Full wwPDB EM Validation Report ⓘ

Sep 6, 2026 – 04:54 PM EDT

PDB ID	:	9PMW / pdb_00009pmw
EMDB ID	:	EMD-71743
Title	:	Structure of HTTQ23-HAP40 complex bound to macrocycles HHL1, HD4 and HL2
Authors	:	Balakrishnan, S.; Deme, J.; Lea, S.M.; Harding, R.J.
Deposited on	:	2025-07-18
Resolution	:	2.10 Å(reported)
Based on initial model	:	6X90

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:

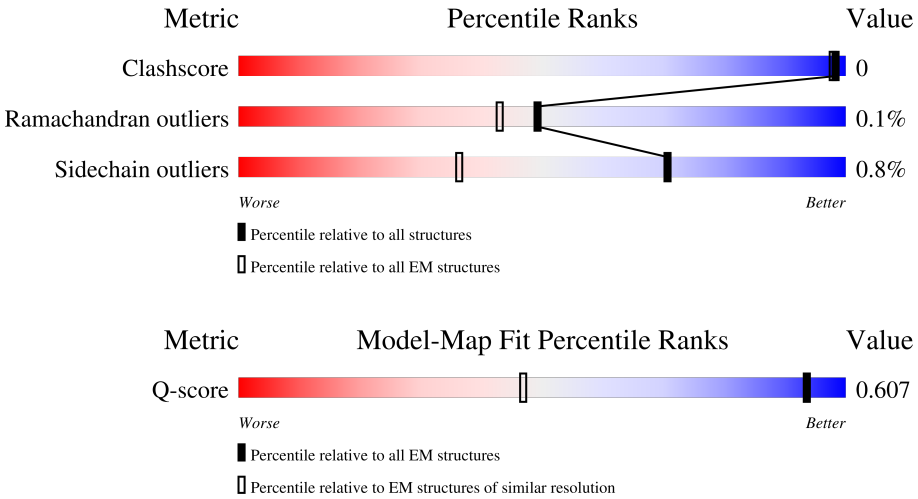
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.10 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2317 (1.60 - 2.60)

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	C	19	11% 95% 5%
2	D	19	16% 84% 16%
3	E	17	6% 76% 12% 12%
4	A	3156	75% 23%

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Mol	Chain	Length	Quality of chain
5	B	389	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 43341 atoms, of which 21953 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 HHL1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	C	19	295	104	143	23	24	1	0	2

- Molecule 2 is a protein called HD4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	D	19	281	91	139	22	27	2	0	1

- Molecule 3 is a protein called HL2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	E	17	261	85	131	22	22	1	0	1

- Molecule 4 is a protein called Huntingtin.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	A	2428	38709	12227	19624	3281	3454	123	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	GLN	-	insertion	UNP P42858
A	40	GLN	-	insertion	UNP P42858
A	1051	PRO	VAL	conflict	UNP P42858
A	1053	LEU	PRO	conflict	UNP P42858
A	2311	HIS	TYR	variant	UNP P42858
A	2788	ILE	VAL	variant	UNP P42858
A	3145	GLY	-	expression tag	UNP P42858
A	3146	GLY	-	expression tag	UNP P42858
A	3147	SER	-	expression tag	UNP P42858

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Chain	Residue	Modelled	Actual	Comment	Reference
A	3148	GLY	-	expression tag	UNP P42858
A	3149	ASP	-	expression tag	UNP P42858
A	3150	TYR	-	expression tag	UNP P42858
A	3151	LYS	-	expression tag	UNP P42858
A	3152	ASP	-	expression tag	UNP P42858
A	3153	ASP	-	expression tag	UNP P42858
A	3154	ASP	-	expression tag	UNP P42858
A	3155	ASP	-	expression tag	UNP P42858
A	3156	LYS	-	expression tag	UNP P42858

- Molecule 5 is a protein called 40-kDa huntingtin-associated protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	B	250	Total	C	H	N	O	S	0	0
			3795	1189	1916	335	348	7		

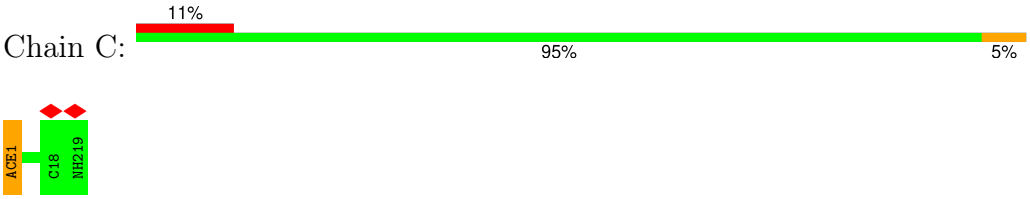
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	expression tag	UNP P23610
B	-16	HIS	-	expression tag	UNP P23610
B	-15	HIS	-	expression tag	UNP P23610
B	-14	HIS	-	expression tag	UNP P23610
B	-13	HIS	-	expression tag	UNP P23610
B	-12	HIS	-	expression tag	UNP P23610
B	-11	HIS	-	expression tag	UNP P23610
B	-10	SER	-	expression tag	UNP P23610
B	-9	SER	-	expression tag	UNP P23610
B	-8	GLY	-	expression tag	UNP P23610
B	-7	ARG	-	expression tag	UNP P23610
B	-6	GLU	-	expression tag	UNP P23610
B	-5	ASN	-	expression tag	UNP P23610
B	-4	LEU	-	expression tag	UNP P23610
B	-3	TYR	-	expression tag	UNP P23610
B	-2	PHE	-	expression tag	UNP P23610
B	-1	GLN	-	expression tag	UNP P23610
B	0	GLY	-	expression tag	UNP P23610

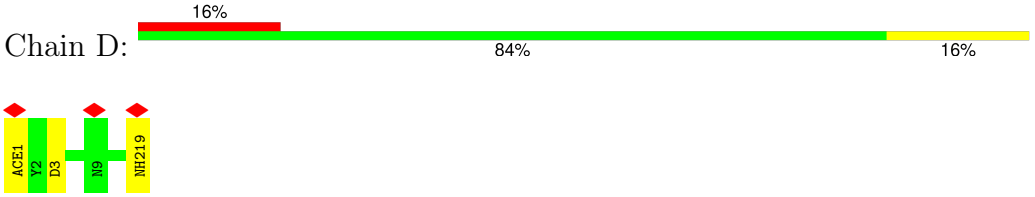
3 Residue-property plots (i)

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.

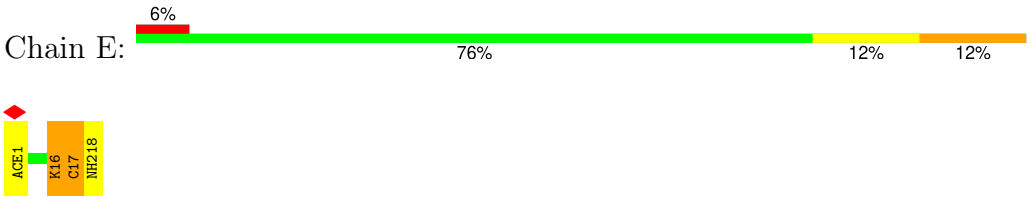
- Molecule 1: HHL1



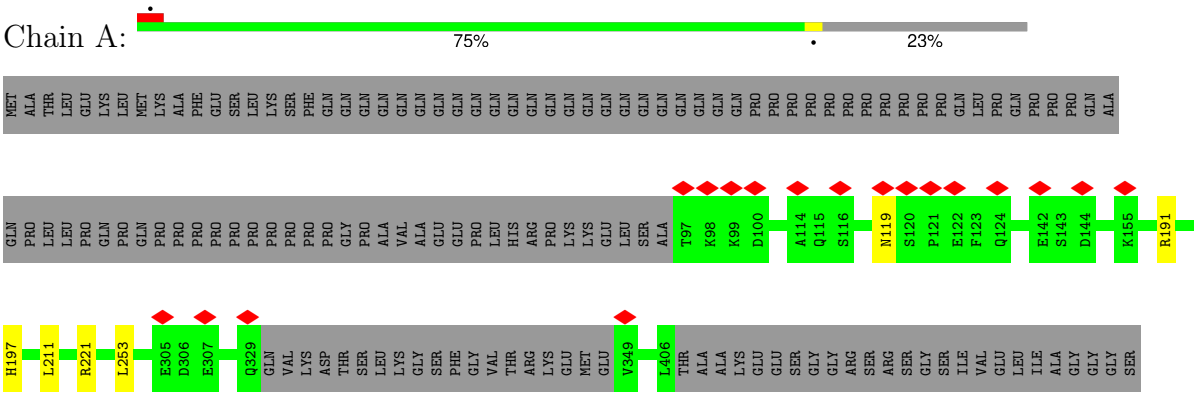
- Molecule 2: HD4

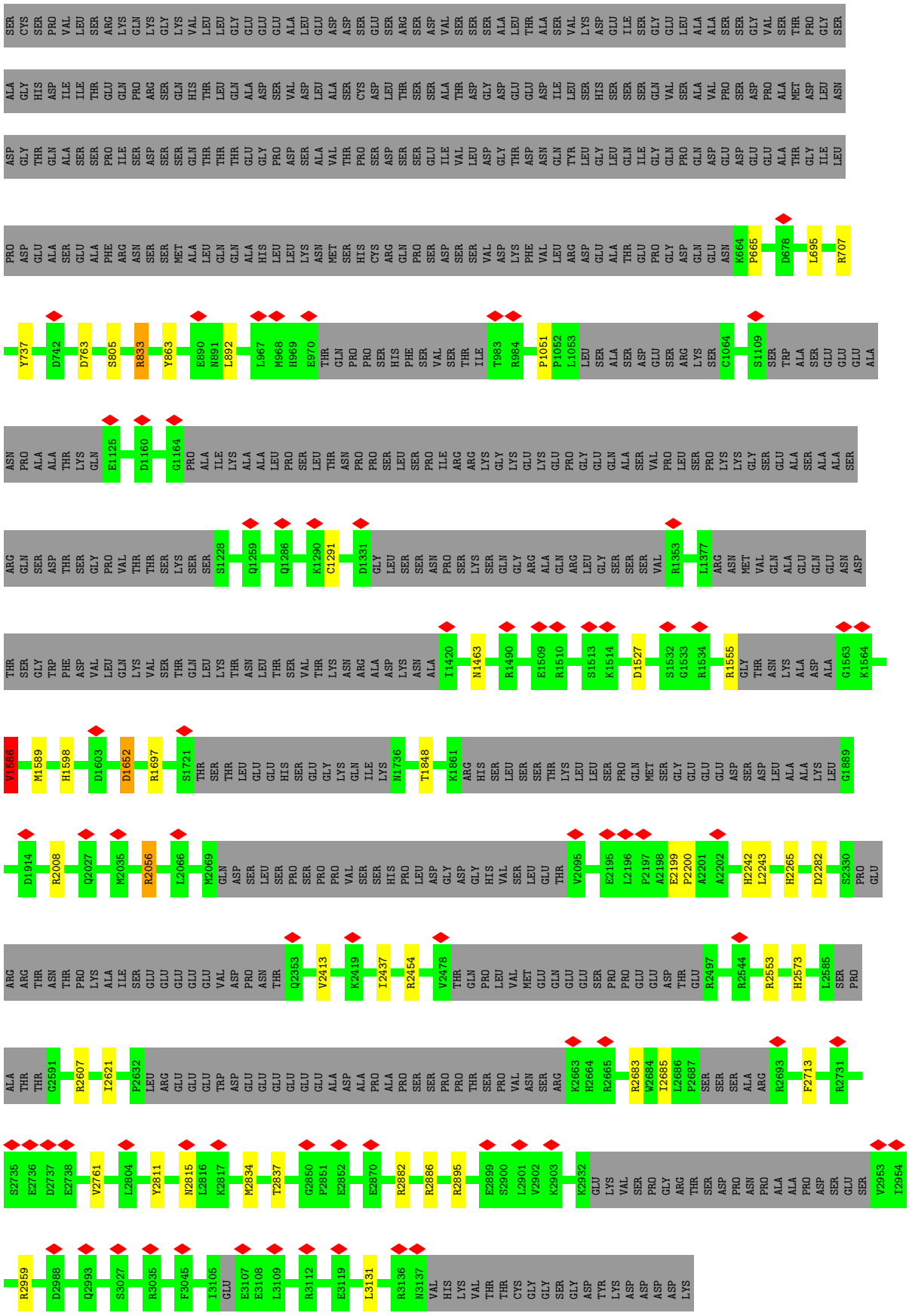


- Molecule 3: HL2



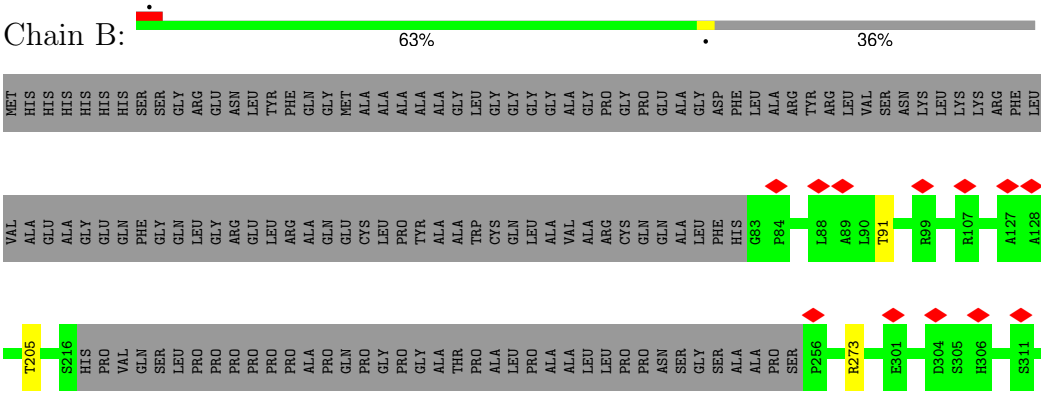
- Molecule 4: Huntingtin





• Molecule 5: 40-kDa huntingtin-associated protein

Chain B:


63%
36%
MET HIS HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN LEU TYR PHE GLN GLY MET ALA ALA ALA ALA ALA GLY LEU GLY GLY GLY GLY ALA GLY PRO GLY PRO GLU ALA GLY ASP PHE LEU ALA ARG TYR ARG LEU VAL SER ASN LYS LEU LYS LYS ARG PHE LEU ARG LYS PRO ASN
VAL ALA GLU ALA GLY GLU GLN PHE GLY GLN LEU GLY ARG GLU LEU ARG ALA GLN GLU CYS LEU PRO TYR ALA ALA TRP CYS GLN LEU ALA VAL ALA ARG CYS GLN GLN ALA LEU PHE HIS G83 P84 L88 A89 L90 T91 R99 R107 A127 A128 L135 L144 L201
T205 S216 HIS PRO VAL GLN SER LEU PRO PRO PRO PRO PRO PRO ALA PRO GLN PRO GLY PRO GLY ALA THR PRO ALA LEU PRO ALA ALA LEU LEU PRO PRO ASN SER GLY SER ALA ALA PRO SER P256 R273 E301 D304 S305 H306 S311 L314 V371

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	230039	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	2.301	Depositor
Minimum map value	-0.185	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.111	Depositor
Map size (Å)	374.784, 374.784, 374.784	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.732, 0.732, 0.732	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: ACE, DTY, NH2

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	C	1.19	1/156 (0.6%)	1.35	0/213
2	D	0.91	0/127	1.37	0/172
3	E	1.48	1/130 (0.8%)	1.82	1/176 (0.6%)
4	A	0.75	0/19460	1.35	30/26429 (0.1%)
5	B	0.76	0/1913	1.36	1/2600 (0.0%)
All	All	0.77	2/21786 (0.0%)	1.35	32/29590 (0.1%)

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
2	D	0	1
4	A	0	4
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1	ACE	C-N	10.89	1.55	1.33
1	C	1	ACE	C-N	7.66	1.48	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	17	CYS	CA-C-O	-17.86	90.44	120.80
4	A	1586	VAL	CA-CB-CG1	8.12	124.21	110.40
4	A	695	LEU	CB-CG-CD1	7.02	131.75	110.70
4	A	1527	ASP	CA-CB-CG	6.75	119.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1051	PRO	N-CA-C	6.66	118.82	110.70
4	A	2056	ARG	NE-CZ-NH2	5.86	124.48	119.20
4	A	2959	ARG	NE-CZ-NH2	5.67	124.30	119.20
4	A	2713	PHE	CA-CB-CG	5.65	119.45	113.80
4	A	2553	ARG	CA-C-N	5.54	126.09	120.00
4	A	2553	ARG	C-N-CA	5.54	126.09	120.00
4	A	191	ARG	NE-CZ-NH2	5.41	124.07	119.20
4	A	763	ASP	CA-C-N	5.40	124.59	118.97
4	A	763	ASP	C-N-CA	5.40	124.59	118.97
4	A	2573	HIS	CB-CG-CD2	-5.39	124.19	131.20
5	B	314	LEU	CB-CG-CD1	5.33	126.70	110.70
4	A	197	HIS	CB-CG-CD2	-5.32	124.28	131.20
4	A	2282	ASP	CA-CB-CG	5.30	117.90	112.60
4	A	221	ARG	NE-CZ-NH2	5.30	123.97	119.20
4	A	1697	ARG	NE-CZ-NH2	5.29	123.96	119.20
4	A	2265	HIS	CB-CG-CD2	-5.27	124.35	131.20
4	A	2886	ARG	NE-CZ-NH2	5.24	123.92	119.20
4	A	833	ARG	NE-CZ-NH2	5.24	123.91	119.20
4	A	1291	CYS	N-CA-CB	-5.23	103.51	111.15
4	A	1555	ARG	NE-CZ-NH2	5.23	123.91	119.20
4	A	2607	ARG	NE-CZ-NH2	5.16	123.84	119.20
4	A	2683	ARG	NE-CZ-NH2	5.14	123.82	119.20
4	A	2895	ARG	NE-CZ-NH2	5.11	123.80	119.20
4	A	2242	HIS	CB-CG-CD2	-5.09	124.58	131.20
4	A	737	TYR	CA-C-N	5.05	127.46	120.29
4	A	737	TYR	C-N-CA	5.05	127.46	120.29
4	A	1598	HIS	CB-CG-CD2	-5.01	124.69	131.20
4	A	1652	ASP	CA-CB-CG	5.00	117.61	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	2811	TYR	Sidechain
4	A	2882	ARG	Sidechain
4	A	833	ARG	Sidechain
4	A	863	TYR	Sidechain
2	D	3	ASP	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	C	152	143	141	1	0
2	D	142	139	136	4	0
3	E	130	131	129	3	0
4	A	19085	19624	19526	9	0
5	B	1879	1916	1905	3	0
All	All	21388	21953	21837	14	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 0.

All (14) 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)
2:D:19:NH2:N	4:A:1463:ASN:HB2	1.80	0.97
3:E:18:NH2:N	4:A:665:PRO:HB2	2.07	0.70
5:B:205:THR:HG22	5:B:273:ARG:HE	1.62	0.65
4:A:2413:VAL:HG13	4:A:2437:ILE:HD11	1.80	0.64
3:E:16:LYS:O	3:E:18:NH2:N	2.31	0.62
2:D:1:ACE:CH3	4:A:119:ASN:OD1	2.56	0.52
5:B:201:LEU:O	5:B:205:THR:HG23	2.10	0.52
3:E:16:LYS:C	3:E:18:NH2:N	2.67	0.51
2:D:19:NH2:N	4:A:1463:ASN:HD22	2.09	0.51
1:C:1:ACE:O	4:A:2056:ARG:HB2	2.12	0.50
2:D:1:ACE:H3	4:A:119:ASN:OD1	2.11	0.49
4:A:1586:VAL:HB	4:A:1589:MET:HE3	1.94	0.49
4:A:2815:ASN:HB2	4:A:2834:MET:HE1	1.96	0.48
5:B:91:THR:HG22	5:B:144:LEU:HD21	2.03	0.41

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	C	17/19 (90%)	15 (88%)	2 (12%)	0	100 100
2	D	16/19 (84%)	15 (94%)	1 (6%)	0	100 100
3	E	15/17 (88%)	13 (87%)	1 (7%)	1 (7%)	1 0
4	A	2388/3156 (76%)	2323 (97%)	64 (3%)	1 (0%)	100 100
5	B	246/389 (63%)	242 (98%)	4 (2%)	0	100 100
All	All	2682/3600 (74%)	2608 (97%)	72 (3%)	2 (0%)	49 50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	17	CYS
4	A	2200	PRO

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	C	17/17 (100%)	17 (100%)	0	100 100
2	D	15/15 (100%)	15 (100%)	0	100 100
3	E	13/13 (100%)	12 (92%)	1 (8%)	12 9
4	A	2146/2778 (77%)	2129 (99%)	17 (1%)	73 81
5	B	189/290 (65%)	189 (100%)	0	100 100
All	All	2380/3113 (76%)	2362 (99%)	18 (1%)	70 81

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	16	LYS
4	A	211	LEU
4	A	253	LEU
4	A	707	ARG
4	A	805	SER
4	A	892	LEU
4	A	1586	VAL
4	A	1652	ASP
4	A	1848	THR
4	A	2008	ARG
4	A	2199	GLU
4	A	2243	LEU
4	A	2454	ARG
4	A	2621	ILE
4	A	2685	ILE
4	A	2761	VAL
4	A	2837	THR
4	A	3131	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	111	ASN
4	A	124	GLN
4	A	164	ASN
4	A	227	GLN
4	A	701	ASN
4	A	757	ASN
4	A	802	ASN
4	A	860	ASN
4	A	1089	GLN
4	A	1315	GLN
4	A	1358	HIS
4	A	1447	GLN
4	A	1449	GLN
4	A	1488	GLN
4	A	1624	GLN
4	A	1626	HIS
4	A	1672	GLN
4	A	1776	GLN
4	A	1840	GLN

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Mol	Chain	Res	Type
4	A	1858	GLN
4	A	1911	ASN
4	A	1924	ASN
4	A	1946	HIS
4	A	2193	GLN
4	A	2270	GLN
4	A	2278	GLN
4	A	2289	GLN
4	A	2561	GLN
4	A	2733	HIS
4	A	2821	HIS
4	A	2878	HIS
4	A	3007	GLN
5	B	100	GLN
5	B	308	GLN
5	B	313	GLN
5	B	323	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

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.

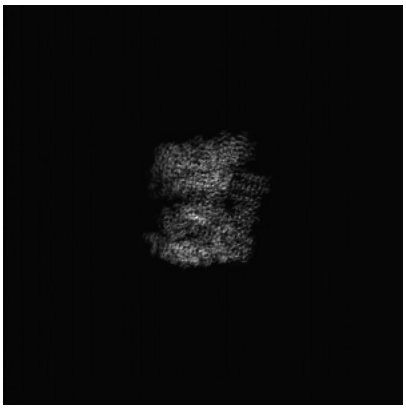
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-71743. These allow visual inspection of the internal detail of the map and identification of artifacts.

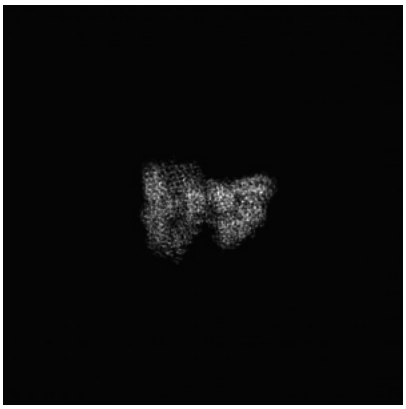
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

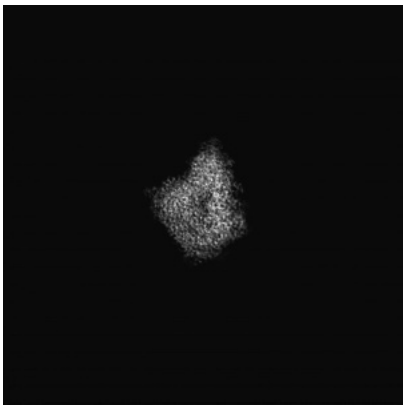
6.1.1 Primary map



X

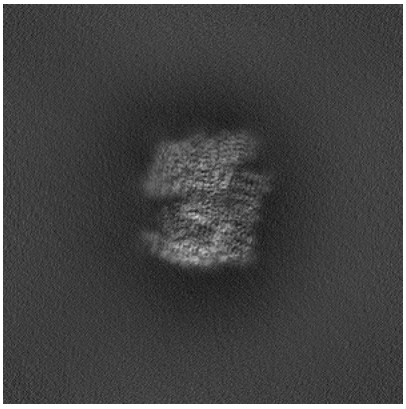


Y

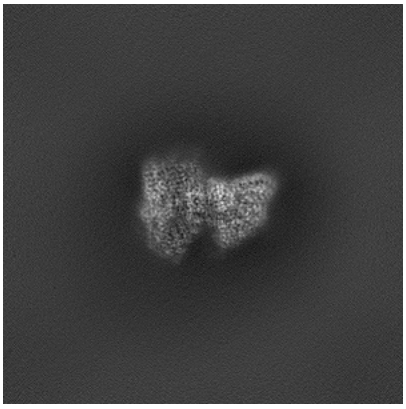


Z

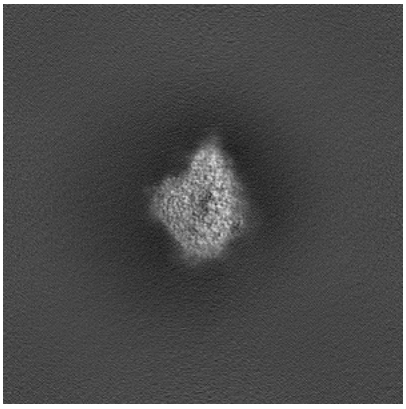
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

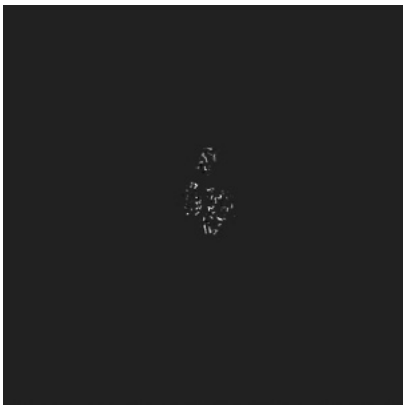
6.2.1 Primary map



X Index: 256

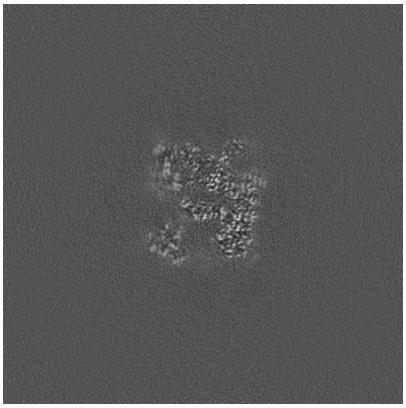


Y Index: 256

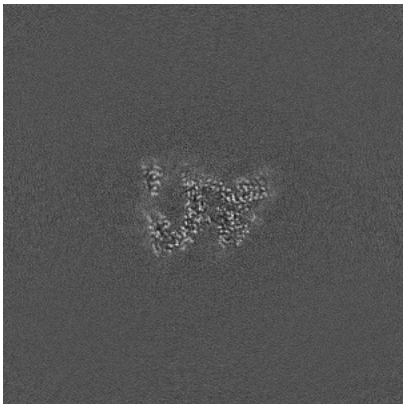


Z Index: 256

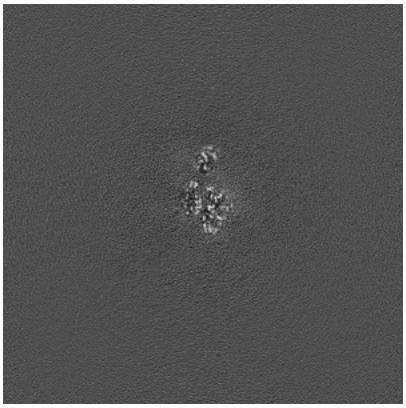
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

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: 273

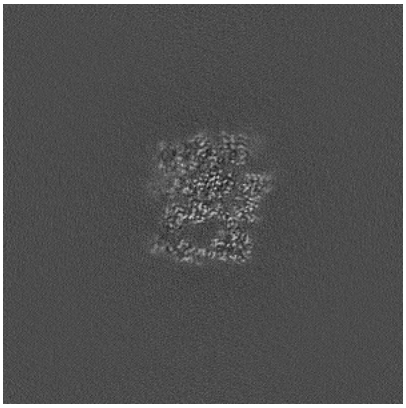


Y Index: 269

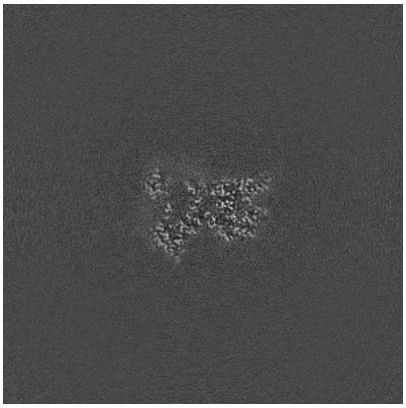


Z Index: 201

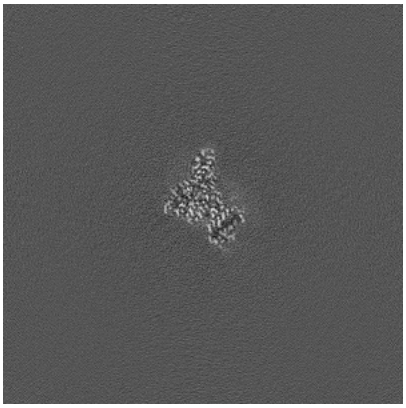
6.3.2 Raw map



X Index: 269



Y Index: 269

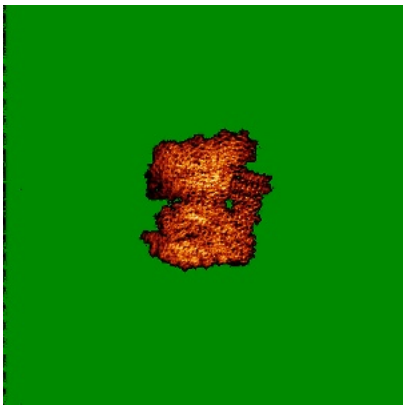


Z Index: 239

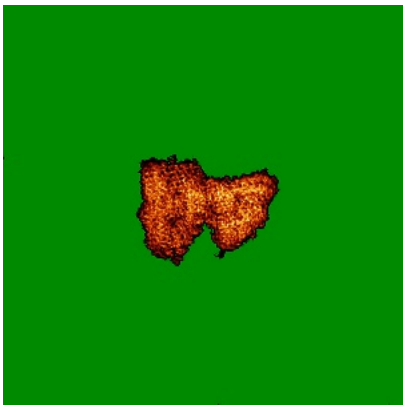
The images above show the largest variance slices of the map in three orthogonal directions.

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

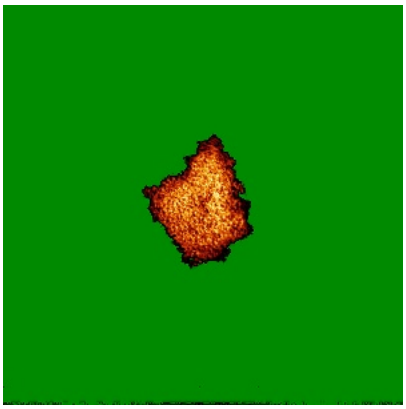
6.4.1 Primary map



X

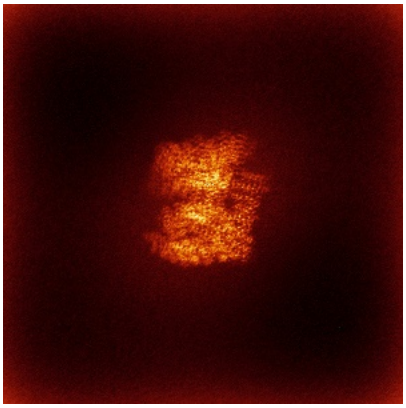


Y

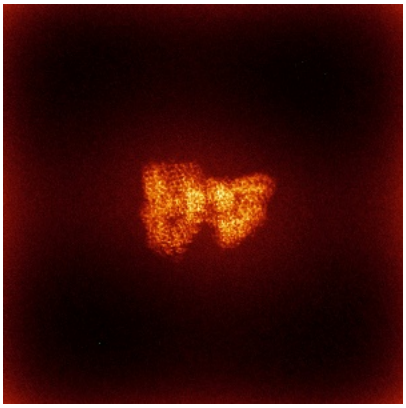


Z

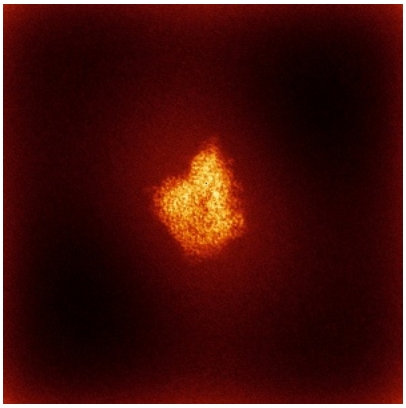
6.4.2 Raw map



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)

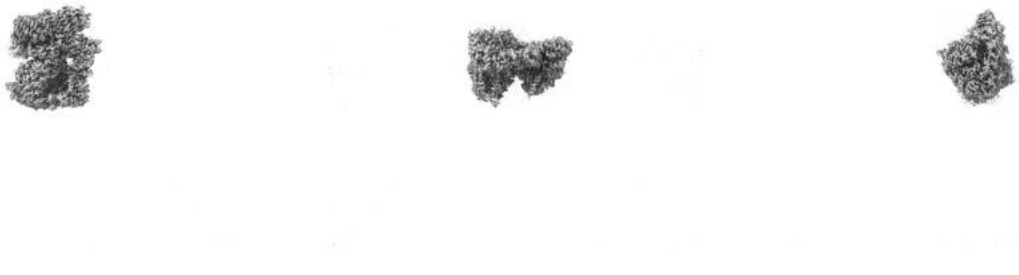
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.111. 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.

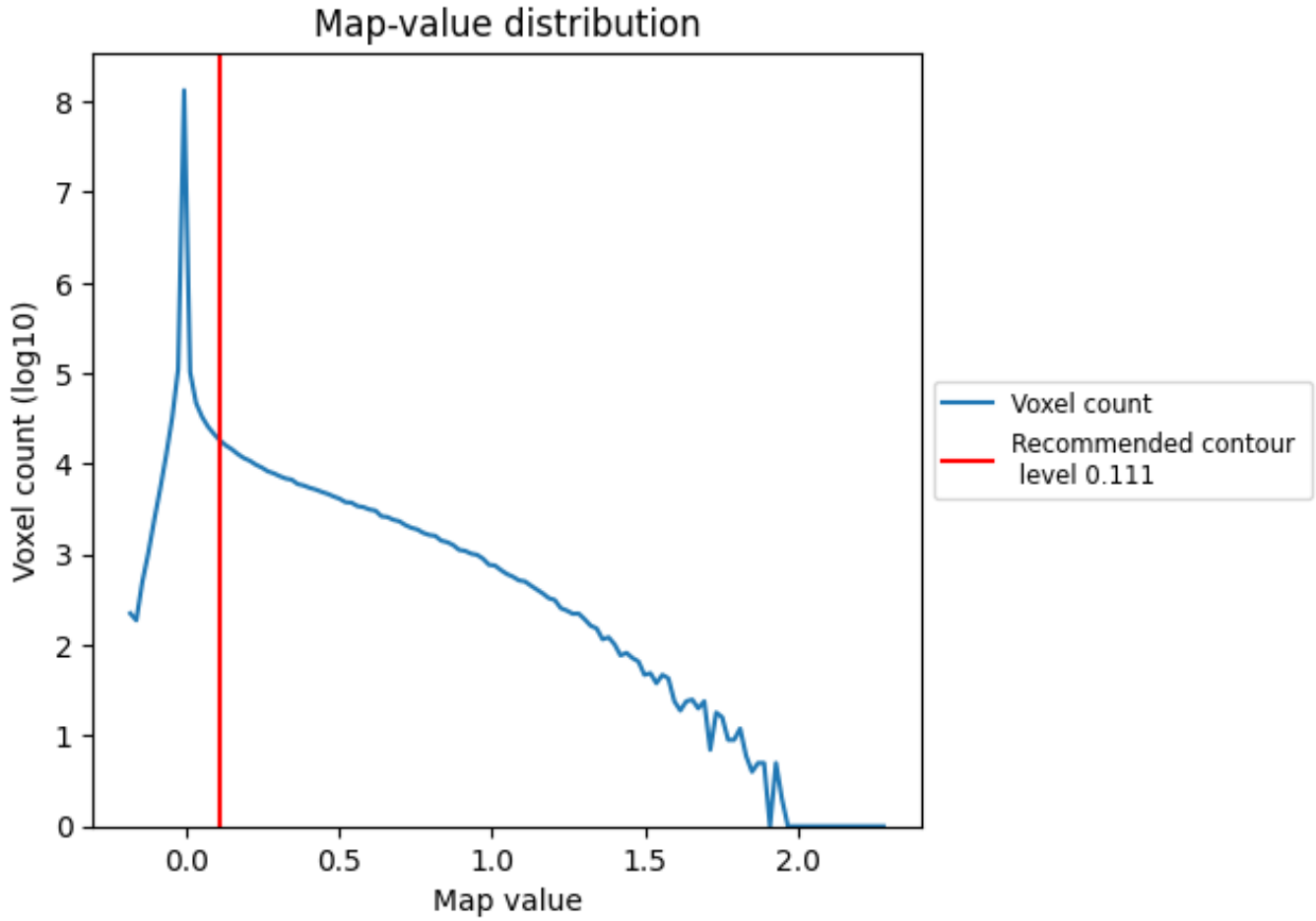
6.6 Mask visualisation (i)

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

7 Map analysis

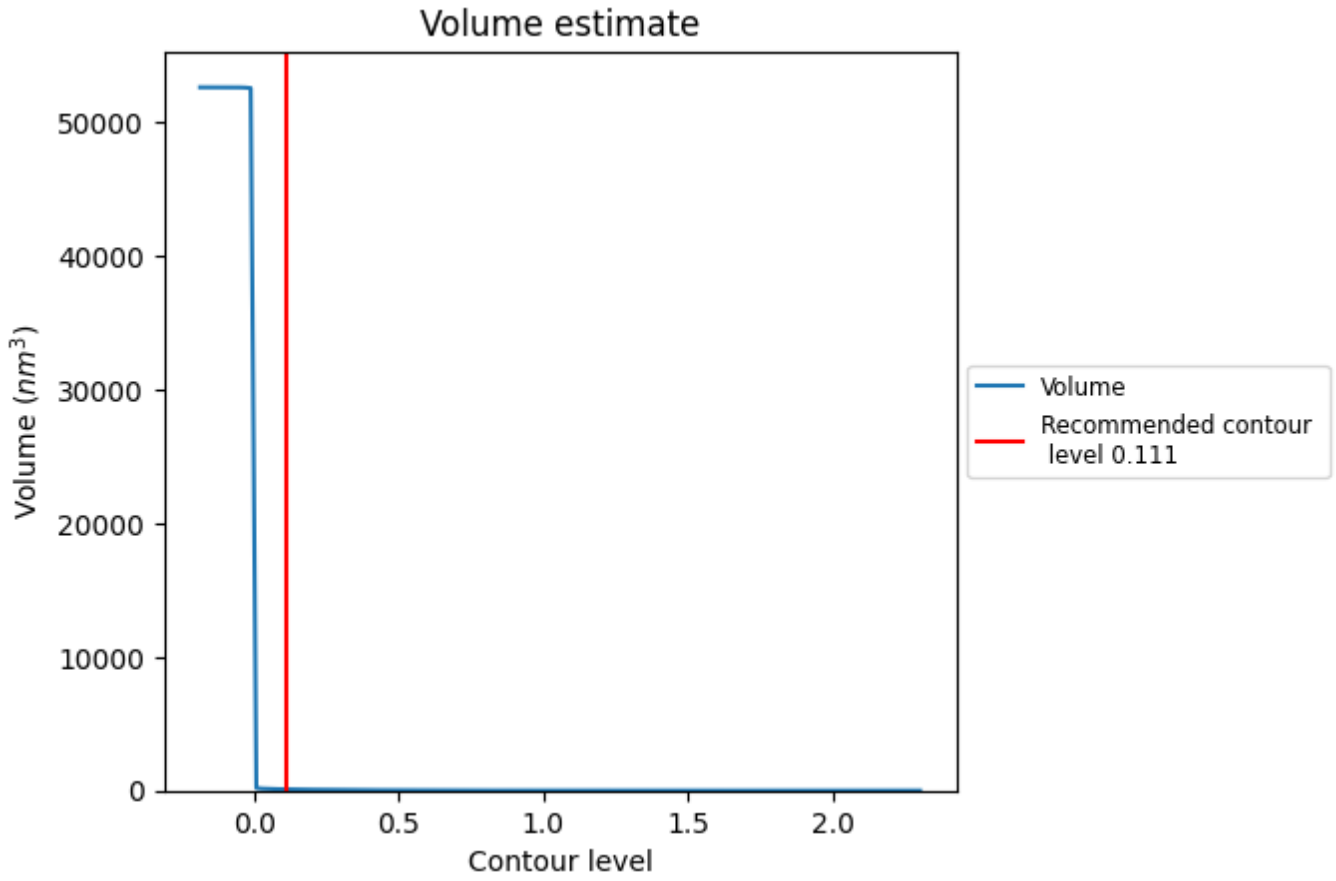
This section contains the results of statistical analysis of the map.

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.

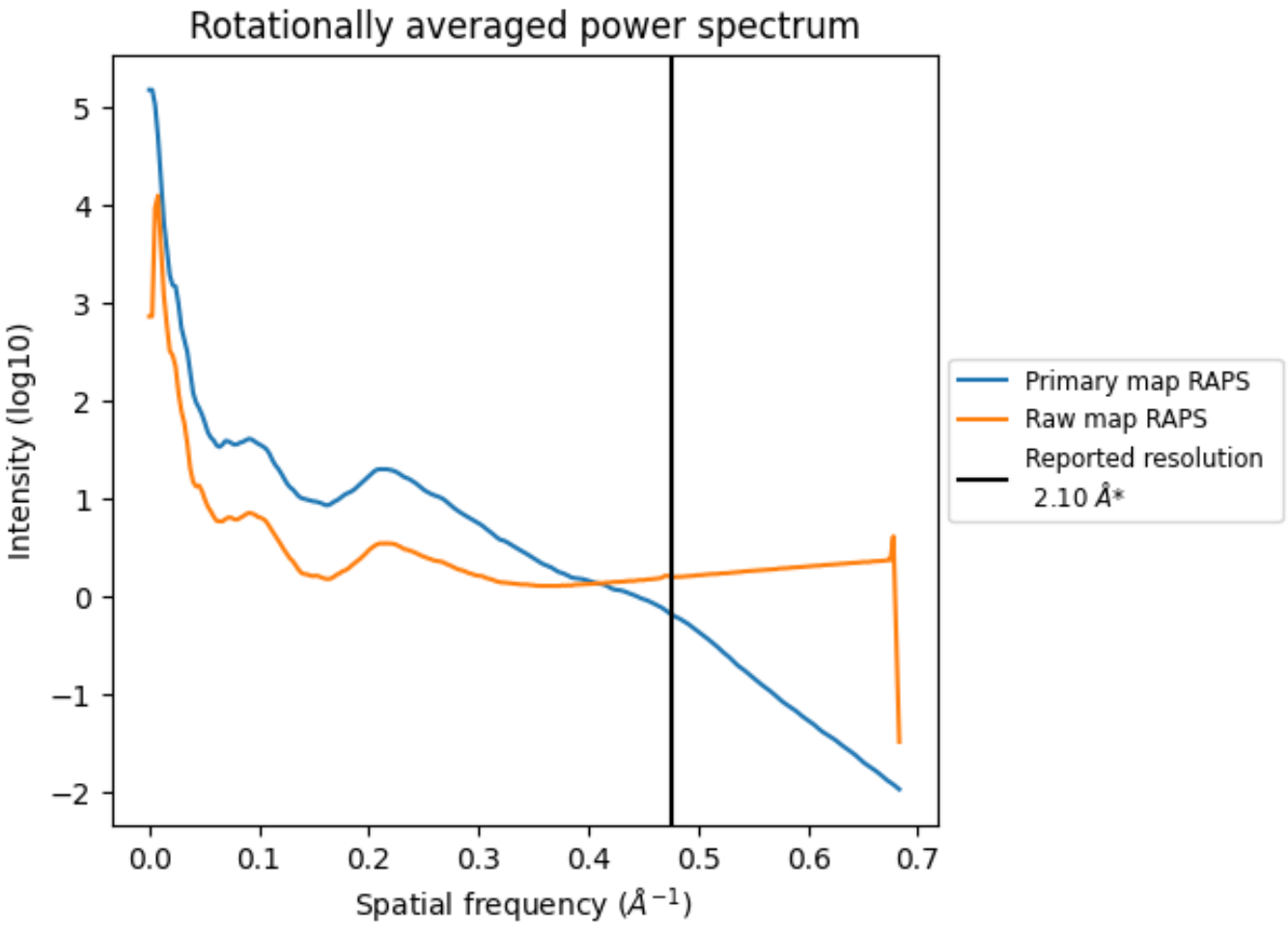
7.2 Volume estimate



The volume at the recommended contour level is 93 nm^3; this corresponds to an approximate mass of 84 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)

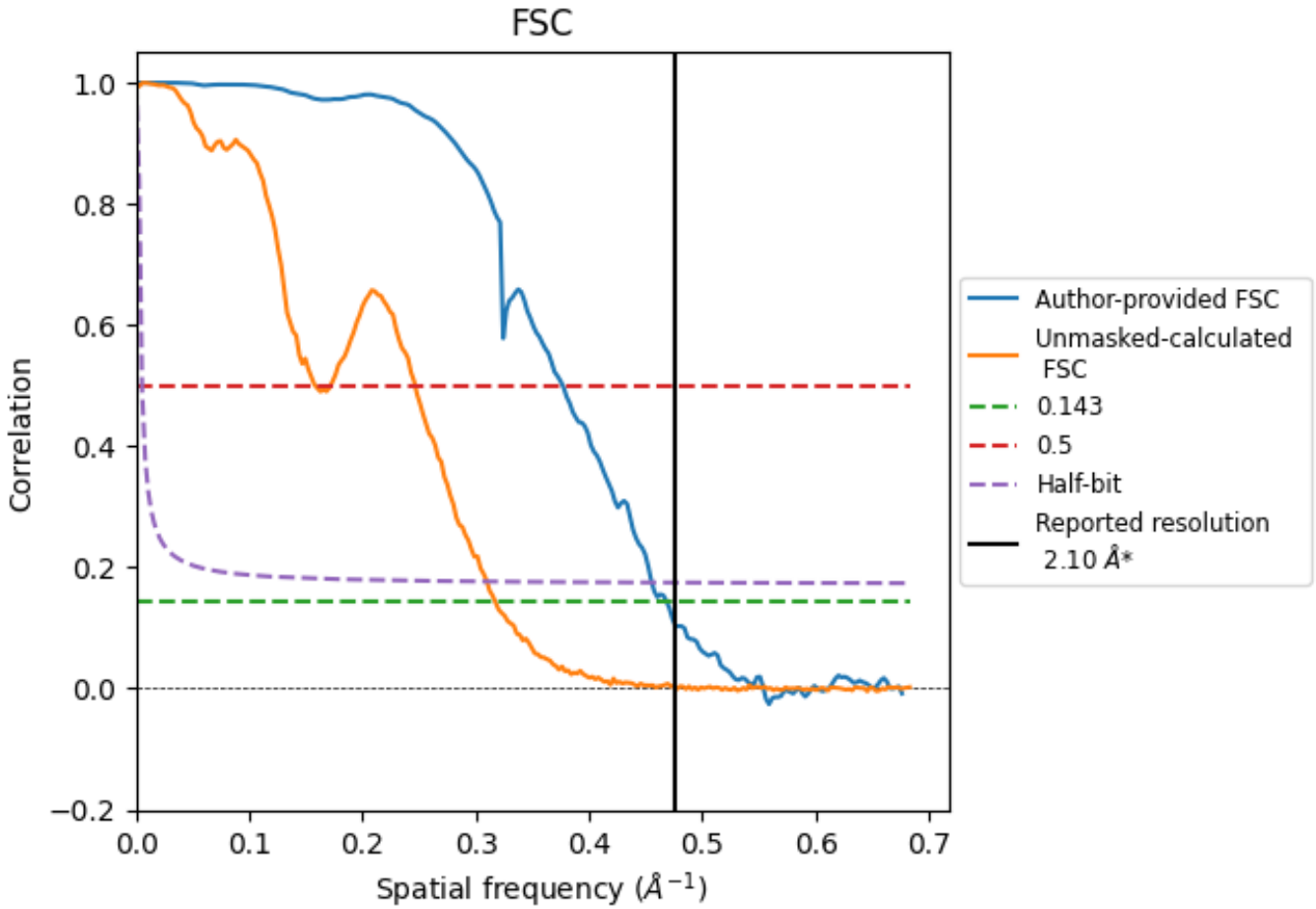


*Reported resolution corresponds to spatial frequency of 0.476 Å^{-1}

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 0.476 Å^{-1}

8.2 Resolution estimates (i)

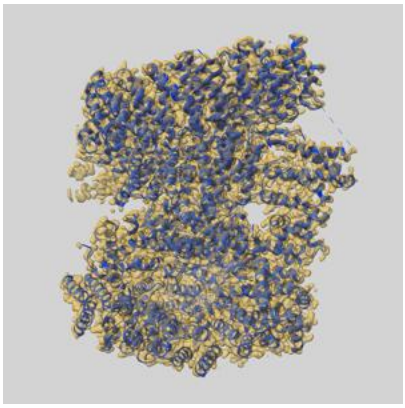
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.13	2.65	2.20
Unmasked-calculated*	3.15	6.32	3.23

*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 3.15 differs from the reported value 2.1 by more than 10 %

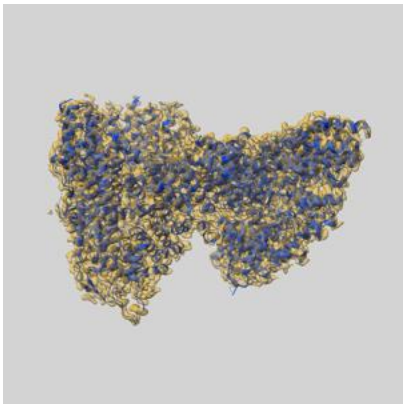
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-71743 and PDB model 9PMW. Per-residue inclusion information can be found in section 3 on page 6.

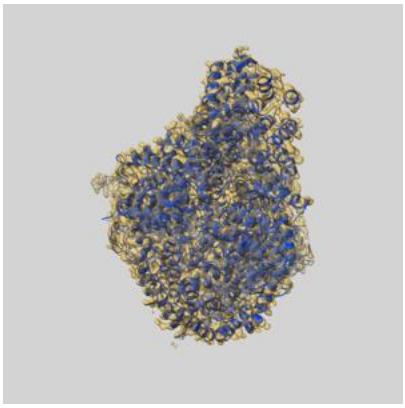
9.1 Map-model overlay



X



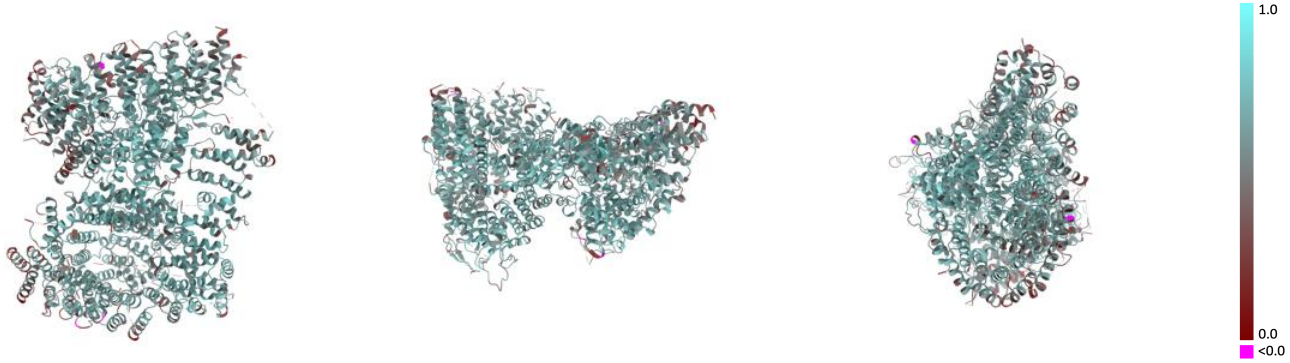
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.111 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.

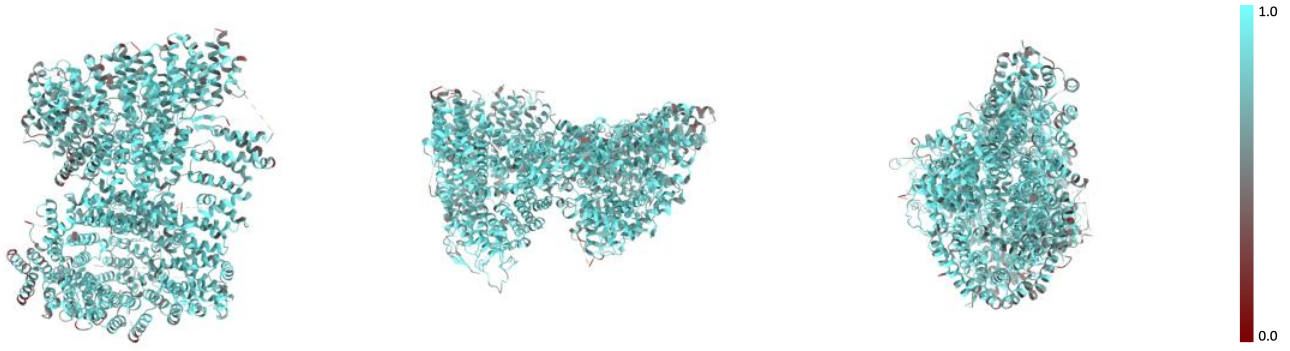
9.2 Q-score mapped to coordinate model (i)



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.

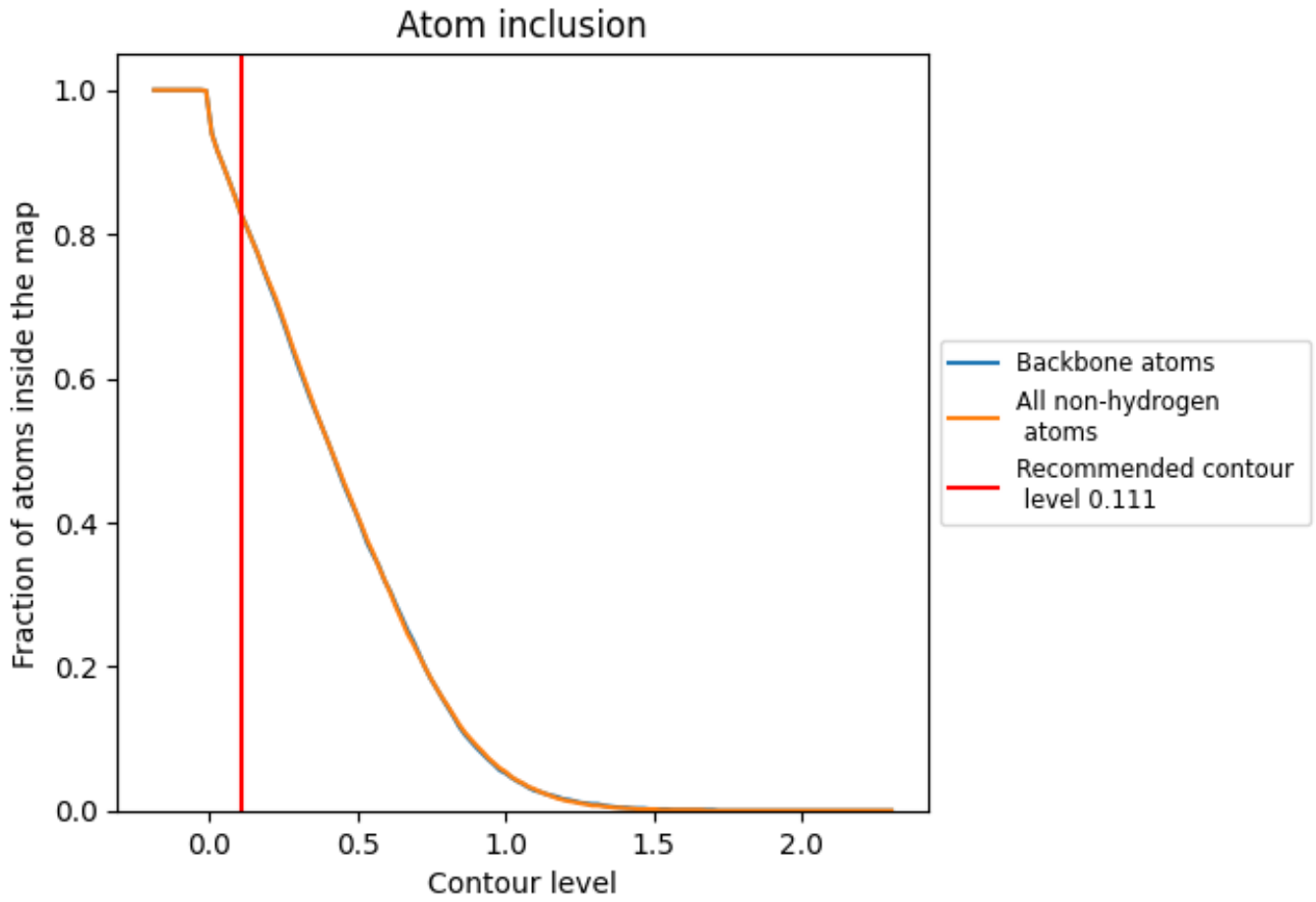
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.111).

9.4 Atom inclusion (i)



At the recommended contour level, 82% 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 (0.111) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8250	0.6070
A	0.8340	0.6060
B	0.8370	0.6270
C	0.8510	0.5910
D	0.6550	0.4650
E	0.7980	0.5800

