Full wwPDB EM Validation Report

May 19, 2025 – 09:59 PM EDT

PDB ID	:	8EDN / pdb_00008edn
EMDB ID	:	EMD-28037
Title	:	Cryo-EM structure of the full-length human NF1 dimer
Authors	:	Darling, J.E.; Merk, A.; Grisshammer, R.; Ognjenovic, J.
Deposited on	:	2022-09-05
Resolution	:	3.80 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 (i) 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 (i)) were used in the production of this report:

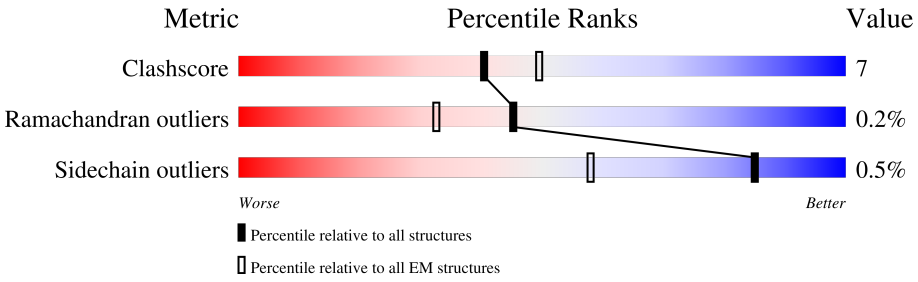
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.80 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	2818	18% 79%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3683 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 Isoform I of Neurofibromin.

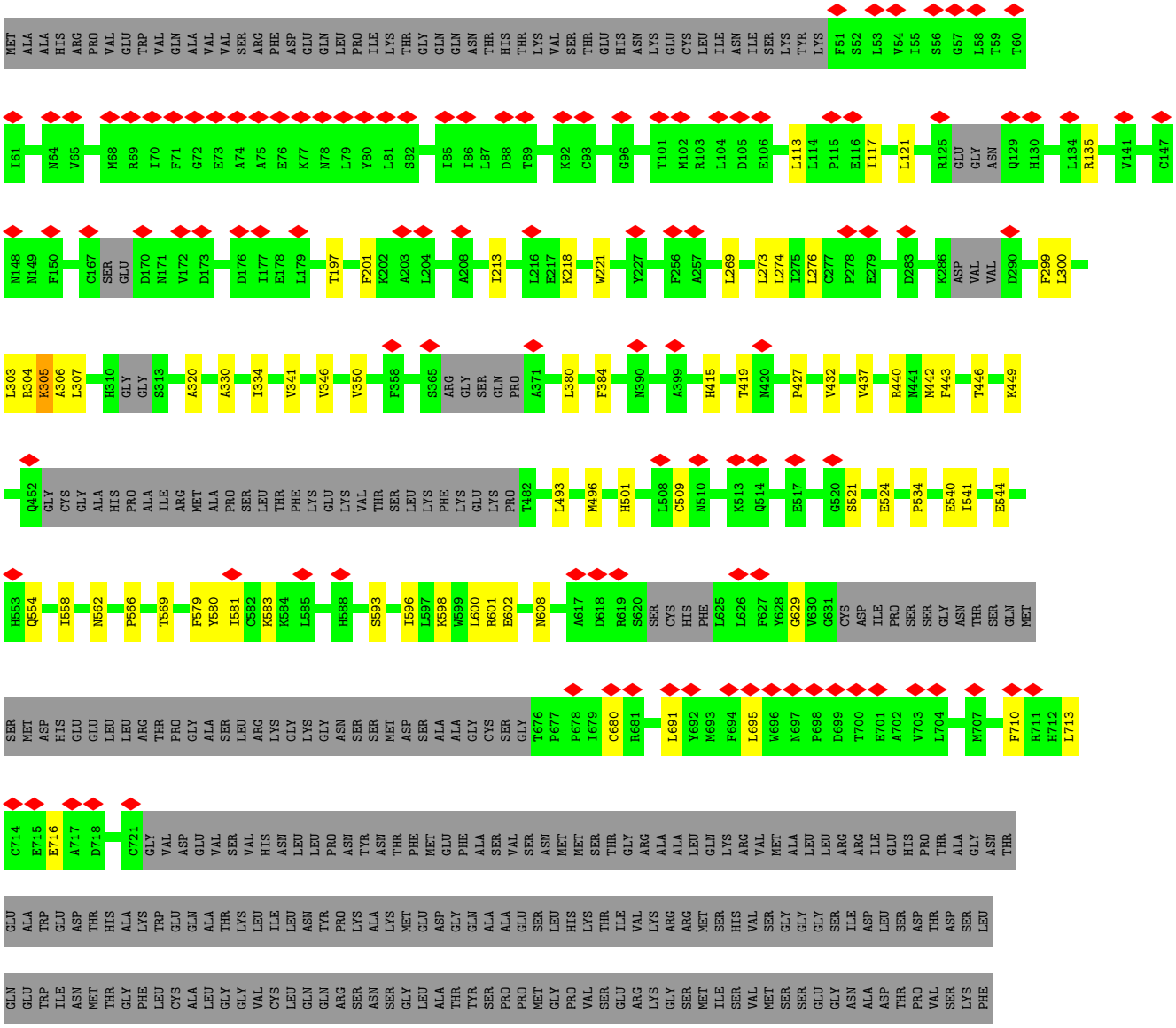
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	579	3683	2360	662	648	13	0	0

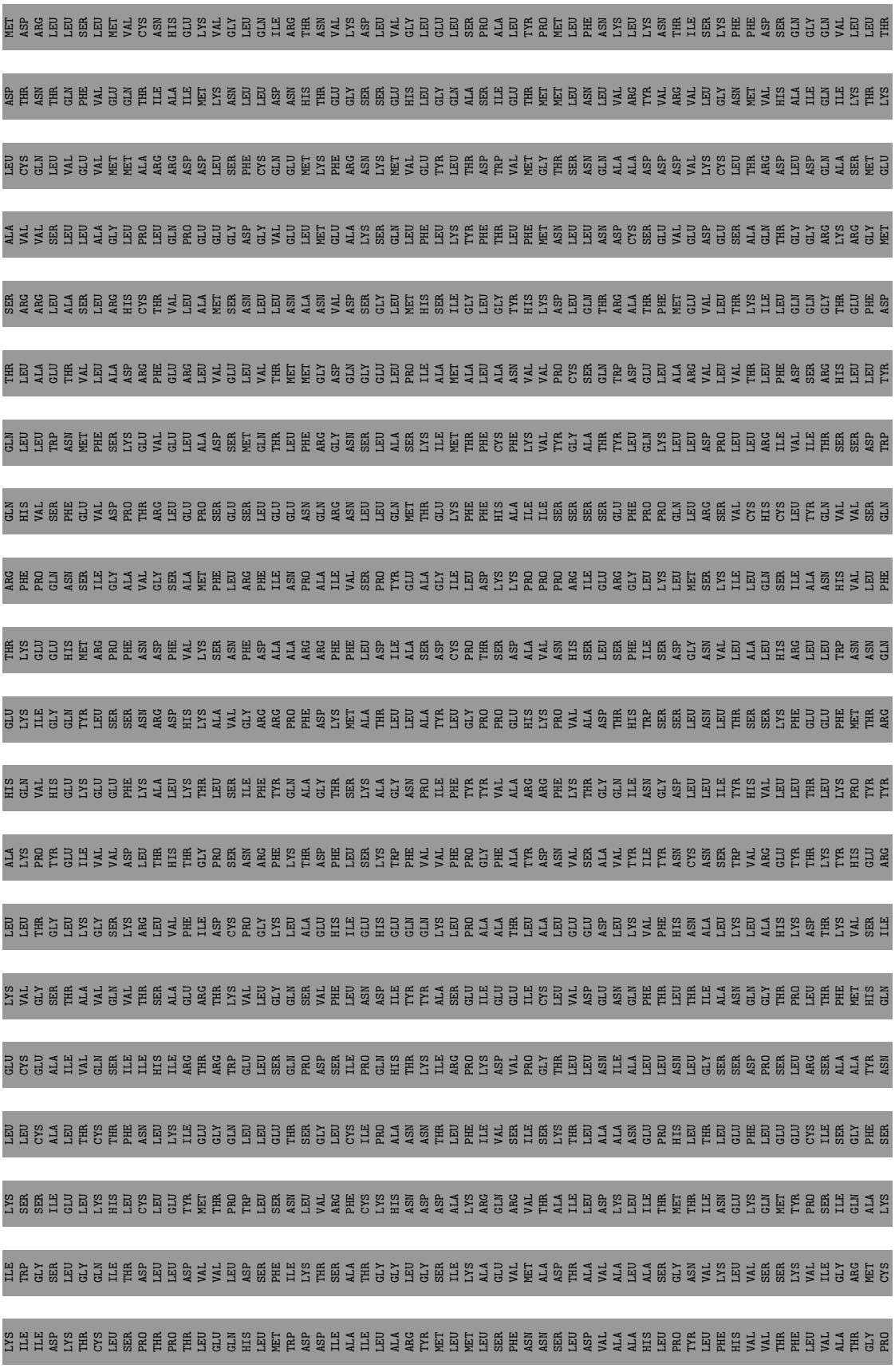
3 Residue-property plots (i)

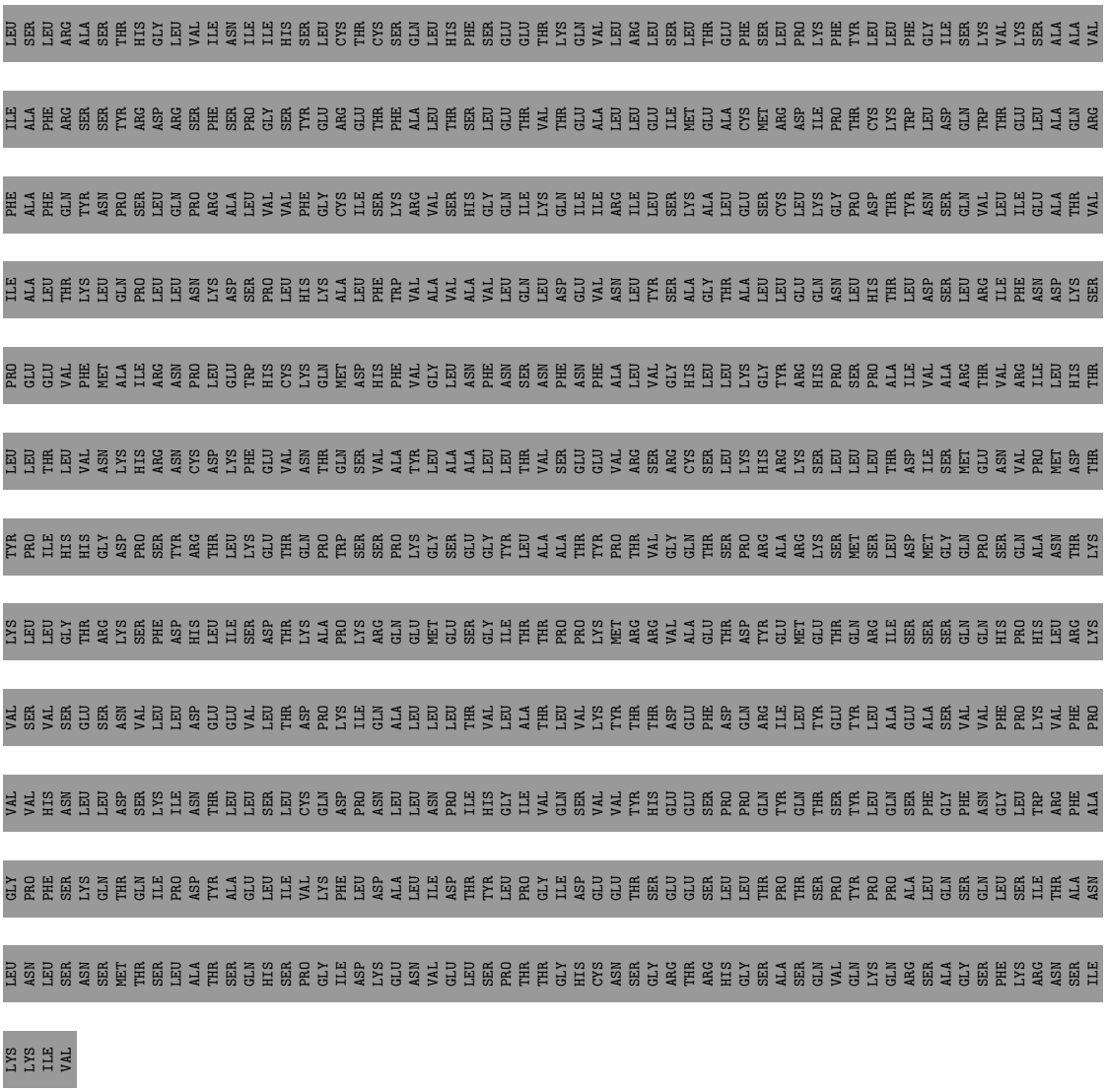
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Isoform I of Neurofibromin

Chain A:




MET ASP ARG LEU LEU SER LEU MET VAL CYS ASN HIS GLU LYS VAL GLY LEU GLN ILE ARG THR ASN VAL LYS ASP LEU VAL GLY LEU GLU LEU GLU LEU SER PRO ALA LEU TYR PRO MET MET LEU PHE ASN LYS LEU LYS ASN THR ILE SER LYS PHE PHE ASP SER GLN GLY GLN VAL LEU LEU THR
ASP THR ASN THR GLN PHE VAL GLU GLN THR ILE ALA ILE MET LYS ASN LEU LEU ASP HIS THR GLU GLY SER GLU HIS LEU GLY GLN ALA SER ILE GLU LEU ASN LEU VAL ARG TYR VAL ARG VAL LEU GLY ASN MET VAL HIS ALA ILE GLN ILE LYS THR LYS
LEU CYS GLN LEU VAL GLU VAL MET MET ALA ARG ARG ASP ASP LEU SER PHE CYS GLN GLU MET LYS PHE ARG ASN LYS MET VAL GLU TYR LEU THR ASP TRP VAL MET GLY THR SER ASN GLN ALA ALA ASP ASP ASP VAL LYS CYS LEU THR ARG ASP LEU ASP GLN ALA SER MET LYS
ALA VAL VAL SER LEU LEU ALA GLY LEU GLN PRO GLU GLU GLY ASP GLY VAL GLU LEU MET GLU ALA LYS SER GLN SER GLU VAL GLU ASP GLU LEU GLY GLY ARG GLY LYS ARG GLY MET
SER ARG ARG LEU ALA SER LEU ARG HIS CYS THR VAL LEU ALA MET SER ASN LEU LEU ASN ALA ASN VAL ASP SER GLY LEU GLU LEU THR LYS ILE LEU GLN GLY THR GLU PHE ASP
THR LEU ALA GLU THR VAL LEU ALA ASP ARG PHE GLU LEU VAL THR MET MET GLY ASP GLN GLY GLU LEU VAL PRO CYS SER GLN THR ARG ALA THR PHE MET GLU VAL LEU THR LYS ILE LEU GLU LEU TYR
GLN LEU LEU TRP ASN MET PHE SER LYS GLU VAL GLU LEU ALA ASP SER MET GLN THR LEU PHE ARG GLY ASN SER LEU ALA SER LYS ILE ALA MET THR GLU GLY ASP GLN TRP ASP GLU LEU GLN LYS LEU LEU ASP PRO LEU LEU VAL ILE THR SER SER ASP TRP
GLN HIS VAL SER PHE GLU VAL ASP PRO THR ARG LEU GLU PRO SER GLU SER LEU GLU GLU ASN GLN ARG ASN LEU LEU GLN MET THR GLU LYS PHE PHE HIS SER SER SER GLU PHE PRO GLN LEU LEU ARG SER VAL CYS HIS CYS LEU TYR GLN VAL VAL SER GLN
ARG PHE PRO GLN ASN SER ILE GLY ALA VAL GLY SER ALA MET PHE LEU ARG PHE ILE ASN PRO ALA ILE VAL SER PRO TYR GLU ALA GLY ILE LEU ASP LYS LYS PRO PRO PRO ARG ILE GLU GLY GLY LEU LYS LEU MET SER LYS ILE LEU GLN SER ILE ALA ASN HIS VAL LEU PHE
THR LYS GLU GLU HIS MET ARG PRO PHE ASN ASP PHE VAL LYS SER ASN PHE ASP ALA ALA ARG ARG PHE PHE LEU ASP CYS PRO THR SER ASP GLU HIS LYS PRO VAL ASN HIS SER LEU SER PHE ILE SER ASP GLY ASN VAL LEU ALA LEU HIS ARG LEU LEU LEU TRP ASN ASN GLN
GLU LYS ILE GLY GLN TYR LEU SER SER ASN ARG ASP HIS LYS ALA VAL GLY ARG ARG PRO PHE ASP LYS MET ALA THR LEU LEU ALA TYR LEU GLY PRO PRO GLU HIS LYS PRO VAL ALA ASP THR HIS TRP SER SER LEU LEU ASN LEU THR SER LYS PHE GLU GLU PHE MET THR ARG
HIS GLN VAL HIS GLU LYS GLU GLU PHE LYS ALA LEU LYS THR LEU SER ILE PHE TYR GLN ALA GLY THR SER LYS ALA GLY ASN PRO ILE PHE TYR TYR TYR VAL ALA LEU ASP PHE LYS THR GLY GLN ILE ASN GLY ASP LEU LEU LEU ILE TYR THR LEU SER LYS PRO TYR TYR
ALA LYS PRO TYR GLU ILE VAL VAL ASP LEU THR HIS THR GLY PRO SER ASN ARG PHE LYS THR ASP PHE LEU SER LYS TRP PHE VAL VAL PHE PRO GLY PHE ALA TYR ASP ASN VAL SER ALA VAL TYR ILE TYR ASN CYS ASN SER TRP VAL ARG GLU TYR THR HIS SER ARG GLU HIS
LEU LEU THR GLY LEU LYS ARG LEU VAL PHE ILE ASP CYS PRO GLY LYS LEU ALA GLU HIS ILE GLU HIS GLU GLN GLN LYS LEU PRO ALA ALA THR LEU LEU GLU GLU ASP LEU LYS VAL PHE HIS ASN ALA LEU LYS LEU ALA HIS LYS ASP THR LYS VAL SER ILE
LYS VAL GLY SER THR ALA VAL THR SER ALA GLU ARG THR LYS VAL LEU GLY GLN VAL THR GLN ASP ILE TYR TYR ALA SER GLU ILE GLU CYS LEU VAL ASP GLU ASN GLN PHE THR LEU THR ILE ALA SER ASN GLN GLY THR PRO LEU THR PHE MET HIS GLN
GLU CYS GLU ALA ILE VAL GLN SER ILE ILE ARG THR TRP GLU LEU SER GLN PRO ASP SER ILE PRO GLN HIS THR LYS ILE ARG PRO LYS ASP VAL PRO GLY THR LEU LEU ASN LEU GLY SER SER ASP PRO SER LEU ARG SER ALA ALA TYR TYR ASN
LEU LEU CYS ALA LEU THR CYS THR PHE ASN LEU LYS ILE GLU SER GLU LEU CYS ILE PRO ALA ASN ASN THR LEU PHE ILE VAL SER LYS THR LEU ALA ALA ASN GLU PRO HIS LEU THR LEU GLU PHE LEU GLU GLU CYS ILE SER GLY PHE SER
LYS SER SER ILE GLU LEU HIS LEU CYS LYS HIS ASN ASP ASP ALA LYS ARG GLN ARG VAL THR ALA ILE LEU ILE THR MET THR ILE ASN GLU LYS GLN MET TYR PRO SER ILE GLN ALA ASP
ILE TRP GLY SER LEU GLY GLN ILE THR GLY GLY LEU ALA SER GLY SER ALA THR ALA VAL ALA LEU ALA ASP VAL ALA LEU SER ASN VAL LYS LEU ILE GLY ARG MET CYS
LYS ILE ILE ASP LYS THR CYS LEU SER PRO THR PRO THR LEU GLU GLN HIS LEU MET TRP ASP ASP ILE ALA ILE LEU LEU ALA ARG TYR MET LEU MET LEU SER PHE ASN ASN SER LEU ASP VAL ALA ALA ALA HIS LEU PRO TYR LEU PHE HIS VAL VAL THR PHE LEU VAL ALA THR GLY PRO


LEU SER LEU ARG ALA SER THR HIS GLY LEU VAL ILE ASN ILE ILE HIS SER LEU CYS THR CYS SER GLN LEU HIS PHE SER GLU GLU THR LYS GLN VAL LEU ARG LEU SER LEU THR GLU PHE SER LEU PRO LYS PHE TYR LEU LEU PHE GLY ILE SER LYS VAL LYS SER ALA ALA VAL
ILE ALA PHE ARG SER SER TYR ARG ASP ARG SER PHE SER PRO GLY SER TYR GLU ARG GLU THR VAL THR GLU ALA LEU LEU GLU GLU ILE ILE MET GLU ALA CYS MET ARG ASP ILE PRO THR CYS LYS TRP LEU ASP GLN TRP THR GLU LEU ILE ALA GLN ARG
PHE ALA PHE GLN TYR ASN PRO SER LEU GLN PRO ARG ALA LEU VAL VAL PHE GLY CYS ILE SER LYS ARG VAL SER HIS GLY GLN ILE LYS GLN ILE ILE ARG ILE LEU SER LYS ALA GLU ALA LEU GLU SER CYS LEU LYS GLY PRO ASP THR TYR ASN SER GLN VAL LEU ILE GLU ALA ARG
ILE ALA LEU THR LYS LEU GLN PRO LEU LEU ASN LYS ASP SER PRO LEU HIS LYS ALA LEU PHE TRP VAL ALA VAL ALA VAL GLU GLN LEU ASP GLU VAL ASN LEU TYR SER ALA GLY THR ALA LEU GLU SER GLN ASN LEU HIS THR LEU ASP SER GLN LEU ARG ILE PHE ASN ASP LYS SER
PRO GLU GLU VAL PHE MET ALA ILE ARG ASN PRO LEU GLU TRP HIS CYS LYS GLN MET ASP HIS PHE VAL GLY LEU ASN PHE ASN SER ASN PHE ASN PHE ALA LEU VAL GLY TYR ARG HIS PRO SER PRO ALA ILE VAL ALA ALA ARG THR VAL ARG ILE LEU HIS THR
LEU LEU THR LEU VAL ASN LYS HIS ARG ASN CYS ASP LYS PHE GLU VAL ASN THR GLN SER VAL ALA TYR LEU ALA ALA LEU LEU THR VAL SER GLU GLU VAL ARG SER ARG CYS SER LEU LYS HIS ARG LYS SER LEU LEU THR ASP ILE SER MET GLU ASN VAL PRO MET ASP THR
TYR PRO ILE HIS HIS GLY ASP PRO SER TYR ARG THR LEU LYS GLU THR GLN PRO TRP SER SER PRO LYS GLY SER GLU GLY TYR LEU ALA ALA THR TYR PRO THR VAL SER GLU GLU GLU VAL ARG SER ARG CYS SER LEU LYS HIS ARG LYS SER LEU LEU THR ASP MET GLY GLN PRO SER GLN ALA ASN THR LYS
LYS LEU LEU GLY THR ARG LYS SER PHE ASP HIS LEU ILE SER ASP THR LYS ALA PRO LYS ARG GLN GLU MET GLU SER GLY ILE THR THR PRO PRO LYS MET ARG ARG VAL ALA GLU THR ASP TYR GLU MET GLU THR GLN ARG ILE SER SER SER GLN GLN HIS PRO HIS LEU ARG LYS
VAL SER VAL SER GLU SER ASN VAL LEU LEU ASP GLU GLU VAL LEU THR ASP PRO LYS ILE GLN ALA LEU LEU LEU THR VAL LEU ALA THR LEU VAL LYS TYR THR THR ASP GLU PHE ASP GLN ARG ILE LEU TYR GLU TYR LEU ALA GLU ALA SER VAL VAL PHE PRO LYS VAL PHE PRO
VAL VAL HIS ASN LEU LEU ASP SER LYS ILE ASN THR LEU LEU SER LEU CYS GLN ASP PRO ASN LEU LEU ASN PRO ILE HIS GLY ILE VAL GLN SER VAL VAL TYR HIS GLU GLU SER PRO PRO GLN TYR GLN THR SER TYR LEU GLN SER PHE GLY PHE ASN GLY LEU TRP ARG PHE ALA
GLY PRO PHE SER LYS GLN THR GLN ILE PRO ASP TYR ALA GLU LEU PHE LEU ASP ALA LEU ILE ASP THR TYR LEU PRO GLY ILE ASP GLU GLU THR SER GLU GLU SER LEU LEU THR PRO THR PRO TYR PRO PRO ALA LEU GLN SER GLN LEU SER ILE THR ALA ASN
LEU ASN LEU SER ASN SER MET THR SER LEU ALA THR SER GLN HIS SER PRO GLY ILE ASP LYS GLU ASN VAL GLU LEU SER PRO THR THR GLY HIS CYS ASN SER GLY ARG THR ARG HIS GLY SER ALA SER GLN VAL GLN LYS GLN ARG SER ALA GLY SER PHE LYS ARG ASN SER ILE
LYS LYS ILE VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	161208	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 200	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	9.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0223	Depositor
Map size (Å)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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	0.16	0/3748	0.36	3/5161 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	305	LYS	CA-C-N	-5.41	112.49	120.38
1	A	305	LYS	C-N-CA	-5.41	112.49	120.38
1	A	432	VAL	N-CA-C	-5.08	108.34	113.47

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	3683	0	2778	44	0
All	All	3683	0	2778	44	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 7.

All (44) 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:A:440:ARG:NH2	1:A:509:CYS:O	2.21	0.74
1:A:598:LYS:HA	1:A:601:ARG:HD3	1.76	0.68
1:A:629:GLY:HA3	1:A:680:CYS:HB3	1.83	0.60
1:A:501:HIS:NE2	1:A:544:GLU:O	2.33	0.59
1:A:197:THR:O	1:A:201:PHE:HB2	2.04	0.58
1:A:534:PRO:HG2	1:A:580:TYR:HE1	1.69	0.58
1:A:415:HIS:O	1:A:419:THR:N	2.38	0.57
1:A:440:ARG:HA	1:A:443:PHE:HD1	1.72	0.54
1:A:113:LEU:O	1:A:117:ILE:N	2.40	0.52
1:A:346:VAL:O	1:A:350:VAL:HG23	2.10	0.52
1:A:713:LEU:O	1:A:716:GLU:HG3	2.10	0.52
1:A:273:LEU:HA	1:A:276:LEU:HD12	1.92	0.51
1:A:598:LYS:O	1:A:602:GLU:HG2	2.10	0.51
1:A:443:PHE:O	1:A:446:THR:OG1	2.25	0.50
1:A:443:PHE:HB2	1:A:496:MET:SD	2.52	0.50
1:A:213:ILE:HG23	1:A:269:LEU:HD22	1.93	0.49
1:A:305:LYS:O	1:A:306:ALA:C	2.53	0.49
1:A:554:GLN:O	1:A:558:ILE:HG12	2.14	0.48
1:A:446:THR:O	1:A:449:LYS:HG2	2.13	0.47
1:A:440:ARG:HA	1:A:443:PHE:CD1	2.49	0.47
1:A:437:VAL:HA	1:A:440:ARG:CZ	2.44	0.47
1:A:121:LEU:HD11	1:A:135:ARG:HA	1.97	0.46
1:A:593:SER:HA	1:A:596:ILE:HD12	1.97	0.46
1:A:579:PHE:O	1:A:583:LYS:HG2	2.16	0.46
1:A:442:MET:O	1:A:446:THR:HG23	2.18	0.44
1:A:562:ASN:HB3	1:A:566:PRO:HA	1.99	0.44
1:A:213:ILE:HG12	1:A:269:LEU:HD22	1.98	0.43
1:A:493:LEU:HA	1:A:496:MET:HE3	2.00	0.43
1:A:274:LEU:HD21	1:A:300:LEU:HD11	2.01	0.43
1:A:540:GLU:HG2	1:A:541:ILE:N	2.34	0.43
1:A:303:LEU:O	1:A:304:ARG:C	2.62	0.42
1:A:521:SER:O	1:A:524:GLU:N	2.52	0.42
1:A:330:ALA:O	1:A:334:ILE:N	2.53	0.42
1:A:493:LEU:HD12	1:A:496:MET:SD	2.59	0.42
1:A:695:LEU:HD11	1:A:710:PHE:HE2	1.85	0.42
1:A:218:LYS:HA	1:A:221:TRP:HB2	2.01	0.41
1:A:691:LEU:HD23	1:A:691:LEU:HA	1.83	0.41
1:A:493:LEU:O	1:A:496:MET:HG2	2.19	0.41
1:A:380:LEU:HD23	1:A:380:LEU:HA	1.87	0.41
1:A:384:PHE:CZ	1:A:427:PRO:HB2	2.56	0.41
1:A:562:ASN:ND2	1:A:569:THR:OG1	2.49	0.41
1:A:608:ASN:CG	1:A:716:GLU:HB3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LEU:HG	1:A:320:ALA:HB1	2.02	0.40
1:A:581:ILE:HG21	1:A:600:LEU:HD13	2.02	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	561/2818 (20%)	528 (94%)	32 (6%)	1 (0%)	44 74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	341	VAL

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	217/2512 (9%)	216 (100%)	1 (0%)	86 90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	PHE

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	510	ASN
1	A	562	ASN
1	A	614	ASN
1	A	682	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.

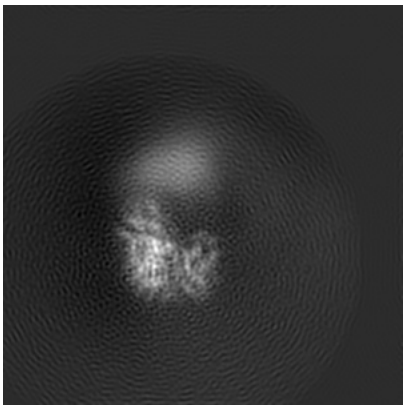
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28037. These allow visual inspection of the internal detail of the map and identification of artifacts.

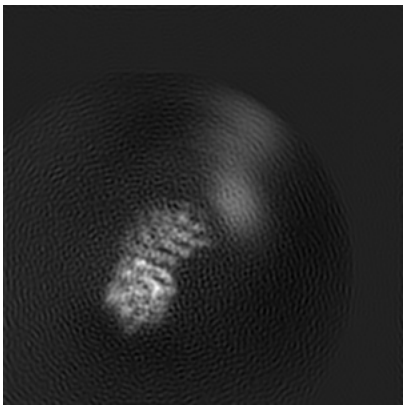
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



X



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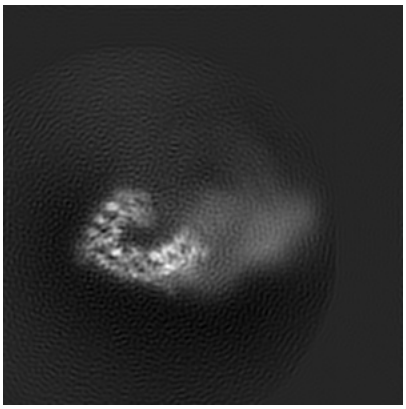
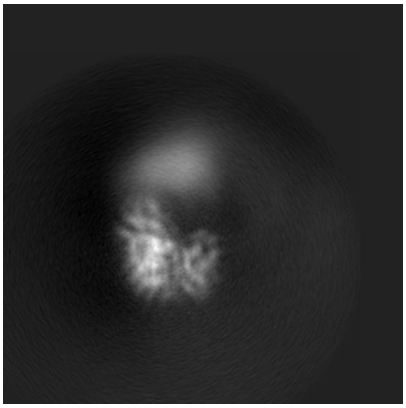
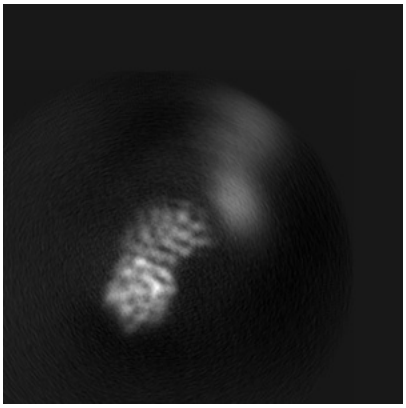


Z

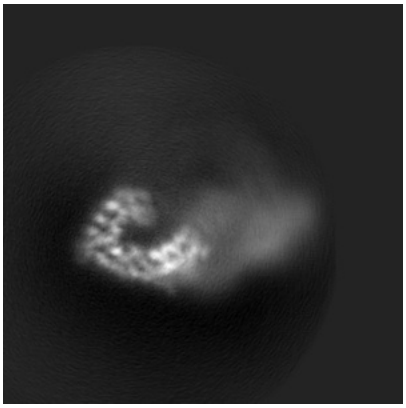
6.1.2 Raw map



X



Y

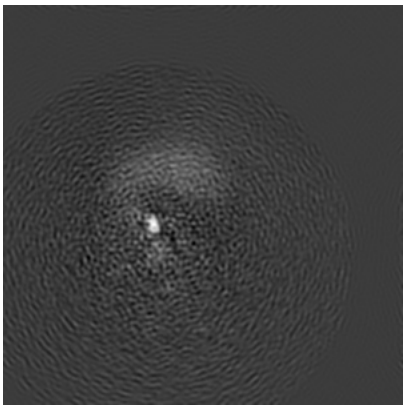


Z

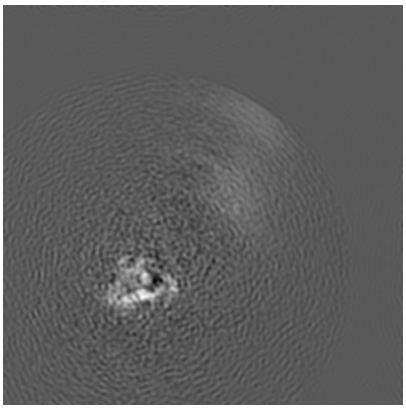
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

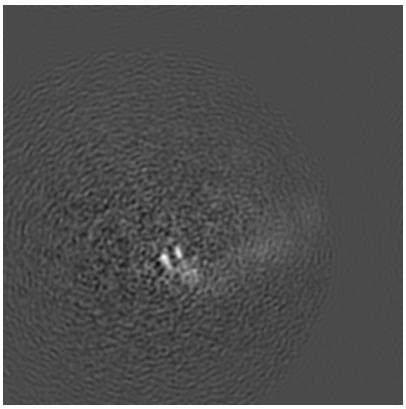
6.2.1 Primary map



X Index: 128

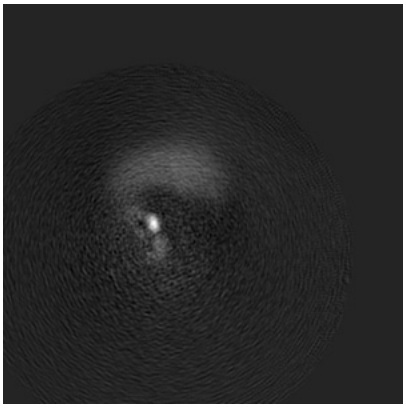


Y Index: 128

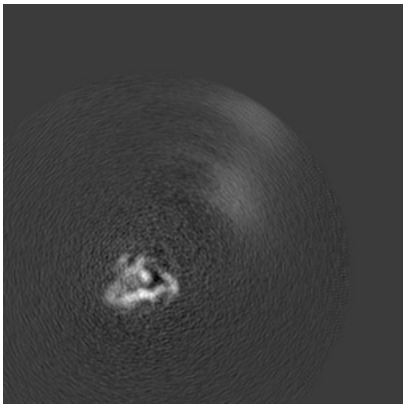


Z Index: 128

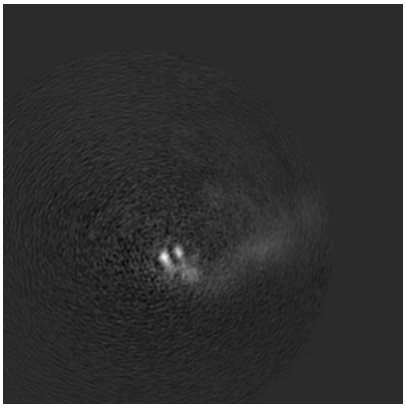
6.2.2 Raw map



X Index: 128



Y Index: 128

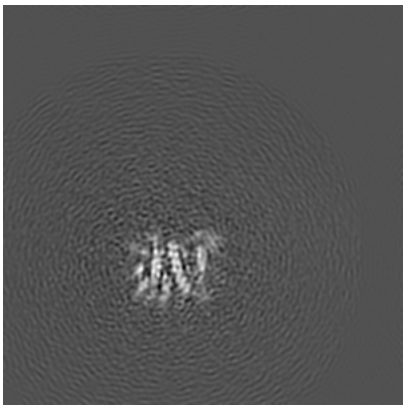


Z Index: 128

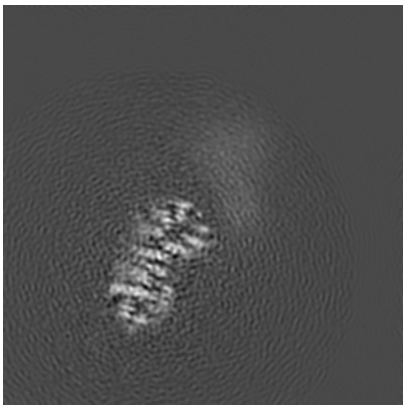
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

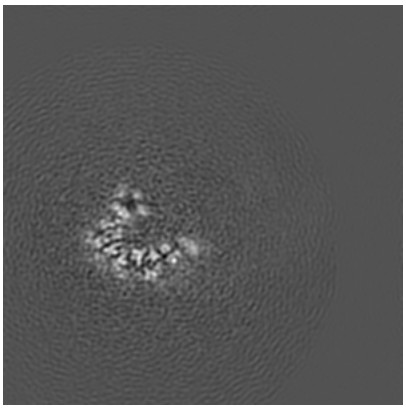
6.3.1 Primary map



X Index: 71

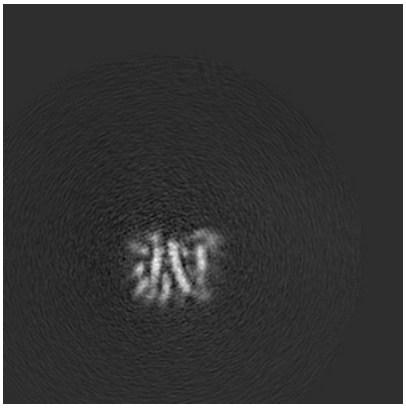


Y Index: 96

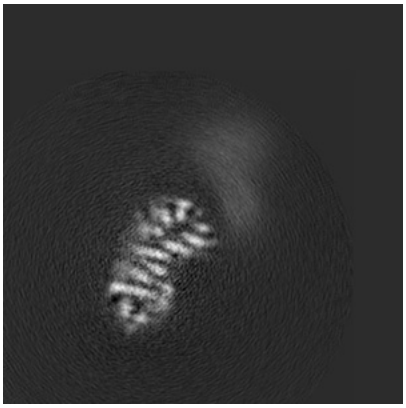


Z Index: 98

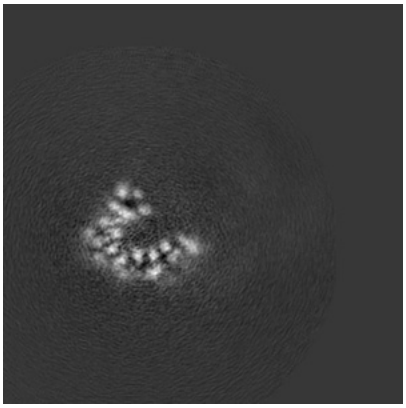
6.3.2 Raw map



X Index: 71



Y Index: 96

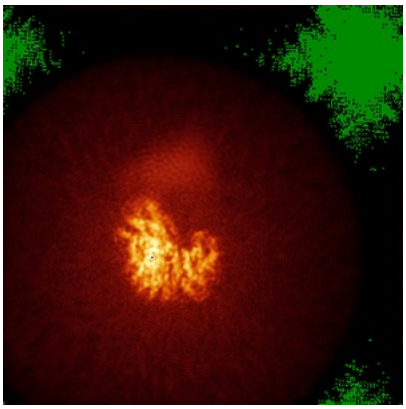


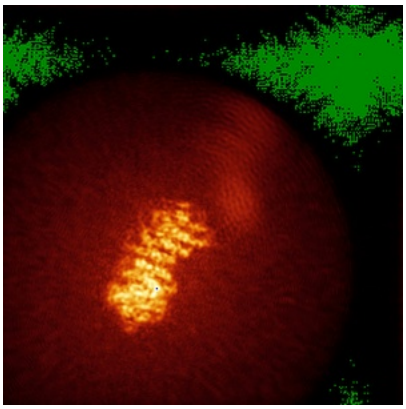
Z Index: 97

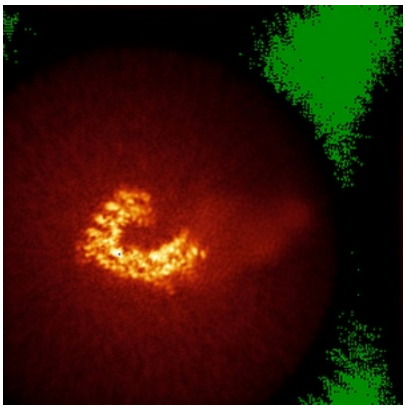
The images above show the largest variance slices of the map in three orthogonal directions.

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

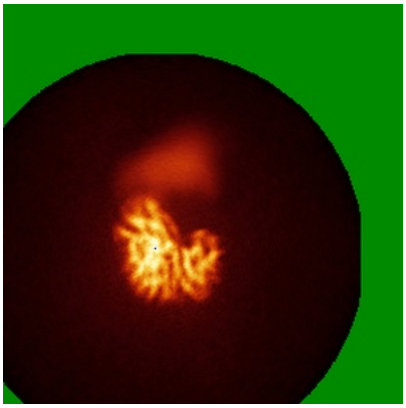
6.4.1 Primary map

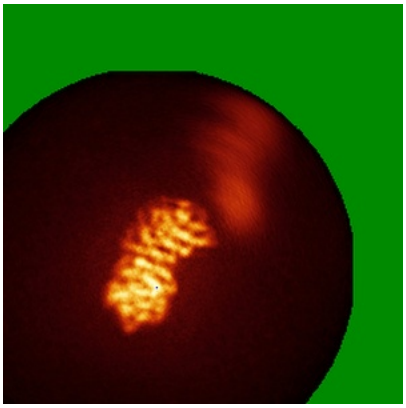

X

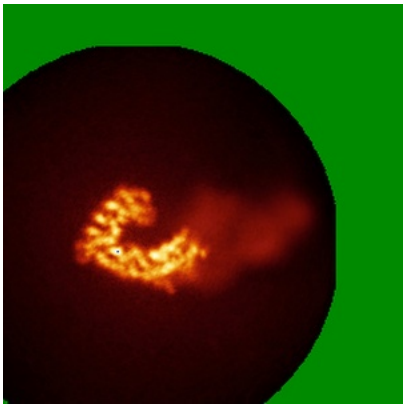

Y


Z

6.4.2 Raw map


X

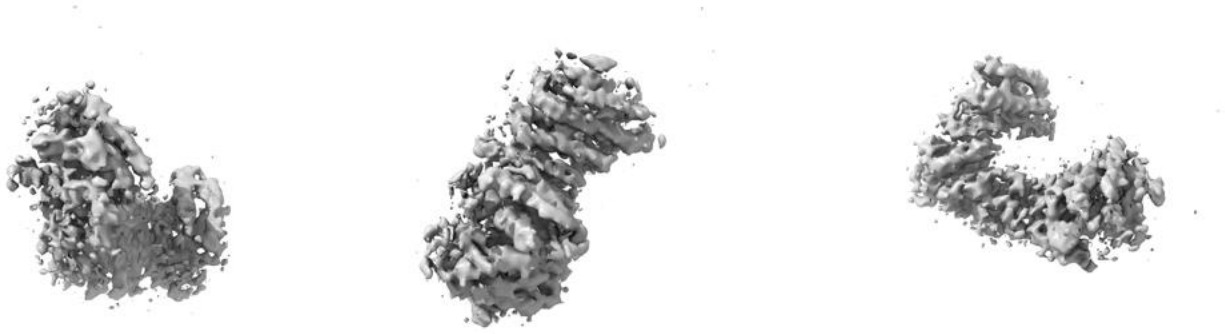

Y


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)

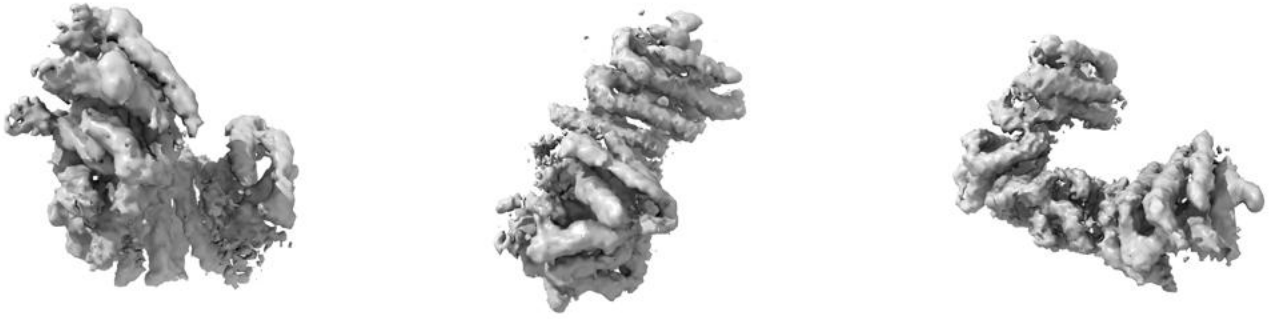
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0223. 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.

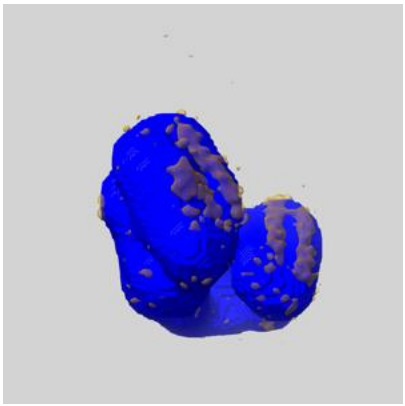
6.6 Mask visualisation (i)

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

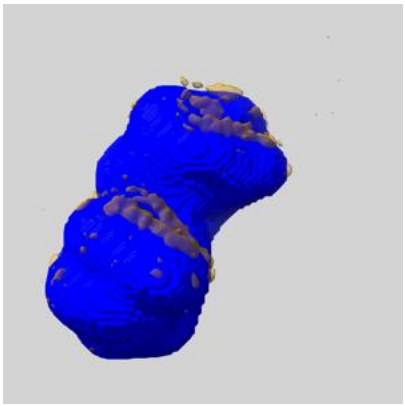
A mask typically either:

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

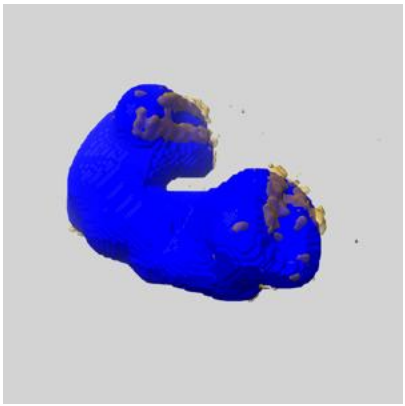
6.6.1 emd_28037_msk_1.map (i)



X



Y

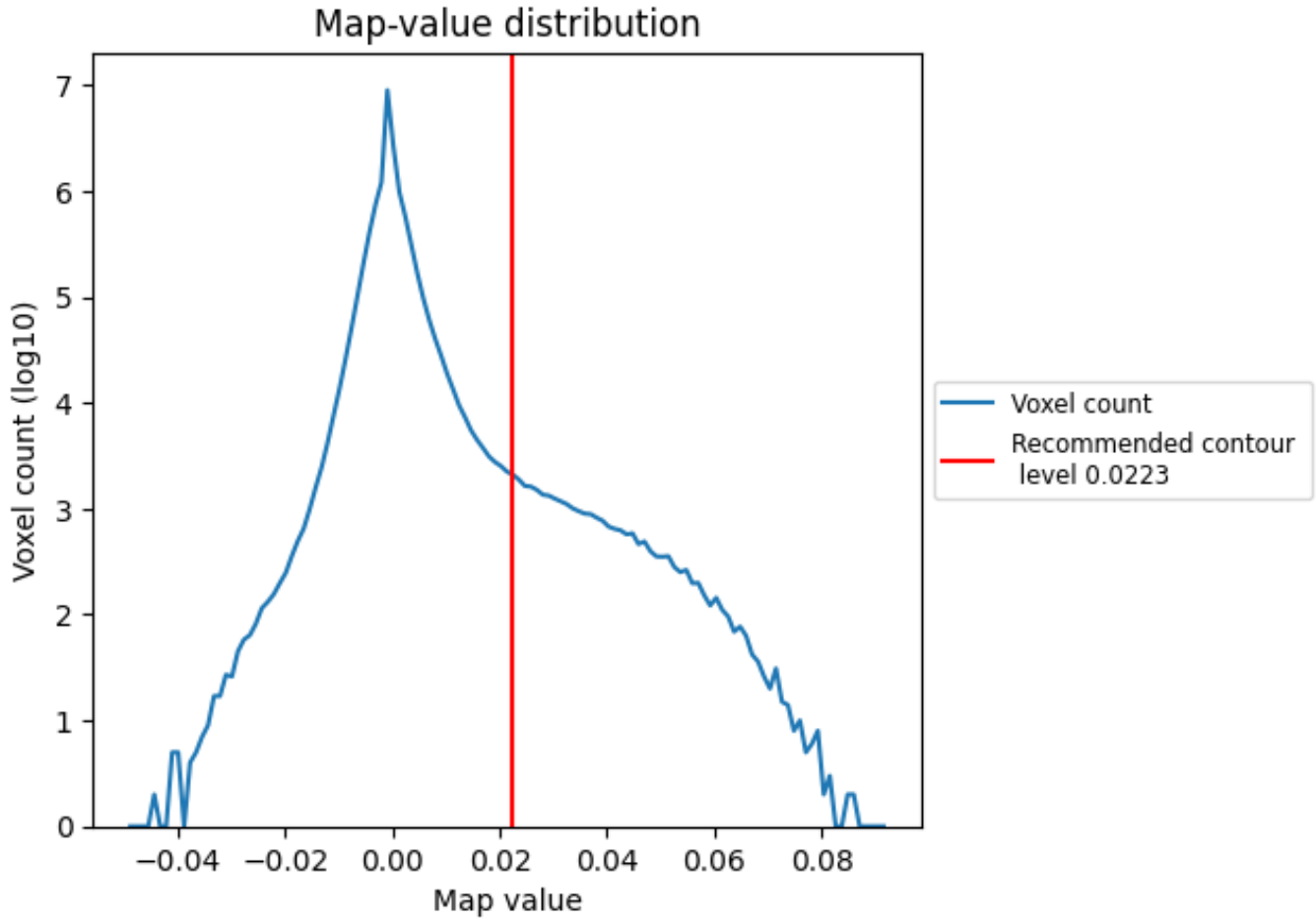


Z

7 Map analysis

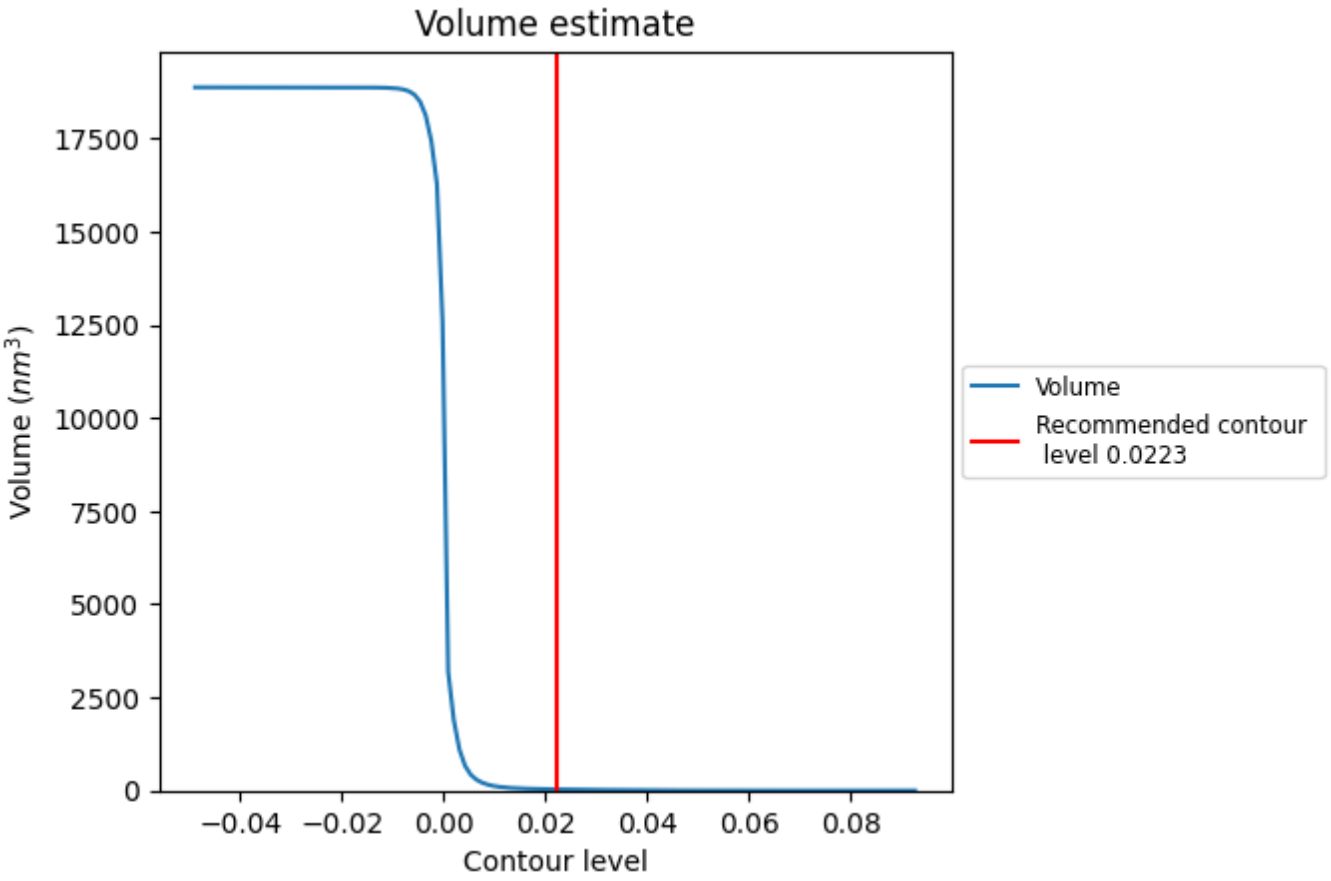
This section contains the results of statistical analysis of the map.

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.

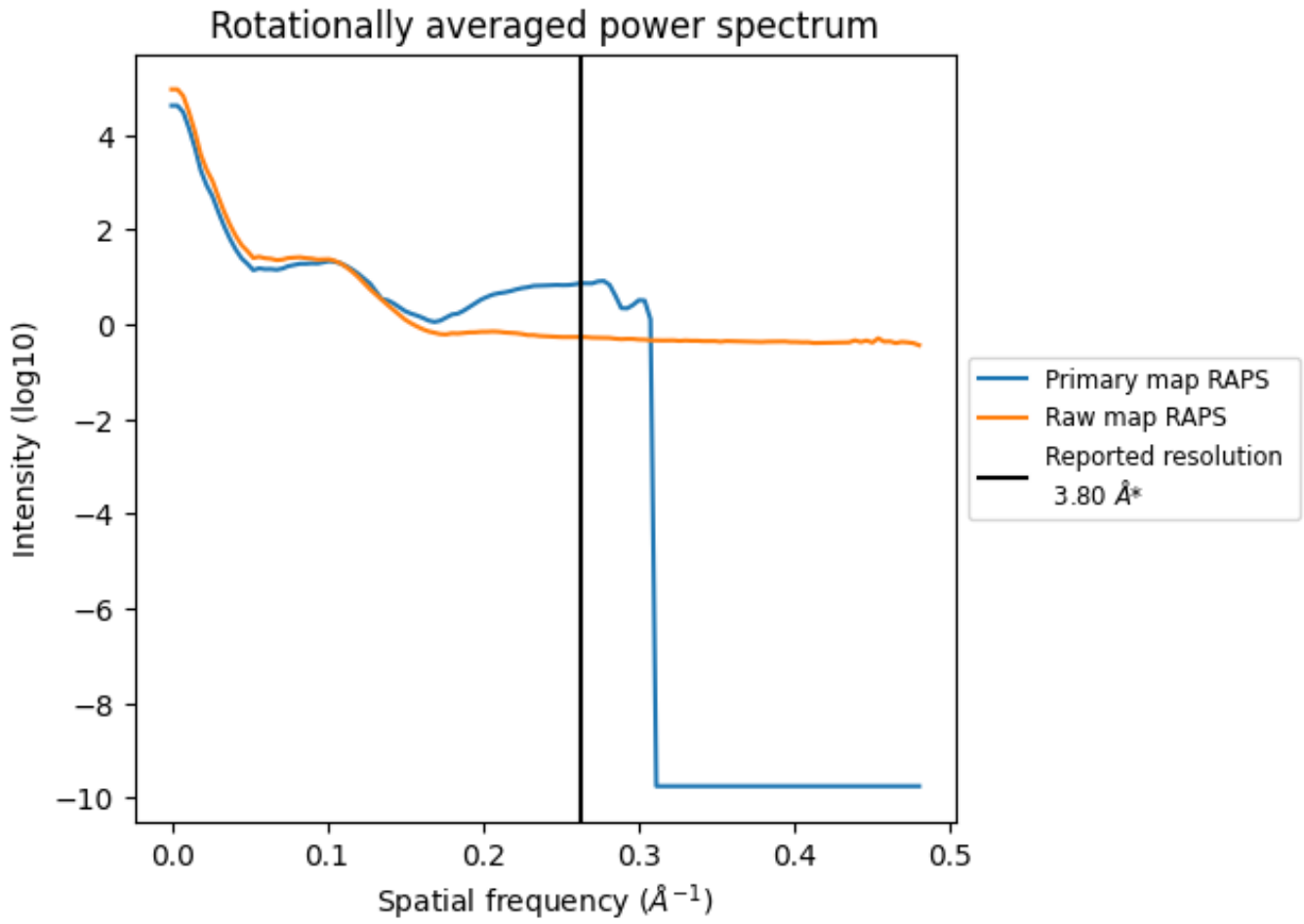
7.2 Volume estimate (i)



The volume at the recommended contour level is 32 nm^3; this corresponds to an approximate mass of 29 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)

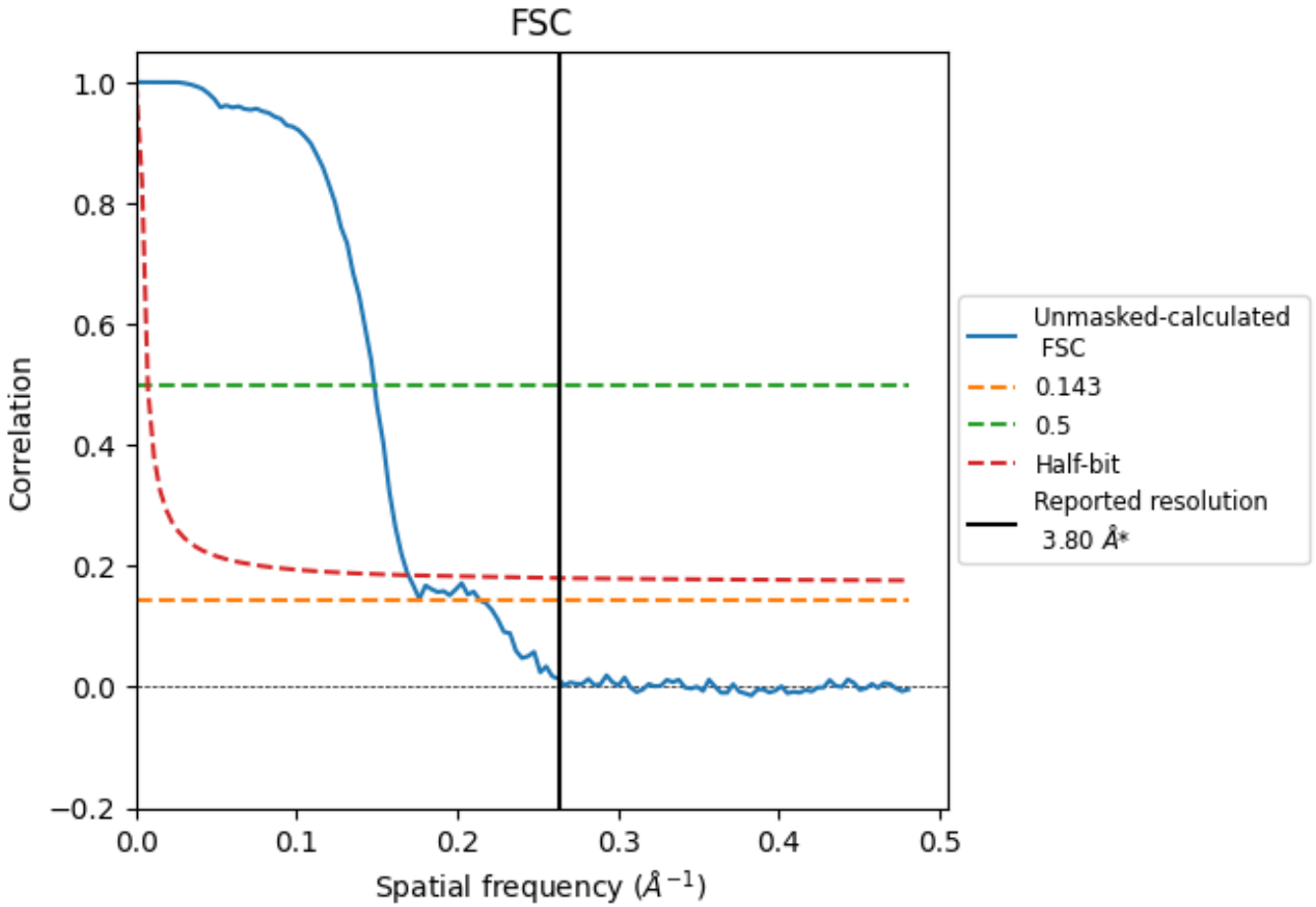


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

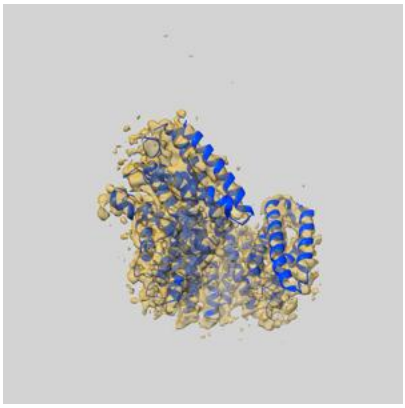
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.67	6.74	5.90

*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 4.67 differs from the reported value 3.8 by more than 10 %

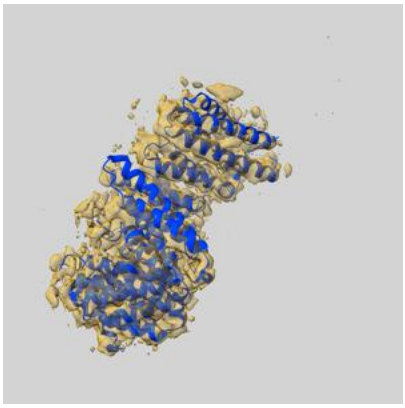
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28037 and PDB model 8EDN. Per-residue inclusion information can be found in section 3 on page 4.

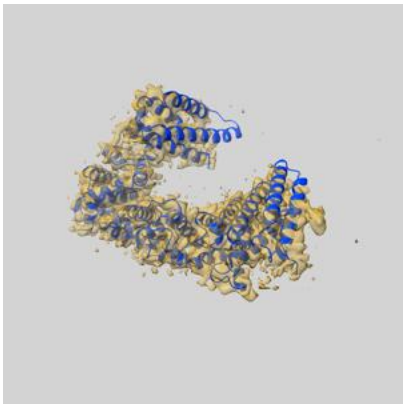
9.1 Map-model overlay



X



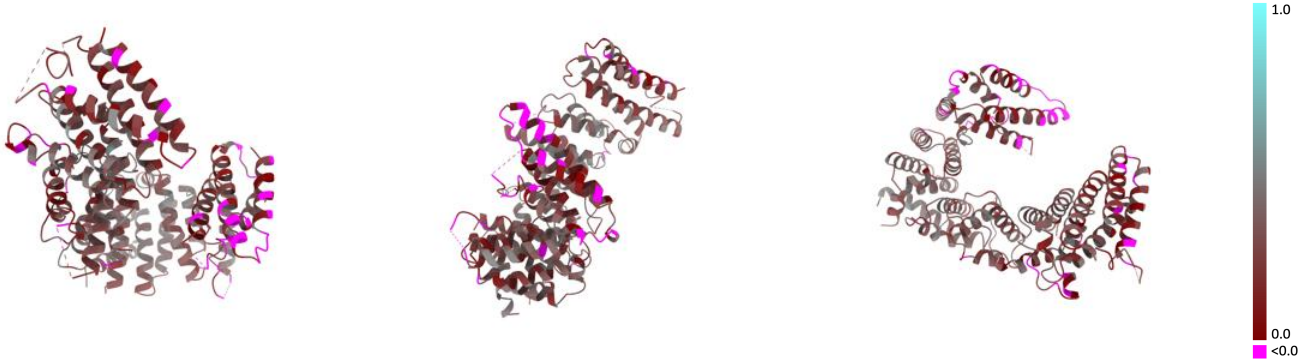
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0223 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.

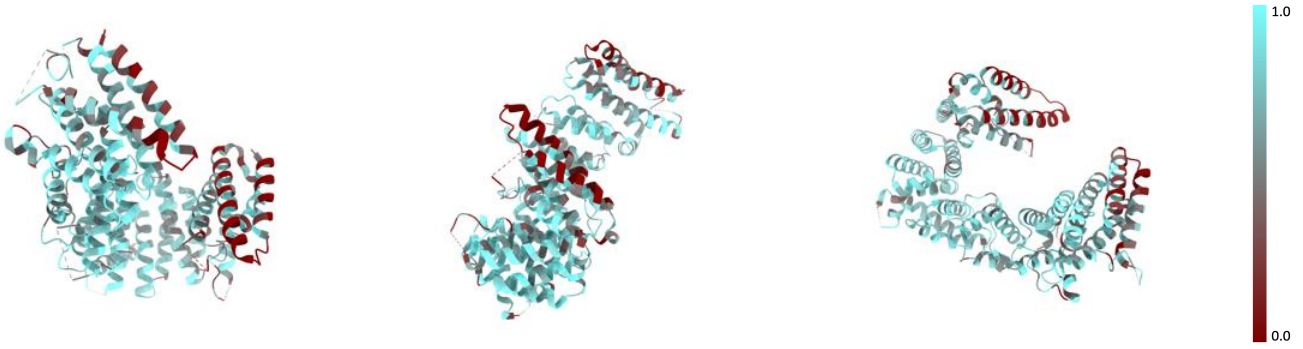
9.2 Q-score mapped to coordinate model (i)



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.

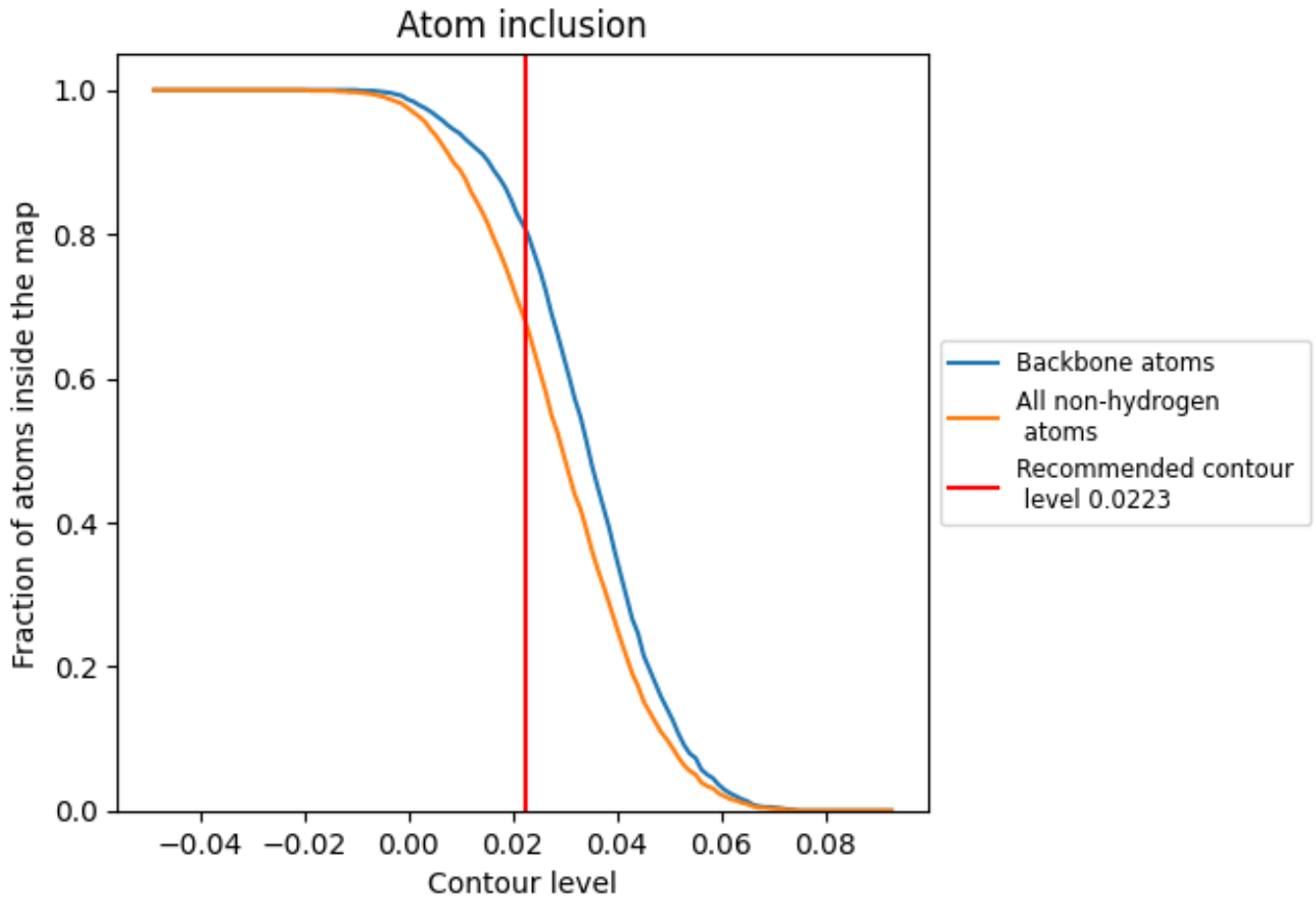
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0223).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 68% 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 (0.0223) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6810	0.2610
A	0.6810	0.2610