970
C	<div></div> 0.6520	<div></div> 0.2650
D	<div></div> 0.6550	<div></div> 0.2620
E	<div></div> 0.4950	<div></div> 0.2130
F	<div></div> 0.4950	<div></div> 0.2140

1.0

0.0

<0.0