W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 07:21 pm GMT

PDB ID	:	7B09
EMDB ID	:	EMD-11964
Title	:	Puumala virus glycoprotein (Gc) in complex with fab fragment P-4G2.
Authors	:	Rissanen, I.; Stass, R.; Huiskonen, J.T.; Bowden, T.A.
Deposited on	:	2020-11-19
Resolution	:	13.40 Å(reported)

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

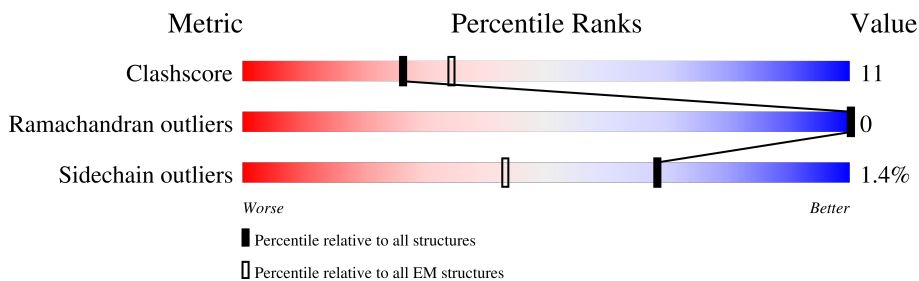|		
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 13.40 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	Percentile Ranks	Value
Clashscore		11
Ramachandran outliers		0
Sidechain outliers		1.4%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

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	H	231	16% / 76% 16% 8%
2	L	216	6% / 87% 12% ·
3	A	460	10% / 80% 11% 8%
4	B	367	10% / 80% 10% · 10%
5	C	2	50% / 50% 50%
6	E	4	75% / 100%

2   Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 9073 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 Heavy chain of fab fragment P-4G2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	212	Total 1607	C 1015	N 267	O 315	S 10	0	0

- Molecule 2 is a protein called Light chain of fab fragment P-4G2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	213	Total 1654	C 1039	N 279	O 329	S 7	0	0

- Molecule 3 is a protein called Envelope polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	422	Total 3203	C 2008	N 535	O 627	S 33	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	656	GLY	-	expression tag	UNP Q9WJ31
A	657	PRO	-	expression tag	UNP Q9WJ31
A	658	GLY	-	expression tag	UNP Q9WJ31
A	1106	GLY	-	expression tag	UNP Q9WJ31
A	1107	THR	-	expression tag	UNP Q9WJ31
A	1108	GLU	-	expression tag	UNP Q9WJ31
A	1109	THR	-	expression tag	UNP Q9WJ31
A	1110	SER	-	expression tag	UNP Q9WJ31
A	1111	GLN	-	expression tag	UNP Q9WJ31
A	1112	VAL	-	expression tag	UNP Q9WJ31
A	1113	ALA	-	expression tag	UNP Q9WJ31
A	1114	PRO	-	expression tag	UNP Q9WJ31
A	1115	ALA	-	expression tag	UNP Q9WJ31

- Molecule 4 is a protein called Envelope polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	331	2517	1599	409	488	21	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	26	GLU	-	expression tag	UNP Q9WJ31
B	27	THR	-	expression tag	UNP Q9WJ31
B	28	GLY	-	expression tag	UNP Q9WJ31
B	384	GLY	-	expression tag	UNP Q9WJ31
B	385	THR	-	expression tag	UNP Q9WJ31
B	386	LYS	-	expression tag	UNP Q9WJ31
B	387	HIS	-	expression tag	UNP Q9WJ31
B	388	HIS	-	expression tag	UNP Q9WJ31
B	389	HIS	-	expression tag	UNP Q9WJ31
B	390	HIS	-	expression tag	UNP Q9WJ31
B	391	HIS	-	expression tag	UNP Q9WJ31
B	392	HIS	-	expression tag	UNP Q9WJ31

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	C	2	28	16	2	10	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gluco pyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	E	4	50	28	2	20	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

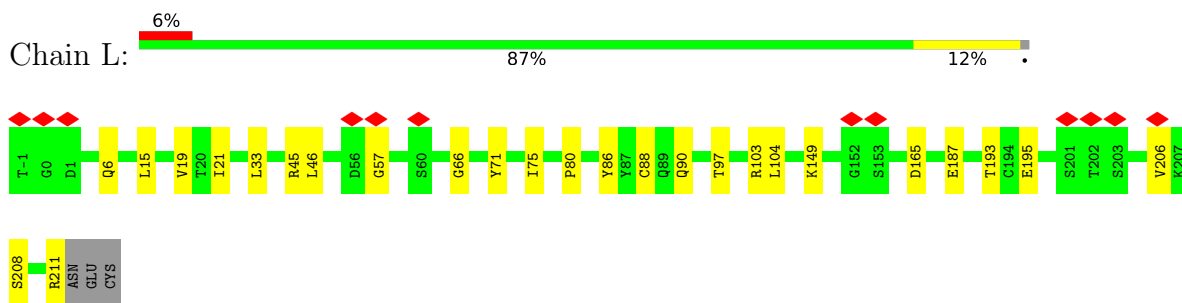| Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	14	8	1	5	0

3 Residue-property plots ⓘ

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: Heavy chain of fab fragment P-4G2
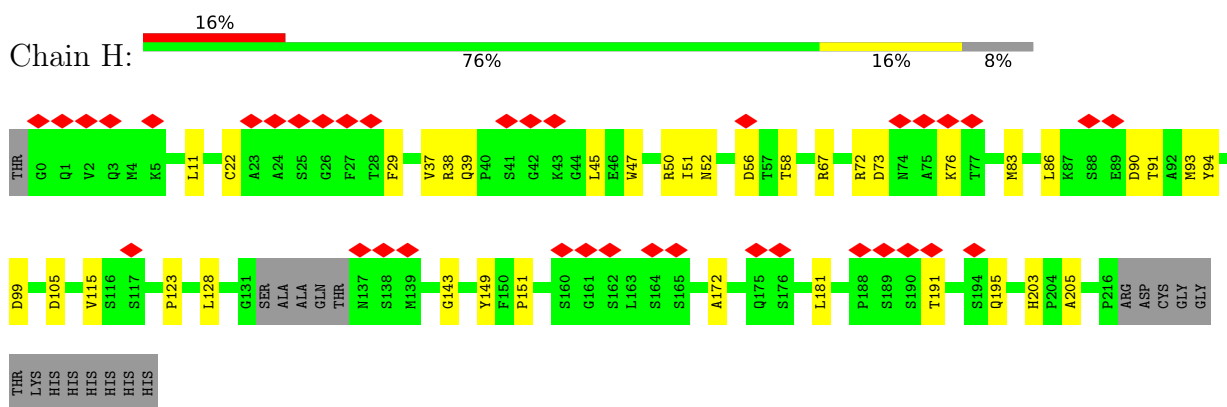
Chain H:

• Molecule 2: Light chain of fab fragment P-4G2

Chain L:

• Molecule 3: Envelope polyprotein

Chain A:

T939 E940 P941 H942 A945 I951 D952 P953 D954 S955 I961 V965 L969 E976 T986 S987 I988 D989 S994 G995 H1040 H1056 K1059 S1062 A1069 PRO HIS LEU ASP ARG VAL THR GLY TYR ASN GLN ALA D1082 S1083 D1084 E1093 I1096 W1099

F1100 T1101 LYS SER GLY GLU GLY THR GLU THR SER GLN VAL ALA PRO ALA
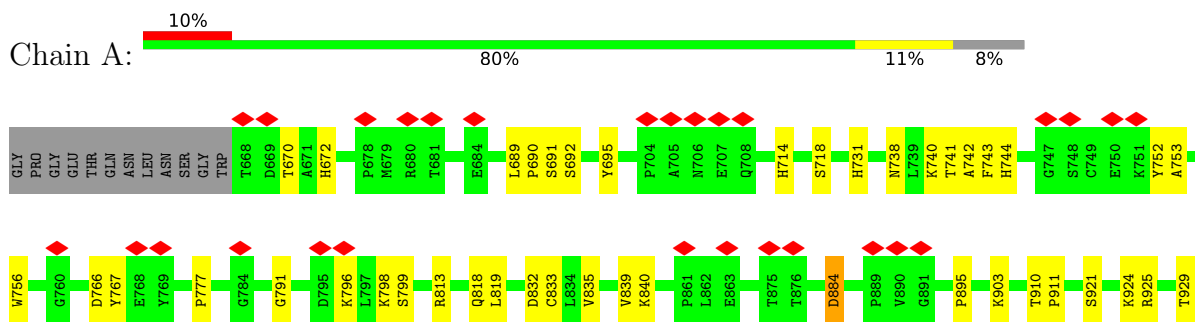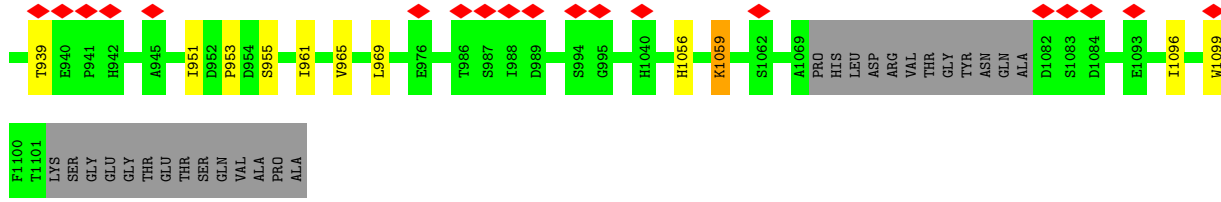
• Molecule 4: Envelope polyprotein

Chain B:

10%

80%   10%   •   10%

GLU T27 G28 E29 L30 K31 I32 E33 H36 G39 L40 G41 Q42 S48 V49 E50 L51 P52 K63 F70 Q80 S91 ASP LEU ALA GLU ASN THR GLN ALA SER SER T102 L113 R131 D171 Q172 R173 I174 Q175 V176 N177 Y178 E179 K180 T181 Y182 C183 L188

V189 E190 G191 V192 C193 S203 GLN PRO SER HIS THR Y209 D210 I211 V212 T213 V214 K224 V225 S226 T227 V241 Q242 K243 T244 S245 Y255 L258 V259 G260 S261 S262 S263 E264 I268 P269 L280 S281 R282 D291 HIS ASP VAL GLU LYS ASN ALA ILE SER A301 M302 R303

I304 I305 G306 K307 S317 S318 L331 Y332 L338 I347 F373 I380 E381 LYS THR GLY THR LYS HIS HIS HIS HIS HIS HIS

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

50%

50%   50%

NAG1 NAG2

• Molecule 6: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

75%

100%

NAG1 NAG2 BMA3 MAN4
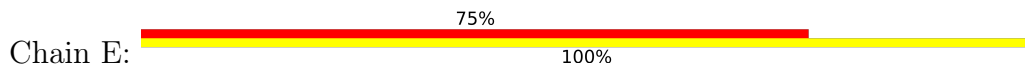
4　Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of subtomograms used	1721	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	4.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.063	Depositor
Minimum map value	-3.815	Depositor
Average map value	-0.042	Depositor
Map value standard deviation	0.497	Depositor
Recommended contour level	1.19	Depositor
Map size (Å)	429.44, 429.44, 429.44	wwPDB
Map dimensions	122, 122, 122	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.52, 3.52, 3.52	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	H	0.24	0/1649	0.44	0/2248
2	L	0.24	0/1694	0.46	0/2302
3	A	0.24	0/3276	0.44	0/4441
4	B	0.60	0/2567	0.80	3/3488 (0.1%)
All	All	0.38	0/9186	0.57	3/12479 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	282	ARG	NE-CZ-NH1	10.00	125.30	120.30
4	B	282	ARG	NE-CZ-NH2	-5.65	117.47	120.30
4	B	131	ARG	NE-CZ-NH1	5.58	123.09	120.30

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	H	1607	0	1567	20	0
2	L	1654	0	1605	14	0
3	A	3203	0	3061	151	0
4	B	2517	0	2509	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	28	0	25	5	0
6	E	50	0	43	0	0
7	A	14	0	13	0	0
All	All	9073	0	8823	198	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 11.

The worst 5 of 198 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)
3:A:752:TYR:CD1	4:B:307:LYS:HE3	1.30	1.64
3:A:910:THR:HB	4:B:303:ARG:CD	1.30	1.56
3:A:777:PRO:CG	4:B:303:ARG:HH22	1.12	1.54
3:A:798:LYS:HE2	4:B:213:THR:CG2	1.10	1.52
3:A:740:LYS:NZ	4:B:302:MET:HE1	1.25	1.49

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	H	208/231 (90%)	191 (92%)	17 (8%)	0	100	100
2	L	211/216 (98%)	200 (95%)	11 (5%)	0	100	100
3	A	418/460 (91%)	404 (97%)	14 (3%)	0	100	100
4	B	323/367 (88%)	316 (98%)	7 (2%)	0	100	100
All	All	1160/1274 (91%)	1111 (96%)	49 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	H	183/198 (92%)	182 (100%)	1 (0%)	88	93
2	L	187/190 (98%)	187 (100%)	0	100	100
3	A	361/390 (93%)	358 (99%)	3 (1%)	81	89
4	B	291/323 (90%)	281 (97%)	10 (3%)	37	60
All	All	1022/1101 (93%)	1008 (99%)	14 (1%)	68	80

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	173	ARG
4	B	209	TYR
4	B	291	ASP
4	B	258	LEU
4	B	282	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	90	GLN
3	A	731	HIS
3	A	744	HIS
3	A	864	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 ⓘ

6 monosaccharides 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	#$|Z| > 2$
5	NAG	C	1	5,4	14,14,15	0.37	0	17,19,21	1.61	4 (23%)
5	NAG	C	2	5	14,14,15	0.44	0	17,19,21	1.08	1 (5%)
6	NAG	E	1	6,4	14,14,15	0.41	0	17,19,21	1.39	3 (17%)
6	NAG	E	2	6	14,14,15	0.56	0	17,19,21	1.45	1 (5%)
6	BMA	E	3	6	11,11,12	0.67	0	15,15,17	1.51	5 (33%)
6	MAN	E	4	6	11,11,12	0.85	1 (9%)	15,15,17	2.35	3 (20%)

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
5	NAG	C	1	5,4	-	2/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
6	NAG	E	1	6,4	-	2/6/23/26	0/1/1/1
6	NAG	E	2	6	-	2/6/23/26	0/1/1/1
6	BMA	E	3	6	-	1/2/19/22	0/1/1/1
6	MAN	E	4	6	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	4	MAN	C4-C5	2.04	1.57	1.53

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	4	MAN	C1-O5-C5	7.63	122.53	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	2	NAG	C1-C2-N2	-4.65	102.54	110.49
5	C	2	NAG	C1-O5-C5	3.64	117.12	112.19
5	C	1	NAG	C1-O5-C5	3.50	116.94	112.19
6	E	1	NAG	O4-C4-C3	-3.15	103.06	110.35

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	2	NAG	O5-C5-C6-O6
5	C	1	NAG	C8-C7-N2-C2
5	C	1	NAG	O7-C7-N2-C2
6	E	3	BMA	O5-C5-C6-O6
6	E	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1	NAG	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings
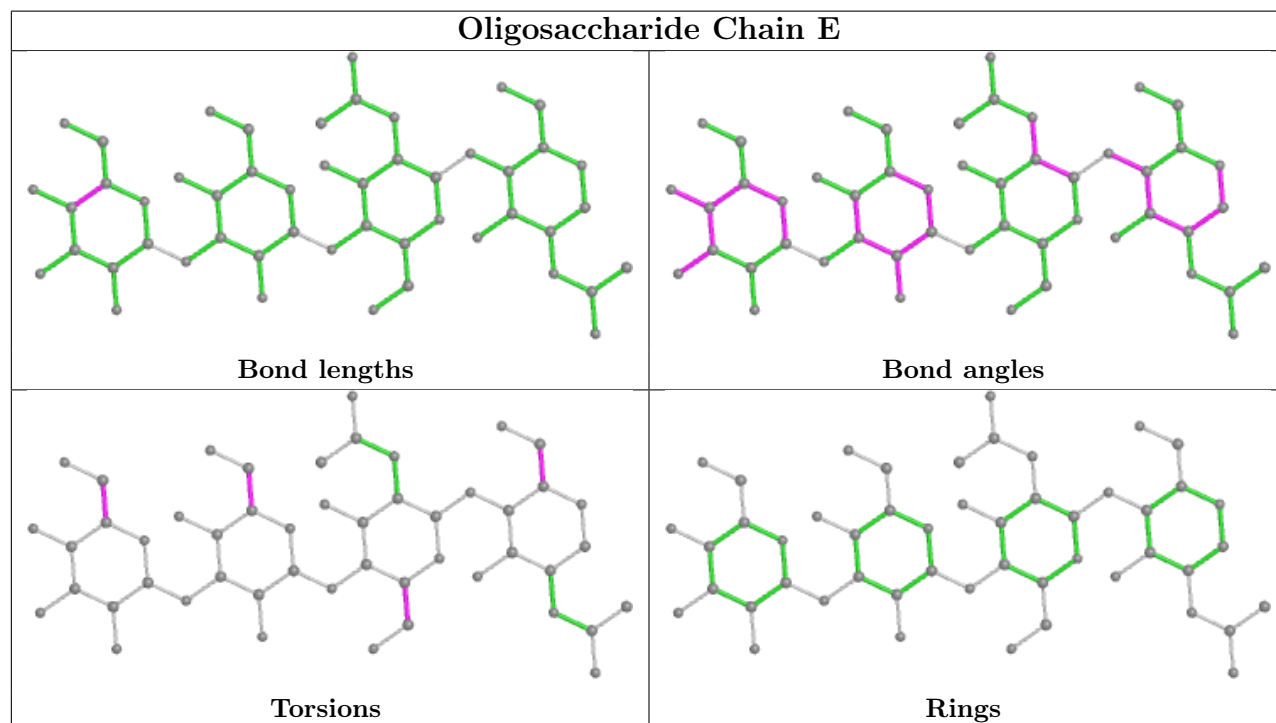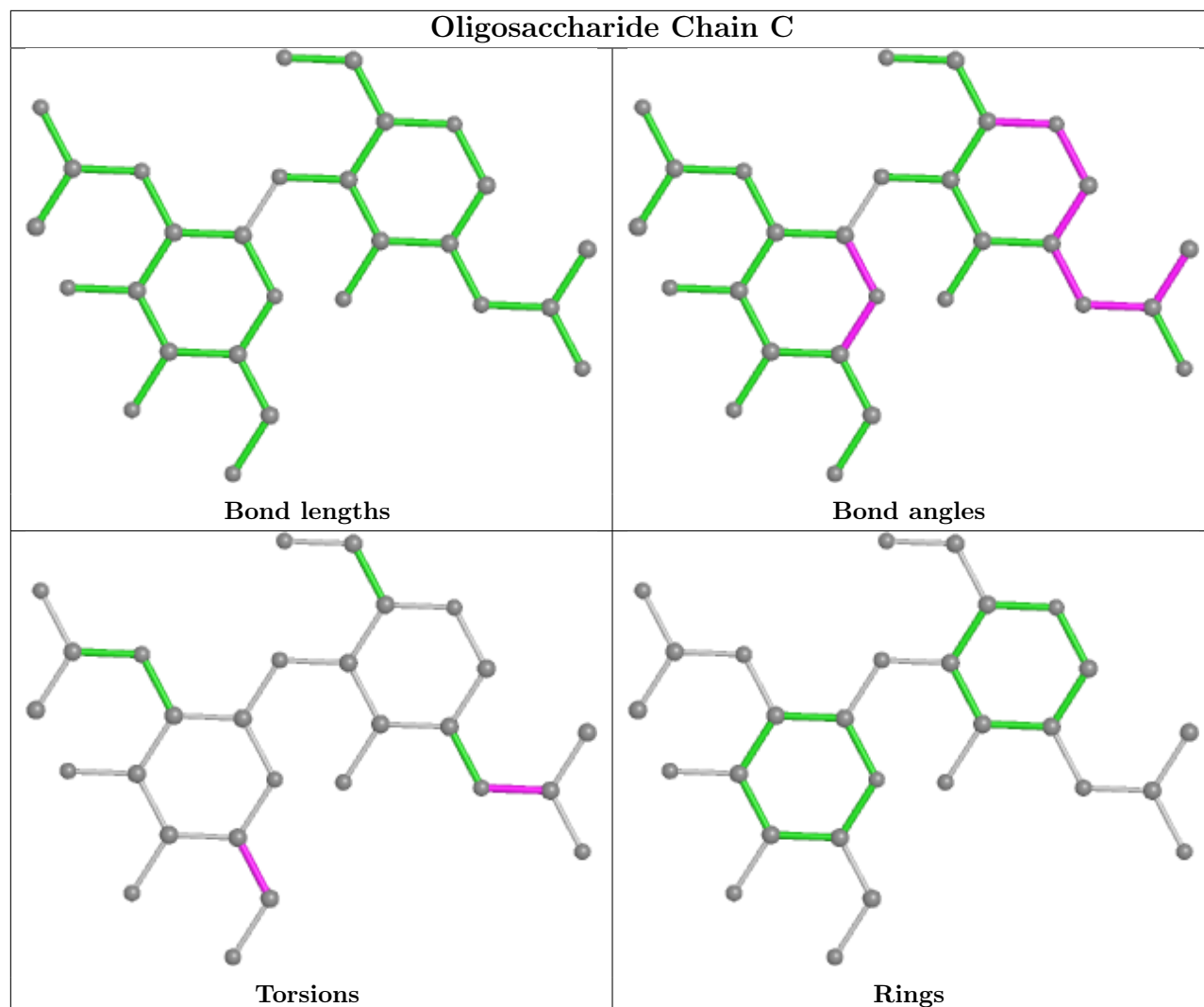
5.6 Ligand geometry (i)

1 ligand is 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	$\#|Z| > 2$
7	NAG	A	1201	3	14,14,15	0.24	0	17,19,21	0.44	0

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
7	NAG	A	1201	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1201	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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-11964. 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 ⓘ
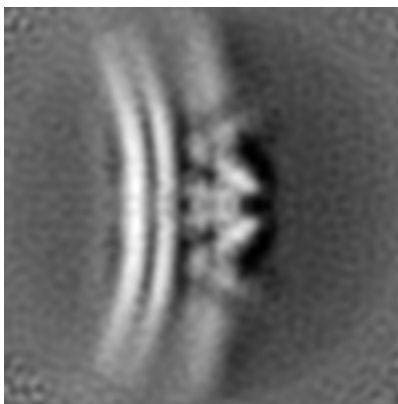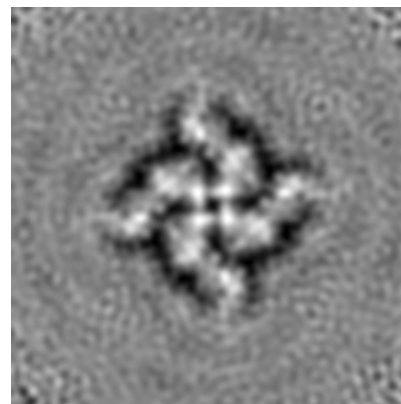
6.1.1   Primary map

X   Y   Z

6.1.2   Raw map

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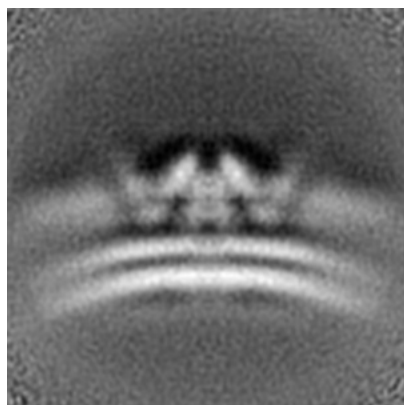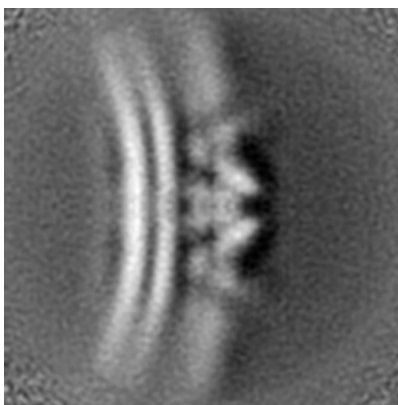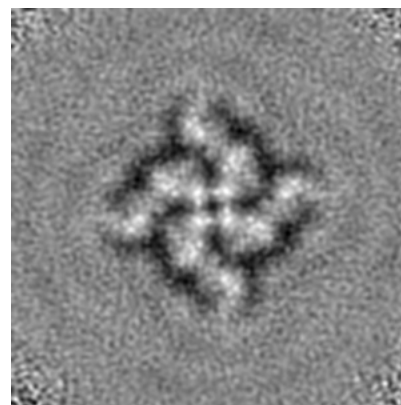
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
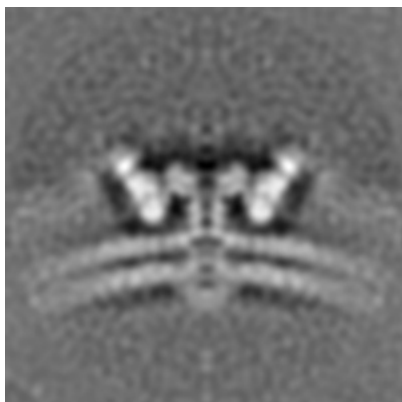
6.2.1   Primary map
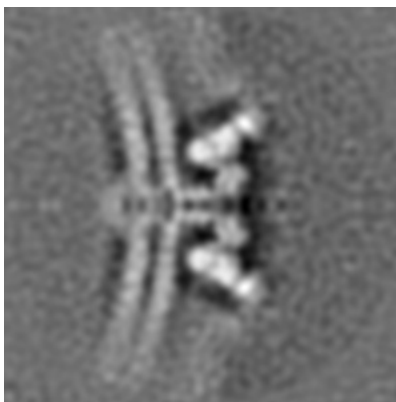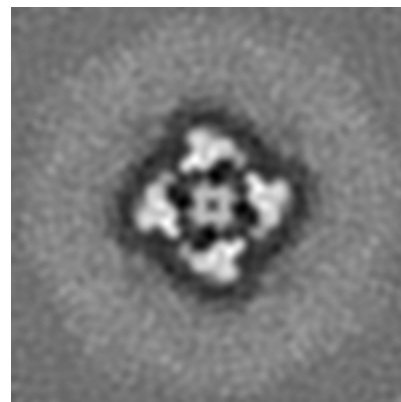
X Index: 61   Y Index: 61   Z Index: 61

6.2.2   Raw map
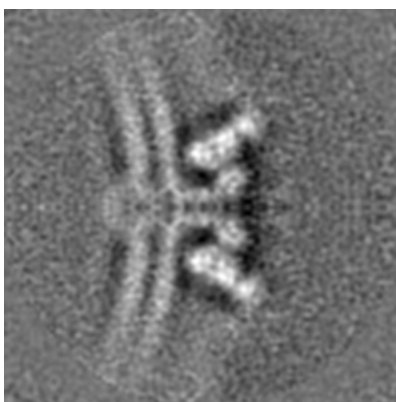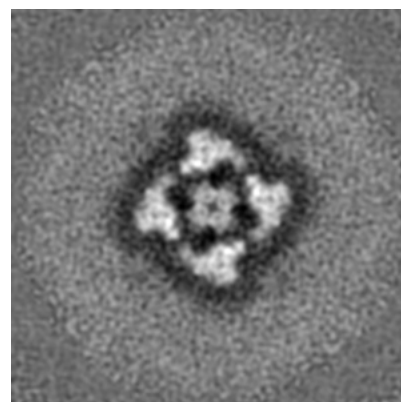
X Index: 61   Y Index: 61   Z Index: 61

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

6.3   Largest variance slices ⓘ

6.3.1   Primary map
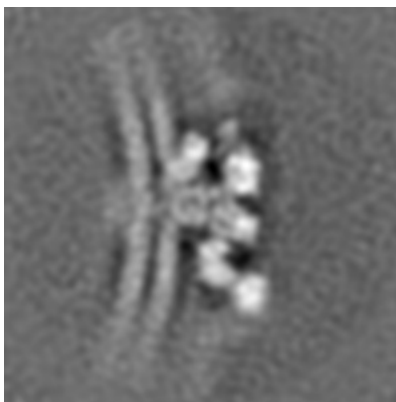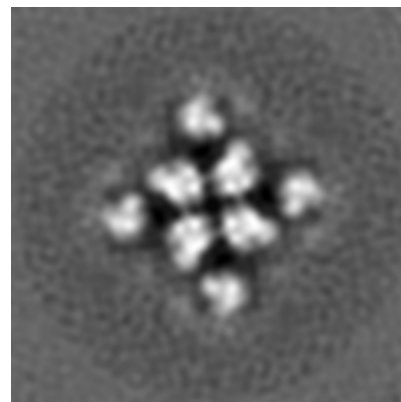
| X Index: 66 | Y Index: 56 | Z Index: 73 |

6.3.2   Raw map
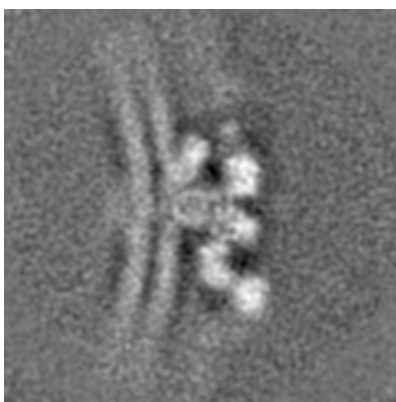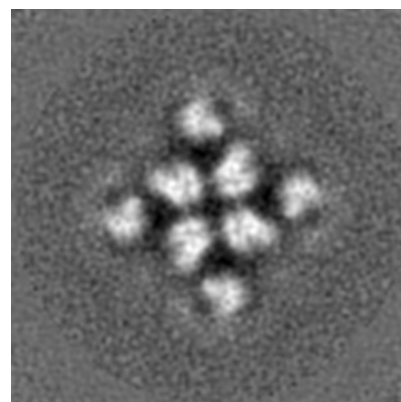
| X Index: 56 | Y Index: 56 | Z Index: 73 |

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

X   Y   Z

The images above show the 3D surface view of the map at the recommended contour level 1.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X   Y   Z
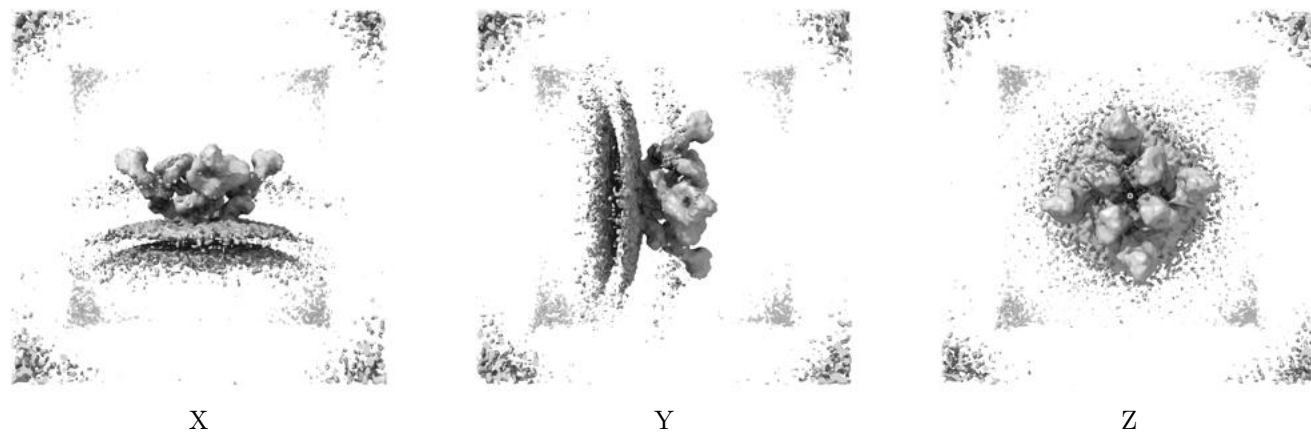
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 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

6.5.1 emd_11964_msk_1.map (i)

X   Y   Z
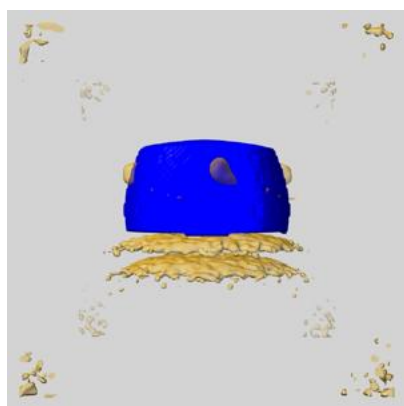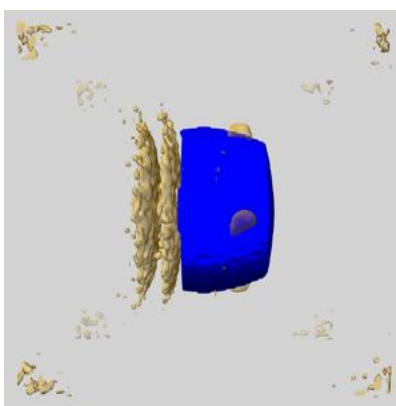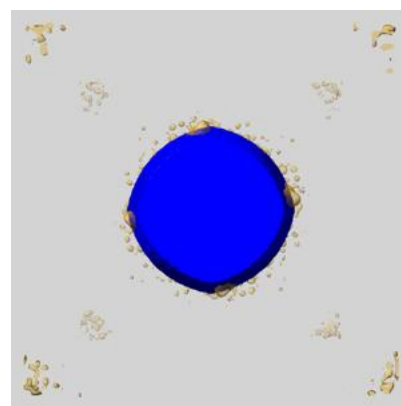
7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ
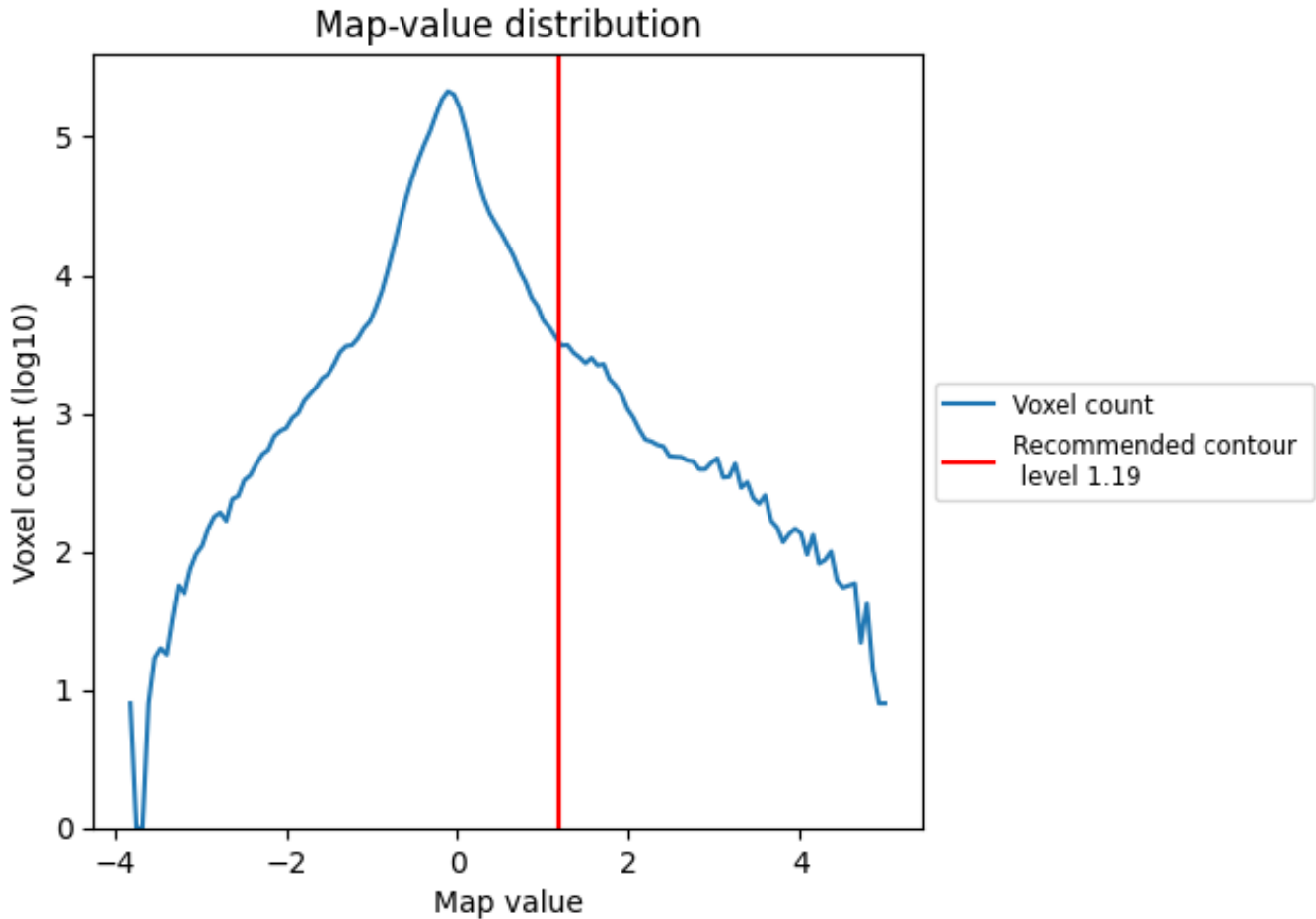
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
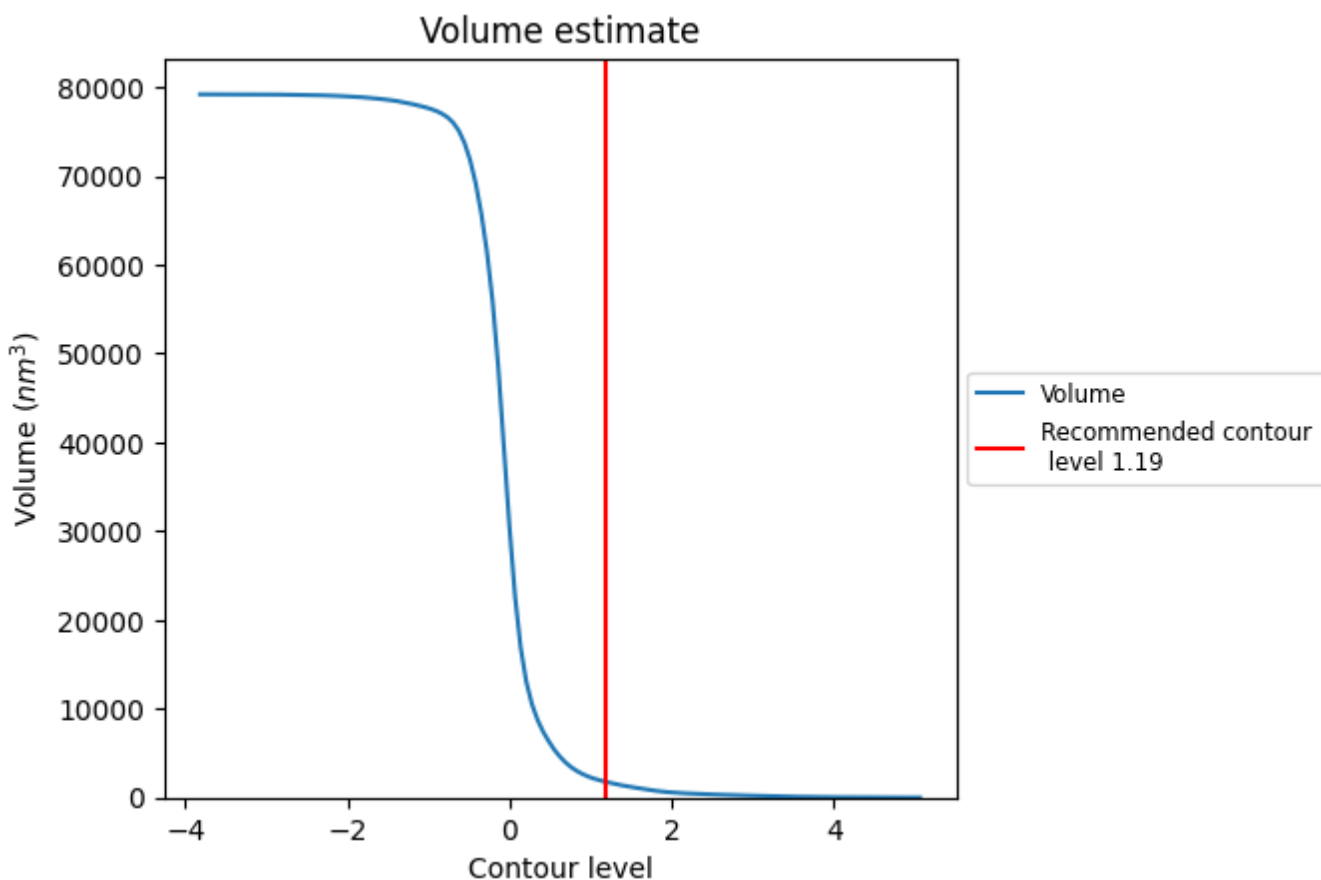
The volume at the recommended contour level is 1760 nm^3; this corresponds to an approximate mass of 1590 kDa.

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 ⓘ
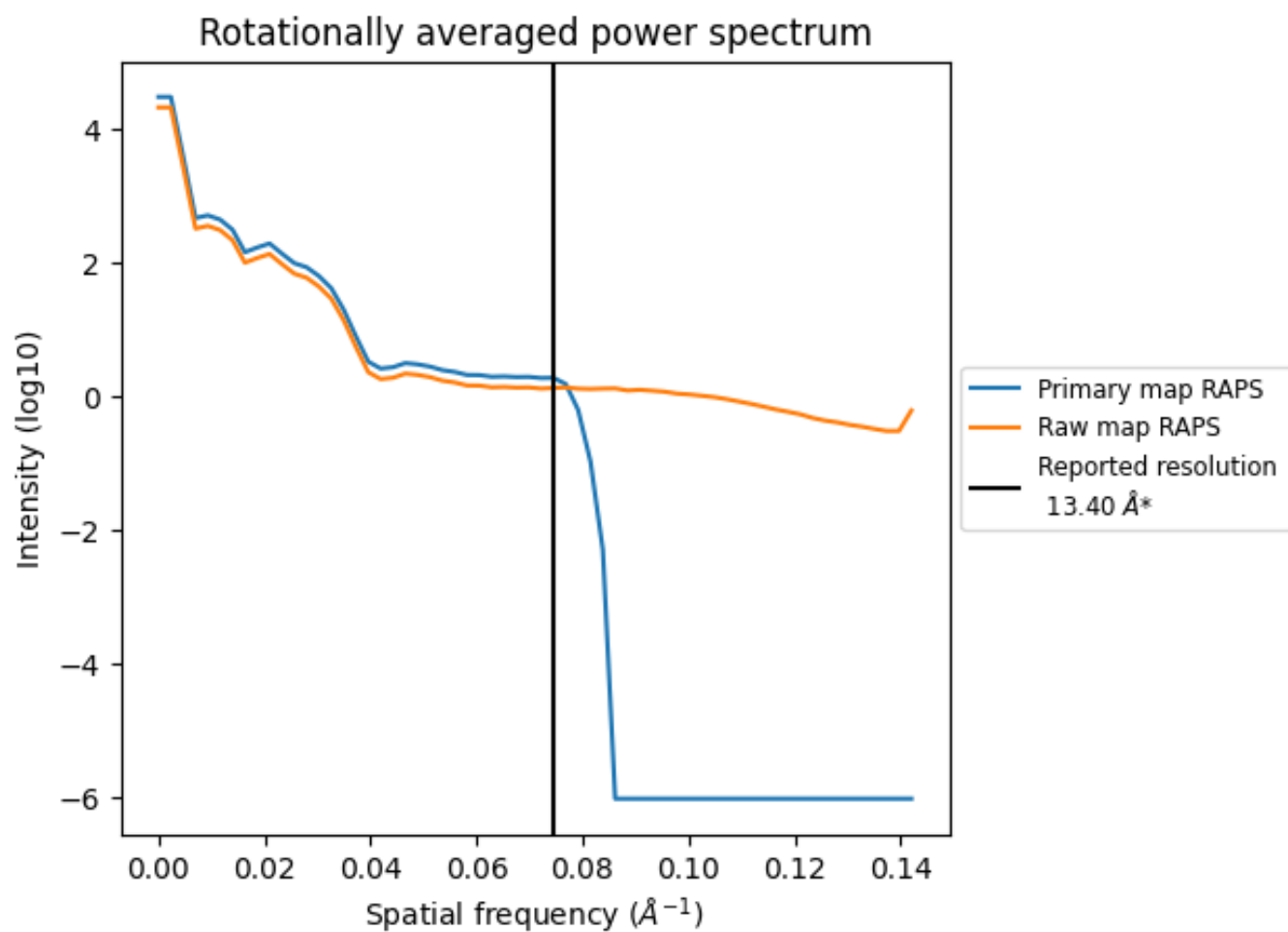
*Reported resolution corresponds to spatial frequency of 0.075 Å^{-1}

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 ⓘ
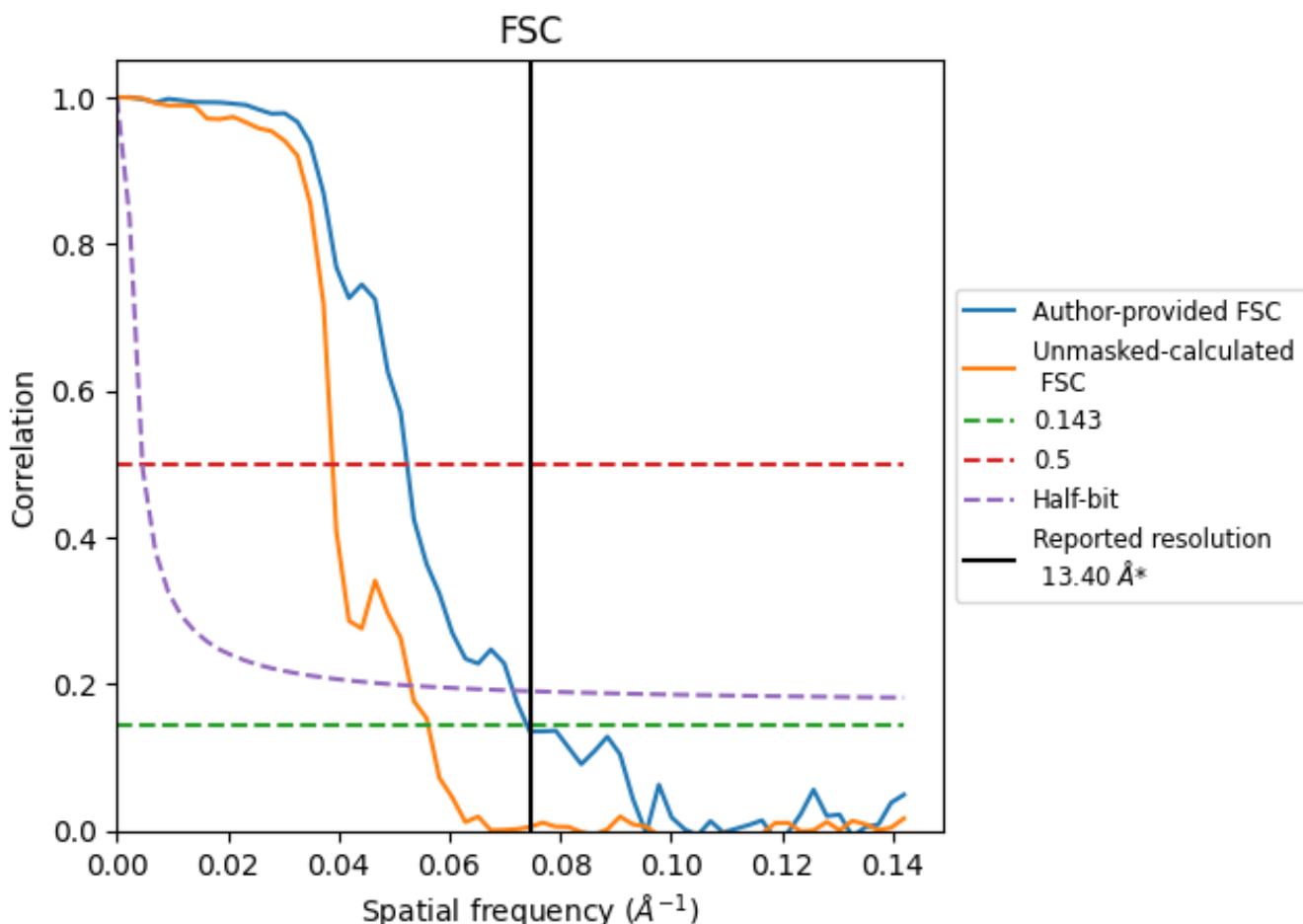
*Reported resolution corresponds to spatial frequency of 0.075 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	13.40	-	-
Author-provided FSC curve	13.51	19.08	13.99
Unmasked-calculated*	17.79	25.71	18.87

*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 17.79 differs from the reported value 13.4 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-11964 and PDB model 7B09. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay ⓘ

X   Y   Z
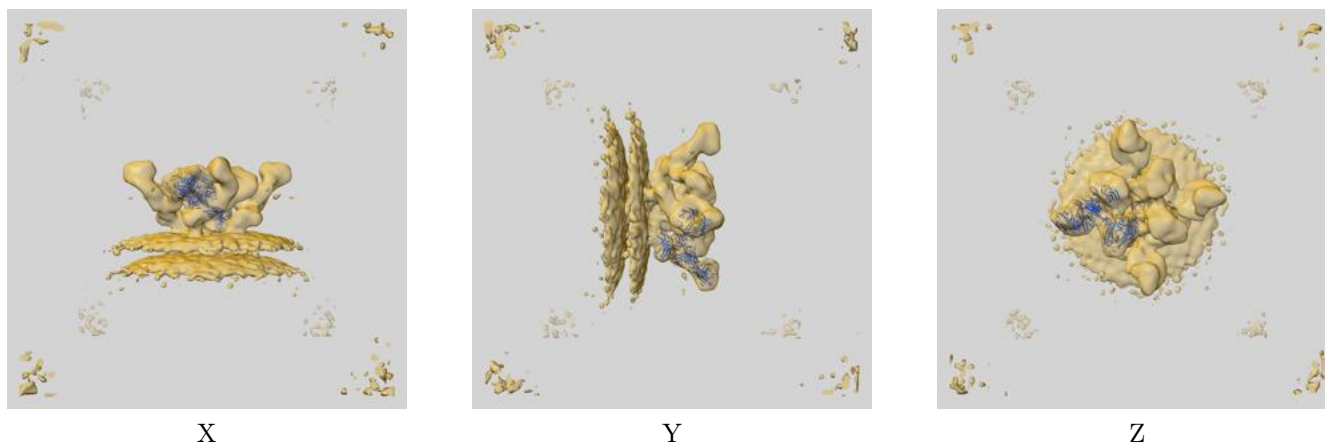
The images above show the 3D surface view of the map at the recommended contour level 1.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

X Y Z
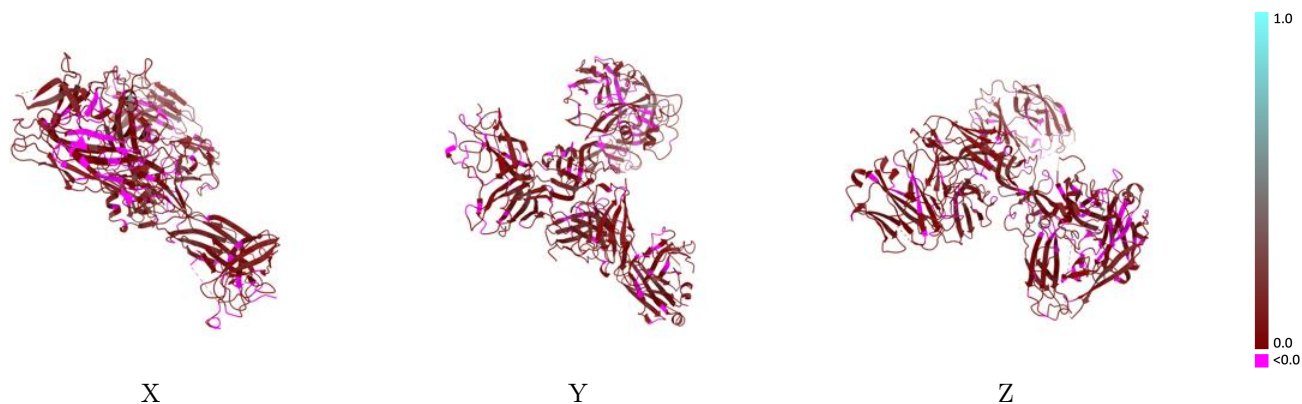
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
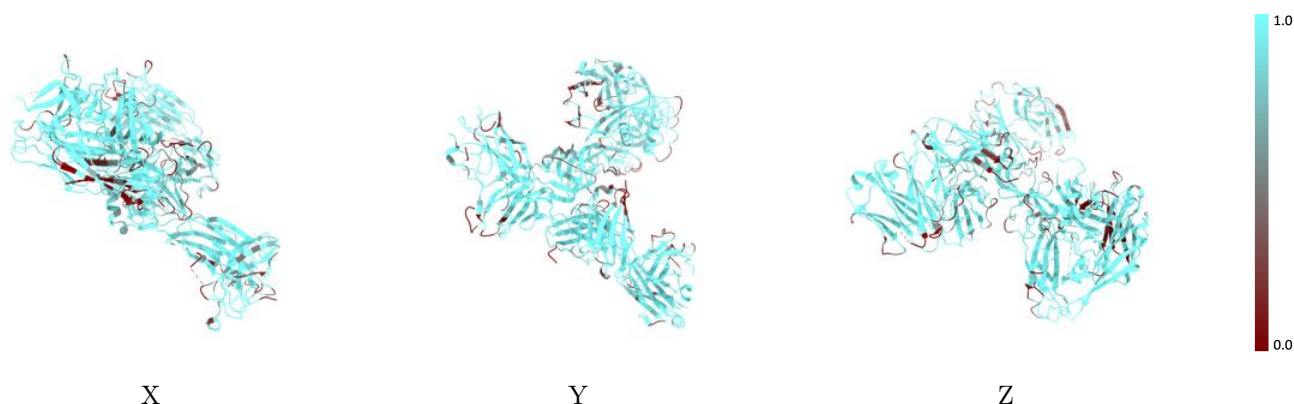
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.19).

9.4   Atom inclusion ⓘ
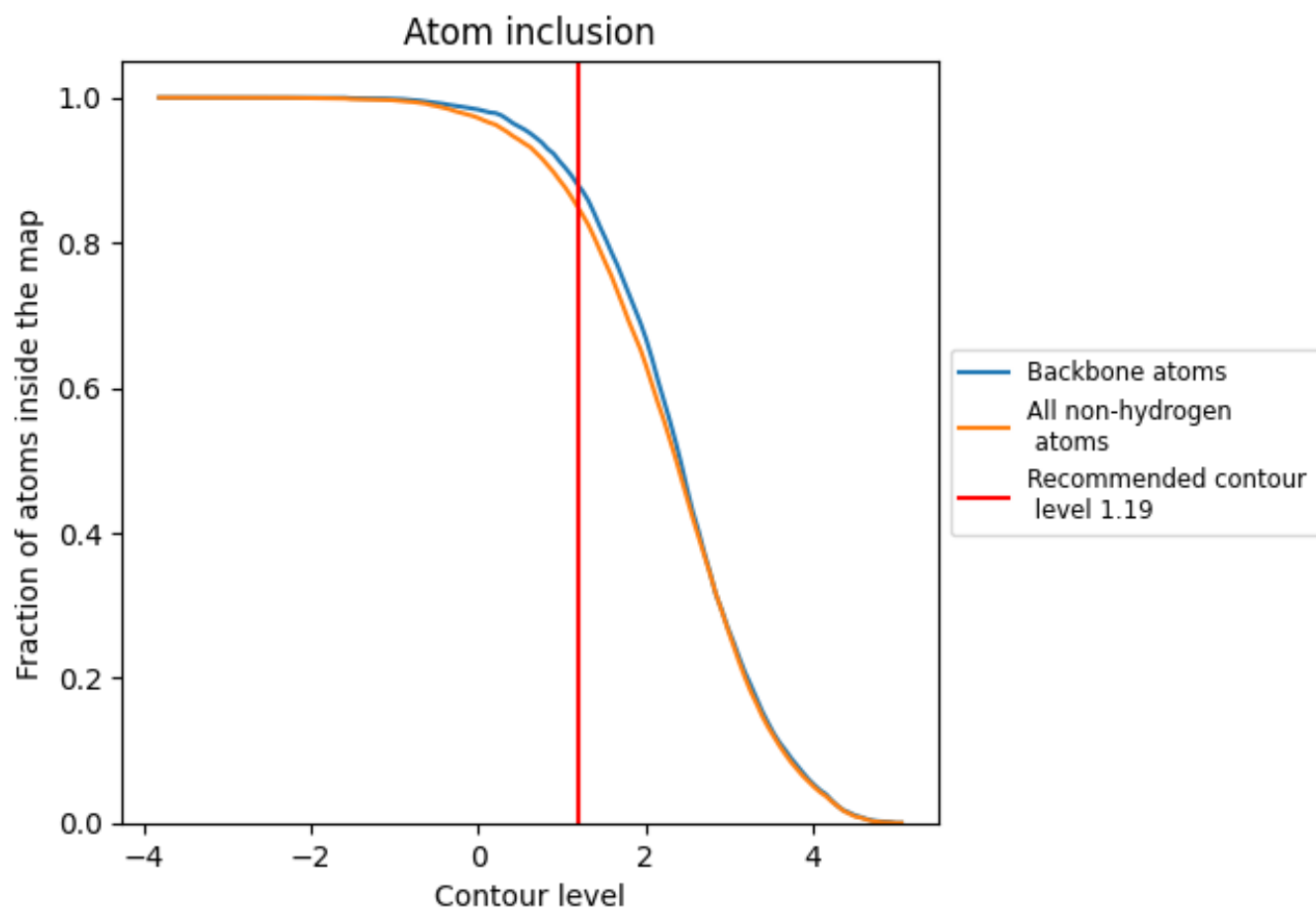
At the recommended contour level, 88% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5　Map-model fit summary　ⓘ

The table lists the average atom inclusion at the recommended contour level (1.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8495	0.0770
A	0.8427	0.0810
B	0.8477	0.0730
C	0.6786	0.1220
E	0.3000	0.0150
H	0.8071	0.0710
L	0.9267	0.0860

1.0

0.0
<0.0