wwPDB EM Validation Summary Report

Jul 22, 2023 – 01:08 PM EDT

PDB ID	:	8FY3
EMDB ID	:	EMD-29551
Title	:	Structure of NOT1:NOT10:NOT11 module of the human CCR4-NOT complex
Authors	:	Lea, S.M.; Deme, J.C.; Raisch, T.; Pekovic, F.; Valkov, E.
Deposited on	:	2023-01-25
Resolution	:	2.88 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:

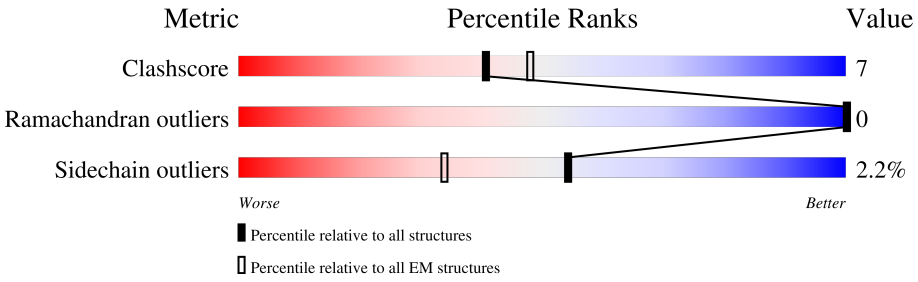
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.88 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 <=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	1000	31% 44% 11% · 44%
2	B	684	17% 62% 14% 23%
3	C	269	· 11% · 86%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8948 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 CCR4-NOT transcription complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	561	Total	C	N	O	S	0	0
			4520	2912	782	805	21		

- Molecule 2 is a protein called CCR4-NOT transcription complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	524	Total	C	N	O	S	0	0
			4114	2625	702	756	31		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	MET	-	initiating methionine	UNP Q9H9A5

- Molecule 3 is a protein called CCR4-NOT transcription complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	38	Total	C	N	O	S	0	0
			314	202	53	56	3		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	256	MET	-	initiating methionine	UNP B3KNB0
C	499	GLY	-	expression tag	UNP B3KNB0
C	500	SER	-	expression tag	UNP B3KNB0
C	501	GLU	-	expression tag	UNP B3KNB0
C	502	ASN	-	expression tag	UNP B3KNB0
C	503	LEU	-	expression tag	UNP B3KNB0
C	504	TYR	-	expression tag	UNP B3KNB0
C	505	PHE	-	expression tag	UNP B3KNB0
C	506	GLN	-	expression tag	UNP B3KNB0
C	507	GLY	-	expression tag	UNP B3KNB0

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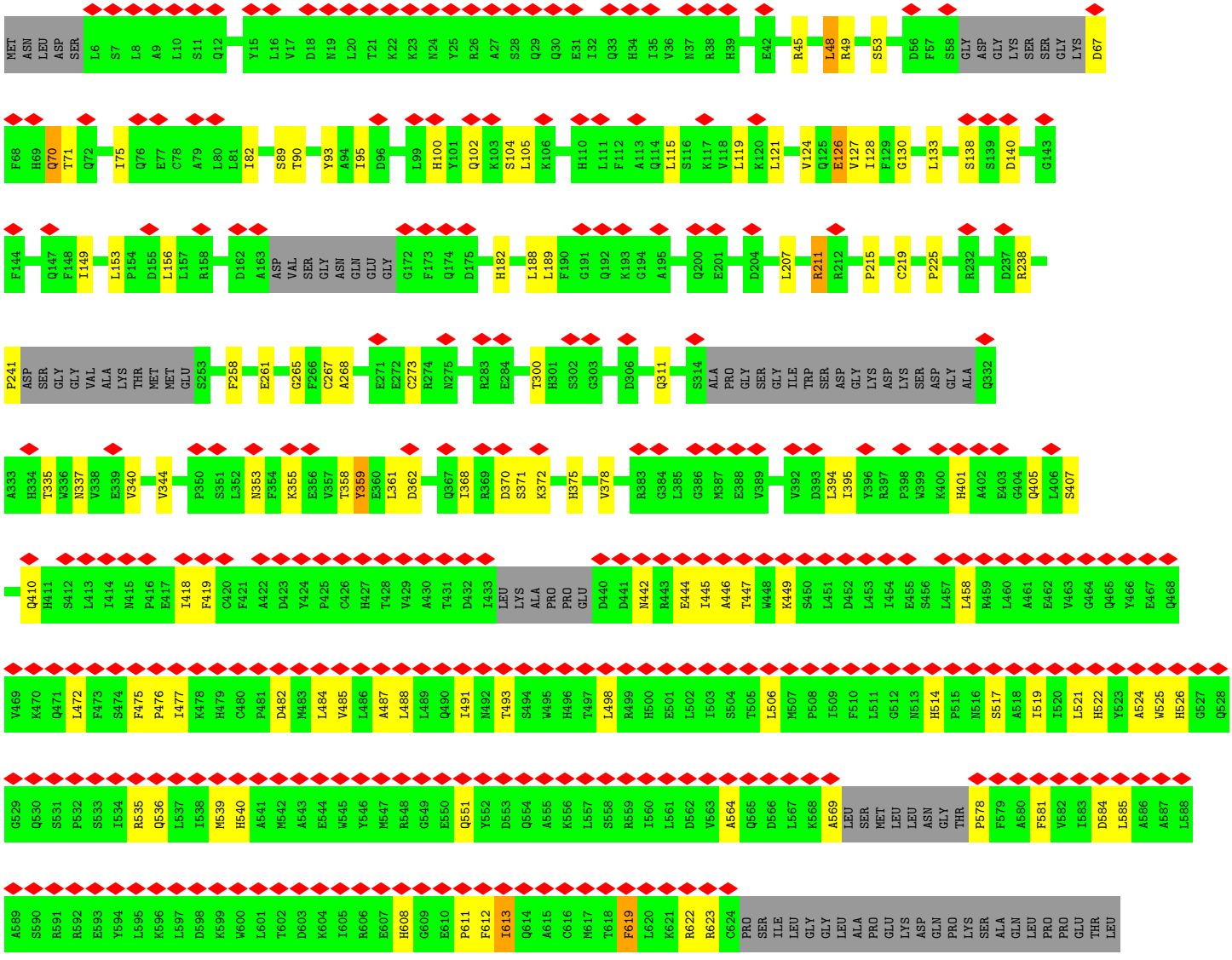
Chain	Residue	Modelled	Actual	Comment	Reference
C	508	SER	-	expression tag	UNP B3KNB0
C	509	GLY	-	expression tag	UNP B3KNB0
C	510	ALA	-	expression tag	UNP B3KNB0
C	511	MET	-	expression tag	UNP B3KNB0
C	512	GLY	-	expression tag	UNP B3KNB0
C	513	SER	-	expression tag	UNP B3KNB0
C	514	GLY	-	expression tag	UNP B3KNB0
C	515	SER	-	expression tag	UNP B3KNB0
C	516	GLY	-	expression tag	UNP B3KNB0
C	517	HIS	-	expression tag	UNP B3KNB0
C	518	HIS	-	expression tag	UNP B3KNB0
C	519	HIS	-	expression tag	UNP B3KNB0
C	520	HIS	-	expression tag	UNP B3KNB0
C	521	HIS	-	expression tag	UNP B3KNB0
C	522	HIS	-	expression tag	UNP B3KNB0
C	523	GLY	-	expression tag	UNP B3KNB0
C	524	THR	-	expression tag	UNP B3KNB0

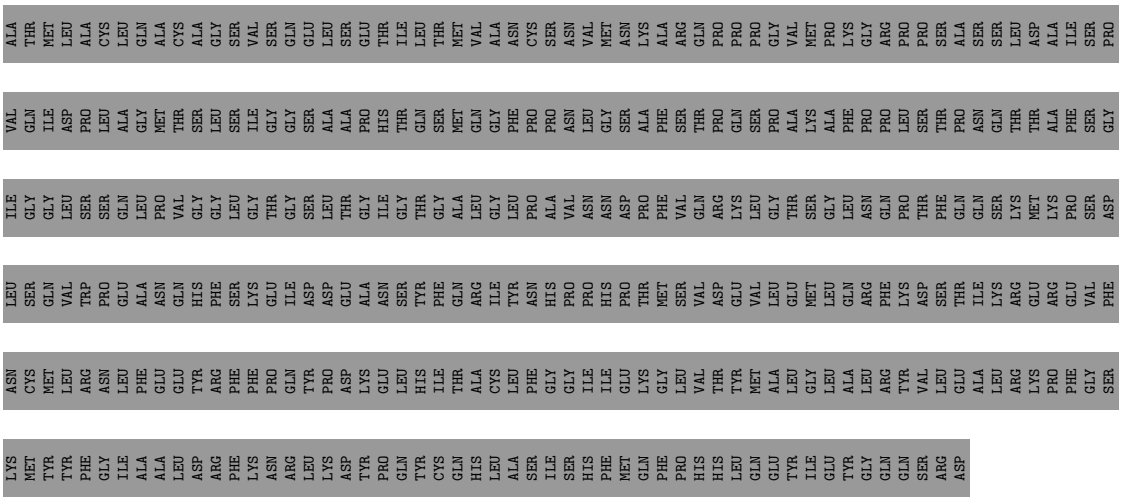
3 Residue-property plots (i)

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: CCR4-NOT transcription complex subunit 1

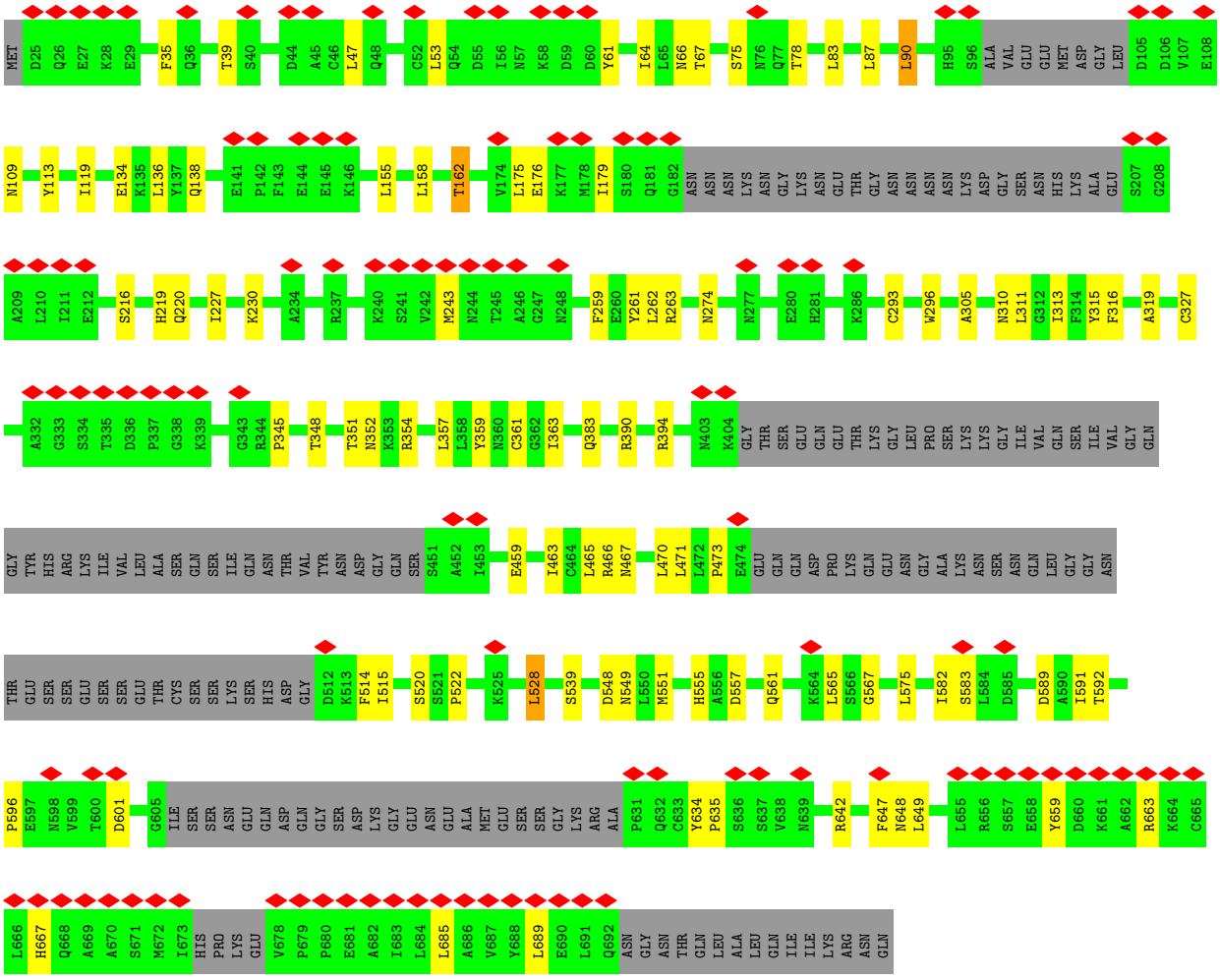
Chain A:





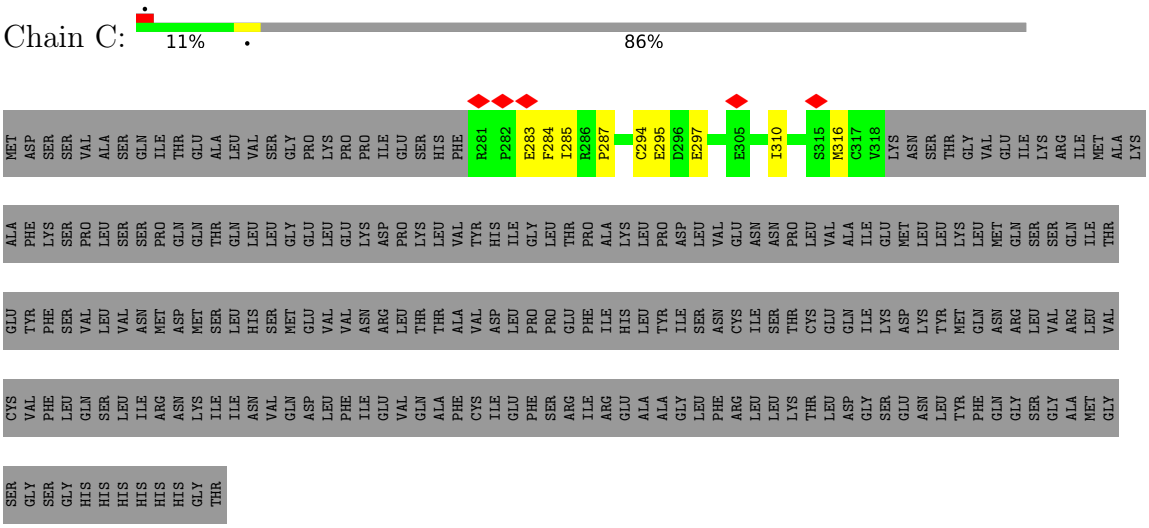
• Molecule 2: CCR4-NOT transcription complex subunit 10

Chain B:



• Molecule 3: CCR4-NOT transcription complex subunit 11

Chain C:


11%
86%
MET ASP SER SER VAL ALA SER GLN ILE THR GLU ALA LEU VAL SER GLY PRO LYS PRO PRO ILE GLU SER HIS PHE R281 P282 E283 F284 I285 R286 P287 C294 E295 D296 E297 E305 I310 S315 M316 C317 V318 LYS ASN SER THR GLY VAL GLU ILE LYS ARG ILE MET ALA LYS
ALA PHE LYS SER PRO LEU SER SER PRO GLN GLN THR GLN LEU LEU GLY GLU LEU GLU LYS ASP PRO LYS LEU VAL TYR HIS ILE GLY LEU THR PRO ALA LYS LEU PRO ASP LEU VAL GLU ASN ASN PRO LEU VAL ALA ILE GLU MET LEU LEU LYS LEU MET GLN SER SER GLN ILE THR
GLU TYR PHE SER VAL LEU VAL ASN MET ASP MET SER LEU HIS SER MET GLU VAL VAL ASN ARG LEU THR THR ALA VAL ASP LEU PRO PRO GLU PHE ILE HIS LEU TYR ILE SER ASN CYS ILE SER THR CYS GLU GLN ILE LYS ASP LYS TYR MET GLN ASN ARG LEU VAL ARG LEU VAL
CYS VAL PHE LEU GLN SER LEU ILE ARG ASN LYS ILE ILE ASN VAL GLN ASP LEU PHE ILE GLU VAL GLN ALA PHE CYS ILE GLU PHE SER ARG ILE ARG GLU ALA ALA GLY LEU PHE ARG LEU LEU LYS THR LEU ASP GLY SER GLU ASN LEU TYR PHE GLN GLY SER GLY ALA MET GLY
SER GLY SER GLY HIS HIS HIS HIS HIS HIS GLY THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	387942	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 ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	250	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	4.511	Depositor
Minimum map value	-3.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.522	Depositor
Map size (Å)	271.656, 271.656, 271.656	wwPDB
Map dimensions	392, 392, 392	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.693, 0.693, 0.693	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	0.25	0/4622	0.44	0/6253
2	B	0.27	0/4188	0.42	0/5654
3	C	0.27	0/327	0.47	0/450
All	All	0.26	0/9137	0.43	0/12357

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4520	0	4543	75	0
2	B	4114	0	4155	66	0
3	C	314	0	296	12	0
All	All	8948	0	8994	134	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.

The worst 5 of 134 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:102:GLN:NE2	1:A:104:SER:OG	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:O	1:A:211:ARG:HG2	1.91	0.70
2:B:390:ARG:NH1	3:C:294:CYS:SG	2.65	0.69
1:A:82:ILE:HG13	1:A:128:ILE:HG21	1.76	0.68
2:B:596:PRO:HB3	2:B:642:ARG:HG3	1.76	0.66

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	547/1000 (55%)	525 (96%)	22 (4%)	0	100	100
2	B	510/684 (75%)	488 (96%)	22 (4%)	0	100	100
3	C	36/269 (13%)	35 (97%)	1 (3%)	0	100	100
All	All	1093/1953 (56%)	1048 (96%)	45 (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	495/860 (58%)	482 (97%)	13 (3%)	46	76
2	B	448/583 (77%)	439 (98%)	9 (2%)	55	81
3	C	36/244 (15%)	36 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	979/1687 (58%)	957 (98%)	22 (2%)	54 80

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	90	LEU
2	B	219	HIS
2	B	175	LEU
2	B	243	MET
1	A	359	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	549	ASN
3	C	308	HIS
1	A	260	GLN
1	A	367	GLN
2	B	85	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 monosaccharides 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.

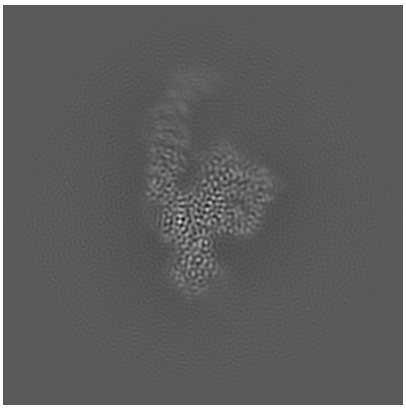
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29551. These allow visual inspection of the internal detail of the map and identification of artifacts.

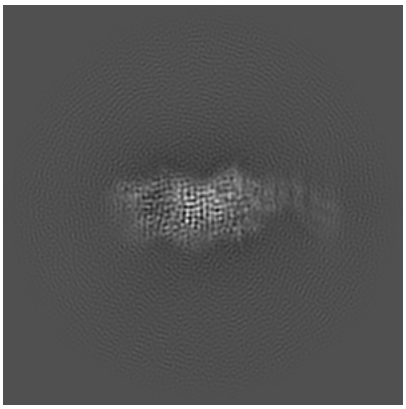
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

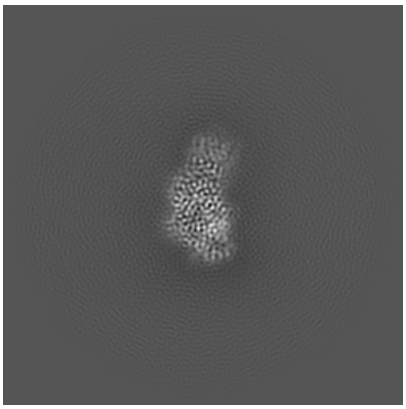
6.1.1 Primary map



X

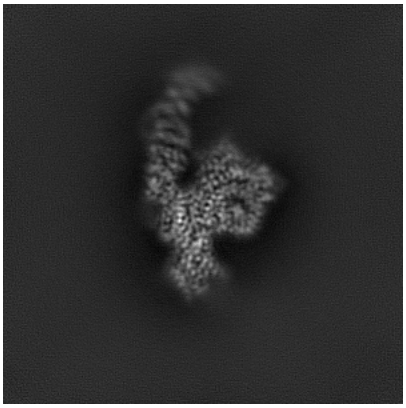


Y

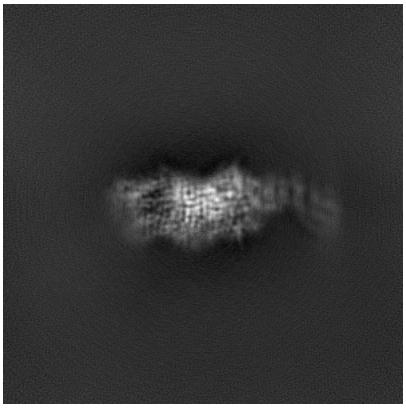


Z

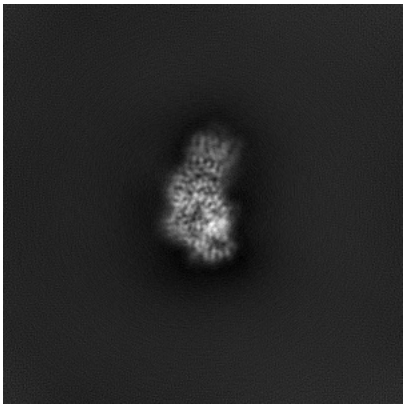
6.1.2 Raw map



X



Y

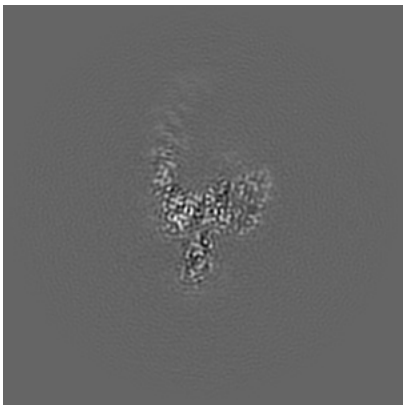


Z

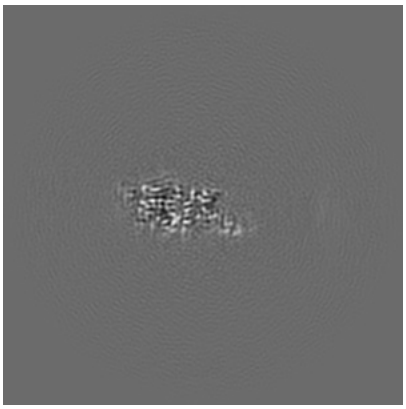
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

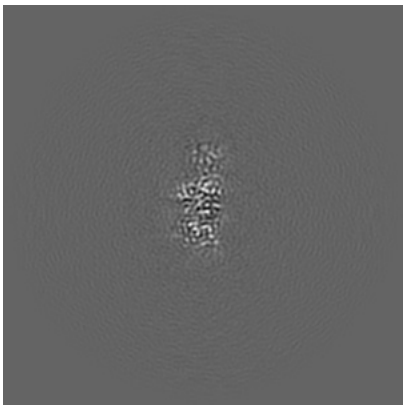
6.2.1 Primary map



X Index: 196

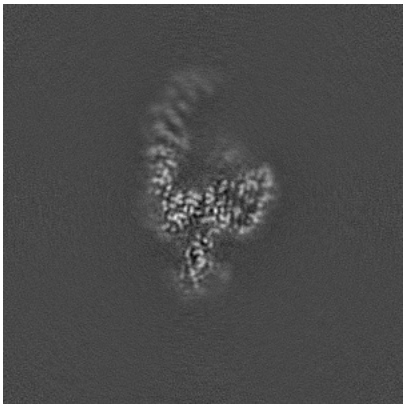


Y Index: 196

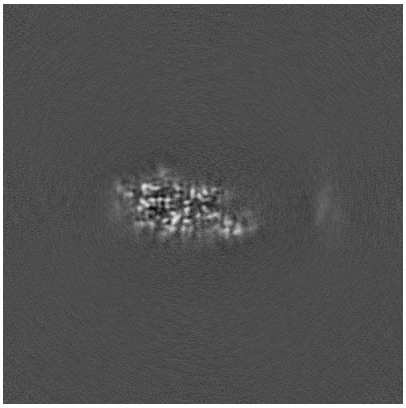


Z Index: 196

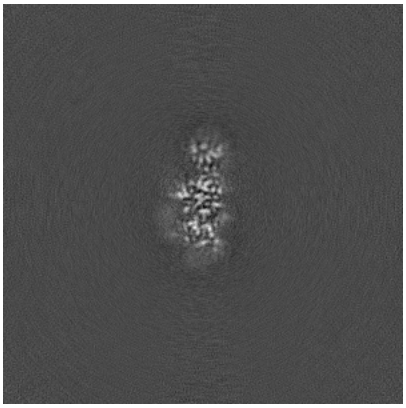
6.2.2 Raw map



X Index: 196



Y Index: 196

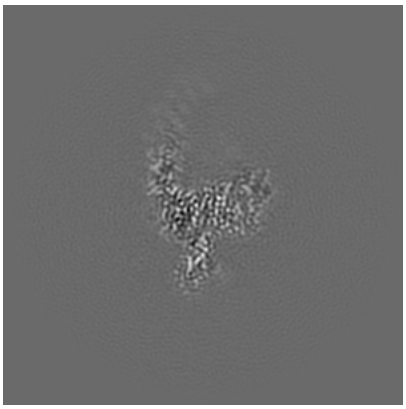


Z Index: 196

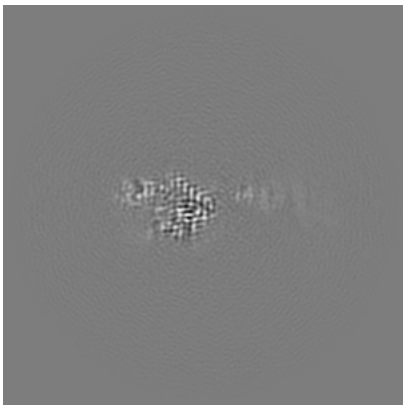
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

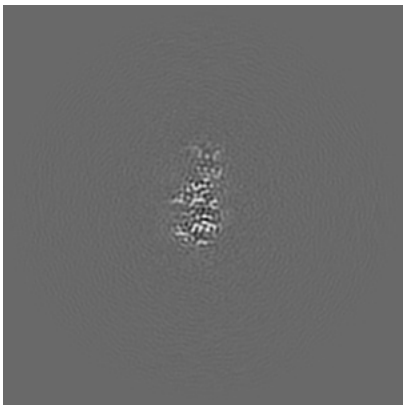
6.3.1 Primary map



X Index: 199

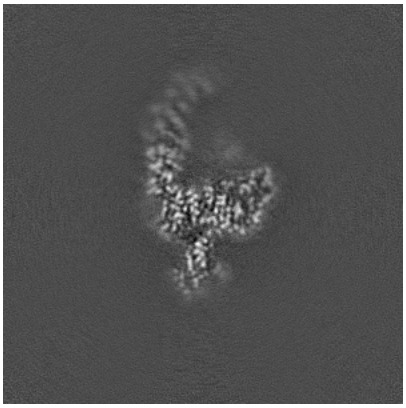


Y Index: 176



Z Index: 191

6.3.2 Raw map



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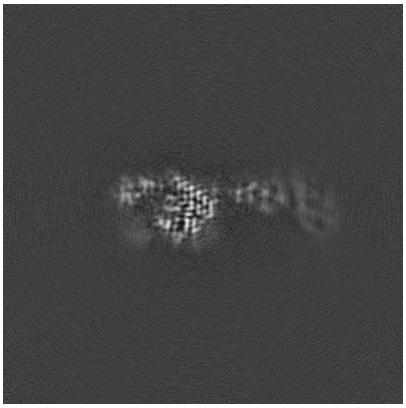
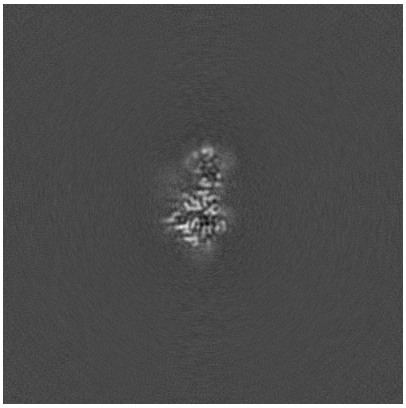


Y Index: 174

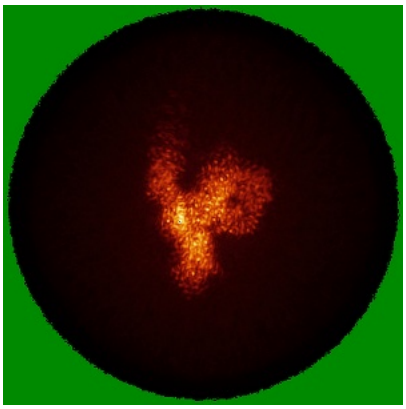


Z Index: 180

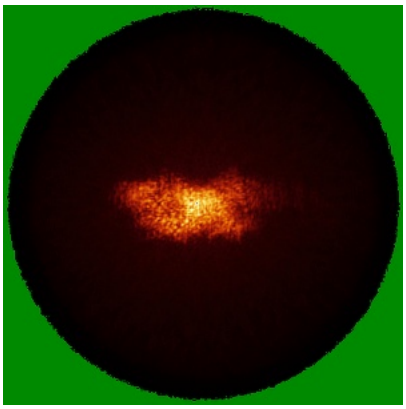
The images above show the largest variance slices of the map in three orthogonal directions.

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

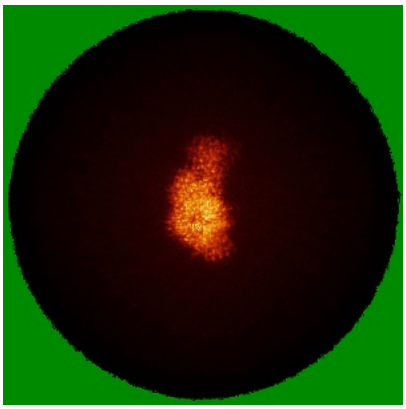
6.4.1 Primary map



X

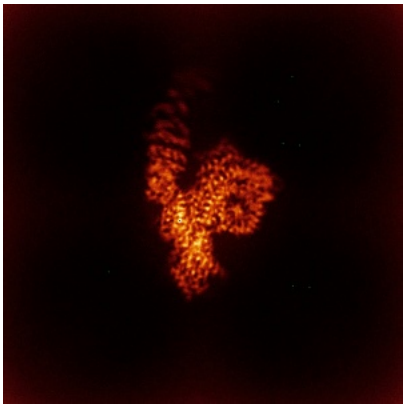


Y

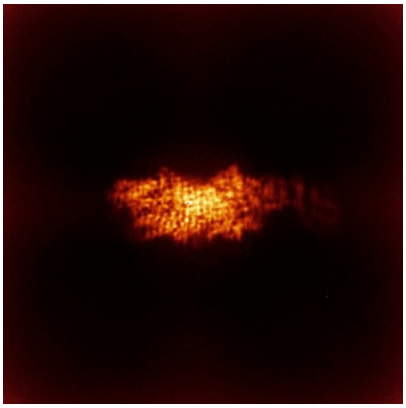


Z

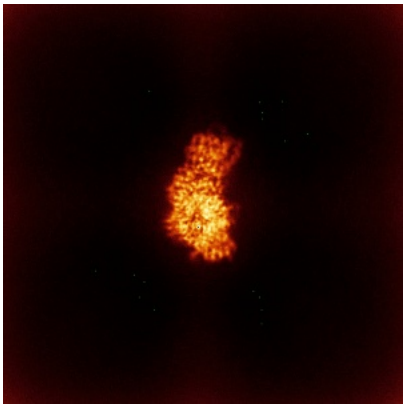
6.4.2 Raw map



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 0.522. 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.

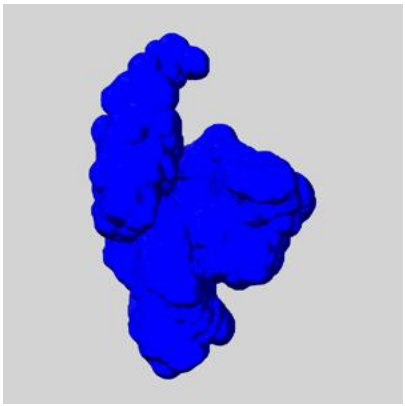
6.6 Mask visualisation

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

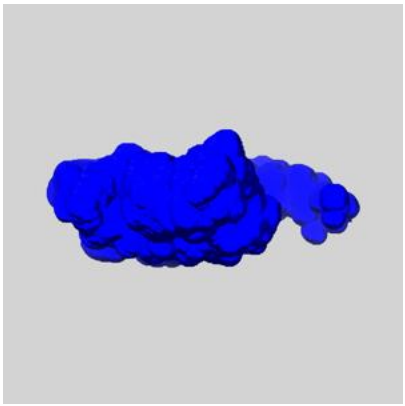
A mask typically either:

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

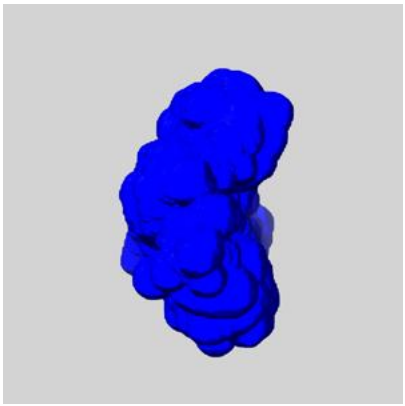
6.6.1 emd_29551_msk_1.map



X



Y

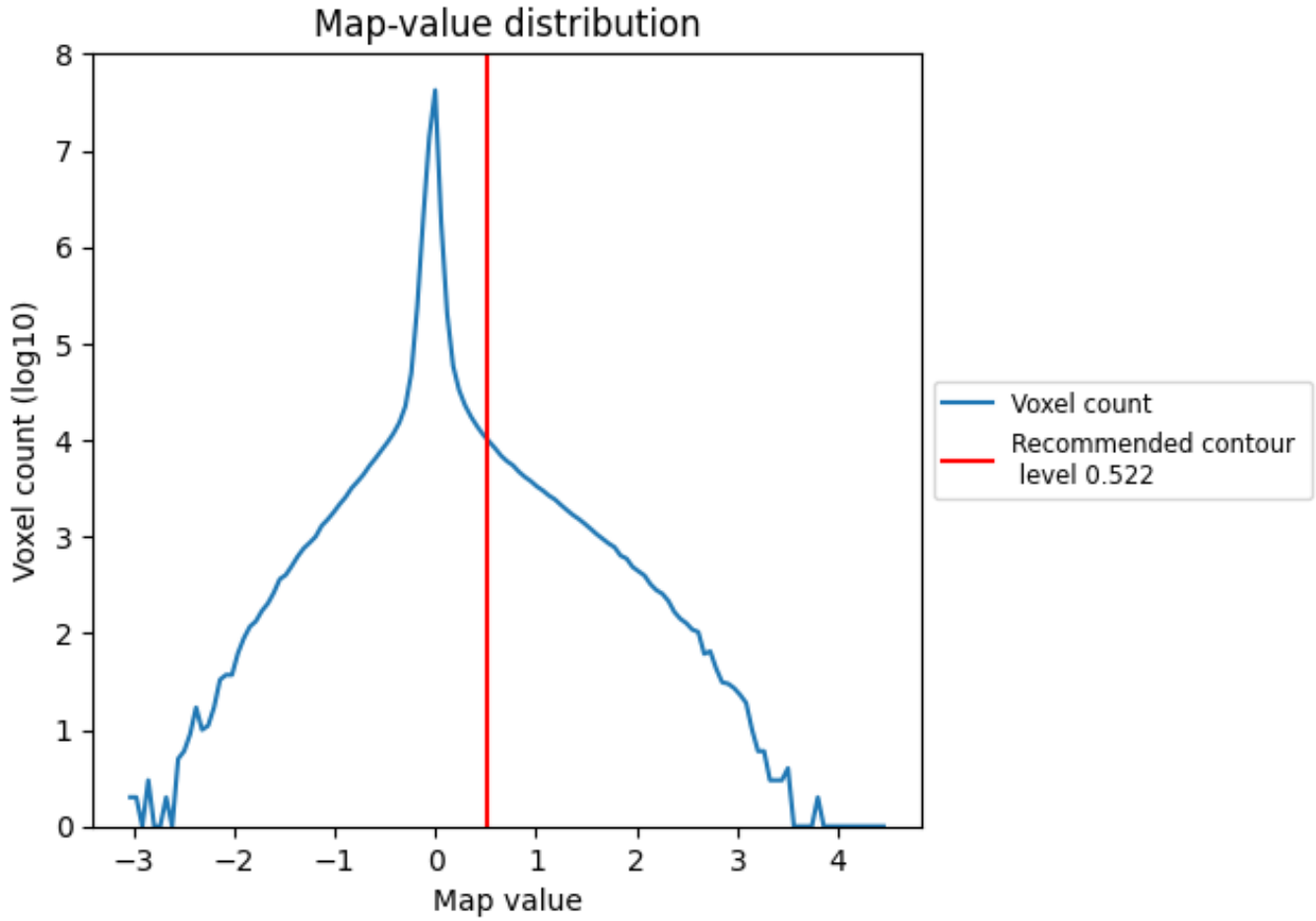


Z

7 Map analysis

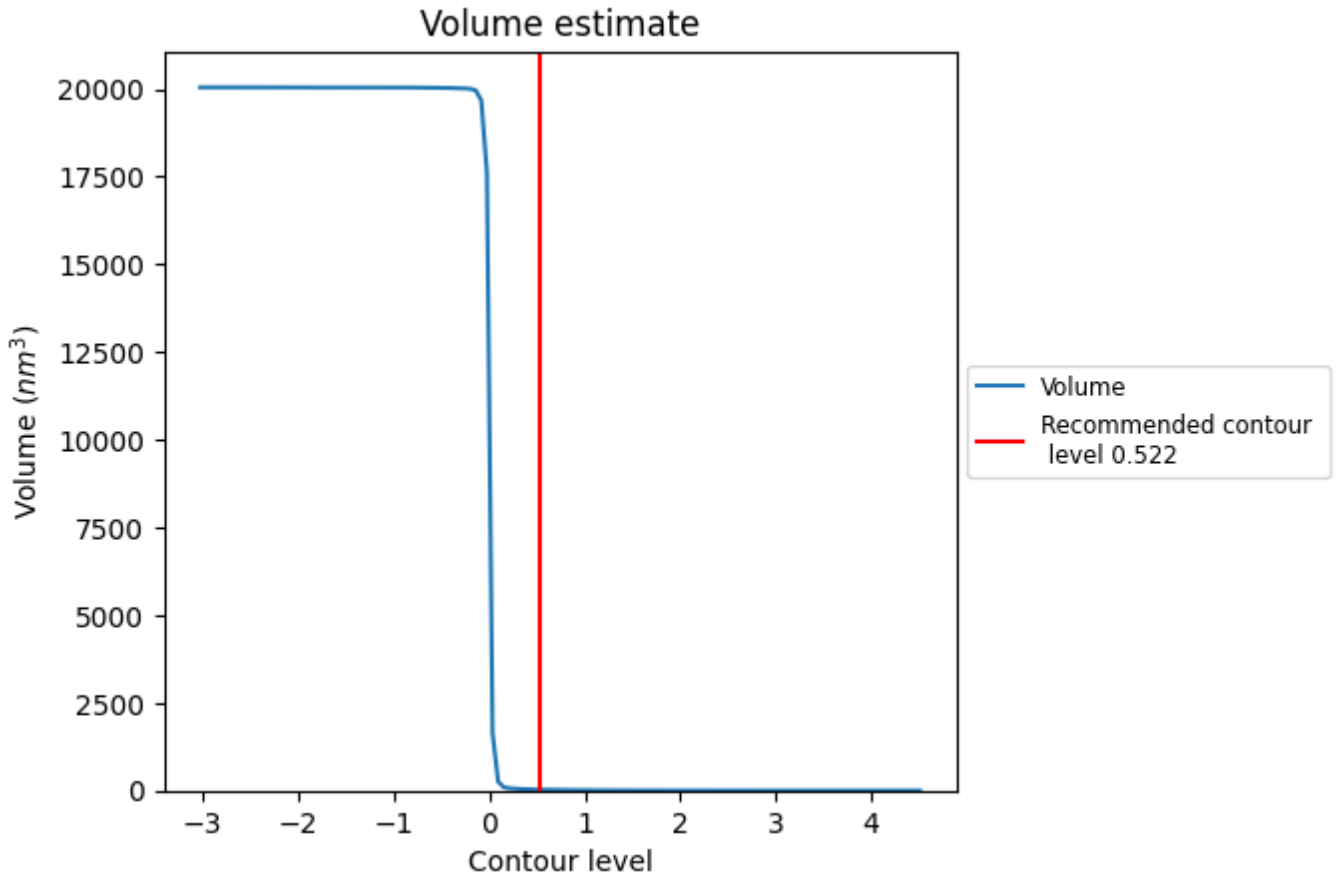
This section contains the results of statistical analysis of the map.

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.

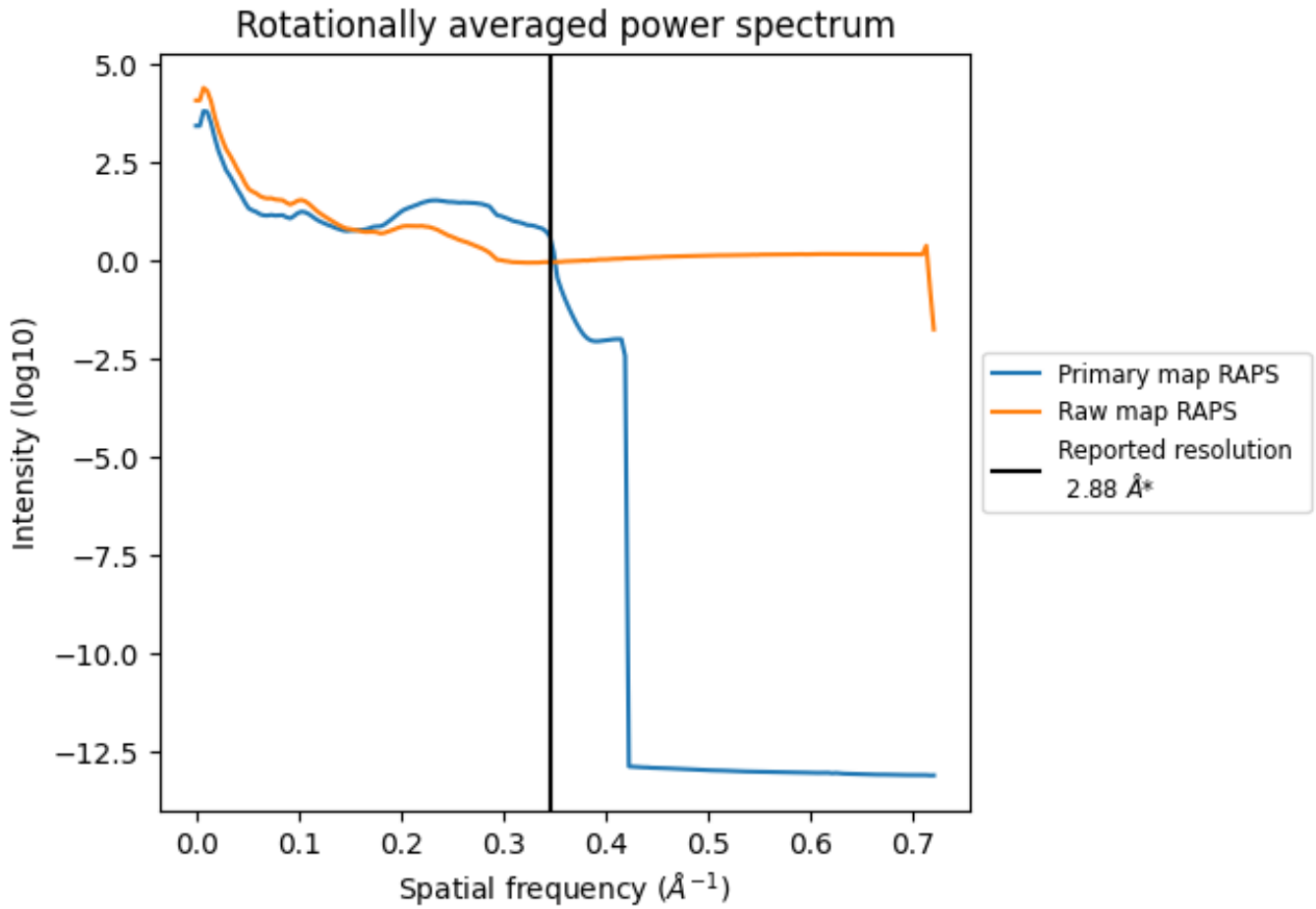
7.2 Volume estimate (i)



The volume at the recommended contour level is 27 nm^3; this corresponds to an approximate mass of 24 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)

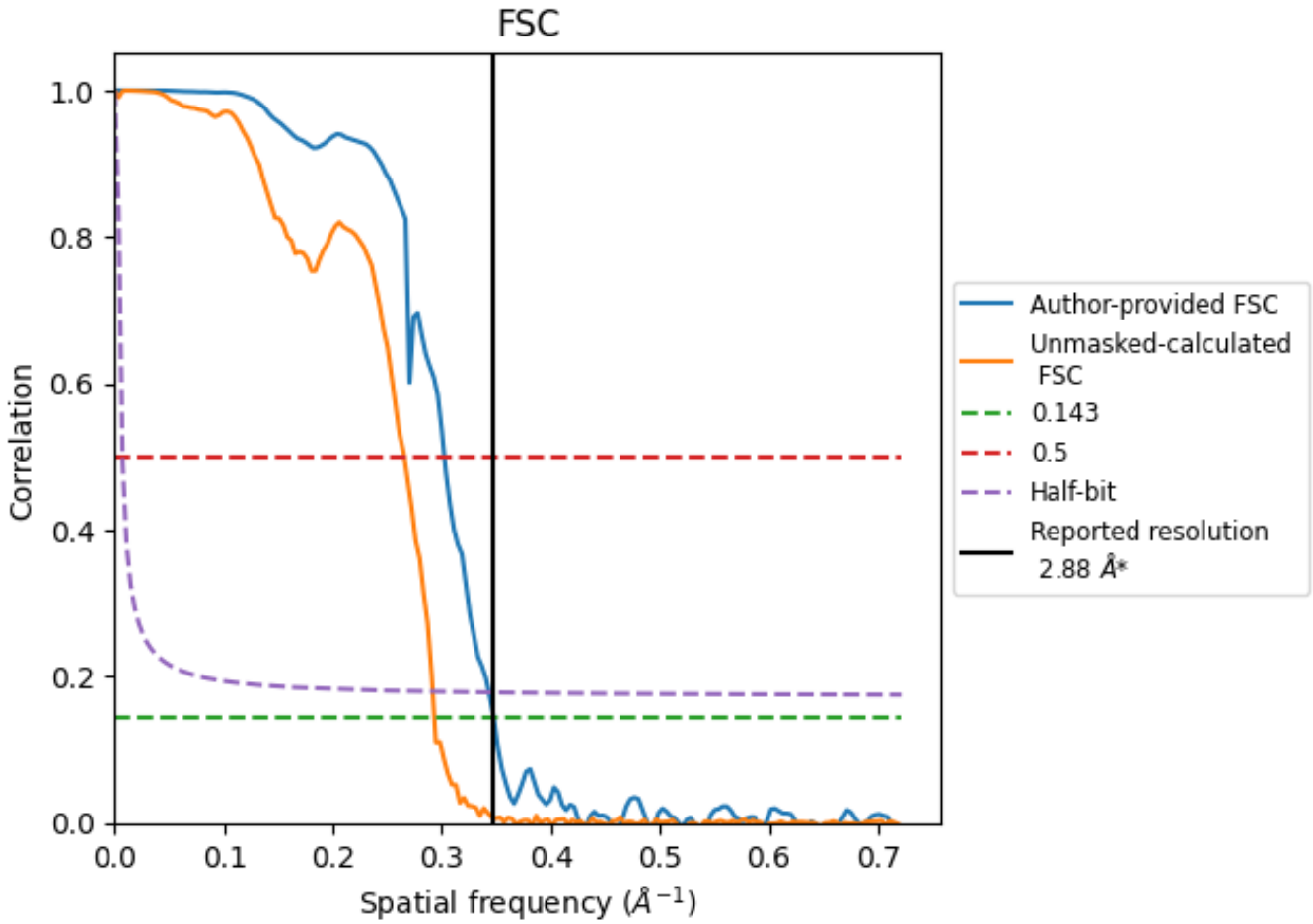


*Reported resolution corresponds to spatial frequency of 0.347 Å^{-1}

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 0.347 Å^{-1}

8.2 Resolution estimates (i)

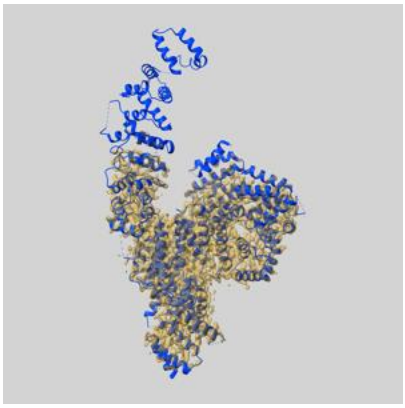
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.88	3.31	2.91
Unmasked-calculated*	3.41	3.77	3.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.41 differs from the reported value 2.88 by more than 10 %

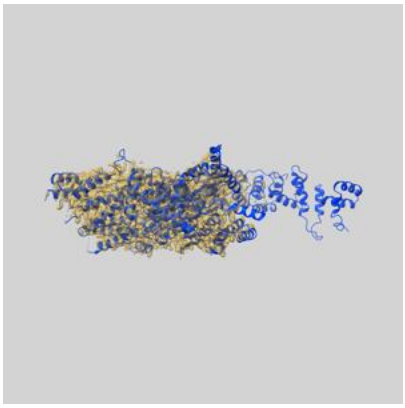
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29551 and PDB model 8FY3. Per-residue inclusion information can be found in section 3 on page 5.

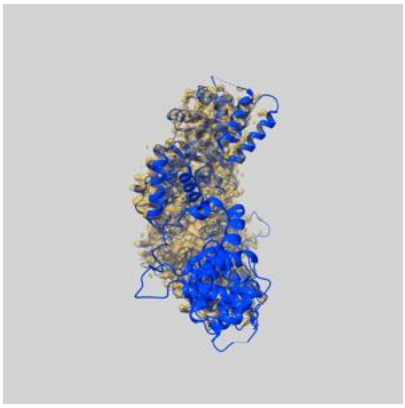
9.1 Map-model overlay



X



Y



Z

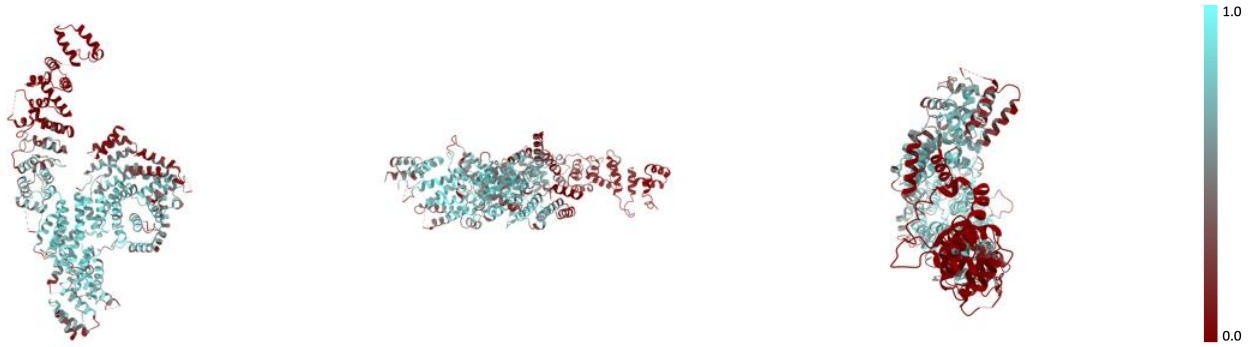
The images above show the 3D surface view of the map at the recommended contour level 0.522 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

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.

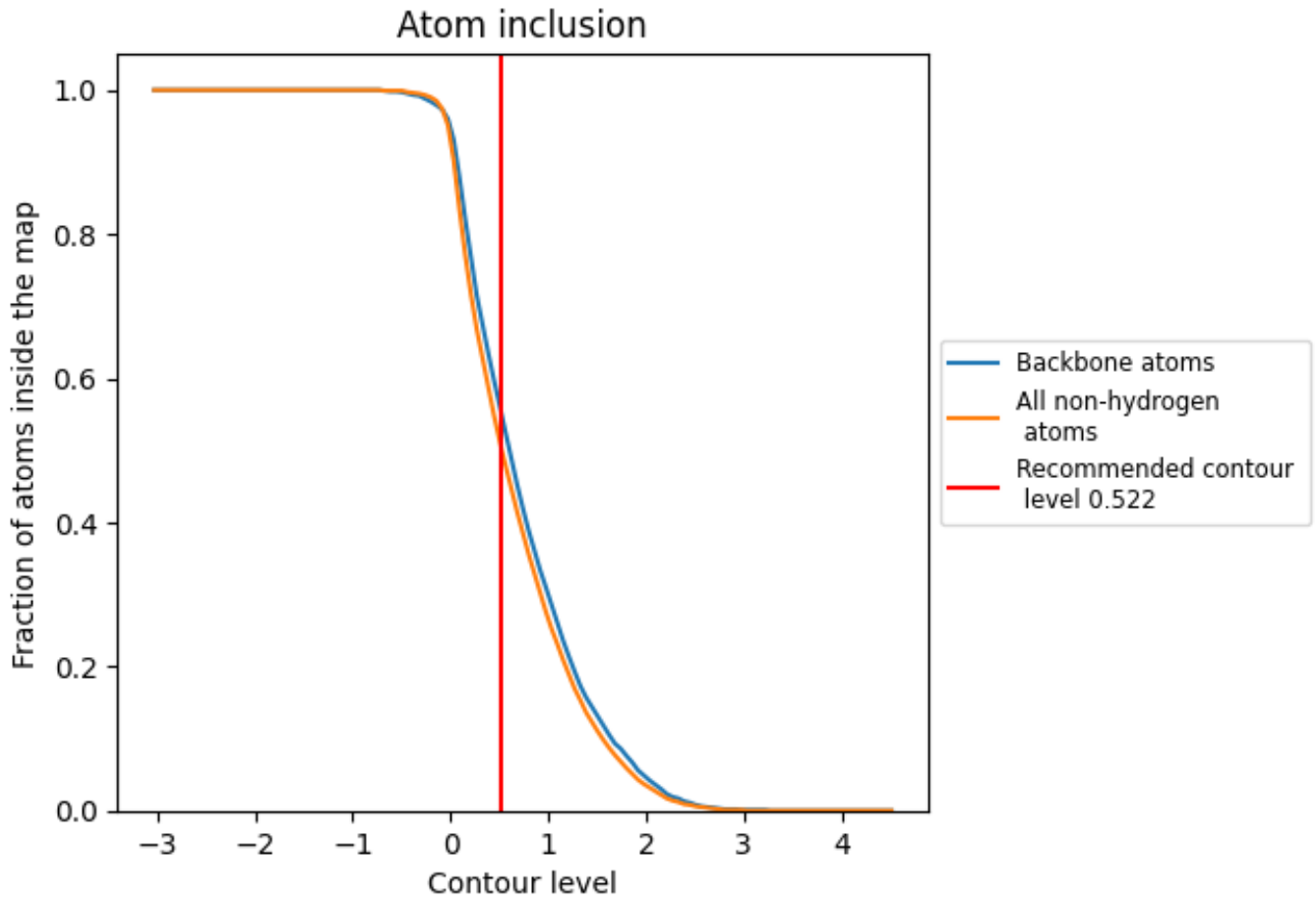
9.3 Atom inclusion mapped to coordinate model



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 (0.522).

9.4 Atom inclusion (i)



At the recommended contour level, 55% of all backbone atoms, 50% 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 (0.522) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5020	0.4290
A	0.3560	0.3700
B	0.6460	0.4870
C	0.7110	0.5060