wwPDB EM Validation Summary Report

Dec 29, 2024 – 08:42 AM EST

PDB ID	:	7MP6
EMDB ID	:	EMD-23930
Title	:	Neurofibromin homodimer
Authors	:	Lupton, C.J.; Bayly-Jones, C.; Ellisdon, A.M.
Deposited on	:	2021-05-04
Resolution	:	6.25 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

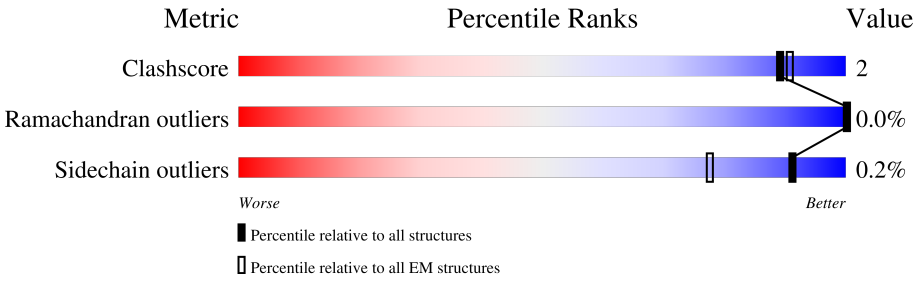
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 6.25 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	2826	53% · 43%
1	B	2826	53% · 43%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 25464 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
1	A	1600	Total	C	N	O	S	0	0
			12704	8190	2127	2296	91		
1	B	1609	Total	C	N	O	S	0	0
			12760	8223	2136	2310	91		

There are 18 discrepancies between the modelled and reference sequences:

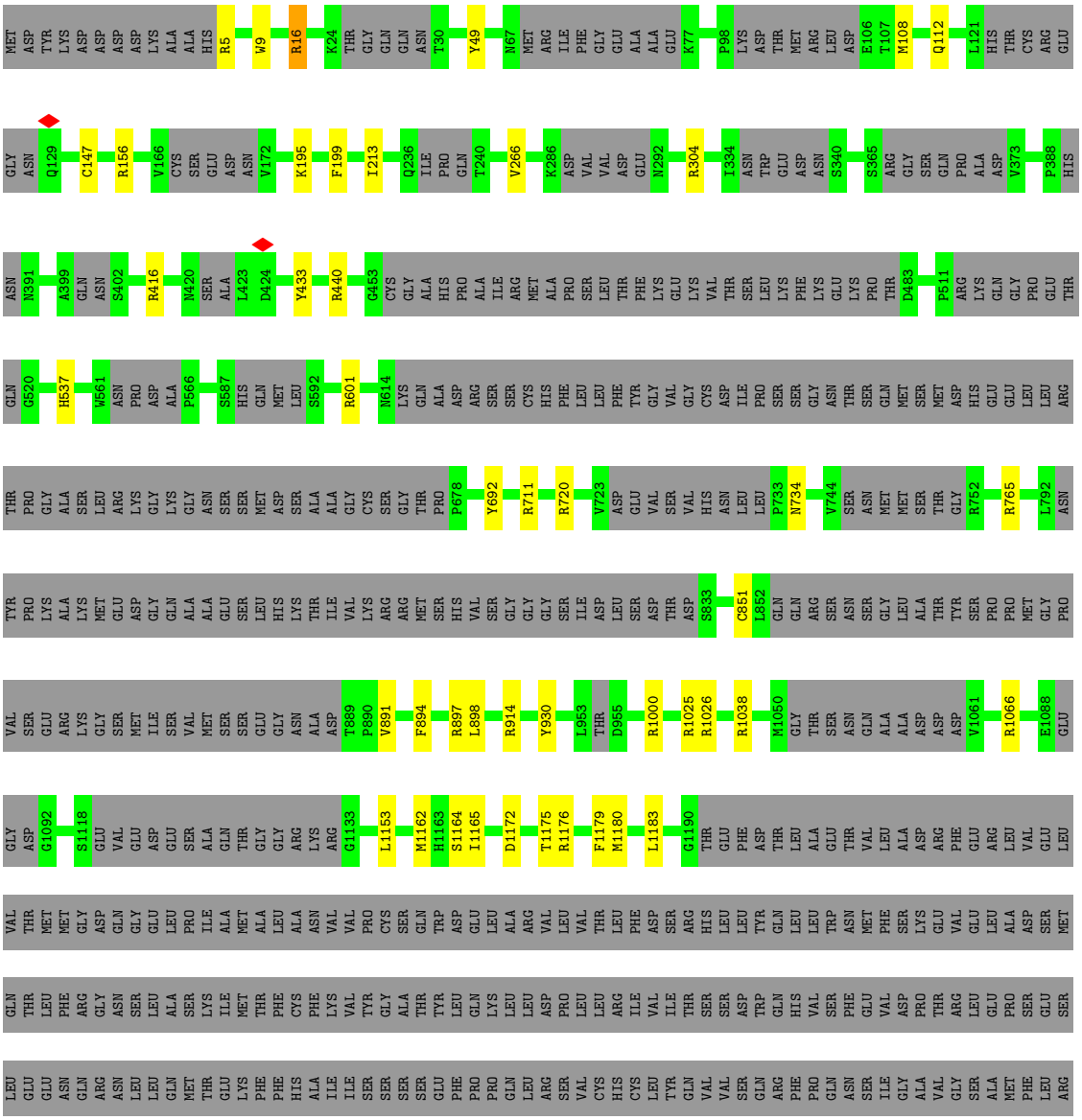
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP P21359
A	-6	ASP	-	expression tag	UNP P21359
A	-5	TYR	-	expression tag	UNP P21359
A	-4	LYS	-	expression tag	UNP P21359
A	-3	ASP	-	expression tag	UNP P21359
A	-2	ASP	-	expression tag	UNP P21359
A	-1	ASP	-	expression tag	UNP P21359
A	0	ASP	-	expression tag	UNP P21359
A	1	LYS	-	expression tag	UNP P21359
B	-7	MET	-	initiating methionine	UNP P21359
B	-6	ASP	-	expression tag	UNP P21359
B	-5	TYR	-	expression tag	UNP P21359
B	-4	LYS	-	expression tag	UNP P21359
B	-3	ASP	-	expression tag	UNP P21359
B	-2	ASP	-	expression tag	UNP P21359
B	-1	ASP	-	expression tag	UNP P21359
B	0	ASP	-	expression tag	UNP P21359
B	1	LYS	-	expression tag	UNP P21359

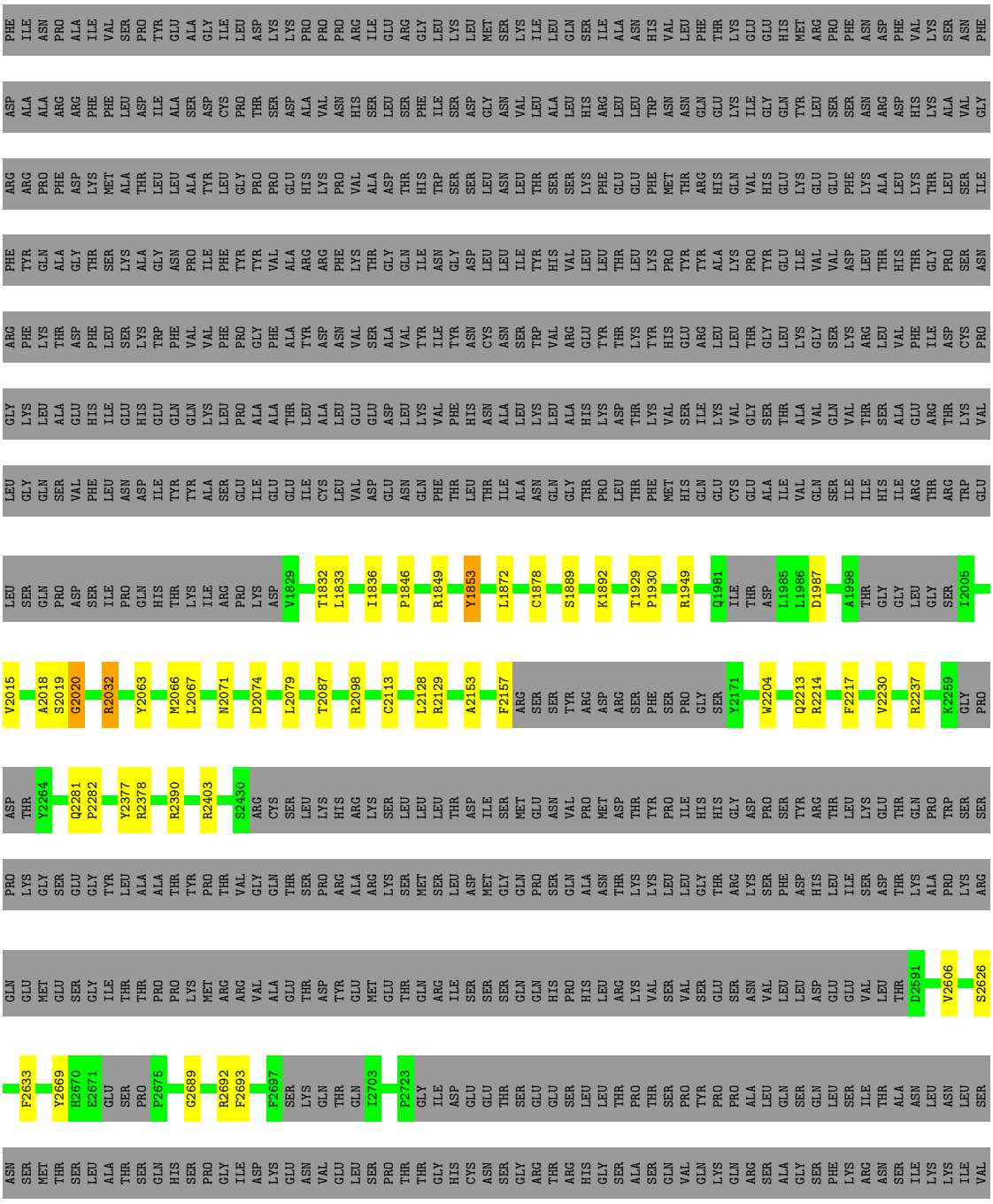
3 Residue-property plots (i)

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

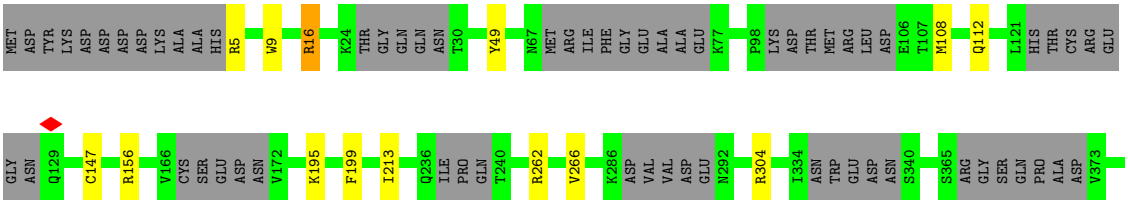
Chain A:

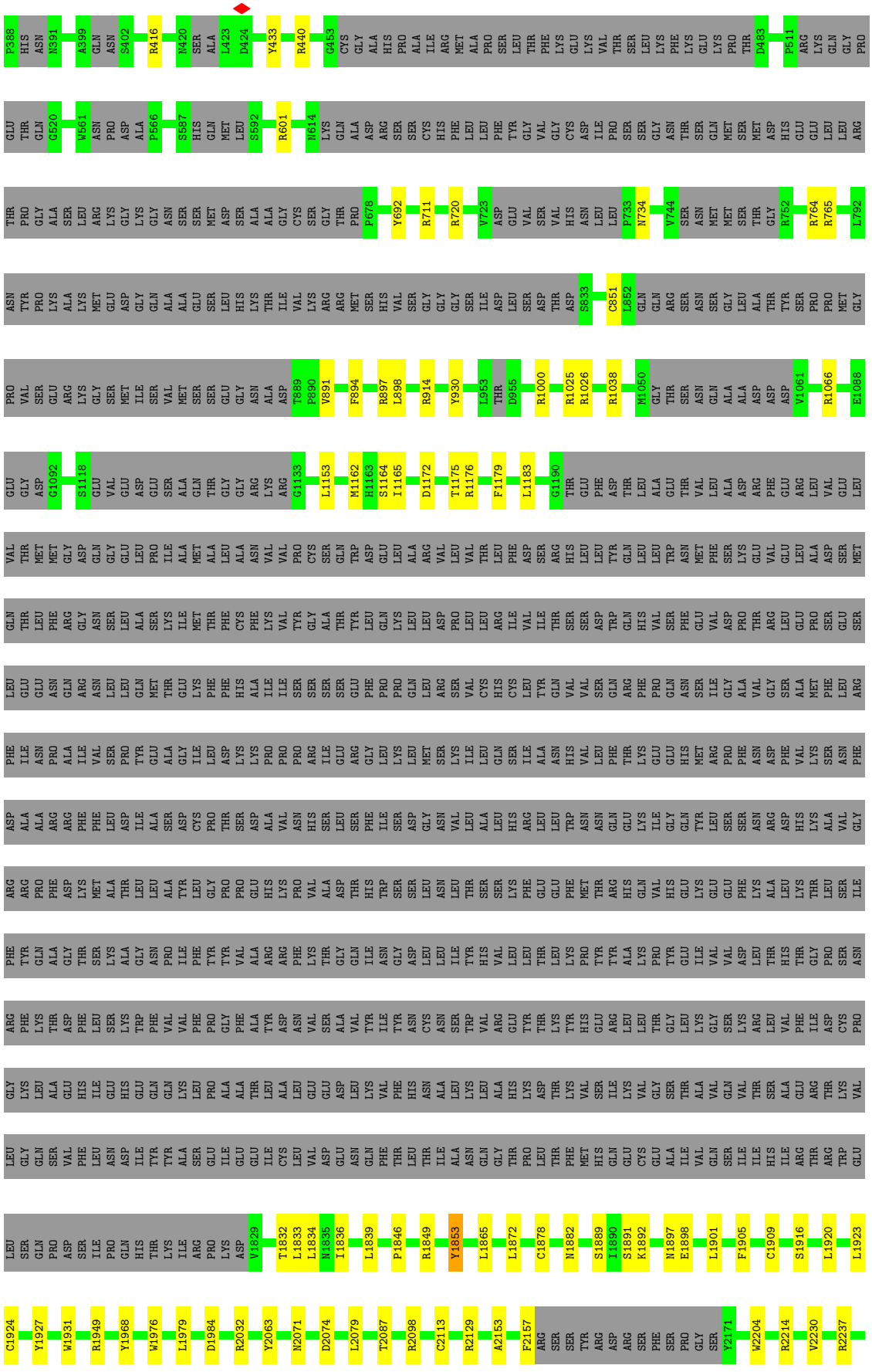


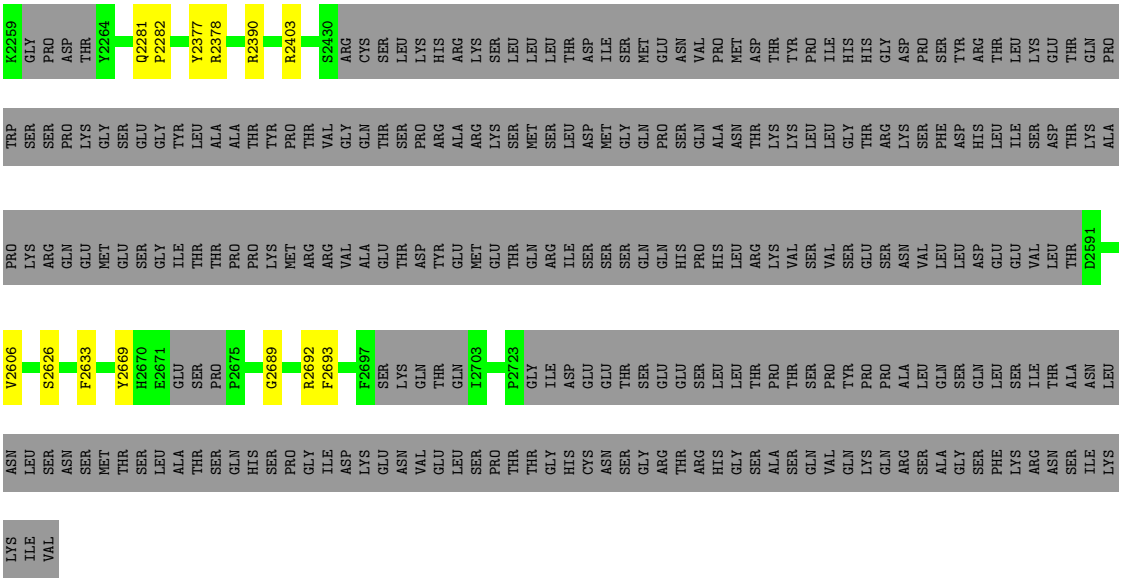


• Molecule 1: Isoform I of Neurofibromin

Chain B:




P388 N391 A399 S402 R416 N420 L423 D424 Y433 R440 G453 D483 P511
G520 W561 S587 P566 R601 N614 S592
P678 Y692 R711 R720 V723 P733 N734 V744 R752 R764 R765 L792
S833 C851 L852
T889 P890 V891 F894 R897 L898 R914 Y930 L953 D955 R1000 R1025 R1026 R1038 M1050 V1061 R1066 E1088
G1092 S1118 G1133 L1153 M1162 H1163 S1164 I1165 D1172 T1175 R1176 F1179 L1183 G1190
V1829 T1832 L1833 L1834 N1835 I1836 L1839 P1846 R1849 Y1863 L1865 L1872 C1878 N1882 S1889 I1890 S1891 K1892 N1897 E1898 L1901 F1905 C1909 S1916 L1920 L1923
C1924 Y1927 W1931 R1949 Y1968 W1976 L1979 D1984 R2032 Y2063 N2071 D2074 L2079 T2087 R2098 C2113 R2129 A2153 F2157 Y2171 W2204 R2214 V2230 R2237


R2259 GLY PRO ASP THR Y2264 Q2281 P2282 Y2377 R2378 R2390 R2403 S2430 ARG CYS SER LEU LYS HIS ARG LYS SER LEU 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 GLY GLN THR SER PRO ARG ALA ARG LYS SER MET SER LEU 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 GLN HIS PRO HIS LEU ARG LYS VAL SER VAL SER GLU SER ASN VAL LEU LEU LEU ASP GLU GLU VAL LEU THR D2591
V2606 S2626 F2633 Y2669 H2670 E2671 GLU SER PRO P2675 G2689 R2692 F2693 P2697 SER LYS GLN THR GLN I2703 P2723 GLY ILE ASP GLU GLU THR SER GLU GLU SER LEU LEU THR PRO THR SER 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, C2	Depositor
Number of particles used	95564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.365	Depositor
Minimum map value	-0.873	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	515.808, 515.808, 515.808	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.388, 2.388, 2.388	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	0.61	0/12925	0.98	39/17476 (0.2%)
1	B	0.61	1/12983 (0.0%)	0.98	42/17558 (0.2%)
All	All	0.61	1/25908 (0.0%)	0.98	81/35034 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1897	ASN	C-N	8.97	1.54	1.34

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	304	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	2669	TYR	CB-CG-CD2	-7.55	116.47	121.00
1	B	304	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	B	2669	TYR	CB-CG-CD2	-7.53	116.48	121.00
1	B	156	ARG	NE-CZ-NH1	7.18	123.89	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	CYS	Mainchain
1	A	1853	TYR	Sidechain
1	A	2693	PHE	Sidechain
1	A	49	TYR	Sidechain
1	B	49	TYR	Sidechain

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	12704	0	13032	48	0
1	B	12760	0	13087	50	0
All	All	25464	0	26119	89	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 89 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:B:1916:SER:CB	1:B:1920:LEU:HD23	1.67	1.24
1:B:1865:LEU:HA	1:B:1898:GLU:OE1	1.46	1.15
1:B:1916:SER:HB3	1:B:1920:LEU:HD23	1.14	1.09
1:A:1987:ASP:OD1	1:A:2032:ARG:NH2	1.94	0.99
1:A:1987:ASP:OD1	1:A:2032:ARG:CZ	2.18	0.92

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	1532/2826 (54%)	1504 (98%)	27 (2%)	1 (0%)	48 83
1	B	1545/2826 (55%)	1518 (98%)	27 (2%)	0	100 100
All	All	3077/5652 (54%)	3022 (98%)	54 (2%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2020	GLY

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	1438/2520 (57%)	1436 (100%)	2 (0%)	92 95
1	B	1444/2520 (57%)	1441 (100%)	3 (0%)	92 94
All	All	2882/5040 (57%)	2877 (100%)	5 (0%)	91 94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TRP
1	A	16	ARG
1	B	9	TRP
1	B	16	ARG
1	B	1984	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	B	112	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

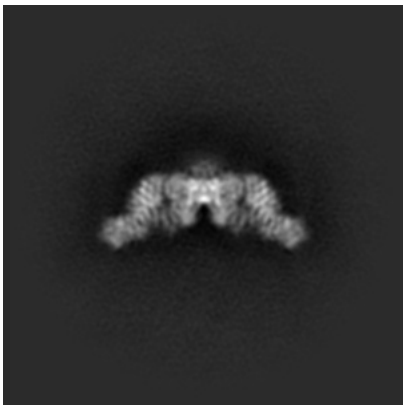
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23930. These allow visual inspection of the internal detail of the map and identification of artifacts.

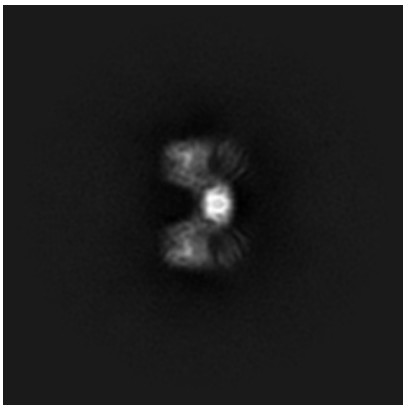
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

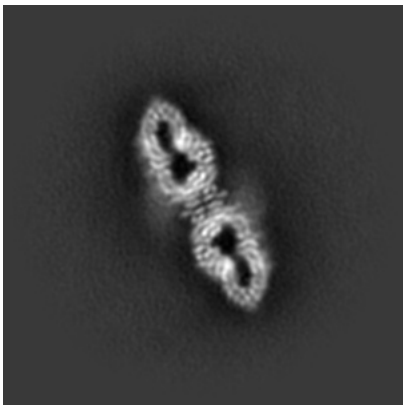
6.1.1 Primary map



X

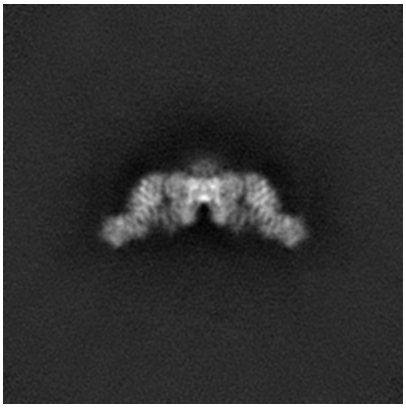


Y

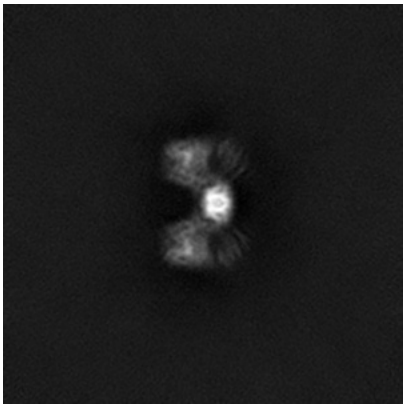


Z

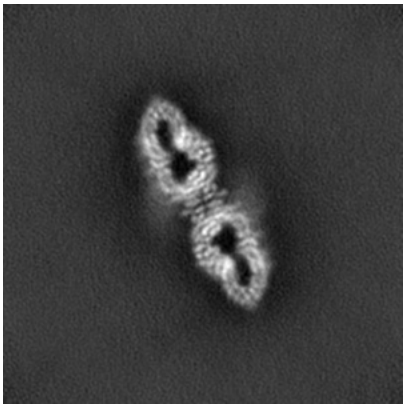
6.1.2 Raw map



X



Y



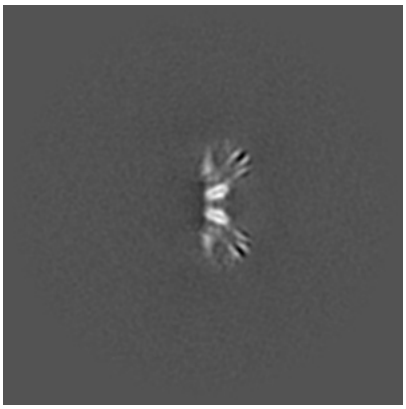
Z

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

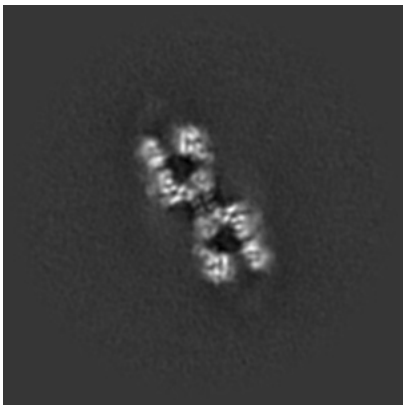
6.2 Central slices (i)

6.2.1 Primary map

X Index: 108



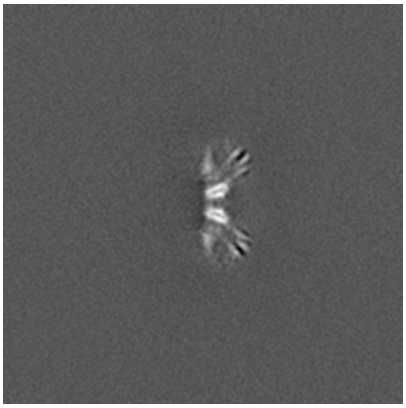
Y Index: 108



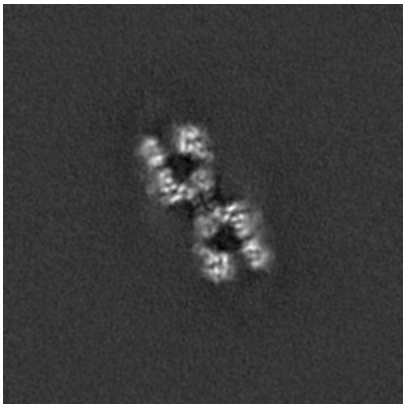
Z Index: 108

6.2.2 Raw map

X Index: 108



Y Index: 108



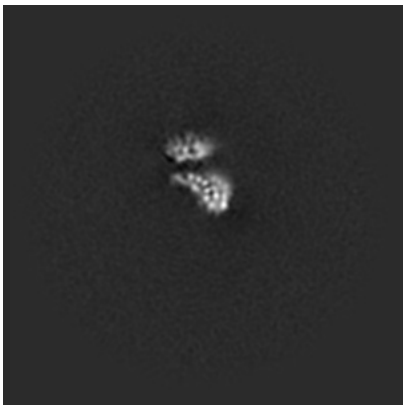
Z Index: 108

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

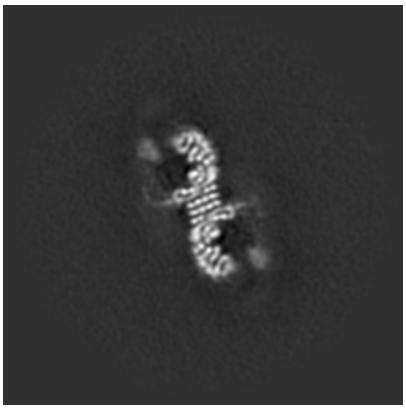
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 105



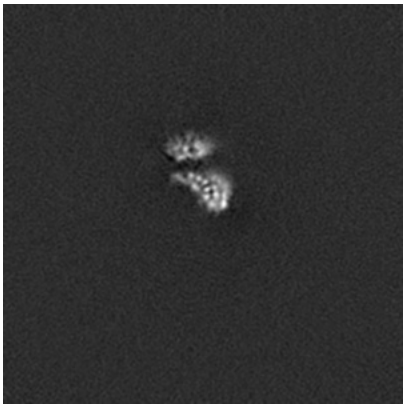
Y Index: 76



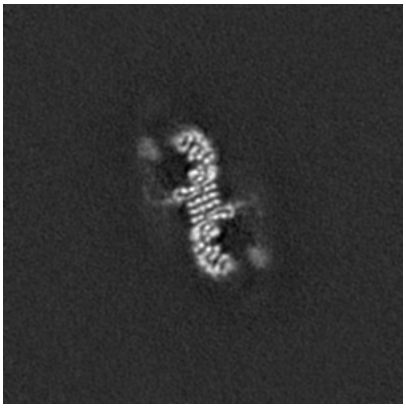
Z Index: 112

6.3.2 Raw map

X Index: 105



Y Index: 76



Z Index: 112

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

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

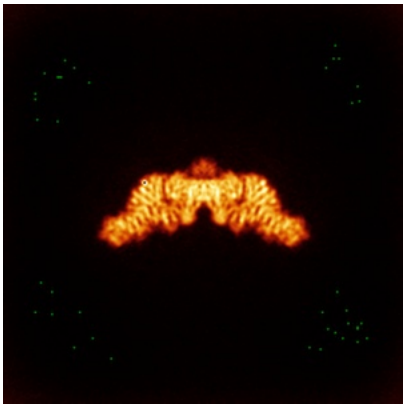
6.4.1 Primary map

X

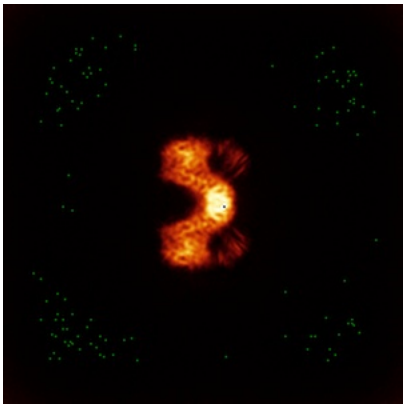
Y

Z

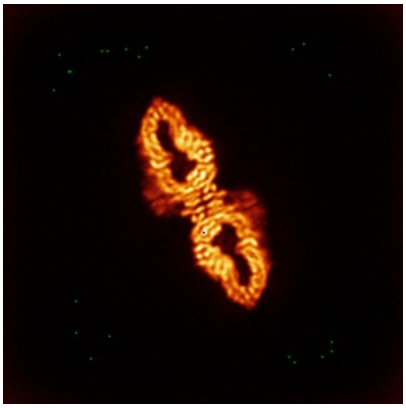
6.4.2 Raw map



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.

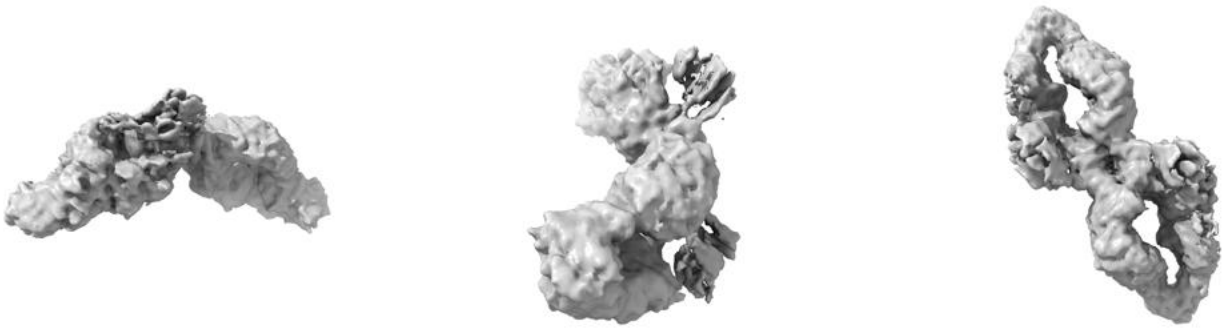
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

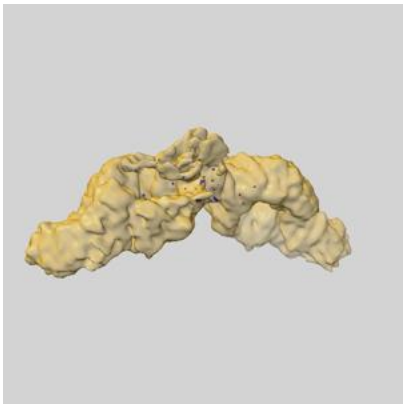
6.6 Mask visualisation (i)

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

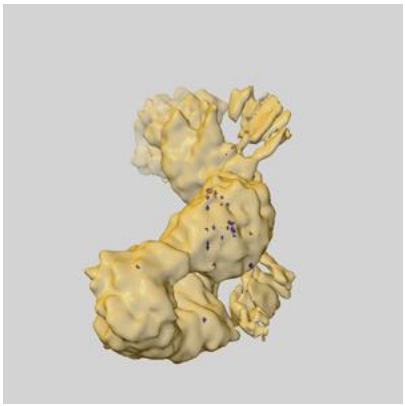
A mask typically either:

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

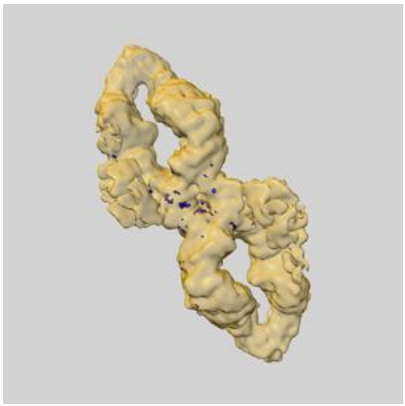
6.6.1 emd_23930_msk_1.map (i)



X



Y

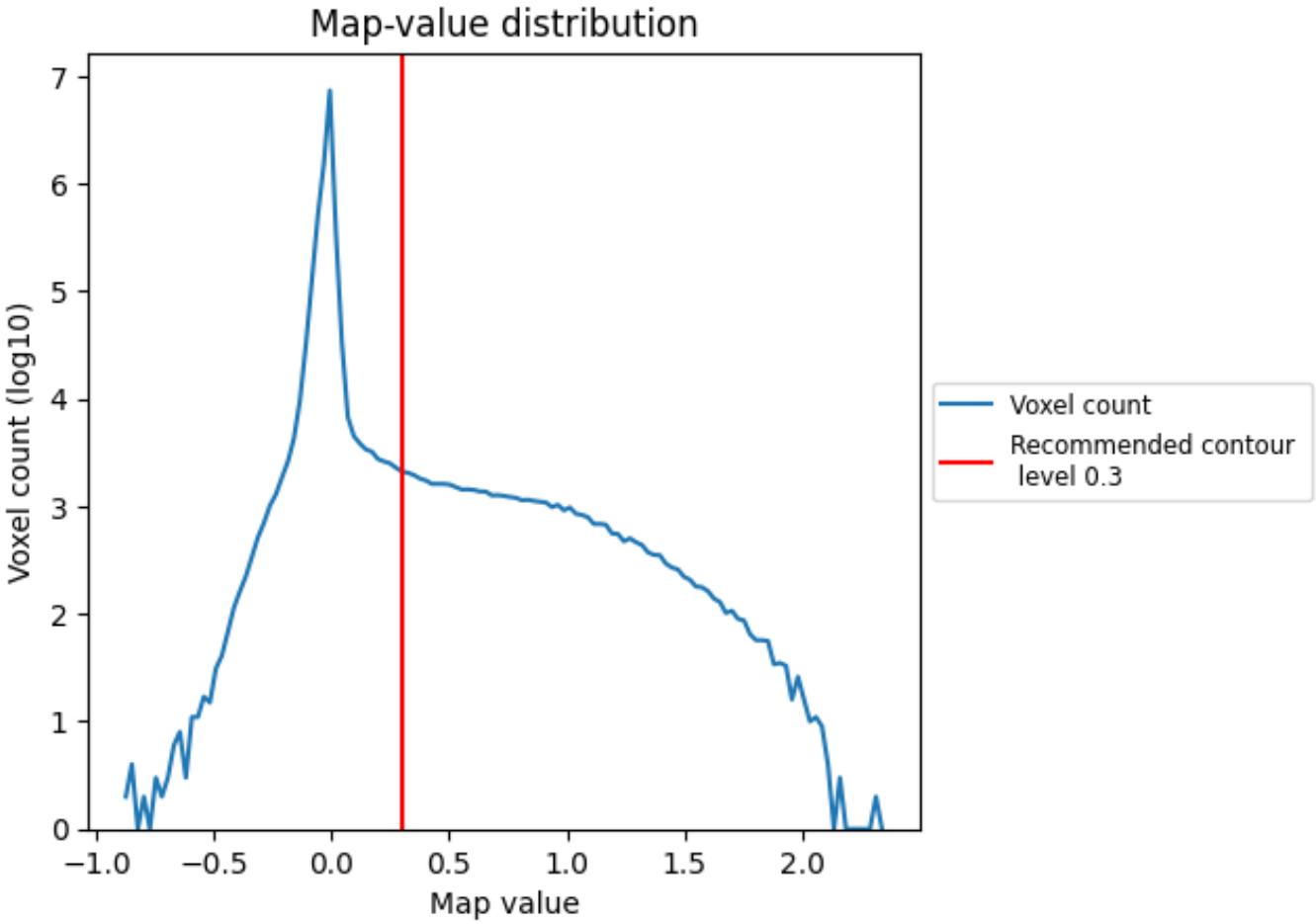


Z

7 Map analysis

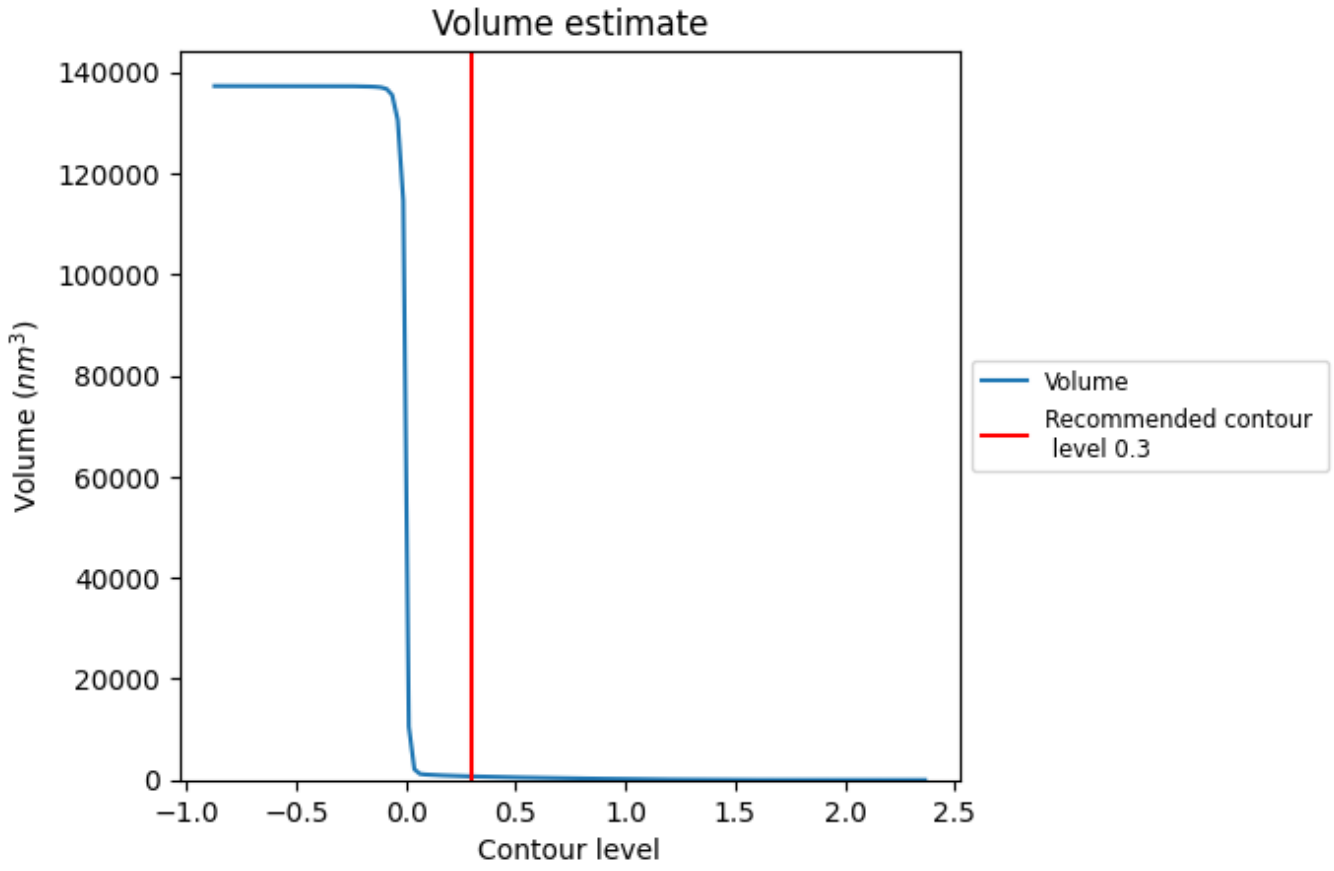
This section contains the results of statistical analysis of the map.

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.

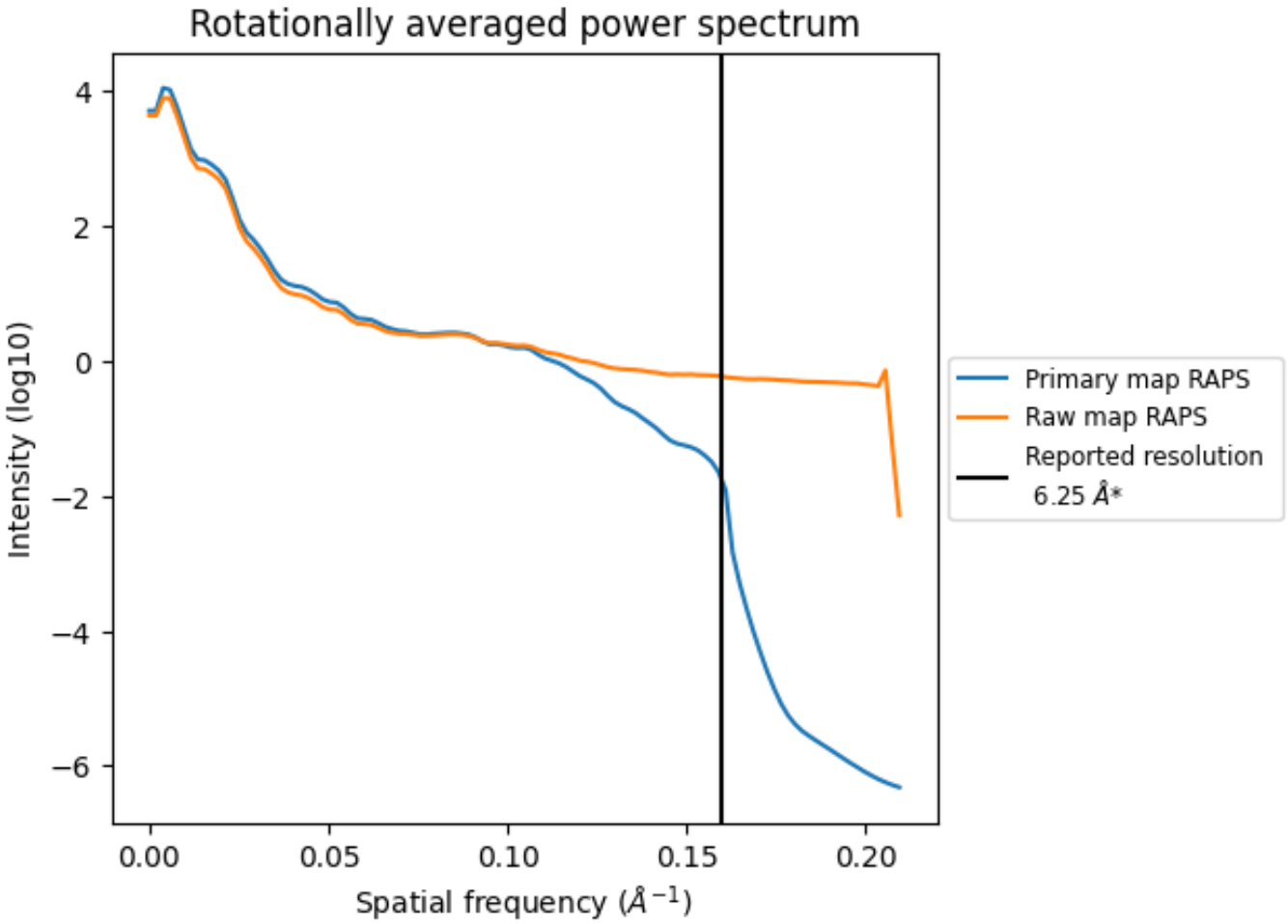
7.2 Volume estimate (i)



The volume at the recommended contour level is 706 nm^3; this corresponds to an approximate mass of 638 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)

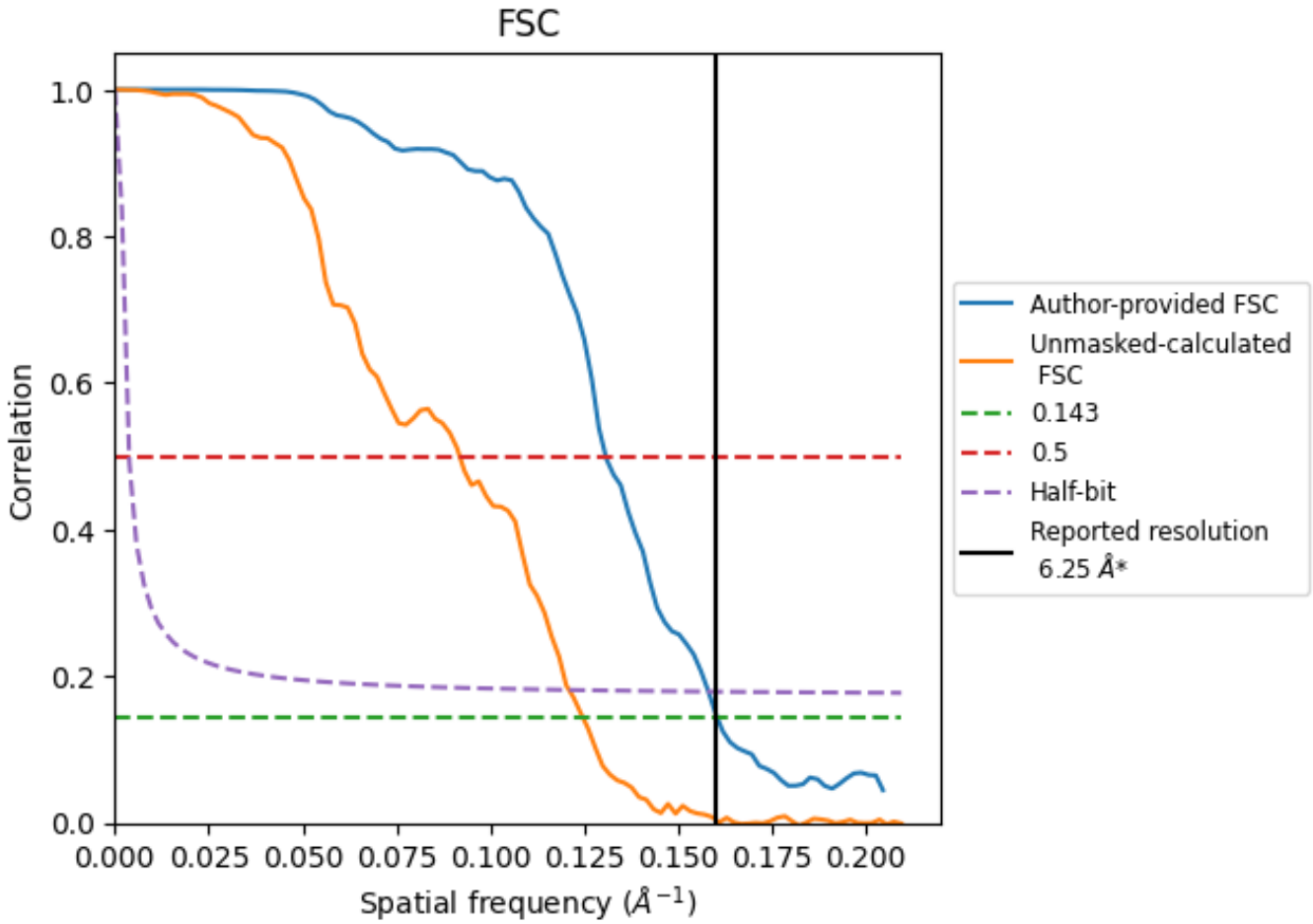


*Reported resolution corresponds to spatial frequency of 0.160 Å^{-1}

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 0.160 Å^{-1}

8.2 Resolution estimates (i)

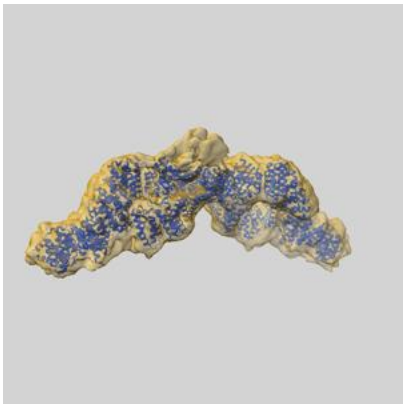
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.25	-	-
Author-provided FSC curve	6.23	7.65	6.33
Unmasked-calculated*	8.03	10.89	8.26

*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 8.03 differs from the reported value 6.25 by more than 10 %

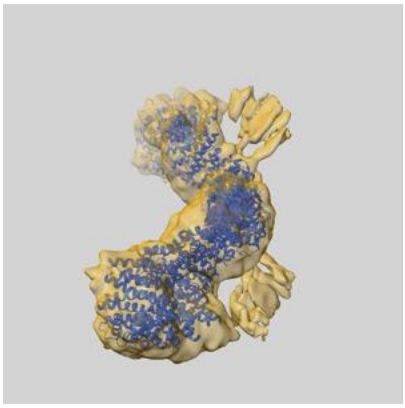
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23930 and PDB model 7MP6. Per-residue inclusion information can be found in section 3 on page 4.

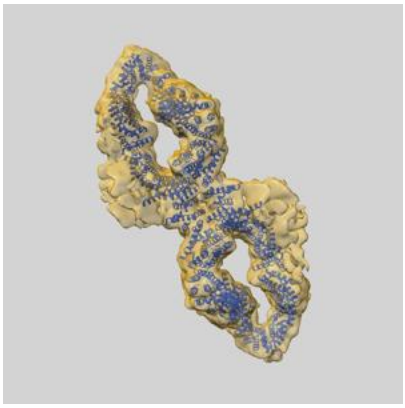
9.1 Map-model overlay



X



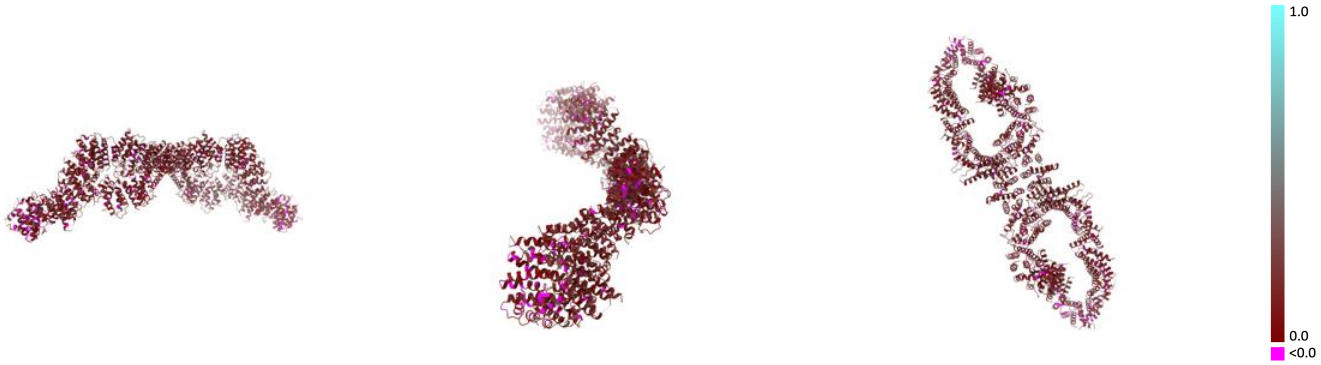
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

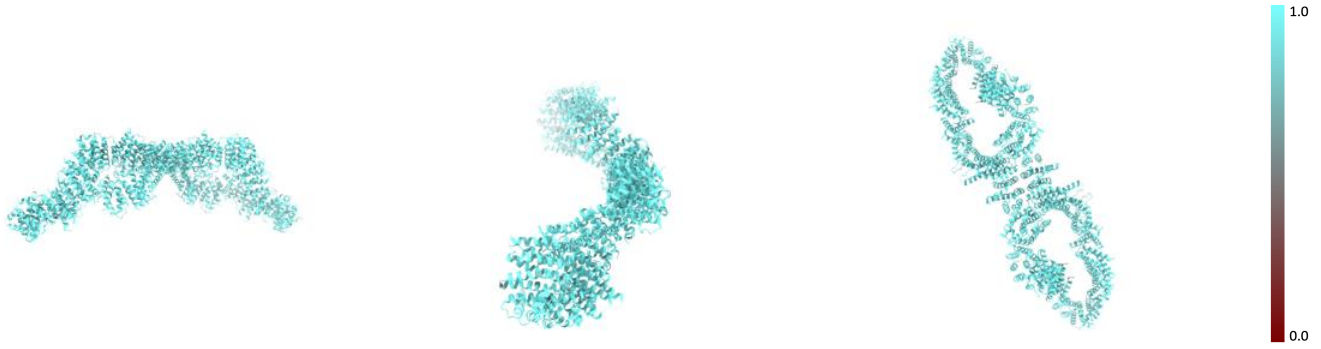
9.2 Q-score mapped to coordinate model



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.

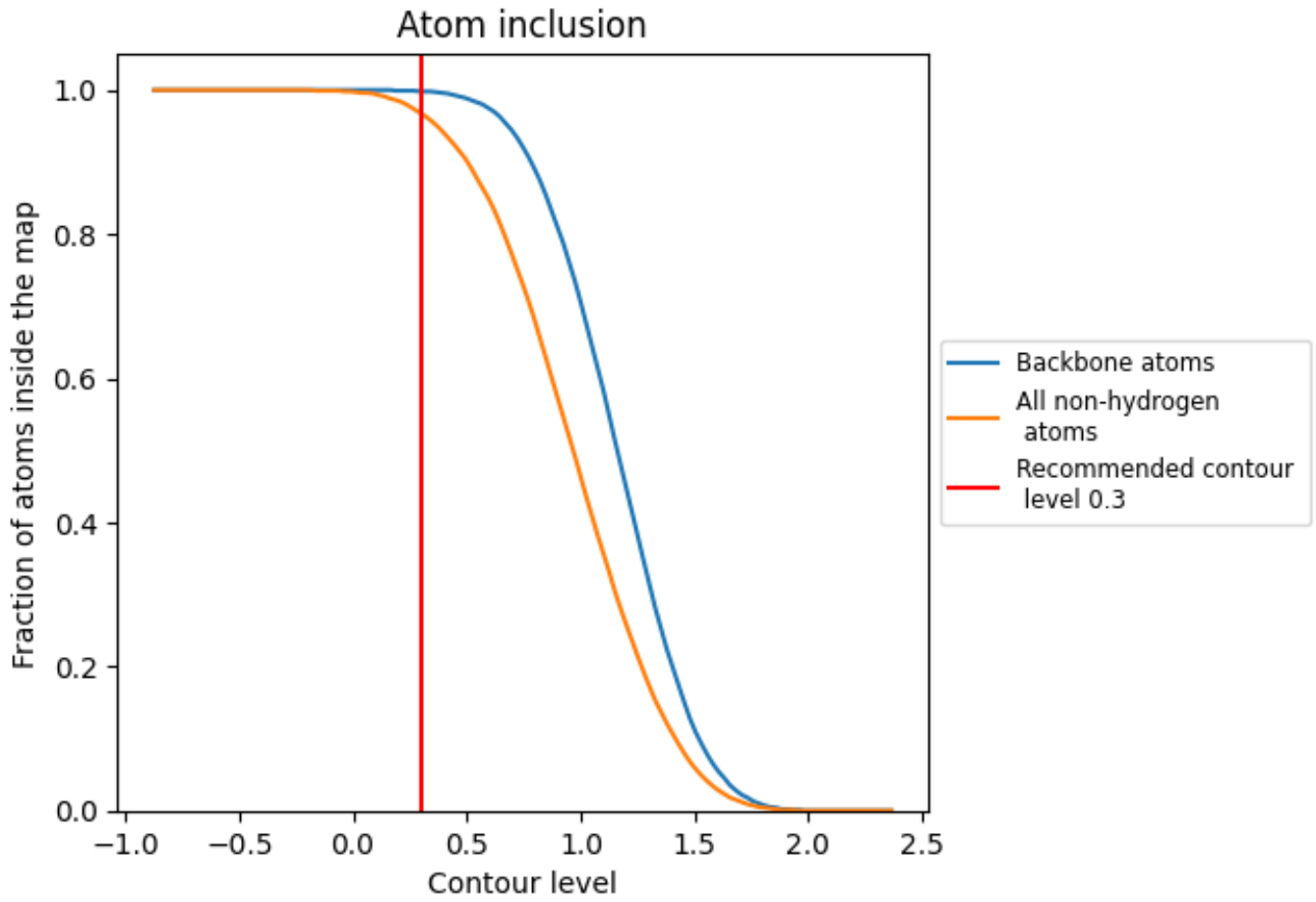
9.3 Atom inclusion mapped to coordinate model



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9670	0.1400
A	0.9690	0.1400
B	0.9660	0.1390