wwPDB EM Validation Summary Report (i)

Oct 26, 2026 – 02:21 PM EDT

PDB ID	:	9ZXV / pdb_00009zxv
EMDB ID	:	EMD-74936
Title	:	HHV6B gB trimer with "deliDoP" mutations and I5350A2h (prefusion conformation) - DII-DV local refinement
Authors	:	McCallum, M.; Veesler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2026-01-05
Resolution	:	4.60 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 (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:

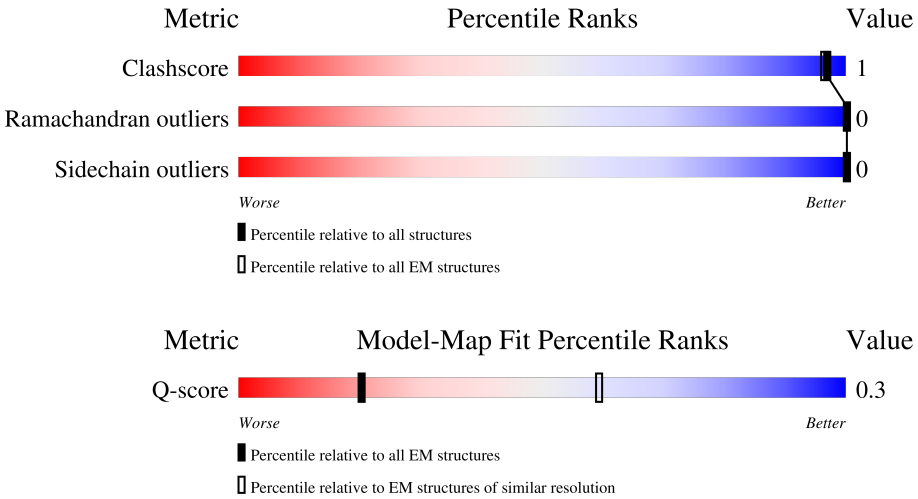
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 4.60 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	2407 (4.10 - 5.10)

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	927	18% 82%
1	B	927	18% 82%
1	C	927	18% 82%

2 Entry composition (i)

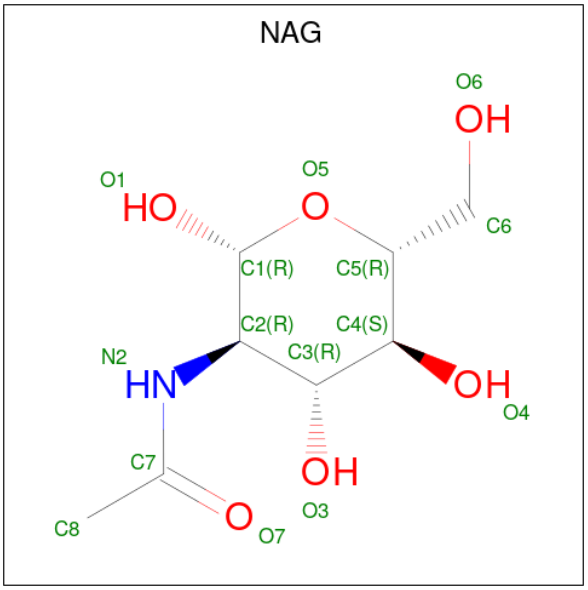
There are 2 unique types of molecules in this entry. The entry contains 2757 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HHV6B gB trimer with "deliDoP" mutations and I5350A2h.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	169	Total	C	N	O	S	0	0
			863	513	173	173	4		
1	A	169	Total	C	N	O	S	0	0
			863	513	173	173	4		
1	C	169	Total	C	N	O	S	0	0
			863	513	173	173	4		

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	

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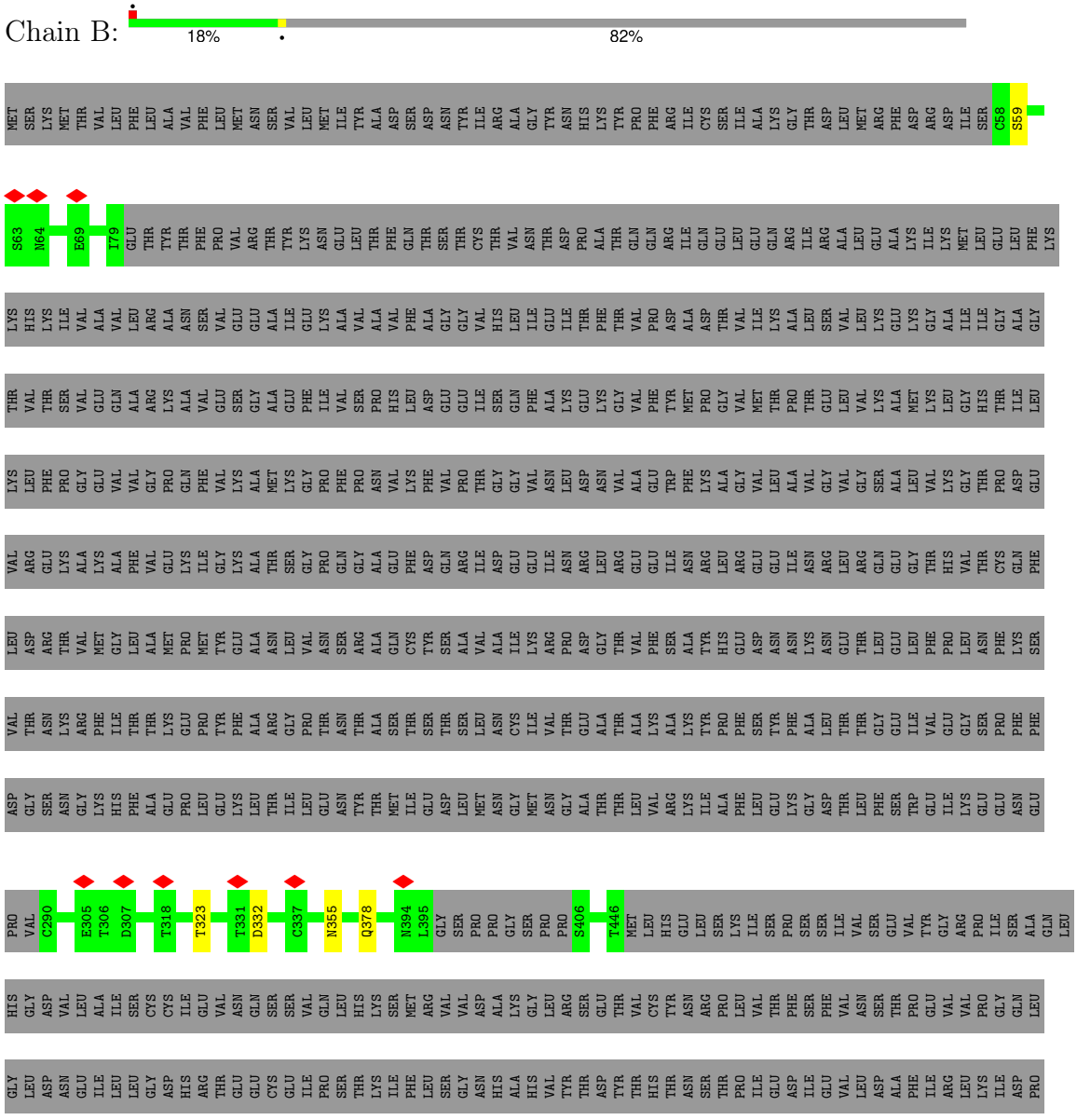
Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	

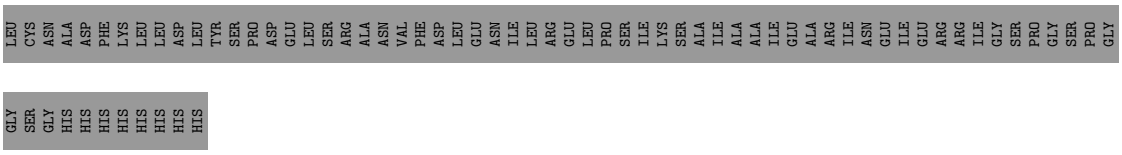
3 Residue-property plots (i)

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: HHV6B gB trimer with "deliDoP" mutations and I5350A2h

Chain B:

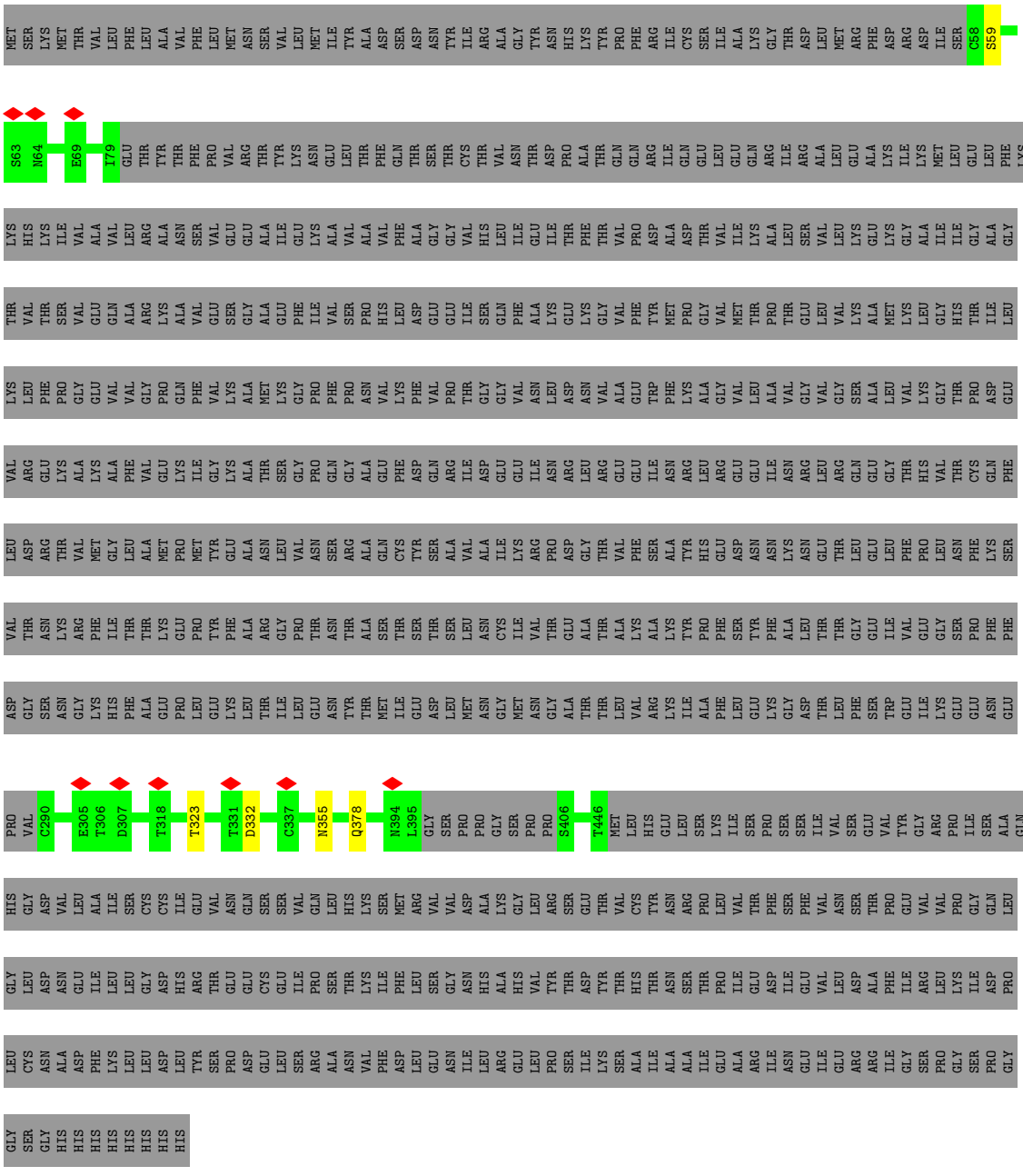




• Molecule 1: HHV6B gB trimer with "deliDoP" mutations and I5350A2h

Chain A:

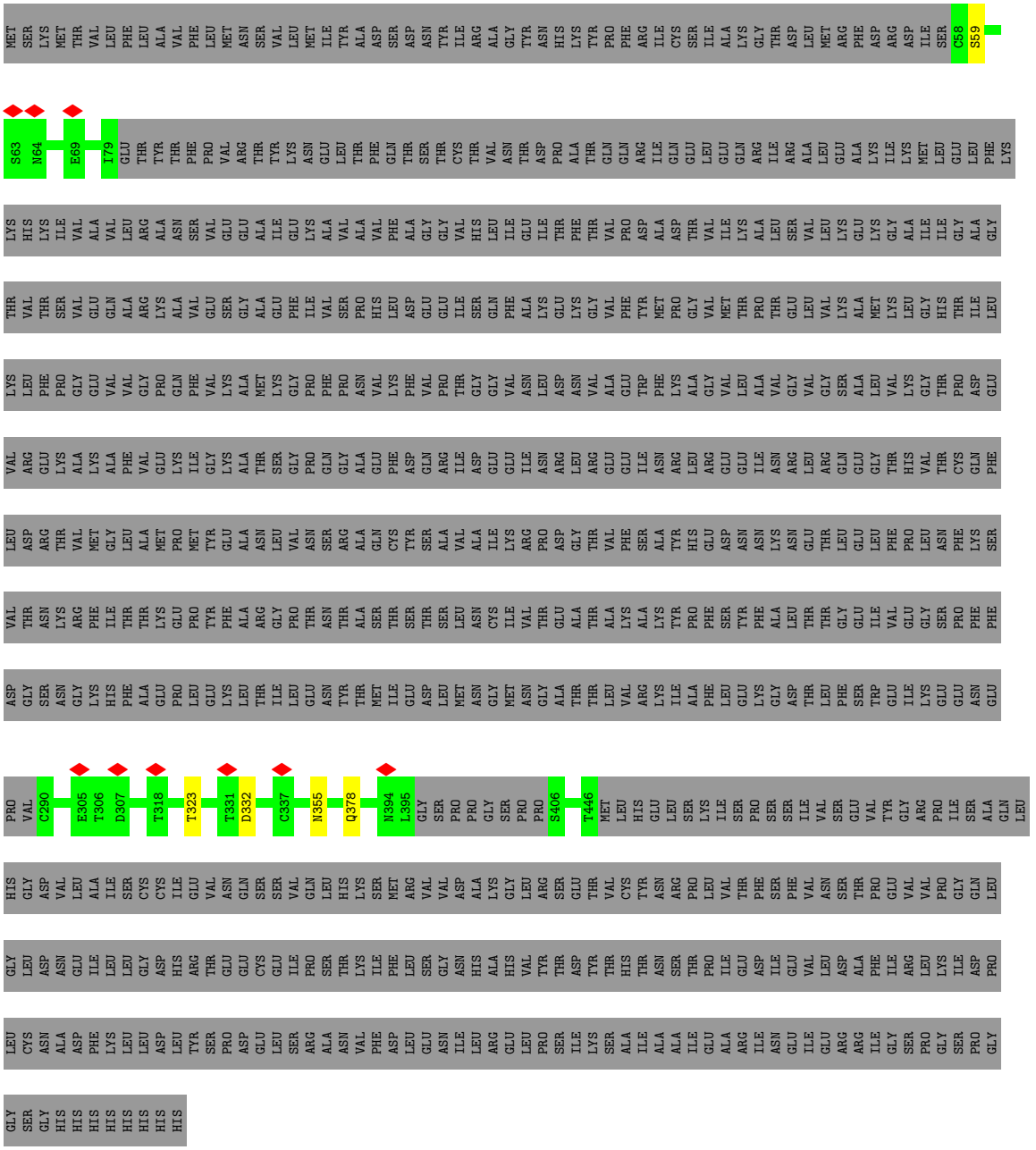




• Molecule 1: HHV6B gB trimer with "deliDoP" mutations and I5350A2h

Chain C:




MET SER LYS MET THR VAL LEU PHE LEU ALA VAL PHE LEU MET ASN SER VAL LEU MET ILE TYR ALA ASP SER ASP ASN TYR ILE ARG ALA GLY TYR ASN HIS LYS TYR PRO PHE ARG ILE CYS SER ILE ALA LYS GLY THR ASP LEU MET ARG PHE ASP ARG ASP ILE SER C58 S59
S63 N64 E69 I79 GLU THR TYR THR PHE PRO VAL ARG THR TYR LYS ASN GLU LEU THR PHE GLN THR SER THR CYS THR VAL ASN THR ASP PRO ALA THR GLN GLN ARG ILE GLN GLU LEU GLU GLN ARG ILE ARG ALA LEU GLU ALA LYS ILE LYS MET LEU GLU LEU PHE LYS
LYS HIS LYS ILE VAL ALA VAL LEU ARG ALA ASN SER VAL GLU GLU ALA ILE GLU LYS ALA VAL ALA VAL PHE ALA GLY GLY VAL HIS LEU ILE GLU ILE THR PHE THR VAL PRO ASP ALA ASP THR VAL ILE LYS ALA LEU SER VAL LEU LYS GLU LYS GLY ALA ILE ILE GLY ALA GLY
THR VAL THR SER VAL GLU GLN ALA ARG LYS ALA VAL GLU SER GLY ALA GLU PHE ILE VAL SER PRO HIS LEU ASP GLU ILE SER GLN PHE ALA LYS GLU LYS GLY VAL PHE TYR MET PRO GLY VAL MET THR PRO THR GLU LEU VAL LYS ALA MET LYS LEU GLY HIS THR ILE LEU
LYS LEU PHE PRO GLY GLU VAL VAL GLY PRO GLN PHE VAL LYS ALA MET LYS GLY PRO PHE PRO ASN VAL LYS PHE VAL PRO THR GLY GLY VAL ASN LEU ASP ASN VAL ALA GLU TRP PHE LYS ALA GLY VAL LEU ALA VAL GLY VAL GLY SER ALA LEU VAL LYS GLY THR PRO ASP GLU
VAL ARG GLU LYS ALA LYS ALA PHE VAL GLU LYS ILE GLY LYS ALA THR SER GLY PRO GLN GLY ALA GLU PHE ASP GLN ARG ILE ASP GLU GLU ILE ASN ARG LEU ARG GLU ILE ASN ARG LEU ARG GLU GLU ILE ASN ARG LEU ARG GLN GLU GLY THR HIS VAL THR CYS GLN PHE
LEU ASP ARG THR VAL MET GLY LEU ALA MET PRO MET TYR GLU ALA ASN LEU VAL ASN SER ARG ALA GLN CYS TYR SER ALA VAL ALA ILE LYS ARG PRO ASP GLY THR VAL PHE SER ALA TYR HIS GLU ASP ASN ASN LYS ASN GLU THR LEU GLU LEU PHE PRO LEU ASN PHE LYS SER
VAL THR ASN LYS ARG PHE ILE THR THR LYS GLU PRO TYR PHE ALA ARG GLY PRO THR ASN THR ALA SER THR SER THR SER LEU ASN CYS ILE VAL THR GLU ALA THR ALA LYS ALA LYS TYR PRO PHE SER TYR PHE ALA LEU THR THR GLY GLU ILE VAL GLU GLY SER PRO PHE PHE
ASP GLY SER ASN GLY LYS HIS PHE ALA GLU PRO LEU GLU LYS LEU THR ILE LEU GLU ASN TYR THR MET ILE GLU ASP LEU MET ASN GLY MET ASN GLY ALA THR THR LEU VAL ARG LYS ILE ALA PHE LEU GLU LYS GLY ASP THR LEU PHE SER TRP GLU ILE LYS GLU GLU ASN GLU
PRO VAL C290 E305 T306 D307 T318 T323 T331 D332 C337 N355 Q378 N394 L395 GLY SER PRO PRO GLY SER PRO PRO S406 T446 MET LEU HIS GLU LEU SER LYS ILE SER PRO SER SER ILE VAL SER GLU VAL TYR GLY ARG PRO ILE SER ALA GLN LEU
HIS GLY ASP VAL LEU ALA ILE SER CYS CYS ILE GLU VAL ASN GLN SER SER VAL GLN LEU HIS LYS SER MET ARG VAL VAL ASP ALA LYS GLY LEU ARG SER GLU THR VAL CYS TYR ASN ARG PRO LEU VAL THR PHE SER PHE VAL ASN SER THR PRO GLU VAL VAL PRO GLY GLN LEU
GLY LEU ASP ASN GLU ILE LEU LEU GLY ASP HIS ARG THR GLU GLU CYS GLU ILE PRO SER THR LYS ILE PHE LEU SER GLY ASN HIS ALA HIS VAL TYR THR ASP TYR THR HIS THR ASN SER THR PRO ILE GLU ASP ILE GLU VAL LEU GLU ASP ALA PHE ILE ARG LEU LYS ILE ASP PRO
LEU CYS ASN ALA ASP PHE LYS LEU LEU ASP LEU TYR SER PRO ASP GLU LEU SER ARG ALA ASN VAL PHE ASP LEU GLU GLU ASN ILE LEU ARG GLU LEU PRO SER ILE LYS SER ALA ILE ALA ALA ILE GLU ALA ARG ILE GLU ASN GLU ILE GLU GLU ARG ARG ILE GLY SER PRO GLY SER PRO GLY
GLY SER GLY HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67753	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.867	Depositor
Minimum map value	-0.228	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	424.448, 424.448, 424.448	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.54	0/864	0.95	8/1202 (0.7%)
1	B	0.54	0/864	0.95	8/1202 (0.7%)
1	C	0.54	0/864	0.95	8/1202 (0.7%)
All	All	0.54	0/2592	0.95	24/3606 (0.7%)

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	378	GLN	CA-C-N	6.78	126.74	119.76
1	B	378	GLN	C-N-CA	6.78	126.74	119.76
1	C	378	GLN	CA-C-N	6.76	126.72	119.76
1	C	378	GLN	C-N-CA	6.76	126.72	119.76
1	A	378	GLN	CA-C-N	6.73	126.69	119.76

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	863	0	399	1	0
1	B	863	0	399	1	0
1	C	863	0	399	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	56	0	52	1	0
2	B	56	0	52	1	0
2	C	56	0	52	1	0
All	All	2757	0	1353	3	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 1.

All (3) 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:355:ASN:O	2:A:702:NAG:H83	2.12	0.50
1:C:355:ASN:O	2:C:702:NAG:H83	2.12	0.50
1:B:355:ASN:O	2:B:702:NAG:H83	2.12	0.49

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	163/927 (18%)	161 (99%)	2 (1%)	0	100	100
1	B	163/927 (18%)	161 (99%)	2 (1%)	0	100	100
1	C	163/927 (18%)	161 (99%)	2 (1%)	0	100	100
All	All	489/2781 (18%)	483 (99%)	6 (1%)	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	12/810 (2%)	12 (100%)	0	100	100
1	B	12/810 (2%)	12 (100%)	0	100	100
1	C	12/810 (2%)	12 (100%)	0	100	100
All	All	36/2430 (2%)	36 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	702	1	14,14,15	1.24	1 (7%)	17,19,21	1.07	2 (11%)
2	NAG	B	703	1	14,14,15	1.11	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	B	704	1	14,14,15	1.13	1 (7%)	17,19,21	1.10	2 (11%)
2	NAG	A	703	1	14,14,15	1.12	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	A	704	1	14,14,15	1.12	1 (7%)	17,19,21	1.10	2 (11%)
2	NAG	B	701	1	14,14,15	1.05	1 (7%)	17,19,21	1.24	2 (11%)
2	NAG	A	701	1	14,14,15	1.05	1 (7%)	17,19,21	1.24	2 (11%)
2	NAG	C	702	1	14,14,15	1.23	1 (7%)	17,19,21	1.07	2 (11%)
2	NAG	B	702	1	14,14,15	1.23	1 (7%)	17,19,21	1.07	2 (11%)
2	NAG	C	703	1	14,14,15	1.11	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	C	704	1	14,14,15	1.13	1 (7%)	17,19,21	1.10	2 (11%)
2	NAG	C	701	1	14,14,15	1.04	1 (7%)	17,19,21	1.24	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	702	1	-	2/6/23/26	0/1/1/1
2	NAG	B	703	1	-	0/6/23/26	0/1/1/1
2	NAG	B	704	1	-	0/6/23/26	0/1/1/1
2	NAG	A	703	1	-	0/6/23/26	0/1/1/1
2	NAG	A	704	1	-	0/6/23/26	0/1/1/1
2	NAG	B	701	1	-	2/6/23/26	0/1/1/1
2	NAG	A	701	1	-	2/6/23/26	0/1/1/1
2	NAG	C	702	1	-	2/6/23/26	0/1/1/1
2	NAG	B	702	1	-	2/6/23/26	0/1/1/1
2	NAG	C	703	1	-	0/6/23/26	0/1/1/1
2	NAG	C	704	1	-	0/6/23/26	0/1/1/1
2	NAG	C	701	1	-	2/6/23/26	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	702	NAG	C1-C2	3.67	1.57	1.52
2	B	702	NAG	C1-C2	3.65	1.57	1.52
2	C	702	NAG	C1-C2	3.64	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	704	NAG	C1-C2	3.48	1.57	1.52
2	C	704	NAG	C1-C2	3.43	1.57	1.52

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	703	NAG	C8-C7-N2	2.83	120.81	116.12
2	C	703	NAG	C8-C7-N2	2.81	120.78	116.12
2	A	703	NAG	C8-C7-N2	2.81	120.77	116.12
2	A	701	NAG	C8-C7-N2	2.79	120.75	116.12
2	B	701	NAG	C8-C7-N2	2.79	120.75	116.12

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	NAG	O5-C5-C6-O6
2	A	701	NAG	O5-C5-C6-O6
2	C	701	NAG	O5-C5-C6-O6
2	A	701	NAG	C4-C5-C6-O6
2	B	701	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	702	NAG	1	0
2	C	702	NAG	1	0
2	B	702	NAG	1	0

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.

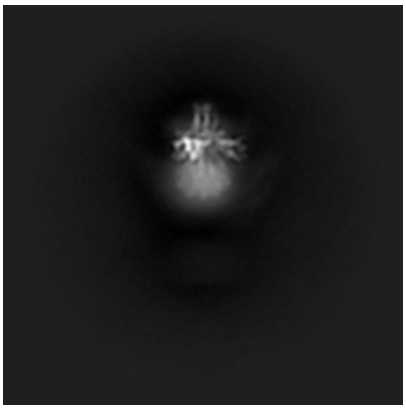
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-74936. These allow visual inspection of the internal detail of the map and identification of artifacts.

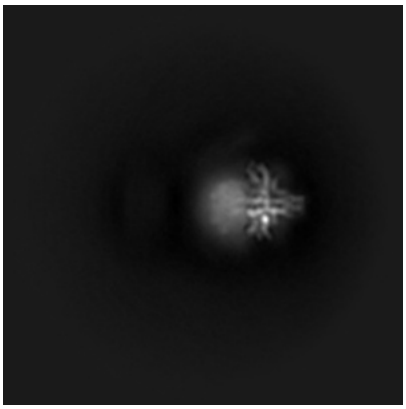
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

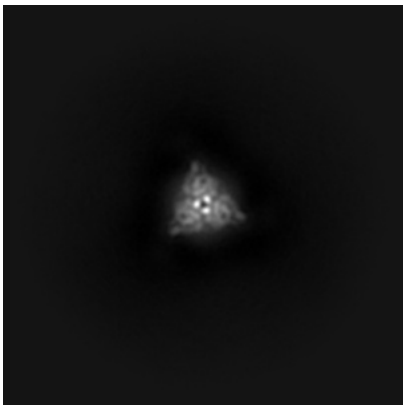
6.1.1 Primary map



X

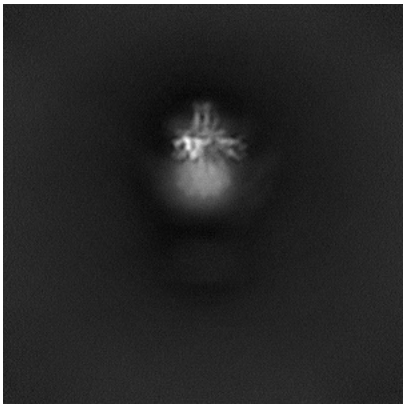


Y

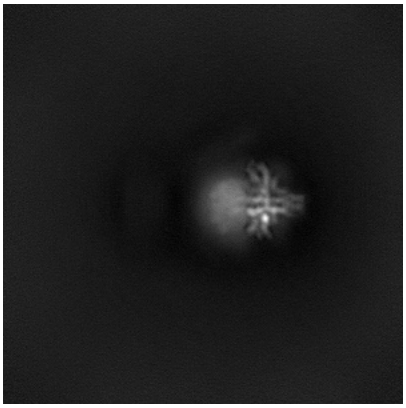


Z

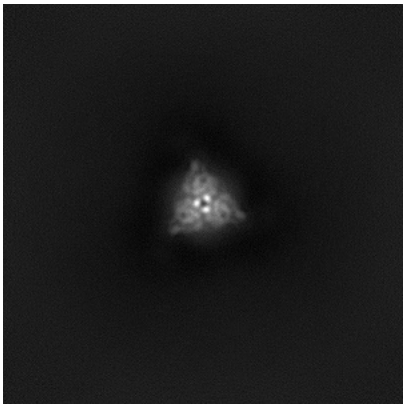
6.1.2 Raw map



X



Y



Z

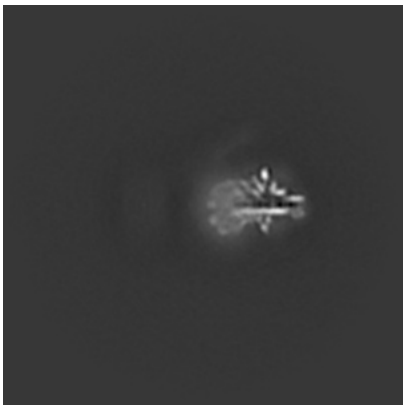
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

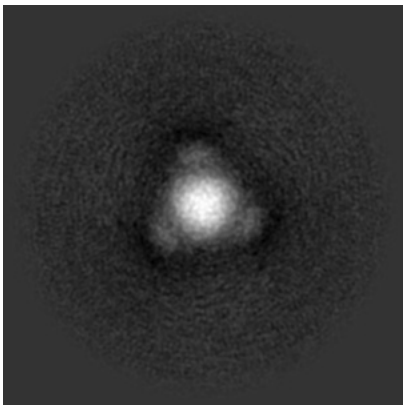
6.2.1 Primary map



X Index: 256

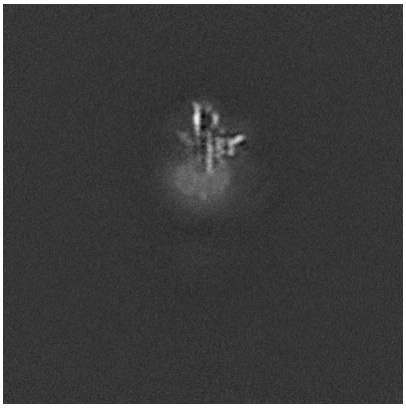


Y Index: 256

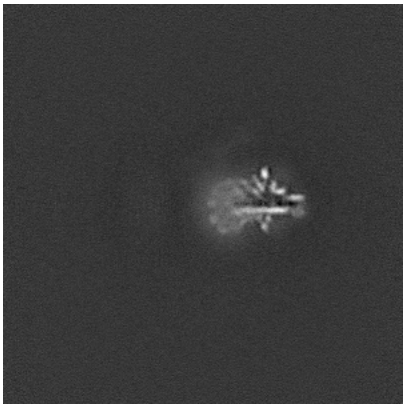


Z Index: 256

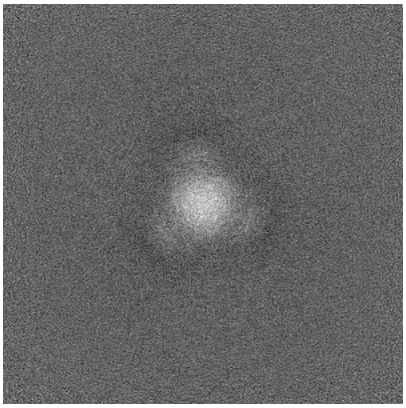
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

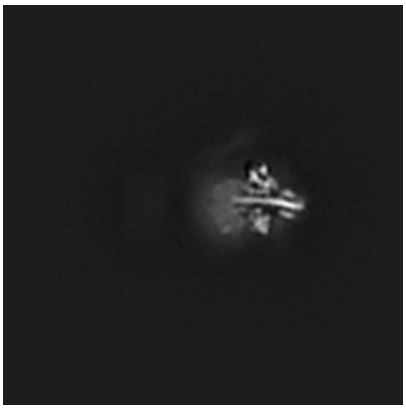
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 248

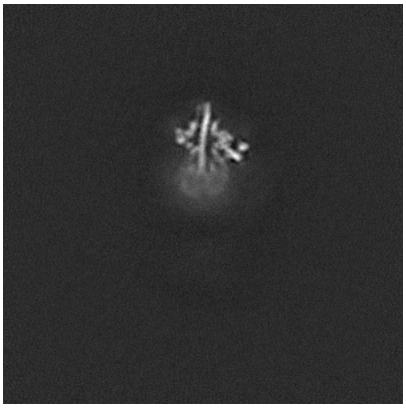


Y Index: 248

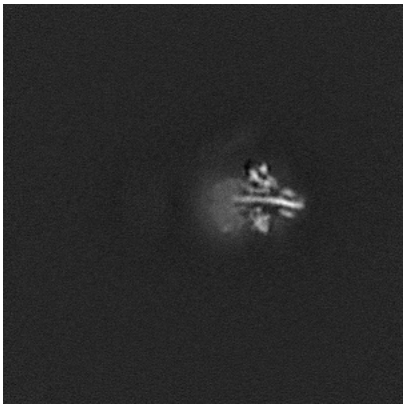


Z Index: 335

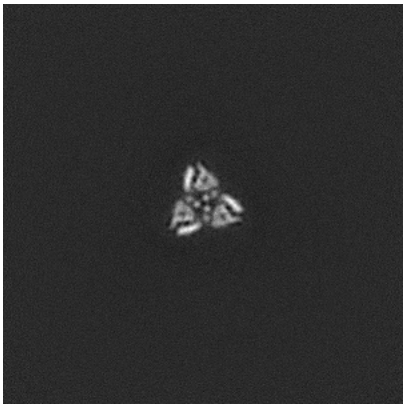
6.3.2 Raw map



X Index: 248



Y Index: 248

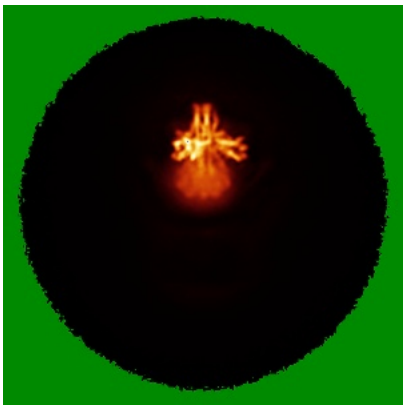


Z Index: 335

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

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

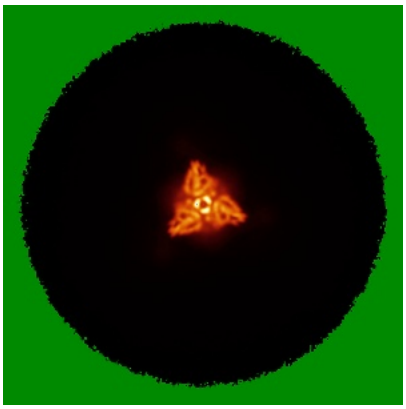
6.4.1 Primary map



X



Y

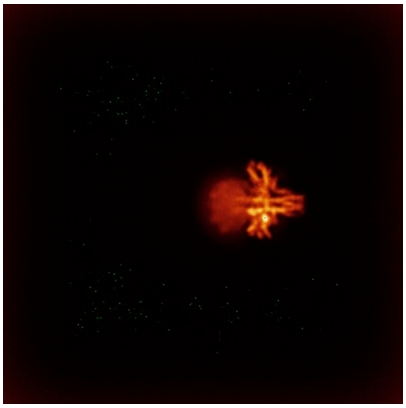


Z

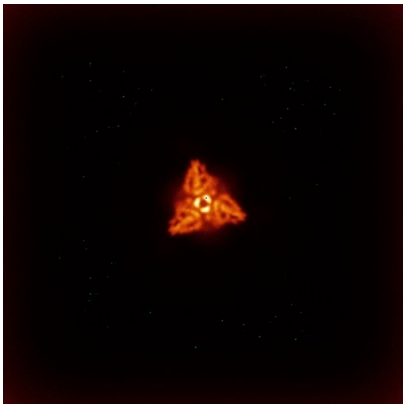
6.4.2 Raw map



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.

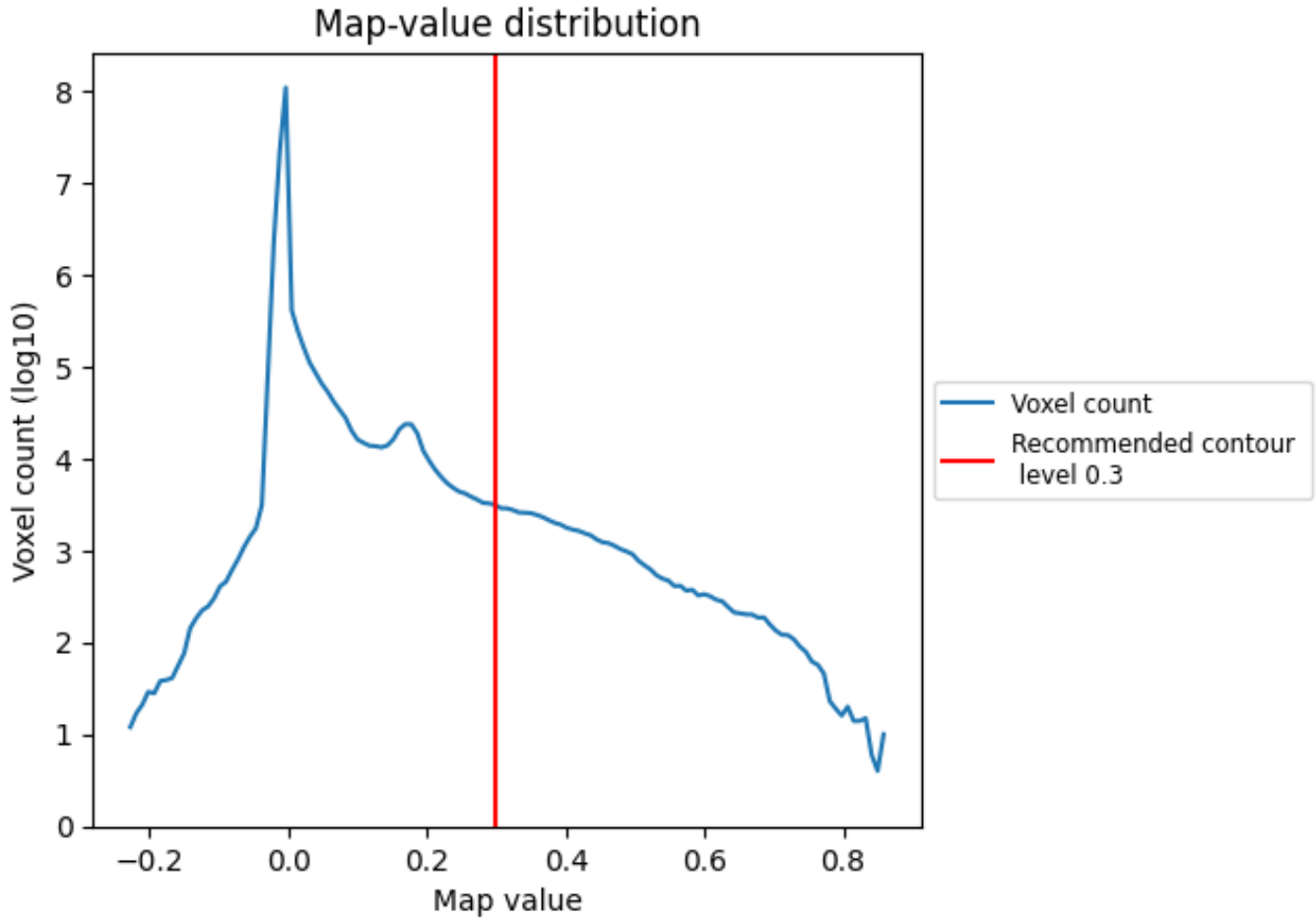
6.6 Mask visualisation (i)

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

7 Map analysis

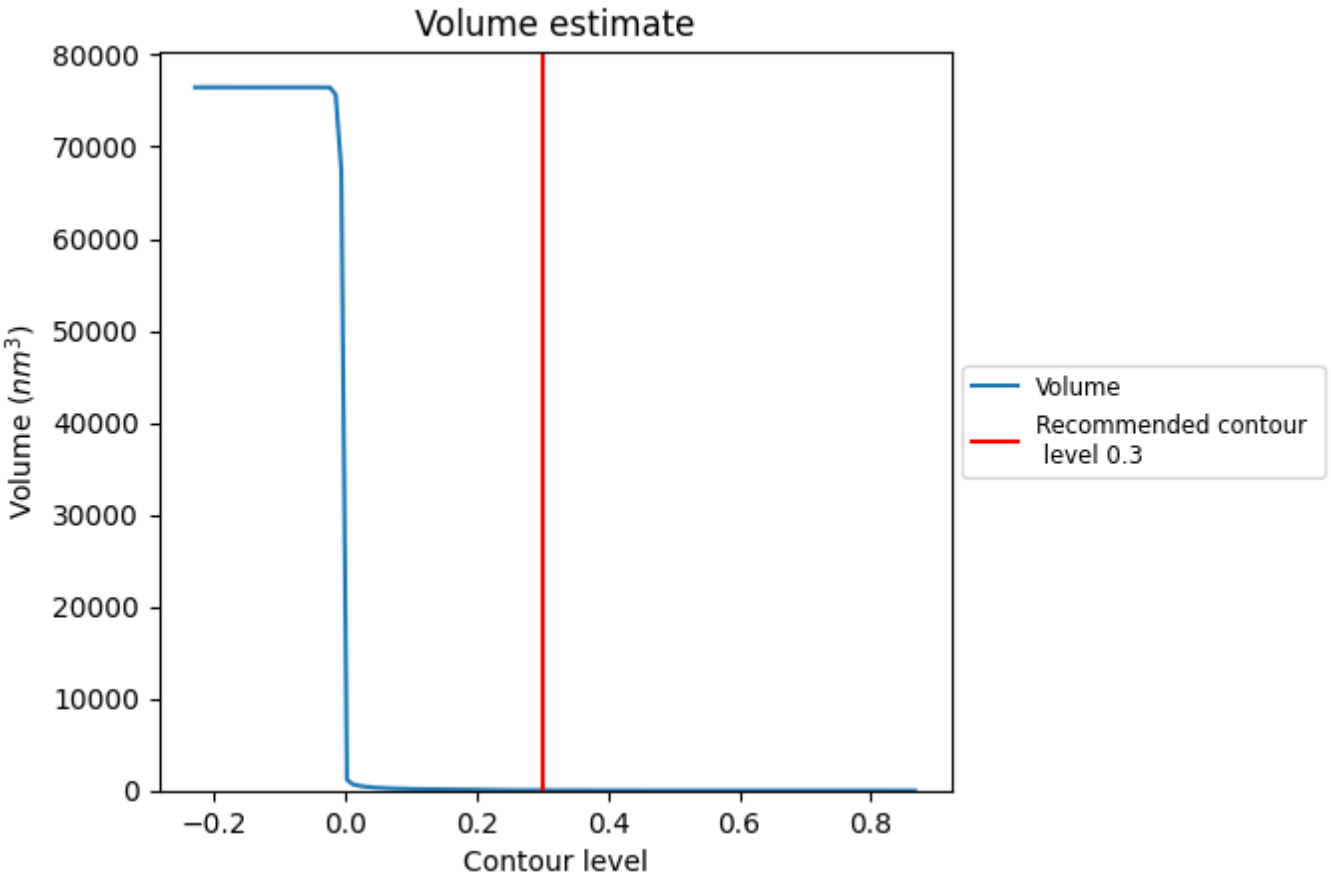
This section contains the results of statistical analysis of the map.

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.

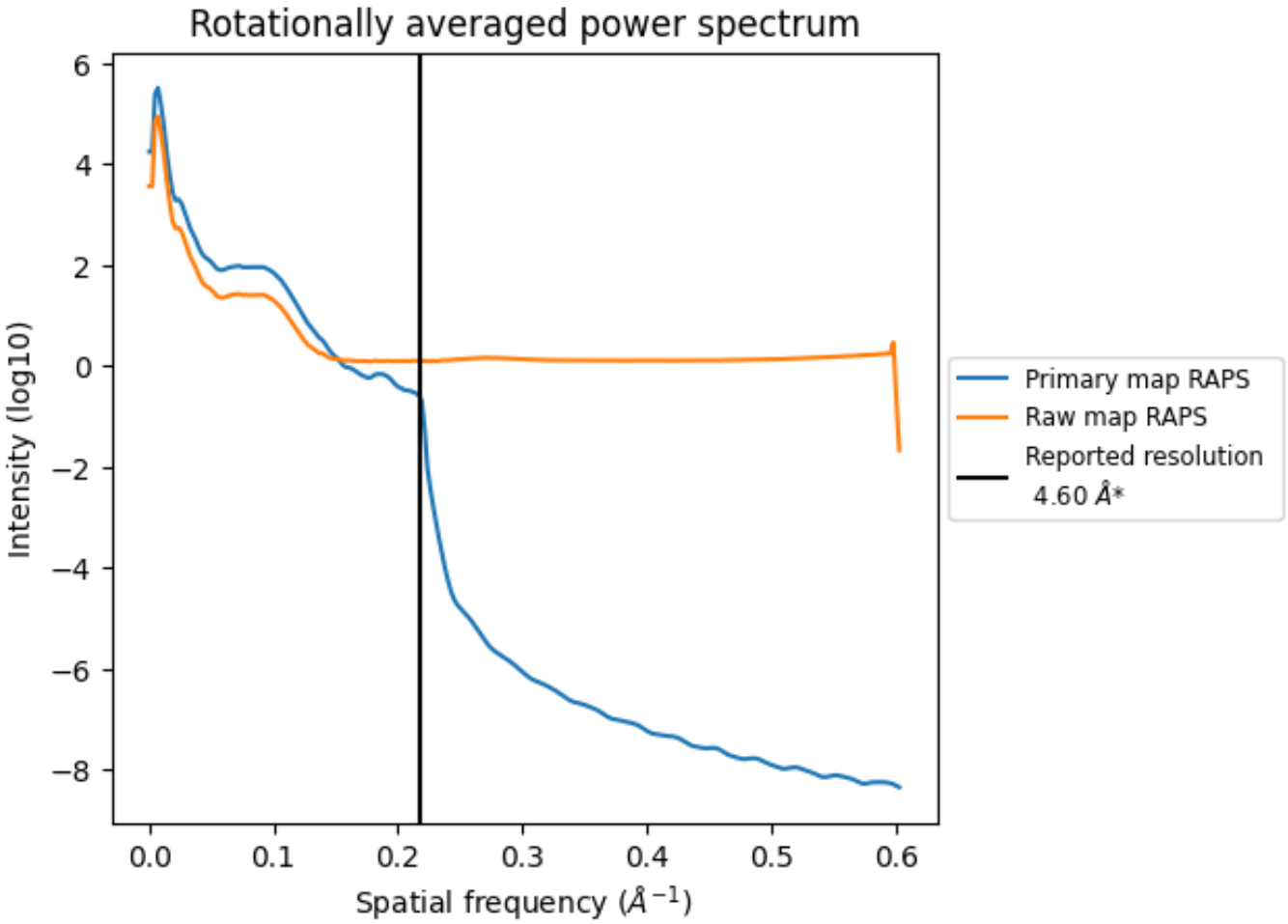
7.2 Volume estimate (i)



The volume at the recommended contour level is 31 nm^3; this corresponds to an approximate mass of 28 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)

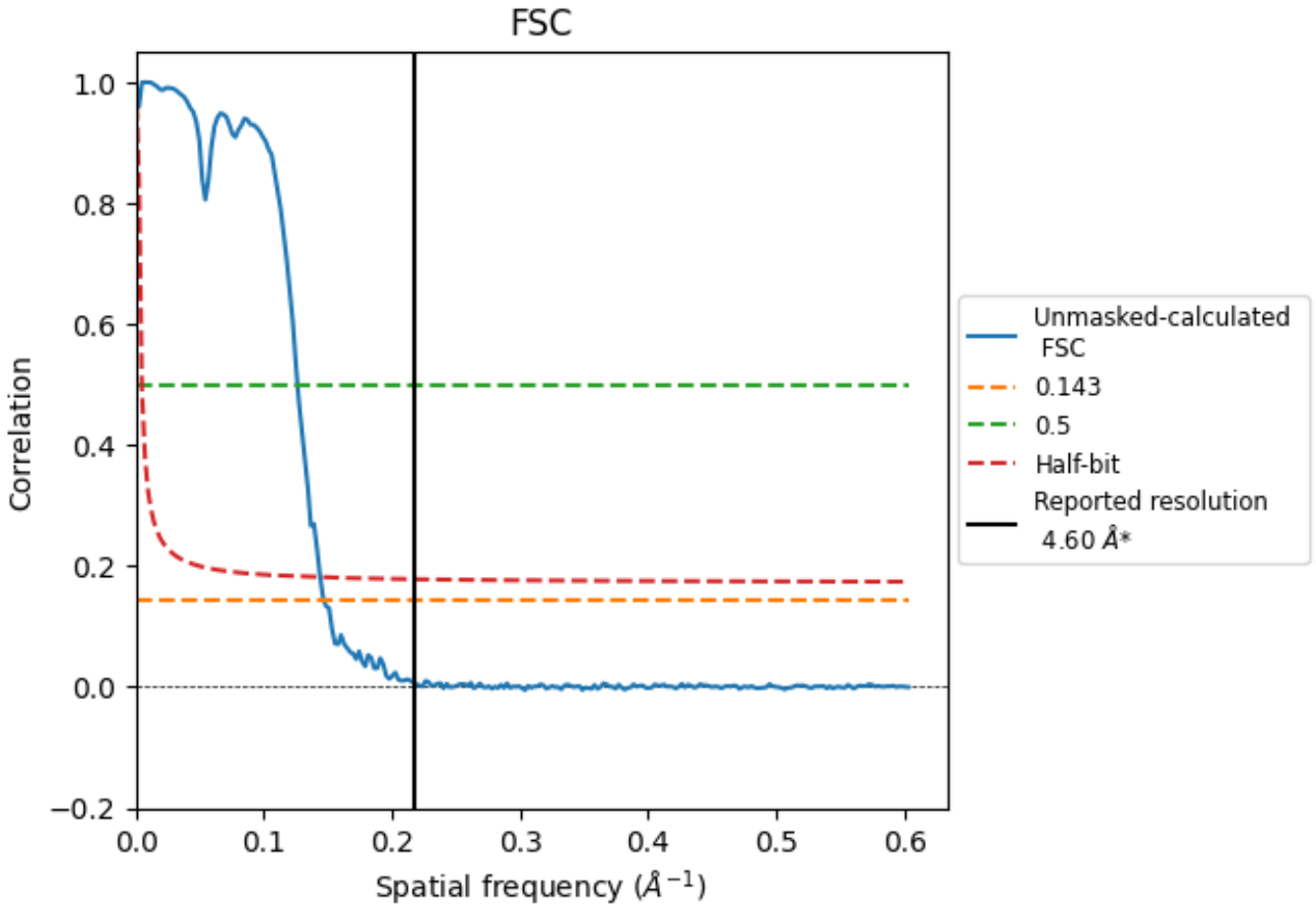


*Reported resolution corresponds to spatial frequency of 0.217 Å^{-1}

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 0.217 Å^{-1}

8.2 Resolution estimates (i)

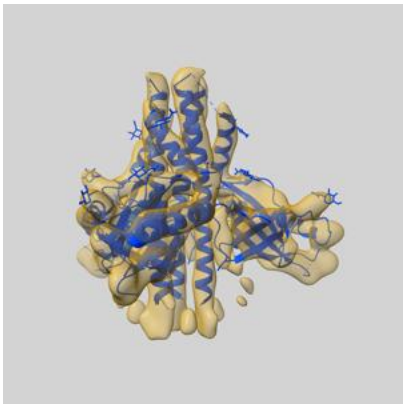
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.81	7.92	6.95

*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 6.81 differs from the reported value 4.6 by more than 10 %

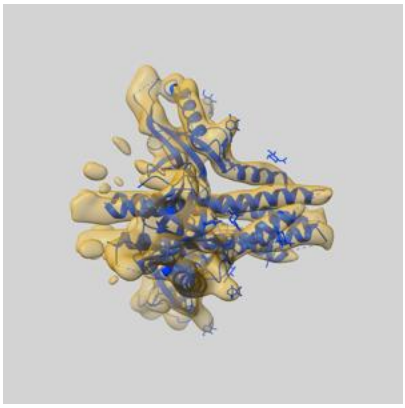
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-74936 and PDB model 9ZXV. Per-residue inclusion information can be found in section 3 on page 5.

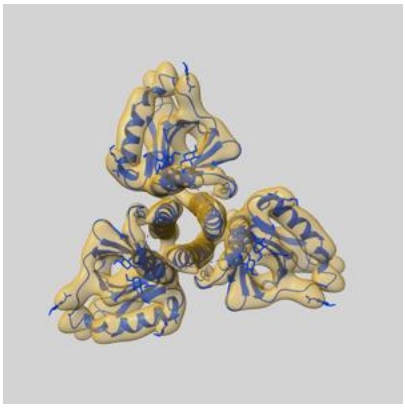
9.1 Map-model overlay



X



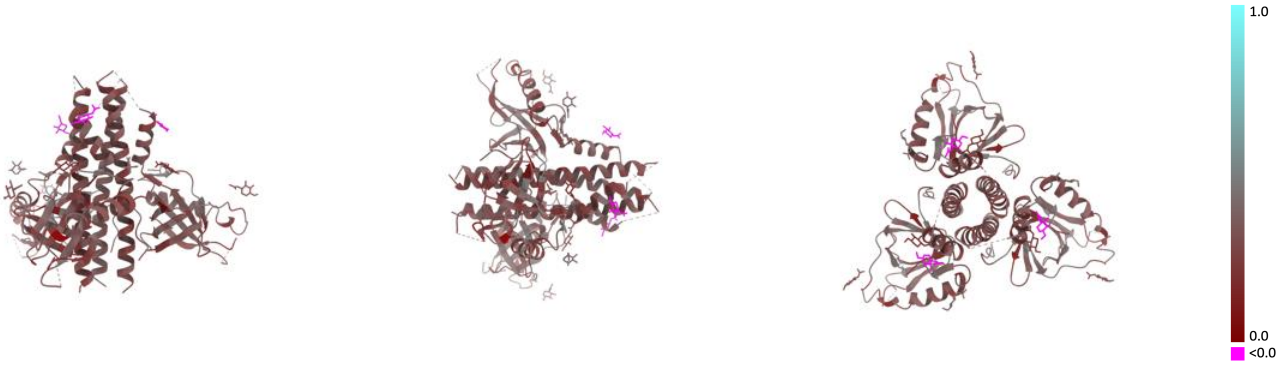
Y



Z

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

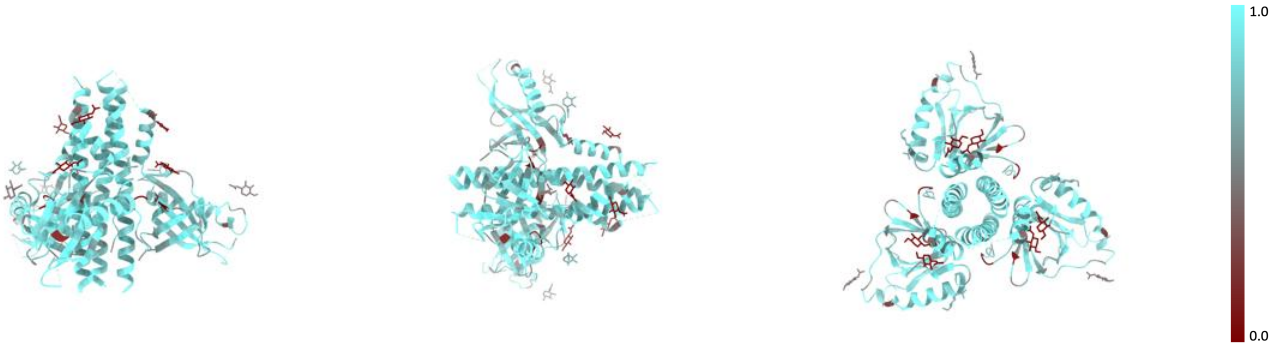
9.2 Q-score mapped to coordinate model (i)



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.

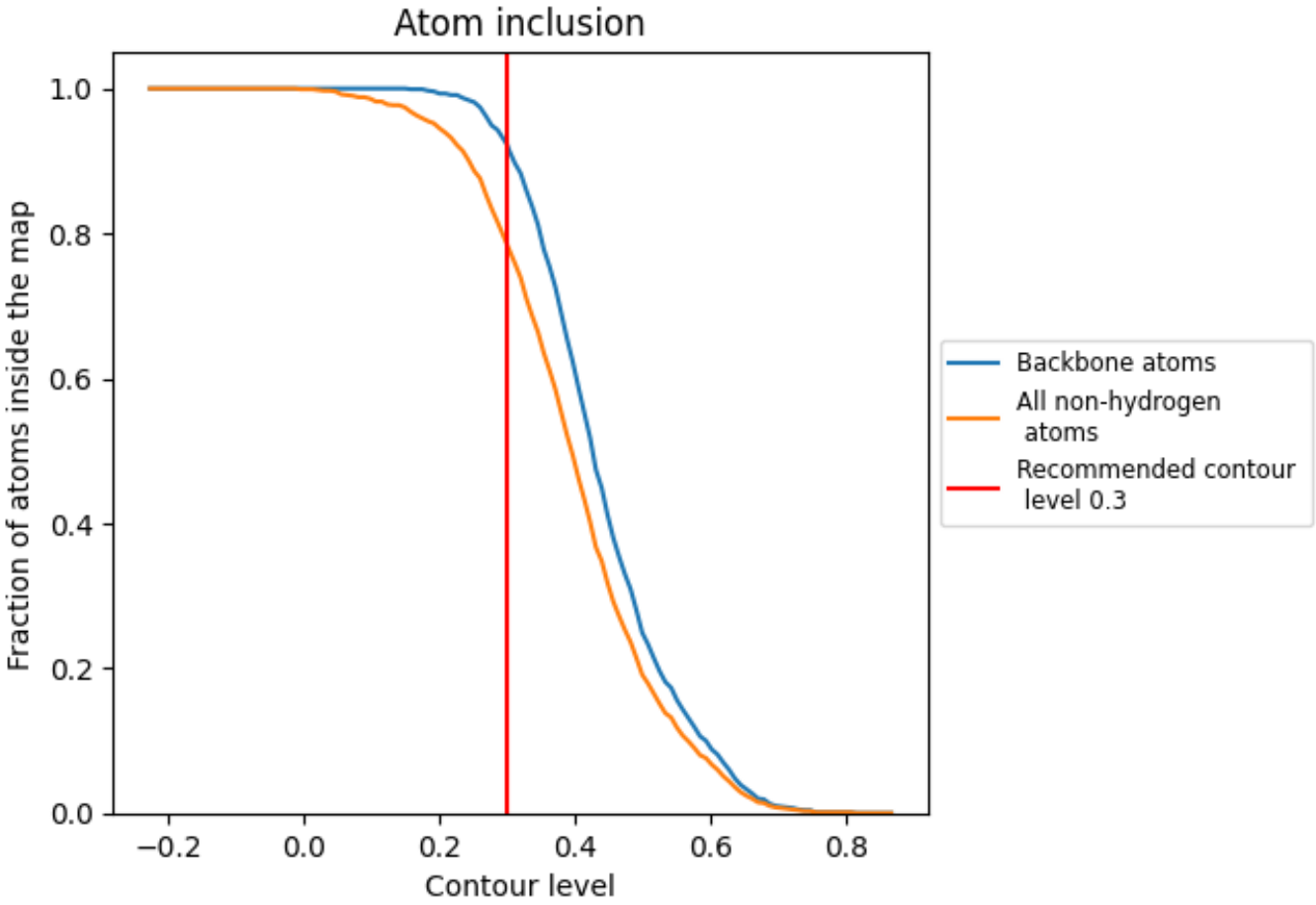
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 78% 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 (0.3) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.7840	0.3000
A	0.7830	0.2980
B	0.7840	0.3020
C	0.7840	0.2990