



Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 07:24 am GMT

PDB ID : 7NDG
EMDB ID : EMD-12286
Title : Cryo-EM structure of the ternary complex between Netrin-1, Neogenin and Repulsive Guidance Molecule B
Authors : Robinson, R.A.; Griffiths, S.C.; van de Haar, L.L.; Malinauskas, T.; van Batum, E.Y.; Zelina, P.; Schwab, R.A.; Karia, D.; Malinauskaite, L.; Brignani, S.; van den Munkhof, M.; Dudukcu, O.; De Ruiter, A.A.; Van den Heuvel, D.M.A.; Bishop, B.; Elegheert, J.; Aricescu, A.R.; Pasterkamp, R.J.; Siebold, C.
Deposited on : 2021-02-01
Resolution : 5.98 Å (reported)

This is a Full wwPDB EM Validation 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
Mogul : 1.8.4, CSD as541be (2020)
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) : 2.31.3

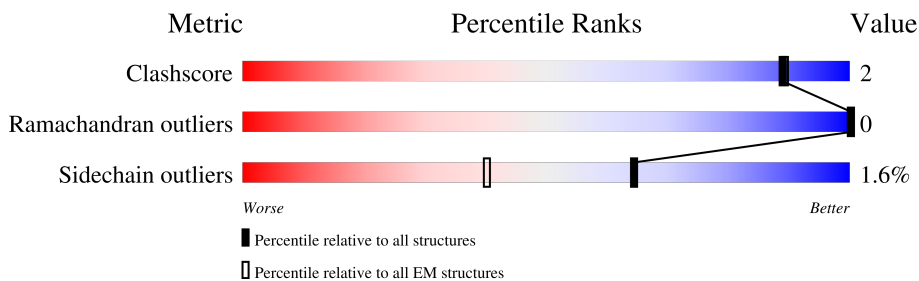
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.98 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.



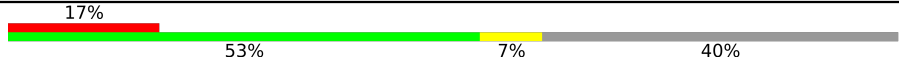
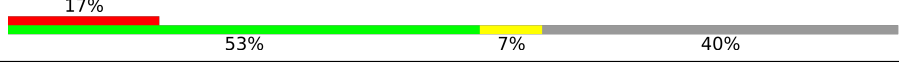
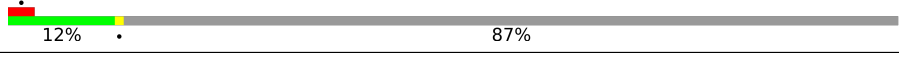


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	441	90% 5% 6%
1	D	441	90% 5% 6%
1	G	441	89% 5% 6%
2	B	354	9% 79% 5% 16%
2	E	354	10% 79% 6% 16%
2	H	354	8% 79% 5% 16%
3	C	252	17% 53% 7% 40%

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Mol	Chain	Length	Quality of chain
3	F	252	
3	I	252	
4	M	119	
4	N	119	
4	O	119	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 20934 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 Netrin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	416	3267	1996	623	608	40	0	0
1	G	416	3267	1996	623	608	40	0	0
1	D	416	3267	1996	623	608	40	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	454	GLY	-	expression tag	UNP O95631
A	455	SER	-	expression tag	UNP O95631
A	456	GLY	-	expression tag	UNP O95631
A	457	THR	-	expression tag	UNP O95631
A	458	GLU	-	expression tag	UNP O95631
A	459	THR	-	expression tag	UNP O95631
A	460	SER	-	expression tag	UNP O95631
A	461	GLN	-	expression tag	UNP O95631
A	462	VAL	-	expression tag	UNP O95631
A	463	ALA	-	expression tag	UNP O95631
A	464	PRO	-	expression tag	UNP O95631
A	465	ALA	-	expression tag	UNP O95631
G	454	GLY	-	expression tag	UNP O95631
G	455	SER	-	expression tag	UNP O95631
G	456	GLY	-	expression tag	UNP O95631
G	457	THR	-	expression tag	UNP O95631
G	458	GLU	-	expression tag	UNP O95631
G	459	THR	-	expression tag	UNP O95631
G	460	SER	-	expression tag	UNP O95631
G	461	GLN	-	expression tag	UNP O95631
G	462	VAL	-	expression tag	UNP O95631
G	463	ALA	-	expression tag	UNP O95631
G	464	PRO	-	expression tag	UNP O95631
G	465	ALA	-	expression tag	UNP O95631

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Chain	Residue	Modelled	Actual	Comment	Reference
D	454	GLY	-	expression tag	UNP O95631
D	455	SER	-	expression tag	UNP O95631
D	456	GLY	-	expression tag	UNP O95631
D	457	THR	-	expression tag	UNP O95631
D	458	GLU	-	expression tag	UNP O95631
D	459	THR	-	expression tag	UNP O95631
D	460	SER	-	expression tag	UNP O95631
D	461	GLN	-	expression tag	UNP O95631
D	462	VAL	-	expression tag	UNP O95631
D	463	ALA	-	expression tag	UNP O95631
D	464	PRO	-	expression tag	UNP O95631
D	465	ALA	-	expression tag	UNP O95631

- Molecule 2 is a protein called Neogenin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	299	2358	1505	402	445	6	0	0
2	H	299	2358	1505	402	445	6	0	0
2	E	299	2358	1505	402	445	6	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	763	GLU	-	expression tag	UNP Q7TQG5
B	764	THR	-	expression tag	UNP Q7TQG5
B	765	GLY	-	expression tag	UNP Q7TQG5
B	1124	GLY	-	expression tag	UNP Q7TQG5
B	1125	THR	-	expression tag	UNP Q7TQG5
B	1126	LYS	-	expression tag	UNP Q7TQG5
B	1127	HIS	-	expression tag	UNP Q7TQG5
B	1128	HIS	-	expression tag	UNP Q7TQG5
B	1129	HIS	-	expression tag	UNP Q7TQG5
B	1130	HIS	-	expression tag	UNP Q7TQG5
B	1131	HIS	-	expression tag	UNP Q7TQG5
B	1132	HIS	-	expression tag	UNP Q7TQG5
H	763	GLU	-	expression tag	UNP Q7TQG5
H	764	THR	-	expression tag	UNP Q7TQG5
H	765	GLY	-	expression tag	UNP Q7TQG5
H	1124	GLY	-	expression tag	UNP Q7TQG5

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Chain	Residue	Modelled	Actual	Comment	Reference
H	1125	THR	-	expression tag	UNP Q7TQG5
H	1126	LYS	-	expression tag	UNP Q7TQG5
H	1127	HIS	-	expression tag	UNP Q7TQG5
H	1128	HIS	-	expression tag	UNP Q7TQG5
H	1129	HIS	-	expression tag	UNP Q7TQG5
H	1130	HIS	-	expression tag	UNP Q7TQG5
H	1131	HIS	-	expression tag	UNP Q7TQG5
H	1132	HIS	-	expression tag	UNP Q7TQG5
E	763	GLU	-	expression tag	UNP Q7TQG5
E	764	THR	-	expression tag	UNP Q7TQG5
E	765	GLY	-	expression tag	UNP Q7TQG5
E	1124	GLY	-	expression tag	UNP Q7TQG5
E	1125	THR	-	expression tag	UNP Q7TQG5
E	1126	LYS	-	expression tag	UNP Q7TQG5
E	1127	HIS	-	expression tag	UNP Q7TQG5
E	1128	HIS	-	expression tag	UNP Q7TQG5
E	1129	HIS	-	expression tag	UNP Q7TQG5
E	1130	HIS	-	expression tag	UNP Q7TQG5
E	1131	HIS	-	expression tag	UNP Q7TQG5
E	1132	HIS	-	expression tag	UNP Q7TQG5

- Molecule 3 is a protein called Repulsive Guidance Molecule B (C-terminal region).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	151	Total	C	N	O	S	0	0
			1175	737	203	228	7		
3	C	151	Total	C	N	O	S	0	0
			1175	737	203	228	7		
3	I	151	Total	C	N	O	S	0	0
			1175	737	203	228	7		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	413	THR	-	expression tag	UNP Q6NW40
F	414	LYS	-	expression tag	UNP Q6NW40
F	415	HIS	-	expression tag	UNP Q6NW40
F	416	HIS	-	expression tag	UNP Q6NW40
F	417	HIS	-	expression tag	UNP Q6NW40
F	418	HIS	-	expression tag	UNP Q6NW40
F	419	HIS	-	expression tag	UNP Q6NW40
F	420	HIS	-	expression tag	UNP Q6NW40

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Chain	Residue	Modelled	Actual	Comment	Reference
C	413	THR	-	expression tag	UNP Q6NW40
C	414	LYS	-	expression tag	UNP Q6NW40
C	415	HIS	-	expression tag	UNP Q6NW40
C	416	HIS	-	expression tag	UNP Q6NW40
C	417	HIS	-	expression tag	UNP Q6NW40
C	418	HIS	-	expression tag	UNP Q6NW40
C	419	HIS	-	expression tag	UNP Q6NW40
C	420	HIS	-	expression tag	UNP Q6NW40
I	413	THR	-	expression tag	UNP Q6NW40
I	414	LYS	-	expression tag	UNP Q6NW40
I	415	HIS	-	expression tag	UNP Q6NW40
I	416	HIS	-	expression tag	UNP Q6NW40
I	417	HIS	-	expression tag	UNP Q6NW40
I	418	HIS	-	expression tag	UNP Q6NW40
I	419	HIS	-	expression tag	UNP Q6NW40
I	420	HIS	-	expression tag	UNP Q6NW40

- Molecule 4 is a protein called RGM domain family member B.

Mol	Chain	Residues	Atoms				AltConf	Trace	
4	N	15	Total	C	N	O	S	0	0
			121	80	18	21	2		
4	M	15	Total	C	N	O	S	0	0
			121	80	18	21	2		
4	O	15	Total	C	N	O	S	0	0
			121	80	18	21	2		

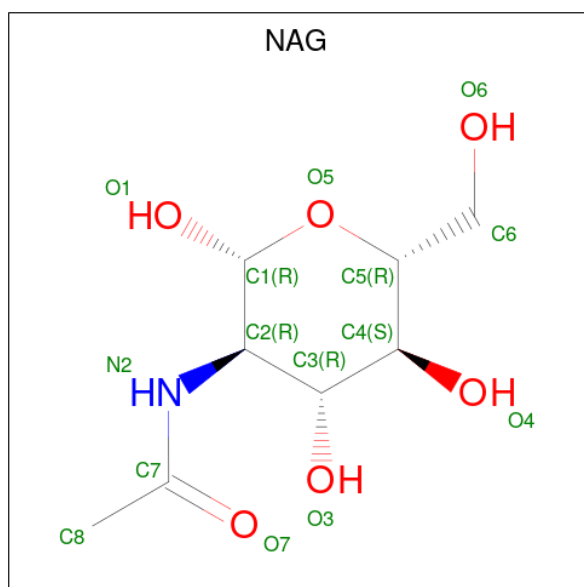
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	50	GLU	-	expression tag	UNP Q6NW40
N	51	THR	-	expression tag	UNP Q6NW40
N	52	GLY	-	expression tag	UNP Q6NW40
M	50	GLU	-	expression tag	UNP Q6NW40
M	51	THR	-	expression tag	UNP Q6NW40
M	52	GLY	-	expression tag	UNP Q6NW40
O	50	GLU	-	expression tag	UNP Q6NW40
O	51	THR	-	expression tag	UNP Q6NW40
O	52	GLY	-	expression tag	UNP Q6NW40

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Ca 1 1	0
5	G	1	Total Ca 1 1	0
5	D	1	Total Ca 1 1	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

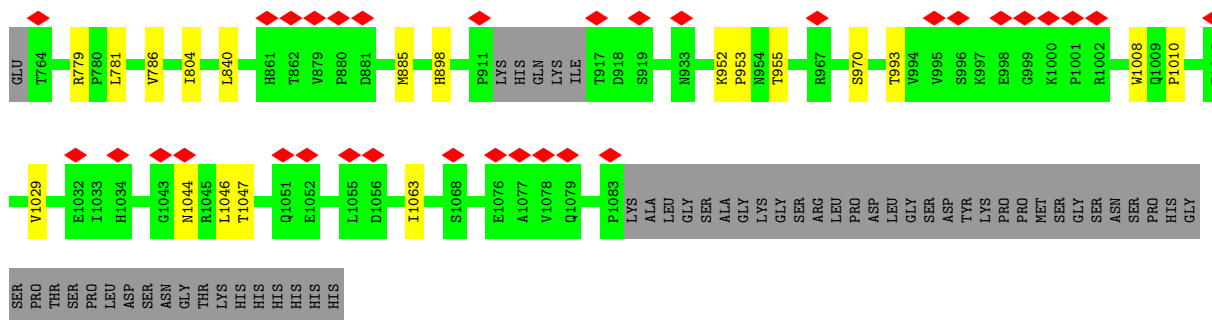


Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C N O 42 24 3 15	0
6	A	1	Total C N O 42 24 3 15	0
6	A	1	Total C N O 42 24 3 15	0
6	B	1	Total C N O 14 8 1 5	0
6	G	1	Total C N O 42 24 3 15	0
6	G	1	Total C N O 42 24 3 15	0
6	G	1	Total C N O 42 24 3 15	0
6	H	1	Total C N O 14 8 1 5	0

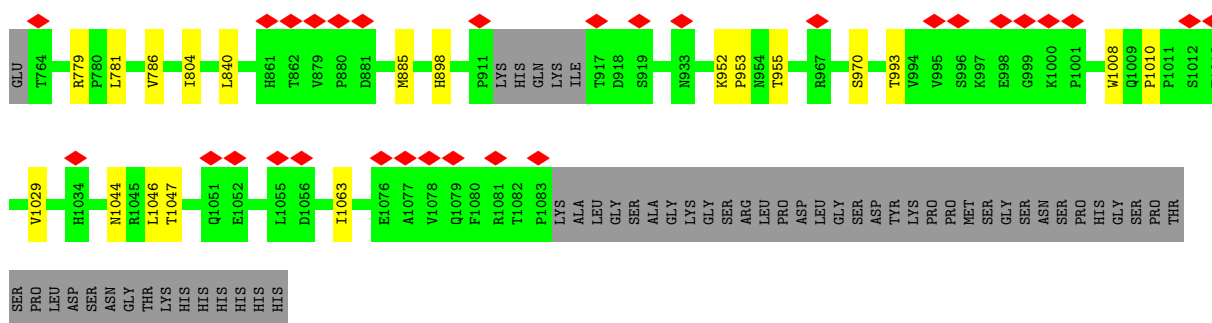
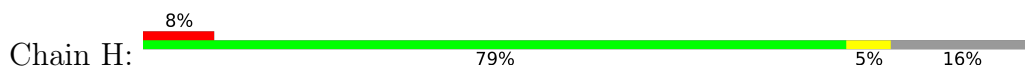
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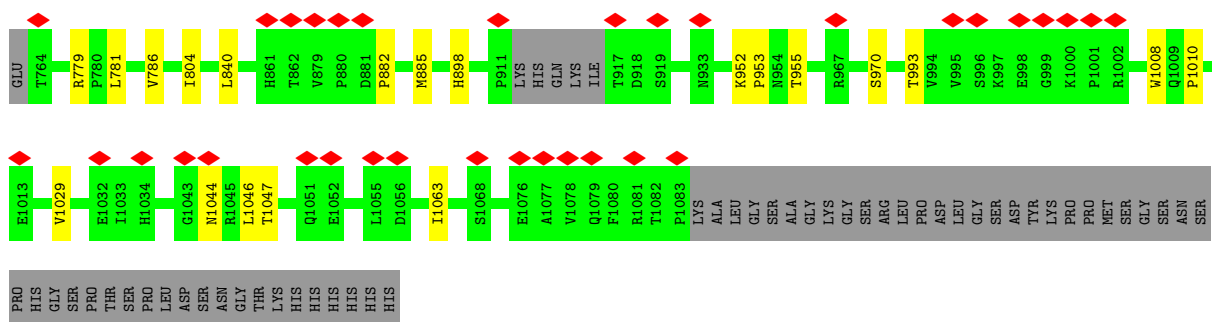
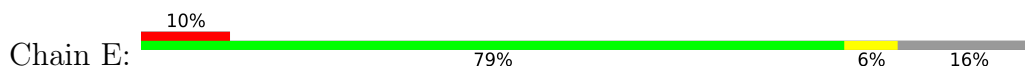
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	D	1	Total 42	C 24	N 3	O 15	0
6	D	1	Total 42	C 24	N 3	O 15	0
6	D	1	Total 42	C 24	N 3	O 15	0
6	E	1	Total 14	C 8	N 1	O 5	0



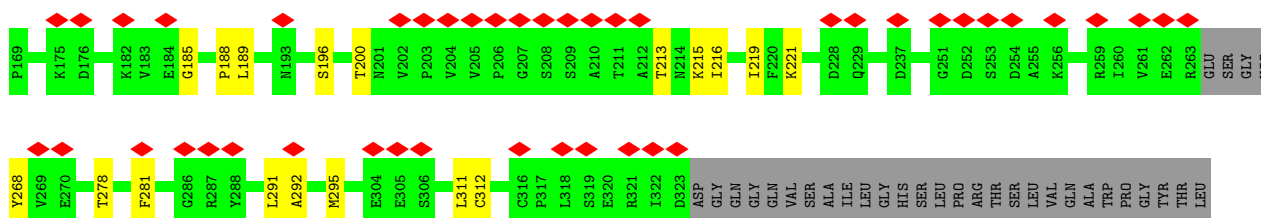
• Molecule 2: Neogenin

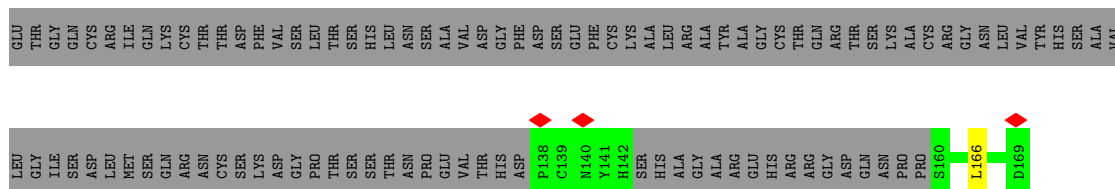


• Molecule 2: Neogenin



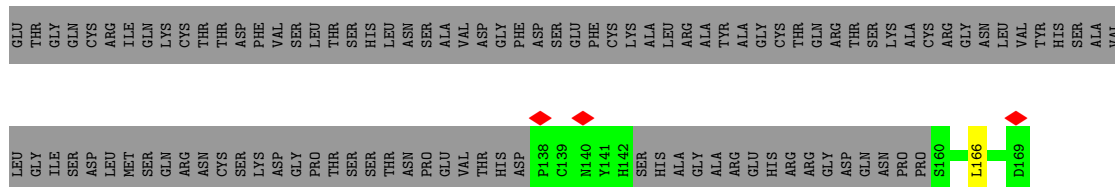
• Molecule 3: Repulsive Guidance Molecule B (C-terminal region)





- Molecule 4: RGM domain family member B

Chain O:  12% . 87%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	68541	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-700	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.018	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	299.2, 299.2, 299.2	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.37	0/3349	0.57	0/4531
1	D	0.37	0/3349	0.57	0/4531
1	G	0.37	0/3349	0.57	0/4531
2	B	0.40	0/2425	0.55	0/3324
2	E	0.40	1/2425 (0.0%)	0.55	0/3324
2	H	0.40	0/2425	0.55	0/3324
3	C	0.39	0/1197	0.53	0/1626
3	F	0.38	0/1197	0.53	0/1626
3	I	0.38	0/1197	0.53	0/1626
4	M	0.34	0/125	0.49	0/166
4	N	0.34	0/125	0.49	0/166
4	O	0.34	0/125	0.49	0/166
All	All	0.38	1/21288 (0.0%)	0.55	0/28941

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	882	PRO	N-CD	5.20	1.55	1.47

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	3267	0	3072	8	0
1	D	3267	0	3072	8	0
1	G	3267	0	3072	10	0
2	B	2358	0	2339	9	0
2	E	2358	0	2339	9	0
2	H	2358	0	2339	9	0
3	C	1175	0	1148	10	0
3	F	1175	0	1148	10	0
3	I	1175	0	1148	10	0
4	M	121	0	100	1	0
4	N	121	0	100	1	0
4	O	121	0	100	1	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
6	A	42	0	39	0	0
6	B	14	0	13	0	0
6	D	42	0	39	0	0
6	E	14	0	13	0	0
6	G	42	0	39	0	0
6	H	14	0	13	0	0
All	All	20934	0	20133	74	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.

All (74) 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:C:188:PRO:HG3	2:H:1047:THR:HG21	1.72	0.72
2:B:1047:THR:HG21	3:F:188:PRO:HG3	1.72	0.71
2:E:1047:THR:HG21	3:I:188:PRO:HG3	1.72	0.71
2:H:885:MET:HB2	2:H:970:SER:HB2	1.80	0.63
2:E:885:MET:HB2	2:E:970:SER:HB2	1.80	0.63
2:B:885:MET:HB2	2:B:970:SER:HB2	1.80	0.61
1:D:221:SER:HB3	1:D:224:ASP:HB2	1.91	0.53
1:G:221:SER:HB3	1:G:224:ASP:HB2	1.91	0.52
1:G:303:VAL:HG13	1:G:313:PRO:HA	1.91	0.52
1:D:303:VAL:HG13	1:D:313:PRO:HA	1.91	0.52
3:I:196:SER:HB3	3:I:219:ILE:HB	1.92	0.52
3:F:189:LEU:HD23	3:F:311:LEU:HB2	1.91	0.52
2:H:779:ARG:HB3	2:H:786:VAL:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:SER:HB3	1:A:224:ASP:HB2	1.91	0.52
3:C:196:SER:HB3	3:C:219:ILE:HB	1.92	0.51
3:I:189:LEU:HD23	3:I:311:LEU:HB2	1.92	0.51
3:F:196:SER:HB3	3:F:219:ILE:HB	1.92	0.51
3:F:213:THR:HG21	4:N:166:LEU:HD21	1.92	0.51
2:B:993:THR:HG21	3:F:185:GLY:HA3	1.92	0.51
3:C:189:LEU:HD23	3:C:311:LEU:HB2	1.92	0.51
2:E:779:ARG:HB3	2:E:786:VAL:HB	1.92	0.51
1:A:303:VAL:HG13	1:A:313:PRO:HA	1.91	0.51
2:E:993:THR:HG21	3:I:185:GLY:HA3	1.92	0.51
3:I:213:THR:HG21	4:O:166:LEU:HD21	1.92	0.51
3:C:213:THR:HG21	4:M:166:LEU:HD21	1.93	0.50
2:B:779:ARG:HB3	2:B:786:VAL:HB	1.92	0.50
2:B:1010:PRO:HD3	2:B:1046:LEU:HD21	1.93	0.50
2:H:1010:PRO:HD3	2:H:1046:LEU:HD21	1.93	0.49
2:E:1010:PRO:HD3	2:E:1046:LEU:HD21	1.93	0.49
3:C:185:GLY:HA3	2:H:993:THR:HG21	1.92	0.49
1:A:429:VAL:HG13	1:A:436:ARG:O	2.14	0.48
1:G:429:VAL:HG13	1:G:436:ARG:O	2.13	0.48
1:G:441:TYR:HB3	1:G:451:CYS:HB3	1.96	0.48
1:A:441:TYR:HB3	1:A:451:CYS:HB3	1.96	0.48
2:H:1008:TRP:HB3	2:H:1063:ILE:HD13	1.96	0.48
2:E:1008:TRP:HB3	2:E:1063:ILE:HD13	1.96	0.48
3:F:200:THR:HG22	3:F:215:LYS:HB3	1.96	0.47
2:B:1008:TRP:HB3	2:B:1063:ILE:HD13	1.96	0.47
1:D:441:TYR:HB3	1:D:451:CYS:HB3	1.96	0.47
1:G:331:THR:HG23	1:G:334:GLU:H	1.79	0.47
1:D:429:VAL:HG13	1:D:436:ARG:O	2.14	0.47
3:C:200:THR:HG22	3:C:215:LYS:HB3	1.96	0.46
1:D:331:THR:HG23	1:D:334:GLU:H	1.79	0.46
1:A:331:THR:HG23	1:A:334:GLU:H	1.80	0.46
1:A:166:ASP:OD2	1:A:170:THR:HG22	2.16	0.46
3:C:216:ILE:HD13	3:C:291:LEU:HD13	1.98	0.46
1:G:166:ASP:OD2	1:G:170:THR:HG22	2.16	0.46
2:E:1044:ASN:HB2	3:I:221:LYS:HD3	1.98	0.46
1:D:166:ASP:OD2	1:D:170:THR:HG22	2.16	0.46
3:I:200:THR:HG22	3:I:215:LYS:HB3	1.96	0.46
3:F:216:ILE:HD13	3:F:291:LEU:HD13	1.98	0.46
3:C:221:LYS:HD3	2:H:1044:ASN:HB2	1.98	0.45
2:B:1044:ASN:HB2	3:F:221:LYS:HD3	1.98	0.44
3:I:216:ILE:HD13	3:I:291:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:898:HIS:HB2	2:H:953:PRO:HB3	2.00	0.44
2:B:898:HIS:HB2	2:B:953:PRO:HB3	2.00	0.43
1:G:344:ASN:ND2	1:G:379:HIS:O	2.51	0.43
3:F:278:THR:HB	3:F:295:MET:HG3	2.01	0.43
3:C:278:THR:HB	3:C:295:MET:HG3	2.01	0.43
2:E:898:HIS:HB2	2:E:953:PRO:HB3	2.00	0.42
1:A:78:CYS:HB2	1:A:271:SER:HB3	2.01	0.42
1:D:78:CYS:HB2	1:D:271:SER:HB3	2.01	0.42
3:F:281:PHE:HB2	3:F:292:ALA:HB3	2.02	0.42
1:G:78:CYS:HB2	1:G:271:SER:HB3	2.01	0.41
3:I:278:THR:HB	3:I:295:MET:HG3	2.01	0.41
2:H:952:LYS:HB2	2:H:955:THR:HG21	2.03	0.41
3:C:281:PHE:HB2	3:C:292:ALA:HB3	2.02	0.41
1:G:236:PRO:HA	1:G:239:GLN:HB2	2.03	0.41
3:I:281:PHE:HB2	3:I:292:ALA:HB3	2.02	0.41
1:G:425:CYS:HB3	1:G:429:VAL:HB	2.03	0.41
2:B:952:LYS:HB2	2:B:955:THR:HG21	2.03	0.40
1:A:236:PRO:HA	1:A:239:GLN:HB2	2.03	0.40
1:D:146:TYR:HA	1:D:220:PHE:O	2.21	0.40
2:E:952:LYS:HB2	2:E:955:THR:HG21	2.03	0.40

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	414/441 (94%)	400 (97%)	14 (3%)	0	100	100
1	D	414/441 (94%)	399 (96%)	15 (4%)	0	100	100
1	G	414/441 (94%)	400 (97%)	14 (3%)	0	100	100
2	B	295/354 (83%)	285 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	295/354 (83%)	285 (97%)	10 (3%)	0	100	100
2	H	295/354 (83%)	285 (97%)	10 (3%)	0	100	100
3	C	147/252 (58%)	137 (93%)	10 (7%)	0	100	100
3	F	147/252 (58%)	137 (93%)	10 (7%)	0	100	100
3	I	147/252 (58%)	137 (93%)	10 (7%)	0	100	100
4	M	11/119 (9%)	11 (100%)	0	0	100	100
4	N	11/119 (9%)	11 (100%)	0	0	100	100
4	O	11/119 (9%)	11 (100%)	0	0	100	100
All	All	2601/3498 (74%)	2498 (96%)	103 (4%)	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	360/375 (96%)	354 (98%)	6 (2%)	60	78
1	D	360/375 (96%)	354 (98%)	6 (2%)	60	78
1	G	360/375 (96%)	354 (98%)	6 (2%)	60	78
2	B	267/313 (85%)	263 (98%)	4 (2%)	65	80
2	E	267/313 (85%)	263 (98%)	4 (2%)	65	80
2	H	267/313 (85%)	263 (98%)	4 (2%)	65	80
3	C	131/217 (60%)	129 (98%)	2 (2%)	65	80
3	F	131/217 (60%)	129 (98%)	2 (2%)	65	80
3	I	131/217 (60%)	129 (98%)	2 (2%)	65	80
4	M	13/101 (13%)	13 (100%)	0	100	100
4	N	13/101 (13%)	13 (100%)	0	100	100
4	O	13/101 (13%)	13 (100%)	0	100	100
All	All	2313/3018 (77%)	2277 (98%)	36 (2%)	64	79

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	CYS
1	A	134	LEU
1	A	166	ASP
1	A	174	PHE
1	A	285	CYS
1	A	404	CYS
2	B	781	LEU
2	B	804	ILE
2	B	840	LEU
2	B	1029	VAL
3	F	268	TYR
3	F	312	CYS
3	C	268	TYR
3	C	312	CYS
1	G	119	CYS
1	G	134	LEU
1	G	166	ASP
1	G	174	PHE
1	G	285	CYS
1	G	404	CYS
2	H	781	LEU
2	H	804	ILE
2	H	840	LEU
2	H	1029	VAL
1	D	119	CYS
1	D	134	LEU
1	D	166	ASP
1	D	174	PHE
1	D	285	CYS
1	D	404	CYS
2	E	781	LEU
2	E	804	ILE
2	E	840	LEU
2	E	1029	VAL
3	I	268	TYR
3	I	312	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS

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Mol	Chain	Res	Type
1	G	47	HIS
1	G	381	HIS
1	D	47	HIS

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](#)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	E	1201	2	14,14,15	0.28	0	17,19,21	0.80	1 (5%)
6	NAG	A	502	1	14,14,15	0.31	0	17,19,21	0.72	0
6	NAG	A	503	1	14,14,15	0.30	0	17,19,21	0.97	2 (11%)
6	NAG	G	503	1	14,14,15	0.30	0	17,19,21	0.97	2 (11%)
6	NAG	D	504	1	14,14,15	0.34	0	17,19,21	0.68	0
6	NAG	H	1201	2	14,14,15	0.27	0	17,19,21	0.81	1 (5%)
6	NAG	G	504	1	14,14,15	0.35	0	17,19,21	0.68	0
6	NAG	B	1201	2	14,14,15	0.28	0	17,19,21	0.81	1 (5%)
6	NAG	G	502	1	14,14,15	0.31	0	17,19,21	0.69	0
6	NAG	A	504	1	14,14,15	0.31	0	17,19,21	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	D	503	1	14,14,15	0.31	0	17,19,21	0.98	2 (11%)
6	NAG	D	502	1	14,14,15	0.32	0	17,19,21	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	E	1201	2	-	0/6/23/26	0/1/1/1
6	NAG	A	502	1	-	1/6/23/26	0/1/1/1
6	NAG	A	503	1	-	2/6/23/26	0/1/1/1
6	NAG	G	503	1	-	2/6/23/26	0/1/1/1
6	NAG	D	504	1	-	1/6/23/26	0/1/1/1
6	NAG	H	1201	2	-	0/6/23/26	0/1/1/1
6	NAG	G	504	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1201	2	-	0/6/23/26	0/1/1/1
6	NAG	G	502	1	-	1/6/23/26	0/1/1/1
6	NAG	A	504	1	-	1/6/23/26	0/1/1/1
6	NAG	D	503	1	-	2/6/23/26	0/1/1/1
6	NAG	D	502	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	503	NAG	C1-C2-N2	2.39	114.57	110.49
6	A	503	NAG	C1-C2-N2	2.38	114.55	110.49
6	G	503	NAG	C1-C2-N2	2.35	114.50	110.49
6	B	1201	NAG	C1-O5-C5	2.32	115.34	112.19
6	H	1201	NAG	C1-O5-C5	2.29	115.30	112.19
6	E	1201	NAG	C1-O5-C5	2.28	115.28	112.19
6	G	503	NAG	C2-N2-C7	2.12	125.92	122.90
6	A	503	NAG	C2-N2-C7	2.06	125.84	122.90
6	D	503	NAG	C2-N2-C7	2.02	125.78	122.90

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	502	NAG	O5-C5-C6-O6
6	A	502	NAG	O5-C5-C6-O6
6	G	502	NAG	O5-C5-C6-O6
6	A	504	NAG	O5-C5-C6-O6
6	G	504	NAG	O5-C5-C6-O6
6	D	504	NAG	O5-C5-C6-O6
6	A	503	NAG	C3-C2-N2-C7
6	G	503	NAG	C3-C2-N2-C7
6	D	503	NAG	C3-C2-N2-C7
6	A	503	NAG	C1-C2-N2-C7
6	G	503	NAG	C1-C2-N2-C7
6	D	503	NAG	C1-C2-N2-C7

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.

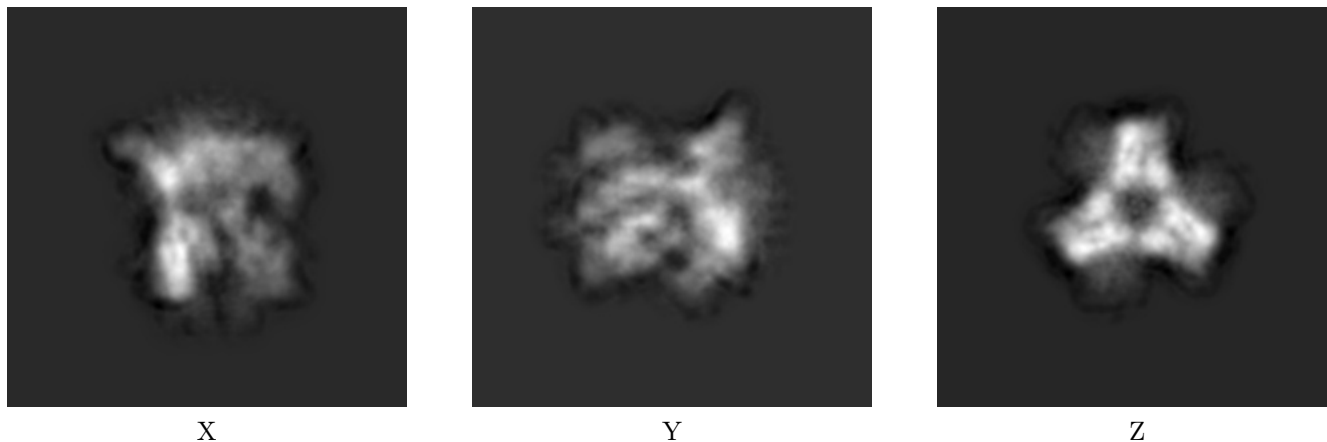
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12286. These allow visual inspection of the internal detail of the map and identification of artifacts.

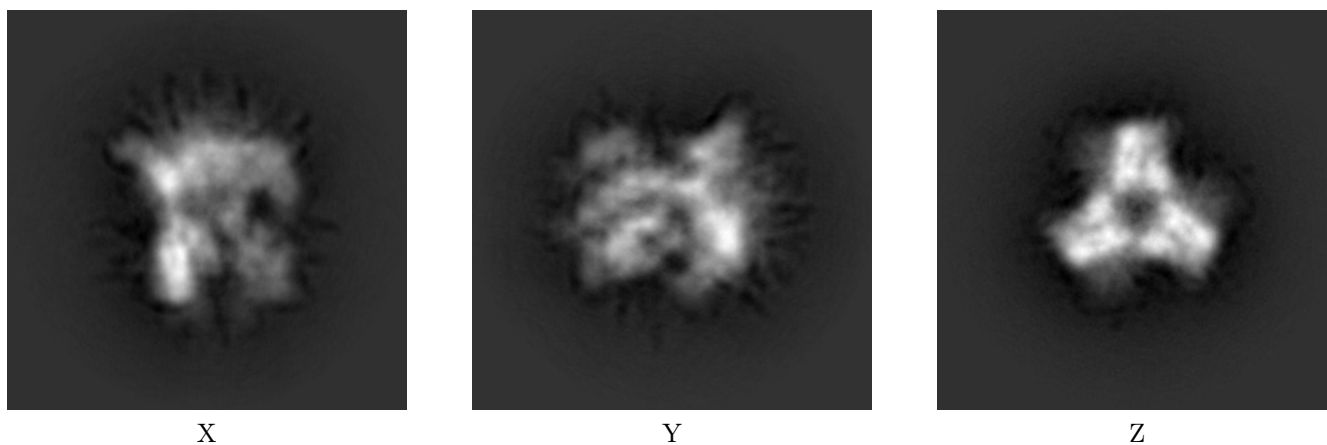
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



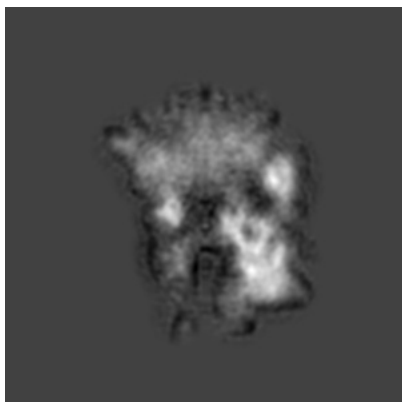
6.1.2 Raw map



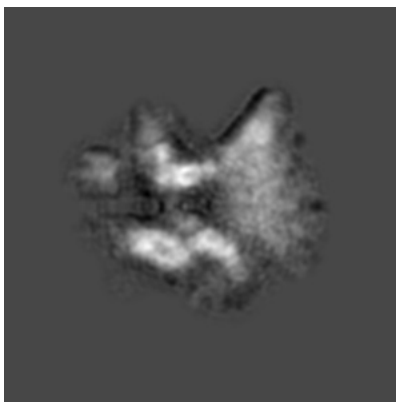
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 176

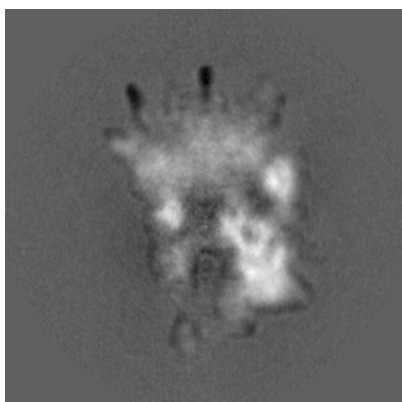


Y Index: 176

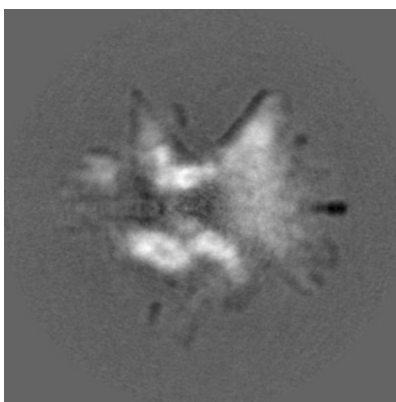


Z Index: 176

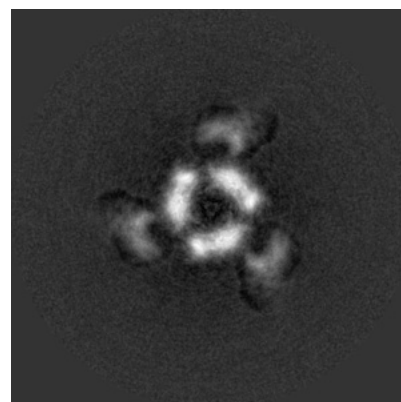
6.2.2 Raw map



X Index: 176



Y Index: 176

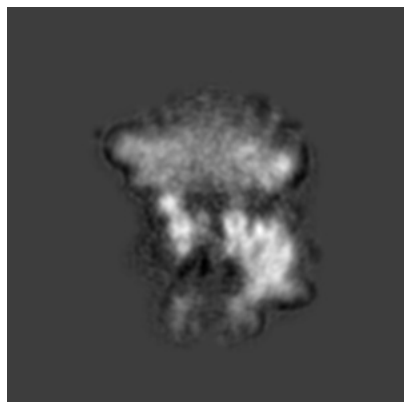


Z Index: 176

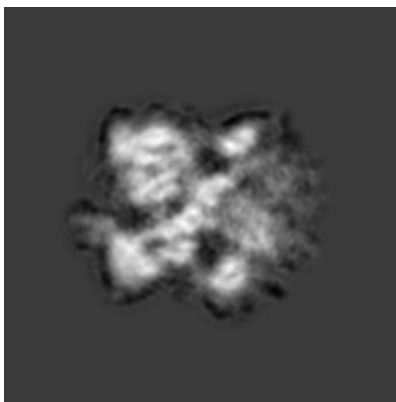
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

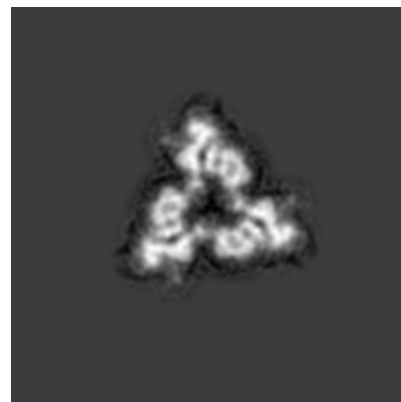
6.3.1 Primary map



X Index: 164

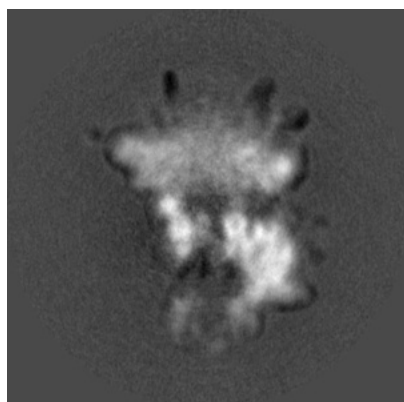


Y Index: 149

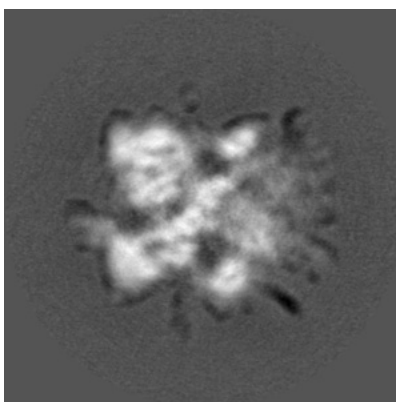


Z Index: 137

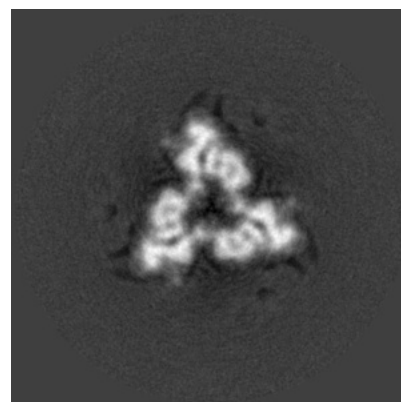
6.3.2 Raw map



X Index: 164



Y Index: 149

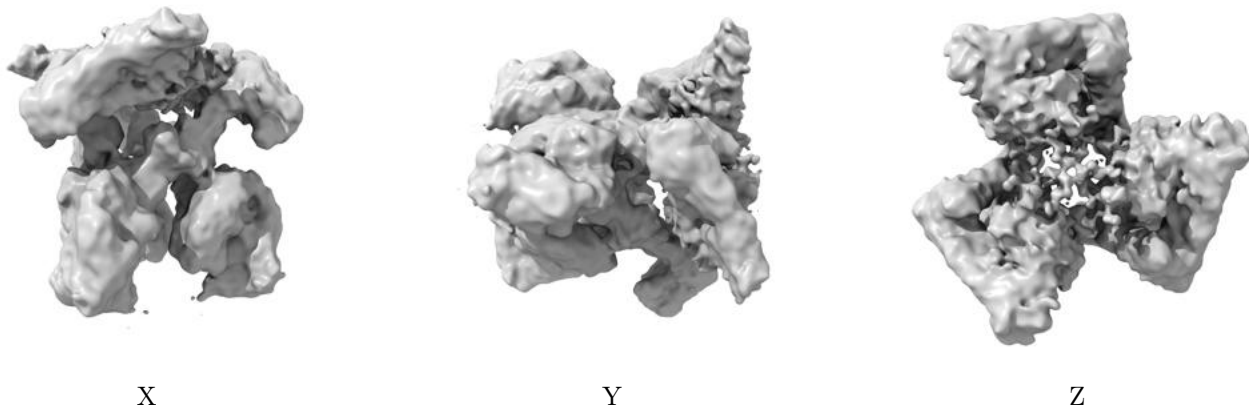


Z Index: 137

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

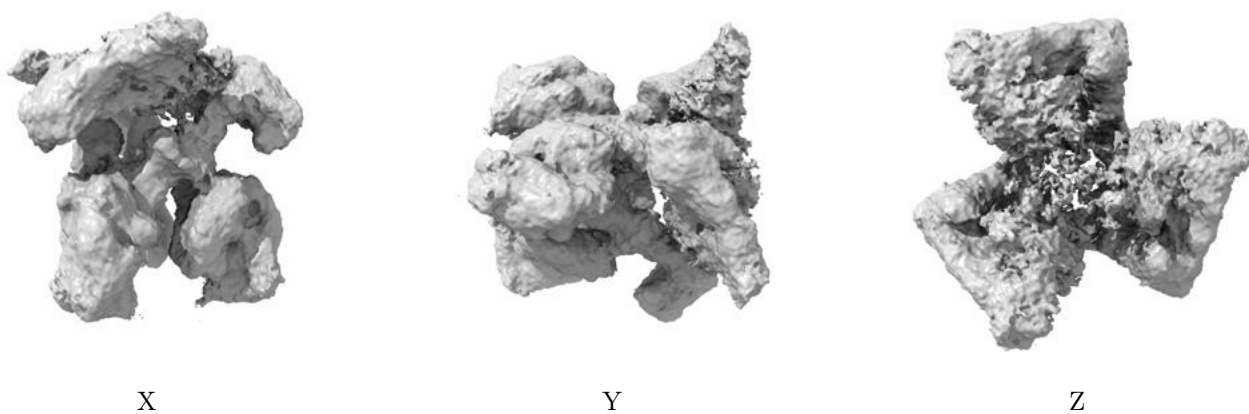
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

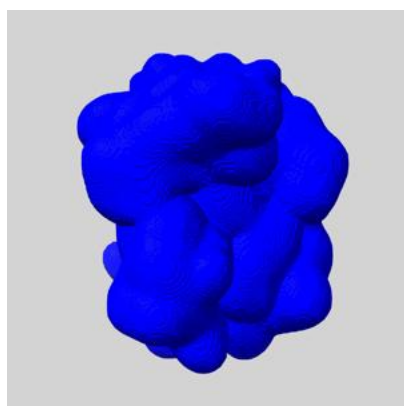
6.5 Mask visualisation [i](#)

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

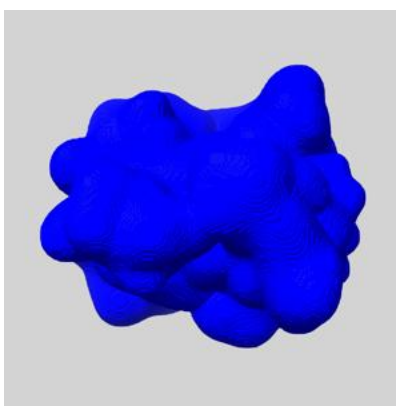
A mask typically either:

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

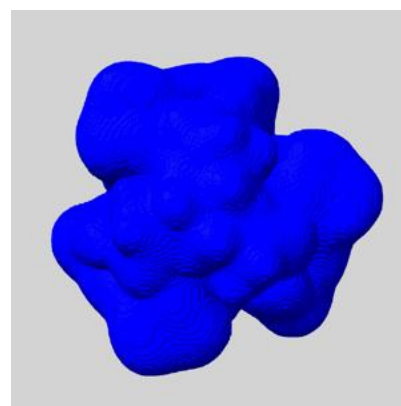
6.5.1 emd_12286_msk_1.map [i](#)



X



Y

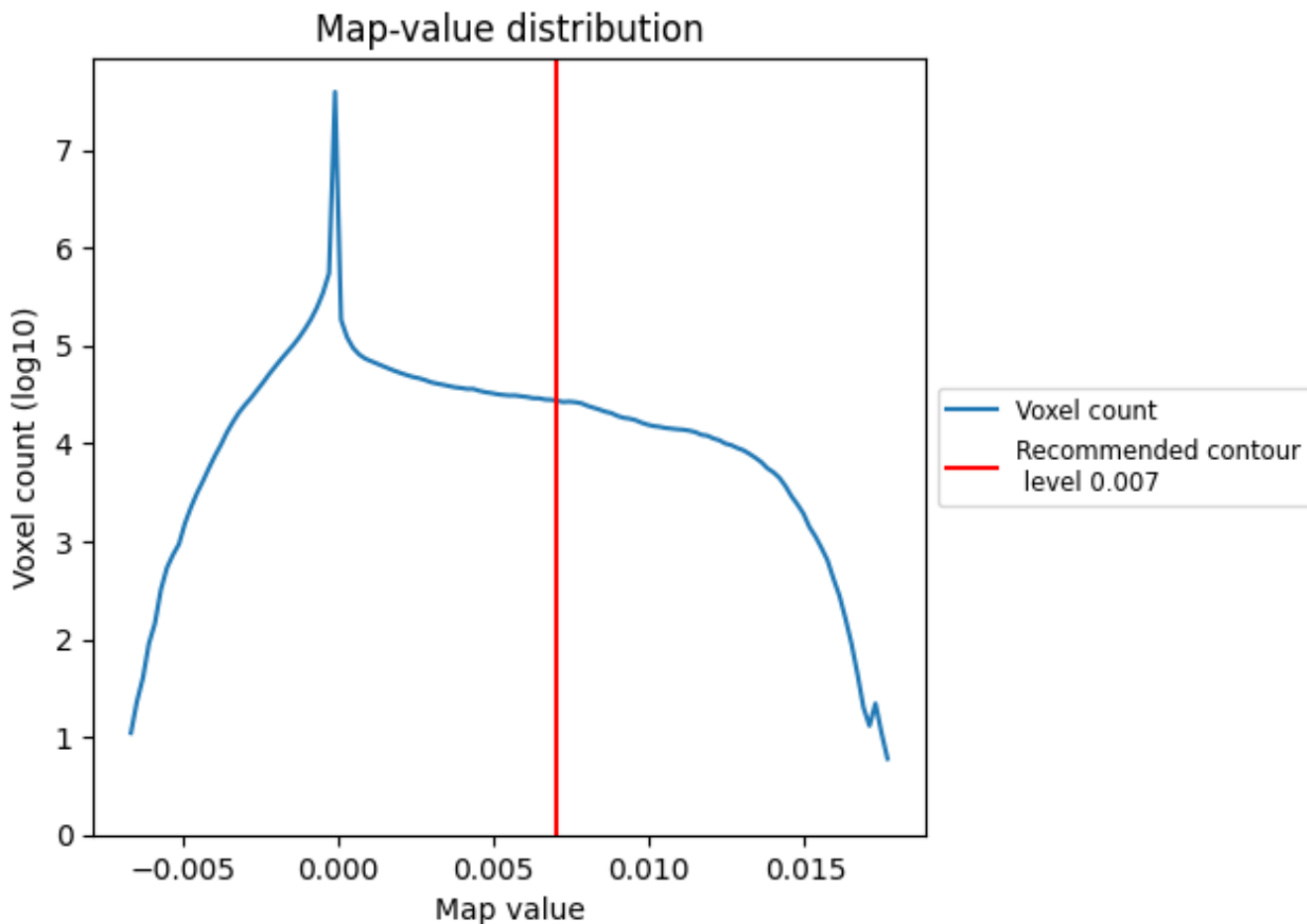


Z

7 Map analysis [i](#)

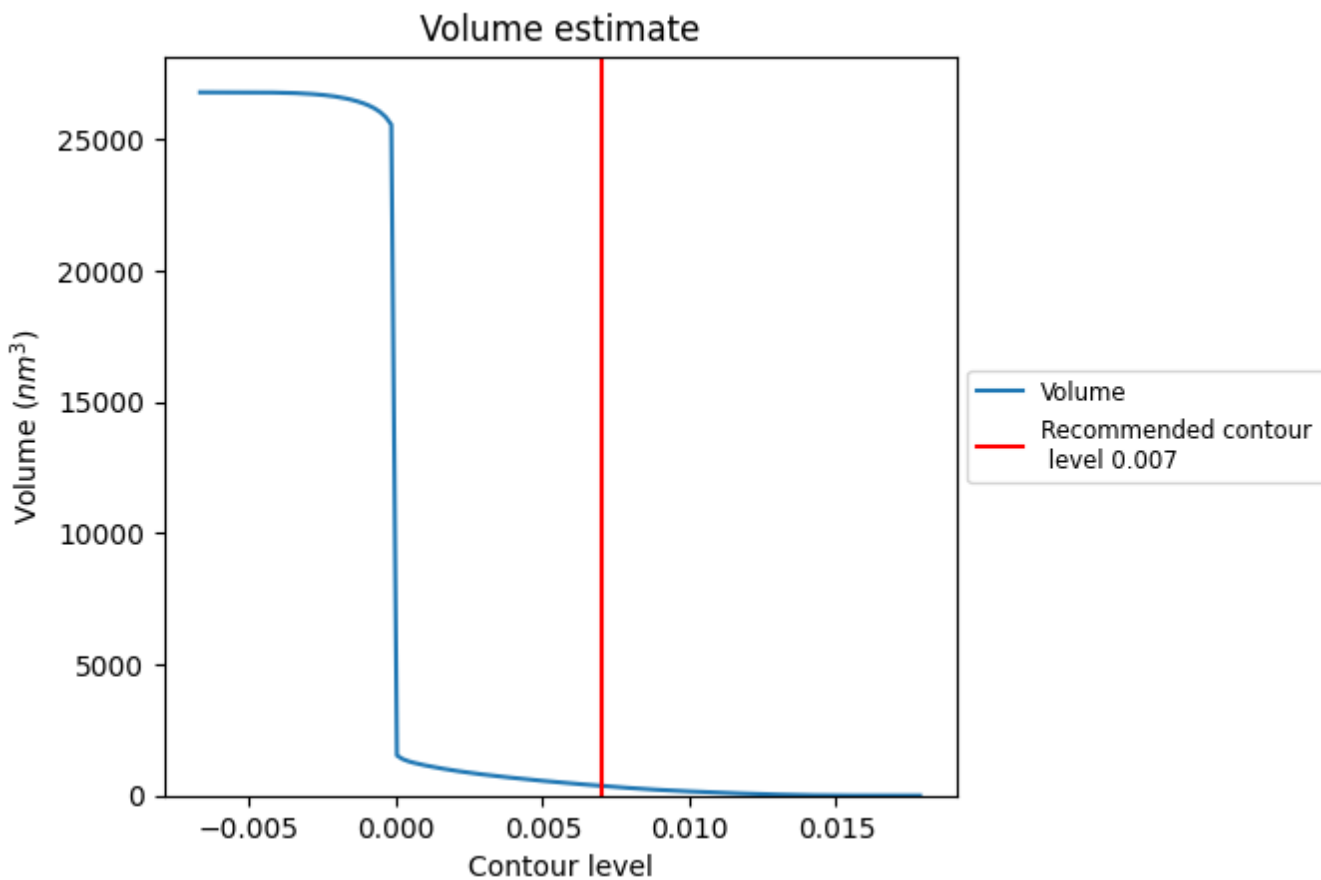
This section contains the results of statistical analysis of the map.

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.

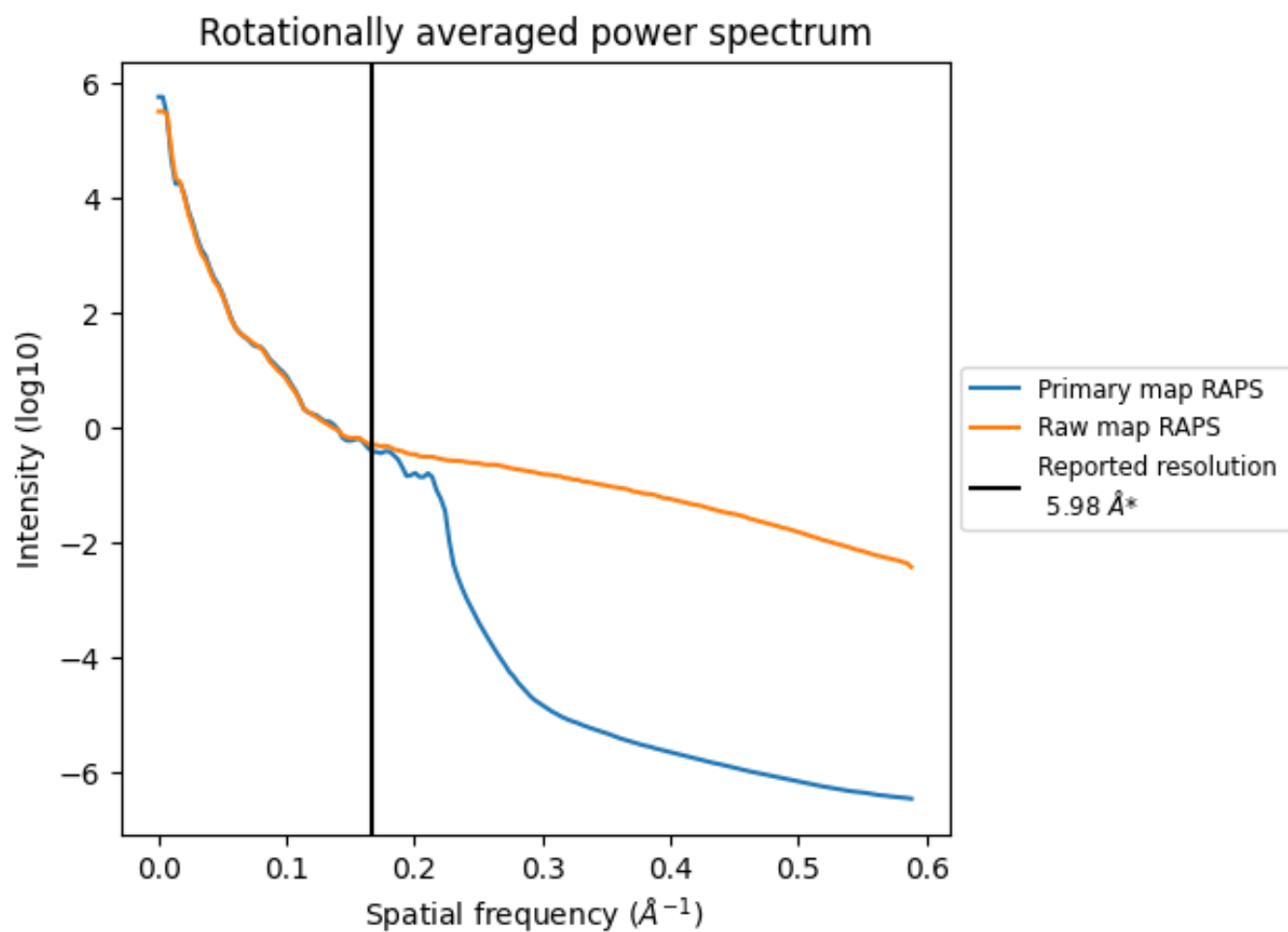
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 370 nm³; this corresponds to an approximate mass of 334 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

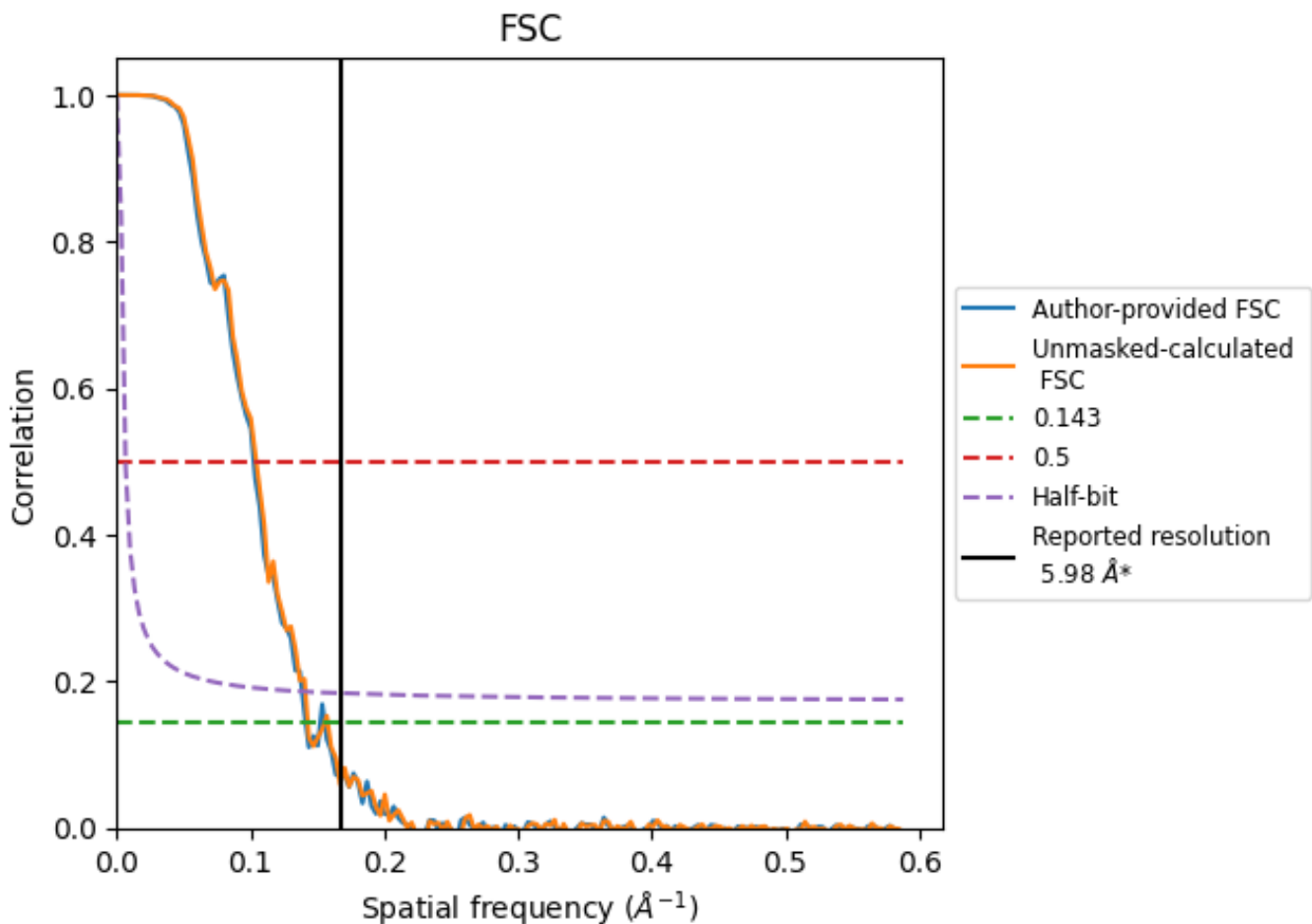


*Reported resolution corresponds to spatial frequency of 0.167 Å⁻¹

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 0.167 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.98	-	-
Author-provided FSC curve	7.08	9.76	7.21
Unmasked-calculated*	7.00	9.59	7.09

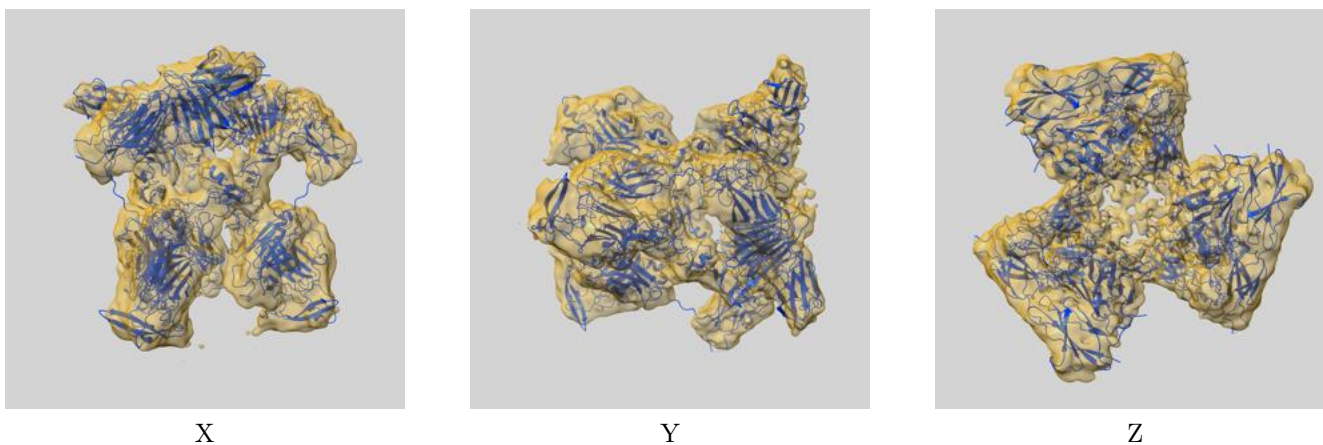
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 7.08 differs from the reported value 5.98 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.00 differs from the reported value 5.98 by more than 10 %

9 Map-model fit [i](#)

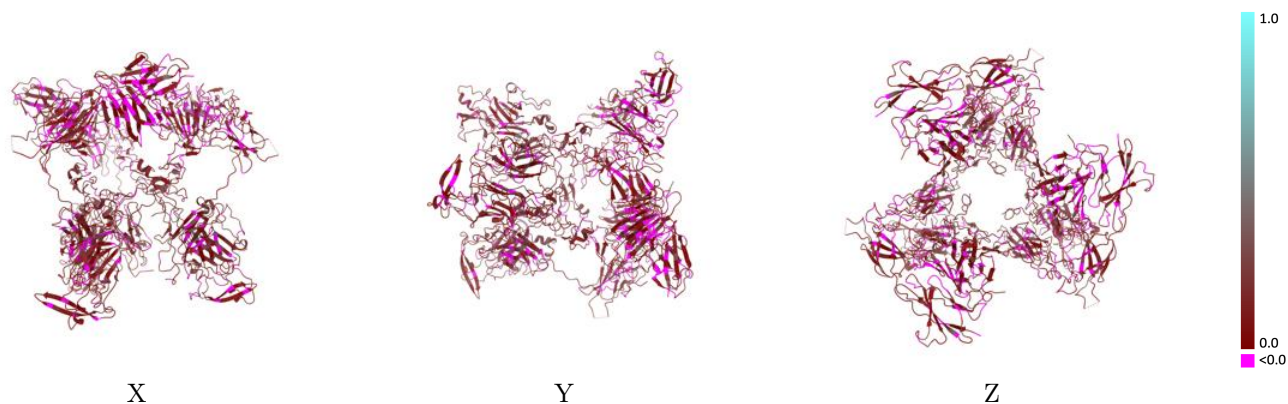
This section contains information regarding the fit between EMDB map EMD-12286 and PDB model 7NDG. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



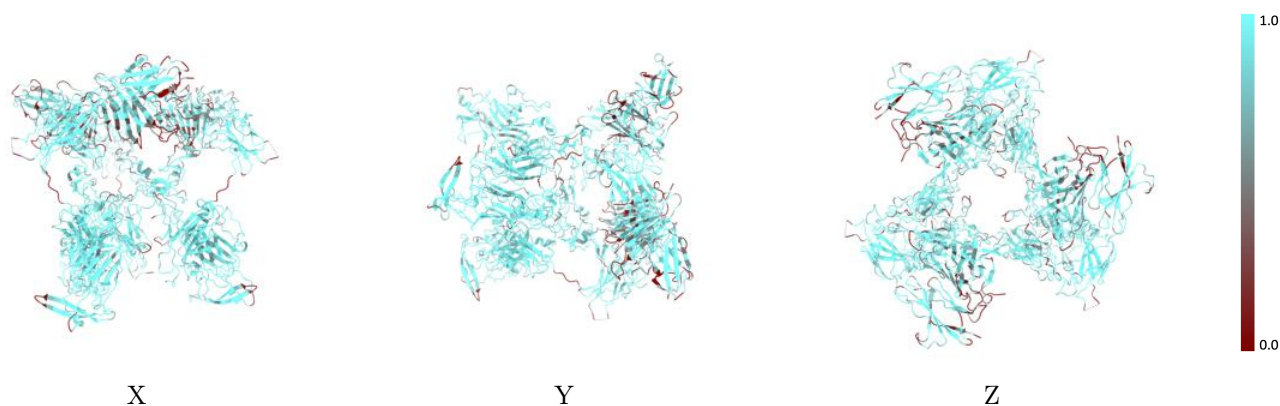
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



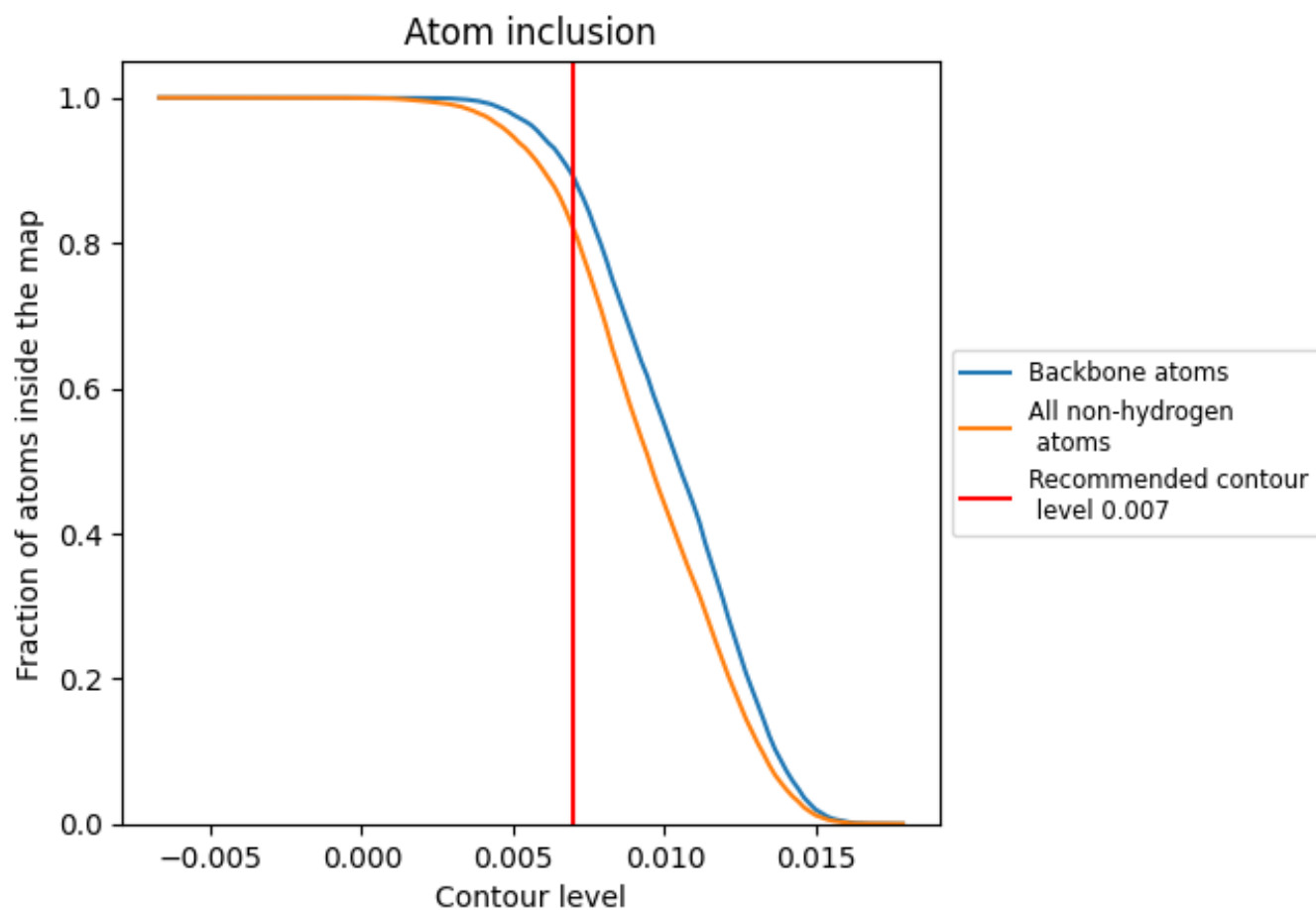
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8187	 0.1050
A	 0.8834	 0.1250
B	 0.8315	 0.1010
C	 0.6302	 0.0520
D	 0.8837	 0.1240
E	 0.8277	 0.1040
F	 0.6424	 0.0590
G	 0.8841	 0.1250
H	 0.8328	 0.1020
I	 0.6389	 0.0620
M	 0.5882	 0.0940
N	 0.5798	 0.0710
O	 0.5882	 0.0840

