



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:05 AM UTC

PDB ID : 7SOC / pdb_00007soc
EMDB ID : EMD-25266
Title : SARS-CoV-2 S RBD B.1.617.1 kappa variant S309 Local Refinement
Authors : McCallum, M.; Veessler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2021-10-29
Resolution : 3.30 Å(reported)

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

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<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.dev132
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) : 2.49

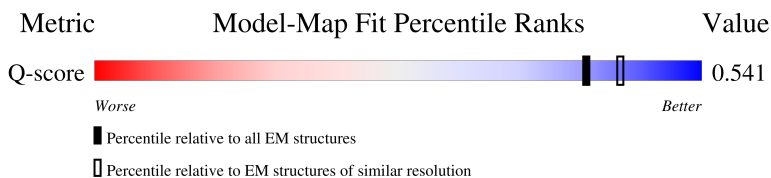
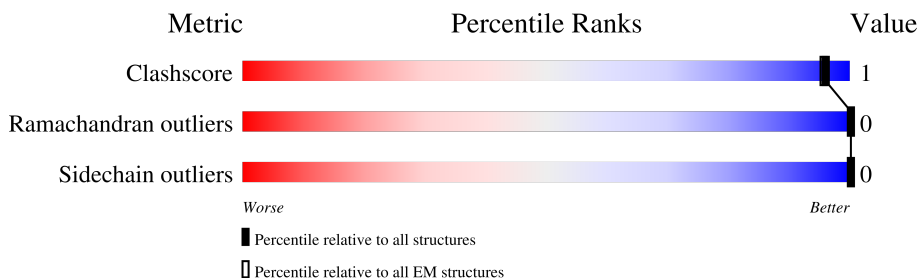
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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 $\leq 5\%$. 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	1277	 15% 84%
2	H	129	 98%
3	L	104	 91% 9%
4	B	6	 33% 50% 17%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3448 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	200	Total	C	N	O	S	0	0
			1589	1019	268	293	9		

There are 85 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	ILE	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	154	LYS	GLU	variant	UNP P0DTC2
A	383	CYS	SER	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	484	GLN	GLU	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	681	ARG	PRO	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	985	CYS	ASP	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1071	HIS	GLN	variant	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	GLY	-	expression tag	UNP P0DTC2
A	1252	GLY	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	ASN	-	expression tag	UNP P0DTC2
A	1255	ASP	-	expression tag	UNP P0DTC2
A	1256	ILE	-	expression tag	UNP P0DTC2
A	1257	PHE	-	expression tag	UNP P0DTC2
A	1258	GLU	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	GLN	-	expression tag	UNP P0DTC2
A	1261	LYS	-	expression tag	UNP P0DTC2
A	1262	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1263	GLU	-	expression tag	UNP P0DTC2
A	1264	TRP	-	expression tag	UNP P0DTC2
A	1265	HIS	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	HIS	-	expression tag	UNP P0DTC2
A	1271	HIS	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	HIS	-	expression tag	UNP P0DTC2
A	1274	HIS	-	expression tag	UNP P0DTC2
A	1275	HIS	-	expression tag	UNP P0DTC2
A	1276	HIS	-	expression tag	UNP P0DTC2
A	1277	HIS	-	expression tag	UNP P0DTC2

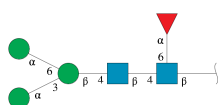
- Molecule 2 is a protein called S309 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	129	Total	C	N	O	S	0	0
			996	625	172	194	5		

- Molecule 3 is a protein called S309 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	104	Total	C	N	O	S	0	0
			778	484	134	158	2		

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	B	6	Total	C	N	O	0	0
			71	40	2	29		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

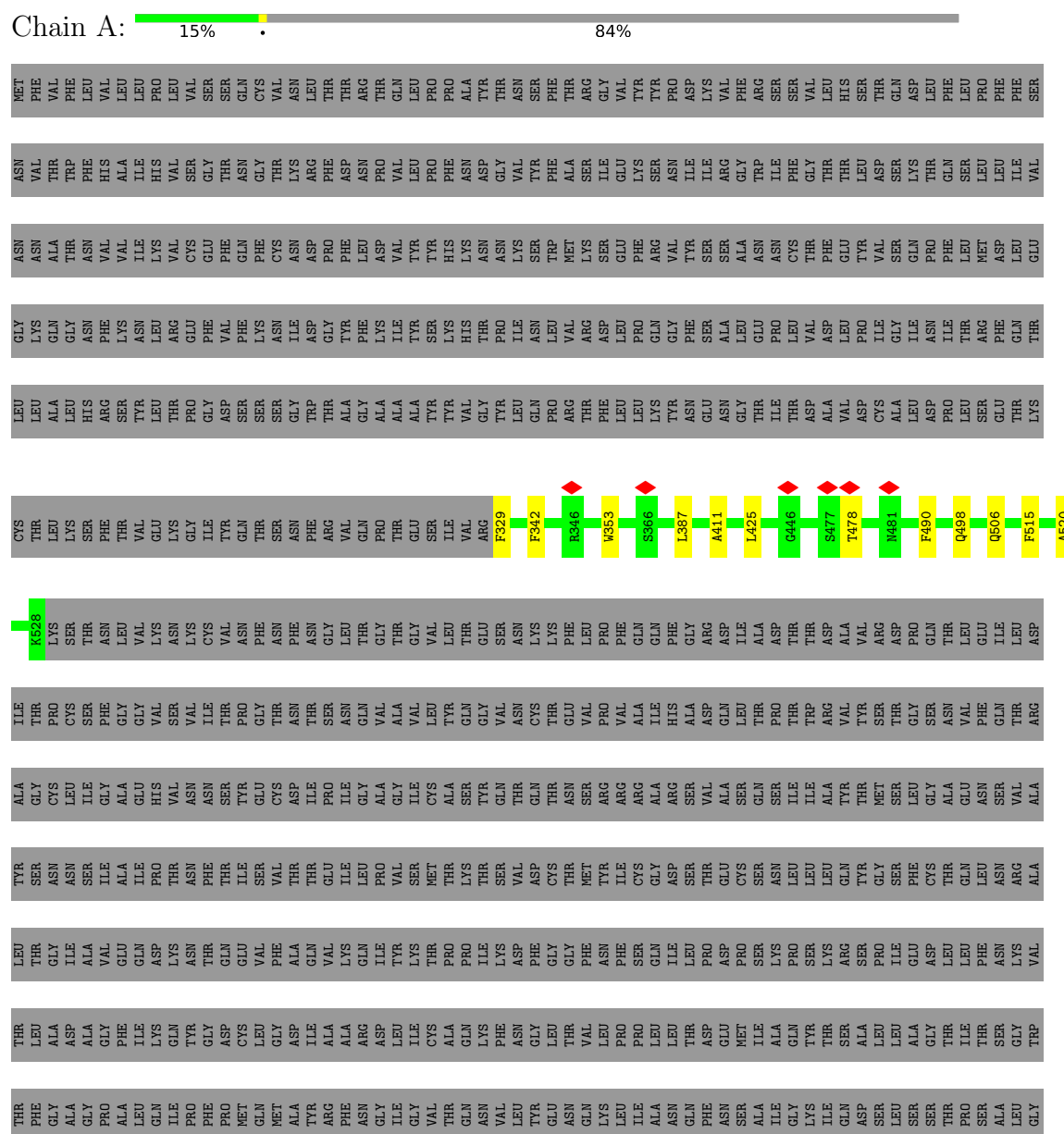


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	14	8	1	5	0

3 Residue-property plots

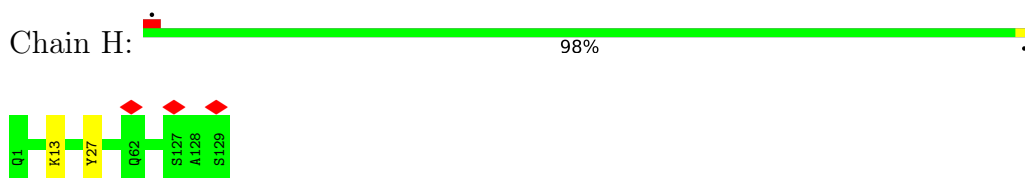
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein

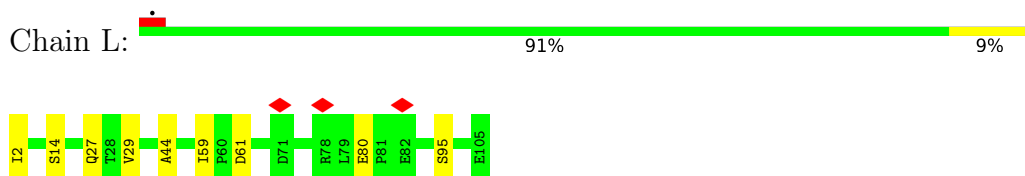


GLY	ASN	ASP	TTR	TTR	LYS
PRO	GLU	VAL	VAL	VAL	GLN
GLY	VAL	VAL	PRO	THR	LEU
SER	ALA	ILE	ALA	GLN	ASP
GLY	LYS	GLY	HIS	GLU	VAL
GLY	ASN	ILE	GLU	LEU	VAL
LEU	LEU	VAL	LYS	ILE	ASN
ASN	ASN	ASN	ASN	ARG	GLN
ASP	GLU	ASN	PHE	ALA	ASN
ILE	SER	THR	THR	ALA	ALA
PHE	LEU	VAL	THR	GLU	GLN
GLU	ILE	TTR	ALA	ILE	ALA
ALA	ASP	ASP	PRO	ARG	LEU
GLN	LEU	PRO	ALA	ALA	ASN
LYS	GLN	LEU	ILE	SER	ASN
ILE	GLU	GLN	CYS	ALA	LEU
GLU	LEU	PRO	HIS	ASN	VAL
TTR	GLY	GLU	ASP	LEU	LYS
HIS	LYS	LEU	GLY	ALA	GLN
GLU	TTR	ASP	LYS	ALA	LEU
GLY	GLU	SER	PHE	THR	SER
SER	GLN	PHE	HIS	LYS	SER
GLY	GLY	GLY	PHE	MET	ASN
HIS	SER	GLU	SER	SER	PHE
HIS	GLY	GLU	ARG	GLU	GLY
HIS	TTR	LEU	GLU	CYS	ALA
HIS	ILE	ASP	GLY	VAL	ILE
HIS	PRO	LYS	VAL	LEU	SER
HIS	GLU	TTR	PHE	GLY	SER
HIS	ALA	PHE	VAL	GLN	VAL
HIS	PRO	LYS	SER	LEU	LEU
	ARG	ASN	LYS	ASN	ASN
	ASP	HIS	GLY	ARG	ASP
	GLY	THR	THR	VAL	ILE
	GLN	SER	HIS	ASP	SER
	ALA	PRO	TTR	PHE	ARG
	TTR	ASP	PHE	CYS	ARG
	VAL	VAL	VAL	GLY	LEU
	ARG	ASP	THR	LYS	CYS
	LYS	LEU	GLN	GLY	PRO
	ASP	GLY	ARG	TTR	PRO
	GLY	ASP	ASN	HIS	GLU
	GLU	ILE	PHE	LEU	ALA
	TTR	SER	TTR	MET	ALA
	VAL	GLY	GLU	SER	VAL
	LEU	ILE	PRO	PHE	GLN
	LEU	ASN	GLN	PRO	ILE
	SER	ALA	ILE	GLN	ASP
	THR	SER	ILE	SER	ARG
	PHE	VAL	THR	ALA	LEU
	LEU	VAL	THR	PRO	ILE
	GLY	THR	ASN	HIS	THR
	SER	ILE	THR	GLY	GLY
	LEU	GLN	THR	VAL	ARG
	LEU	LYS	PHE	VAL	LEU
	GLU	GLU	VAL	PHE	GLN
	VAL	ILE	SER	GLY	SER
	LEU	ASP	GLY	HIS	LEU
	PHE	THR	ASN	VAL	GLN

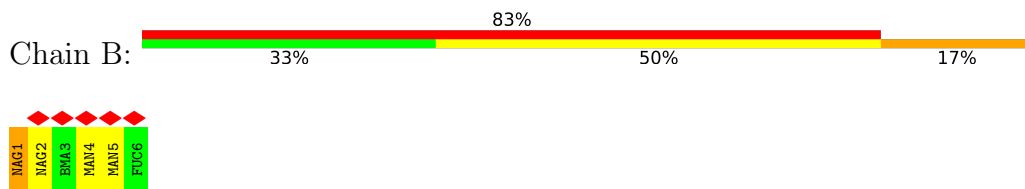
- Molecule 2: S309 Fab heavy chain



- Molecule 3: S309 Fab light chain



- Molecule 4: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-[α -L-fucopyranose-(1-6)]2-acetamido-2-deoxy- β -D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	277827	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	7.835	Depositor
Minimum map value	-5.529	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	1.1	Depositor
Map size (Å)	431.616, 431.616, 431.616	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.843, 0.843, 0.843	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.56	0/1635	0.93	15/2225 (0.7%)
2	H	0.57	0/1020	0.82	4/1384 (0.3%)
3	L	0.57	0/794	0.92	9/1079 (0.8%)
All	All	0.57	0/3449	0.90	28/4688 (0.6%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	PHE	CA-C-N	7.04	126.74	119.56
1	A	490	PHE	C-N-CA	7.04	126.74	119.56
3	L	59	ILE	CA-C-N	6.94	126.97	119.89
3	L	59	ILE	C-N-CA	6.94	126.97	119.89
1	A	425	LEU	CA-C-N	6.90	126.82	119.85
1	A	425	LEU	C-N-CA	6.90	126.82	119.85
1	A	498	GLN	CA-C-N	6.87	126.57	119.56
1	A	498	GLN	C-N-CA	6.87	126.57	119.56
1	A	478	THR	CA-C-N	6.74	126.73	119.78
1	A	478	THR	C-N-CA	6.74	126.73	119.78
3	L	44	ALA	CA-C-N	6.39	126.36	119.78
3	L	44	ALA	C-N-CA	6.39	126.36	119.78
1	A	329	PHE	CA-CB-CG	6.29	120.09	113.80
1	A	506	GLN	CA-C-N	6.04	125.80	119.76
1	A	506	GLN	C-N-CA	6.04	125.80	119.76
1	A	411	ALA	CA-C-N	6.03	125.97	119.76
1	A	411	ALA	C-N-CA	6.03	125.97	119.76
1	A	520	ALA	CA-C-N	5.58	125.90	119.93
1	A	520	ALA	C-N-CA	5.58	125.90	119.93
3	L	14	SER	CA-C-N	5.56	125.57	119.90
3	L	14	SER	C-N-CA	5.56	125.57	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	80	GLU	CA-C-N	5.40	125.73	119.47
3	L	80	GLU	C-N-CA	5.40	125.73	119.47
3	L	95	SER	CB-CA-C	-5.35	110.38	116.54
2	H	13	LYS	CA-C-N	5.21	125.50	119.93
2	H	13	LYS	C-N-CA	5.21	125.50	119.93
2	H	27	TYR	CA-C-N	5.06	126.17	119.84
2	H	27	TYR	C-N-CA	5.06	126.17	119.84

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	1589	0	1508	3	0
2	H	996	0	949	0	0
3	L	778	0	755	3	0
4	B	71	0	61	1	0
5	A	14	0	13	0	0
All	All	3448	0	3286	6	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 (6) 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:L:2:ILE:HG12	3:L:27:GLN:HB2	1.86	0.58
1:A:387:LEU:HD11	1:A:515:PHE:CE2	2.51	0.46
3:L:2:ILE:HG21	3:L:29:VAL:CG2	2.48	0.44
1:A:353:TRP:H	1:A:353:TRP:CD1	2.35	0.43
1:A:342:PHE:HB2	4:B:1:NAG:H82	2.01	0.42
3:L:61:ASP:OD1	3:L:61:ASP:N	2.53	0.42

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	A	198/1277 (16%)	195 (98%)	3 (2%)	0	100	100
2	H	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
3	L	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
All	All	427/1510 (28%)	419 (98%)	8 (2%)	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	A	173/1112 (16%)	173 (100%)	0	100	100
2	H	104/104 (100%)	104 (100%)	0	100	100
3	L	86/86 (100%)	86 (100%)	0	100	100
All	All	363/1302 (28%)	363 (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. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	439	ASN
3	L	90	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
4	NAG	B	1	4,1	14,14,15	0.94	1 (7%)	17,19,21	1.08	2 (11%)
4	NAG	B	2	4	14,14,15	1.43	2 (14%)	17,19,21	1.11	1 (5%)
4	BMA	B	3	4	11,11,12	0.87	0	15,15,17	0.57	0
4	MAN	B	4	4	11,11,12	1.11	1 (9%)	15,15,17	0.67	0
4	MAN	B	5	4	11,11,12	1.06	1 (9%)	15,15,17	0.54	0
4	FUC	B	6	4	10,10,11	1.07	0	14,14,16	0.75	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
4	NAG	B	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	BMA	B	3	4	-	0/2/19/22	0/1/1/1
4	MAN	B	4	4	-	0/2/19/22	0/1/1/1
4	MAN	B	5	4	-	2/2/19/22	0/1/1/1
4	FUC	B	6	4	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2	NAG	C1-C2	4.06	1.57	1.52
4	B	2	NAG	O5-C5	2.30	1.47	1.43
4	B	1	NAG	C1-C2	2.21	1.55	1.52
4	B	4	MAN	O5-C5	2.02	1.47	1.43
4	B	5	MAN	O5-C5	2.01	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2	NAG	C8-C7-N2	3.03	121.14	116.12
4	B	1	NAG	C2-N2-C7	-2.45	119.62	122.90
4	B	1	NAG	C8-C7-N2	2.05	119.52	116.12

There are no chirality outliers.

All (2) torsion outliers are listed below:

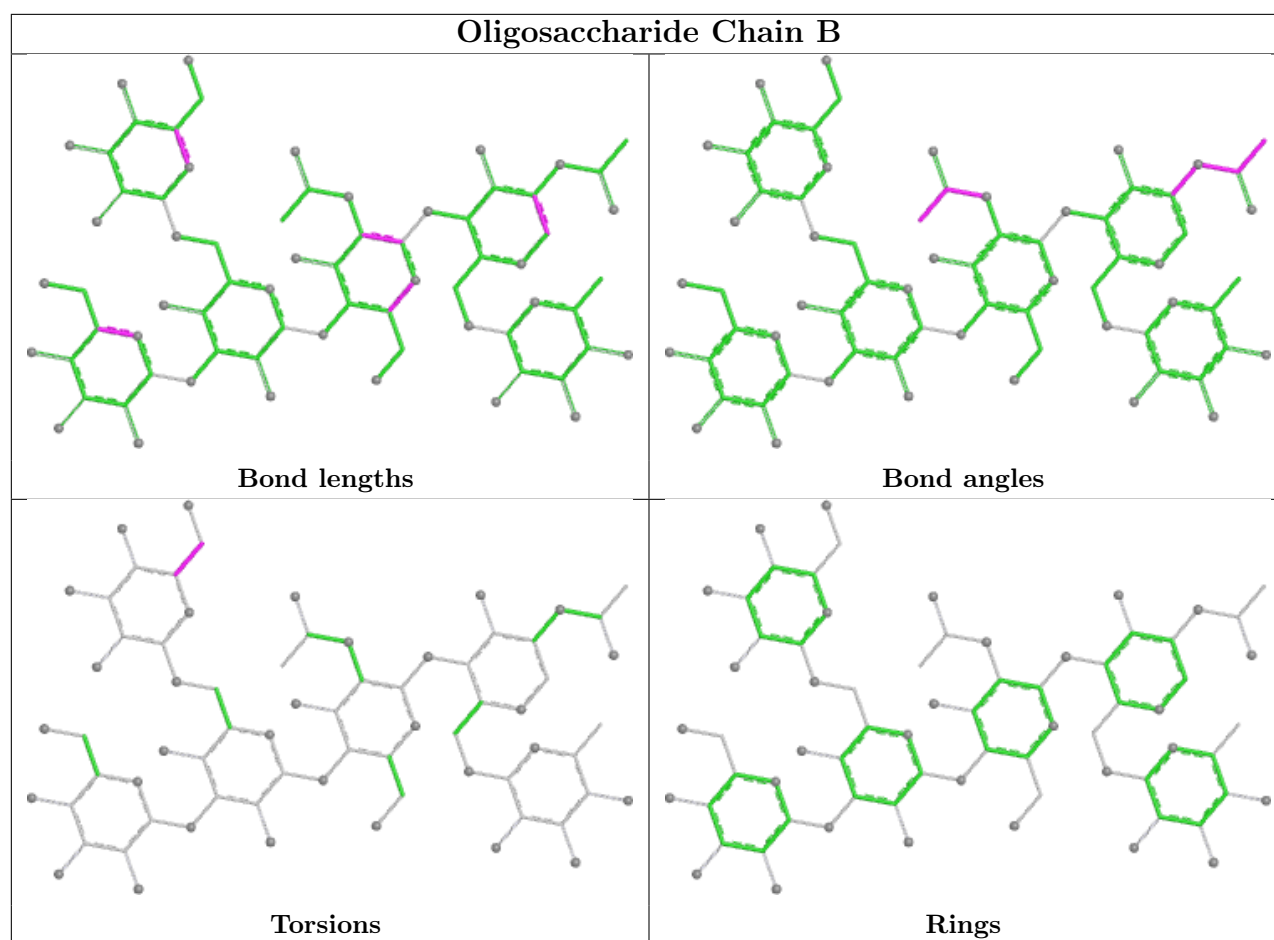
Mol	Chain	Res	Type	Atoms
4	B	5	MAN	O5-C5-C6-O6
4	B	5	MAN	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	NAG	1	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.



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$
5	NAG	A	1301	1	14,14,15	1.28	1 (7%)	17,19,21	1.04	1 (5%)

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	A	1301	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1301	NAG	C1-C2	3.96	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	A	1301	NAG	C8-C7-N2	2.64	120.50	116.12

There are no chirality outliers.

There are no torsion outliers.

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.

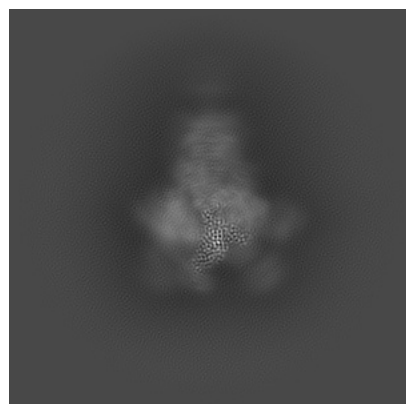
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25266. These allow visual inspection of the internal detail of the map and identification of artifacts.

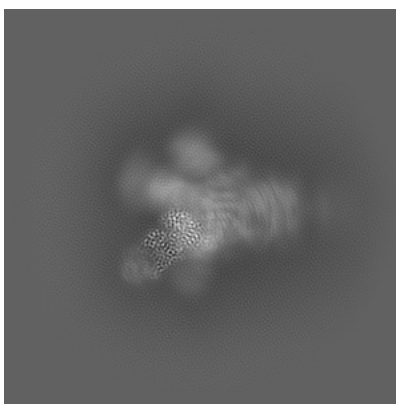
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

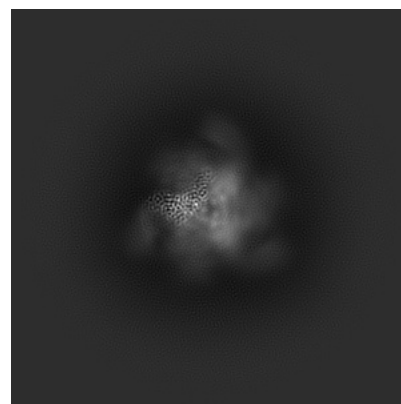
6.1.1 Primary map



X

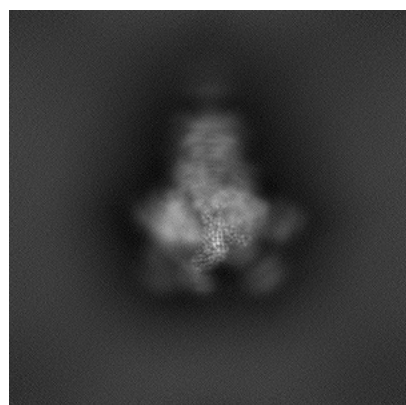


Y

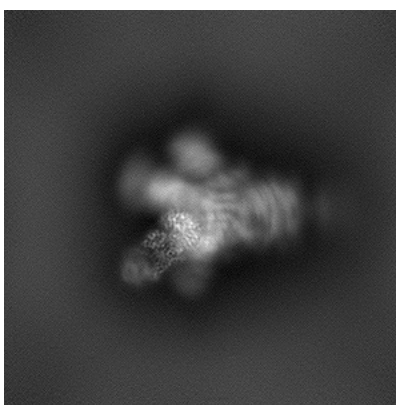


Z

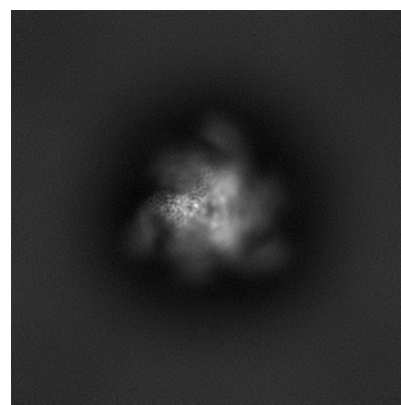
6.1.2 Raw map



X



Y



Z

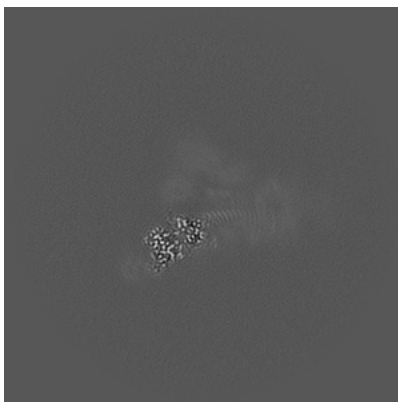
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

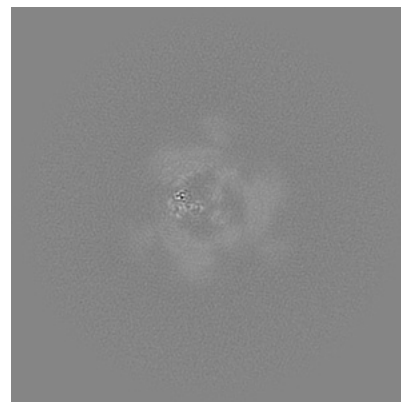
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

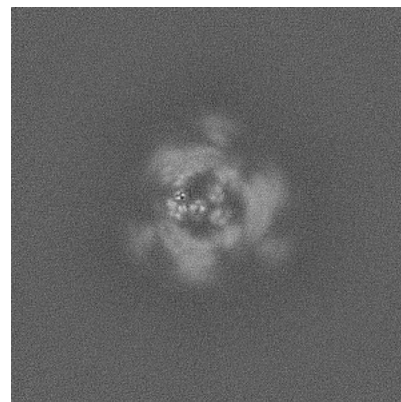
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

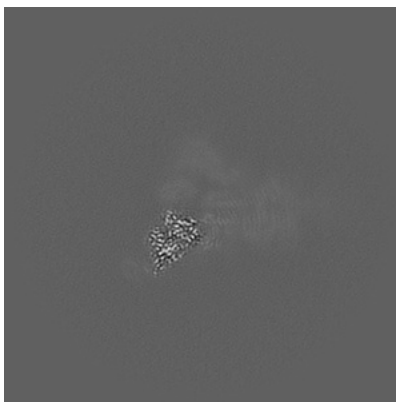
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

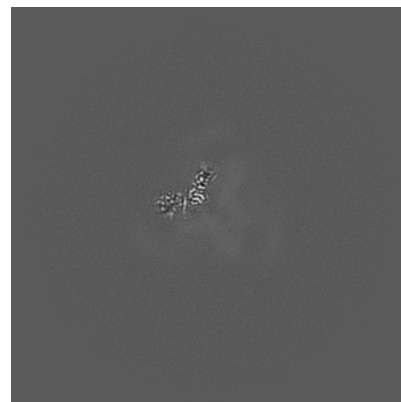
6.3.1 Primary map



X Index: 219



Y Index: 262

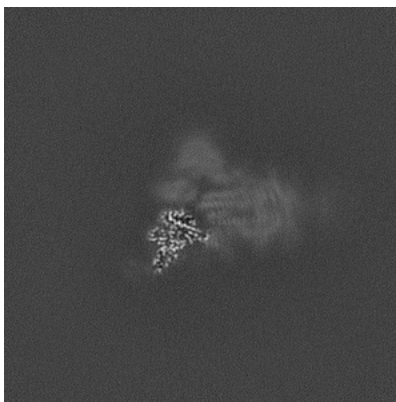


Z Index: 218

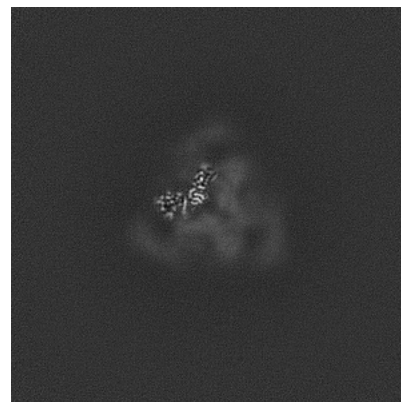
6.3.2 Raw map



X Index: 236



Y Index: 267

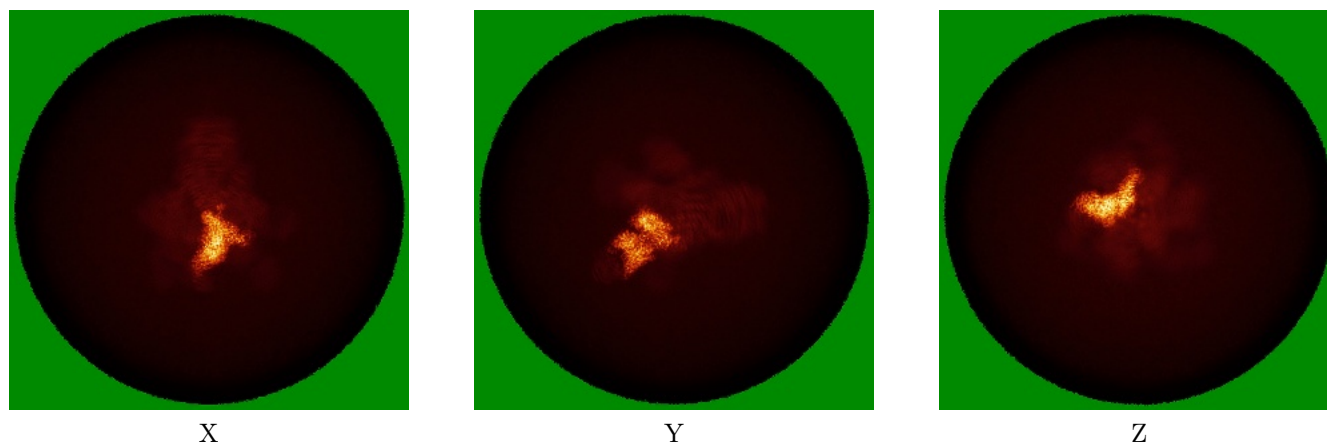


Z Index: 218

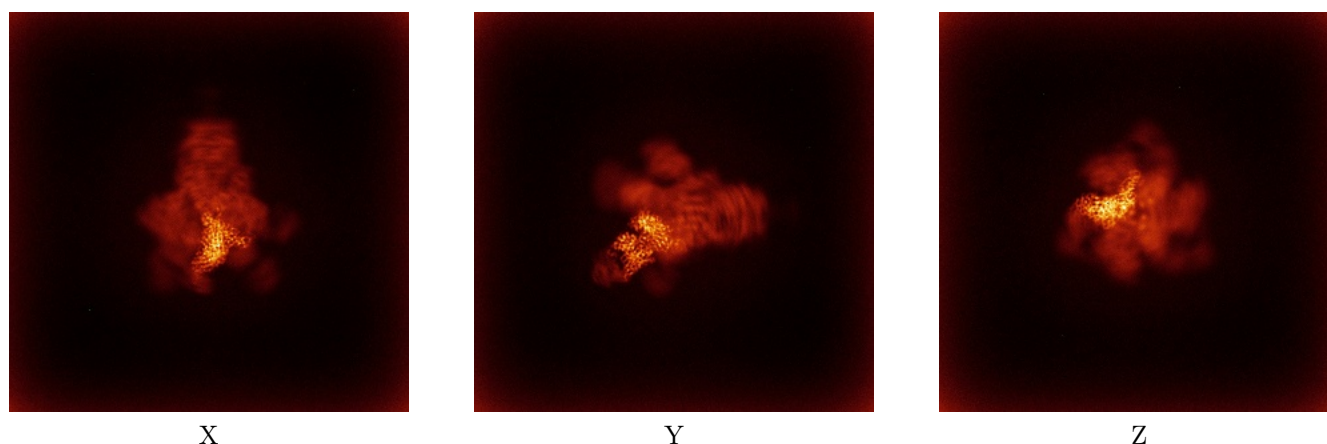
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

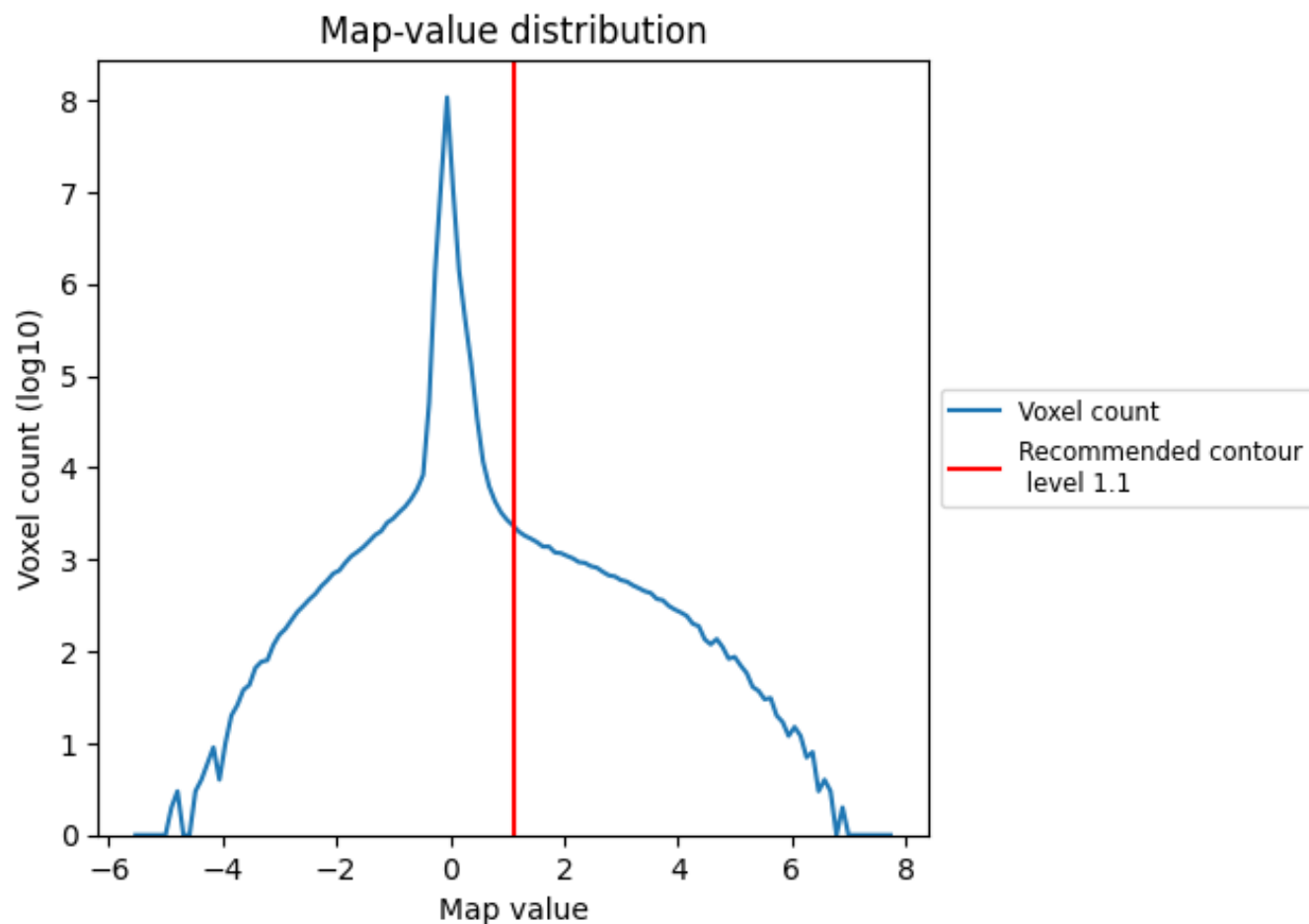
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

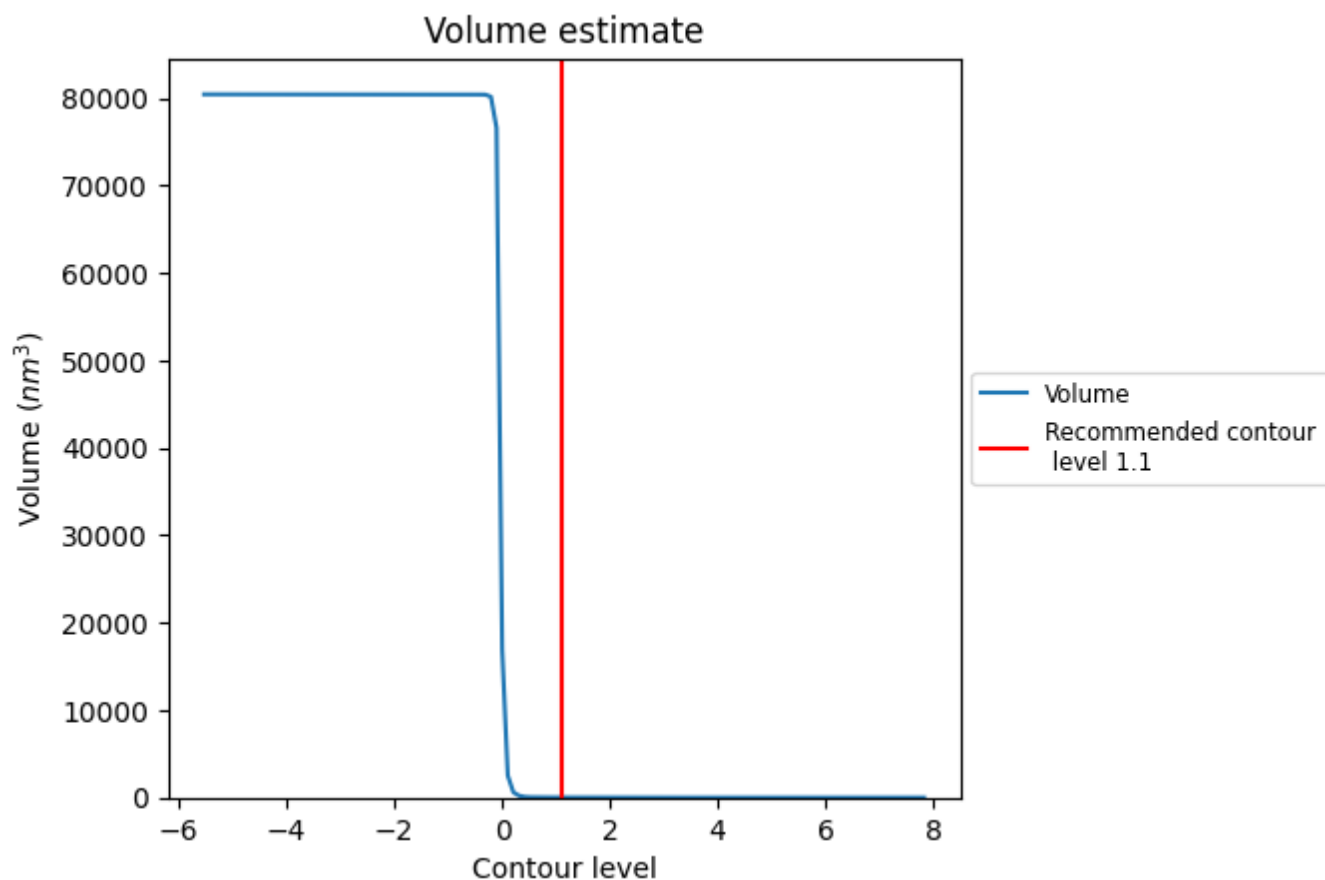
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

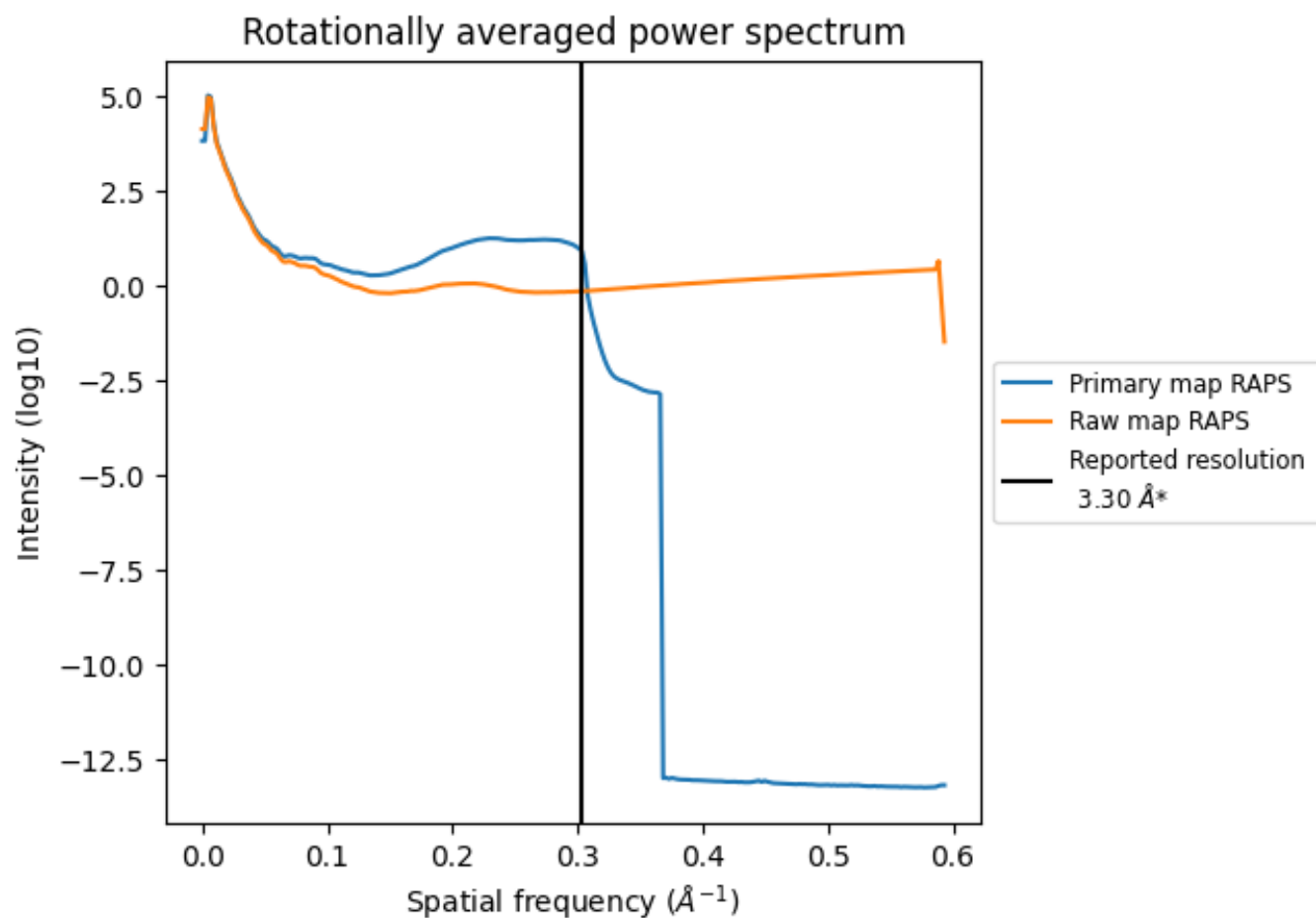
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 17 nm³; this corresponds to an approximate mass of 15 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 ⓘ

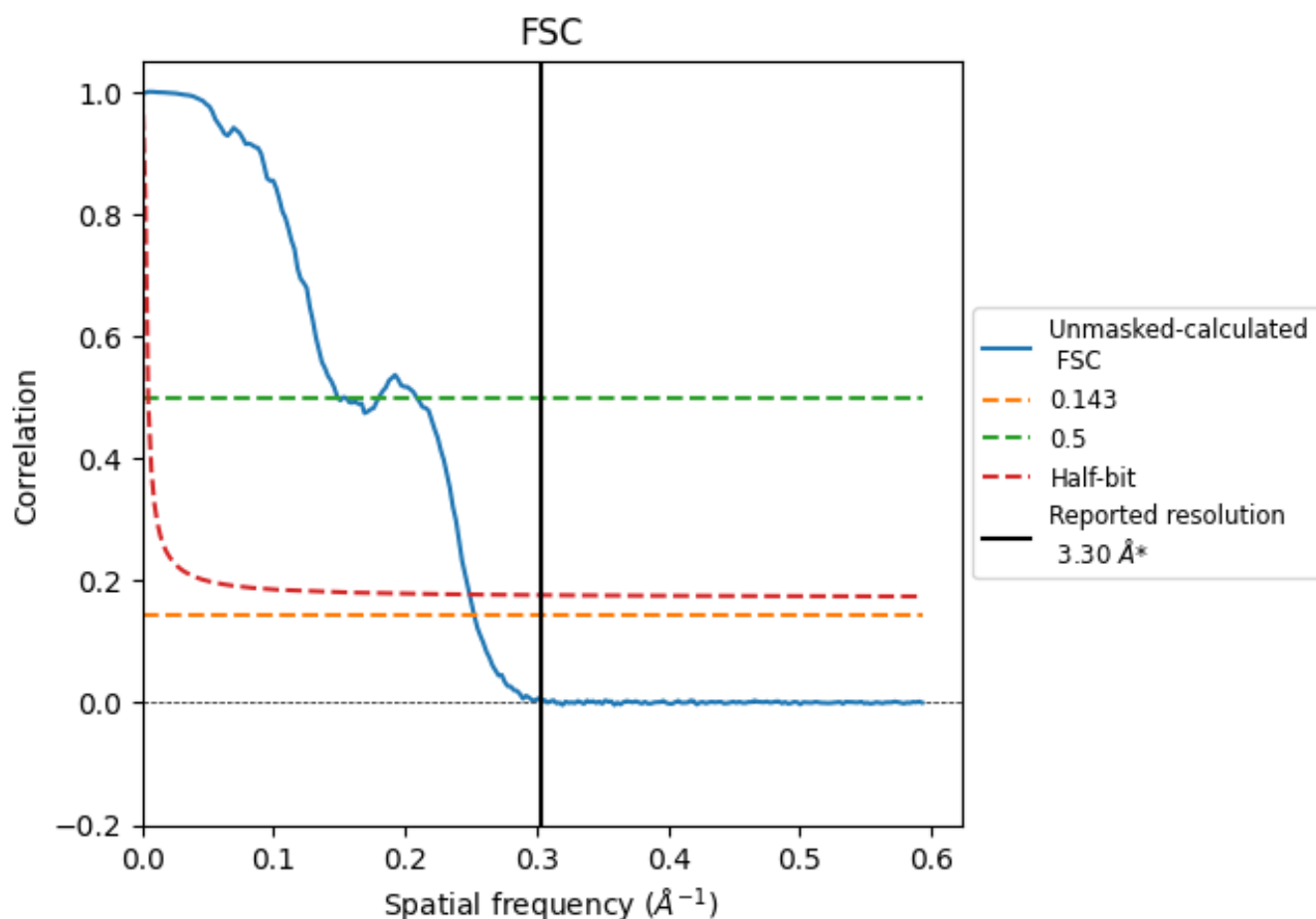


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.96	6.73	4.02

*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 3.96 differs from the reported value 3.3 by more than 10 %

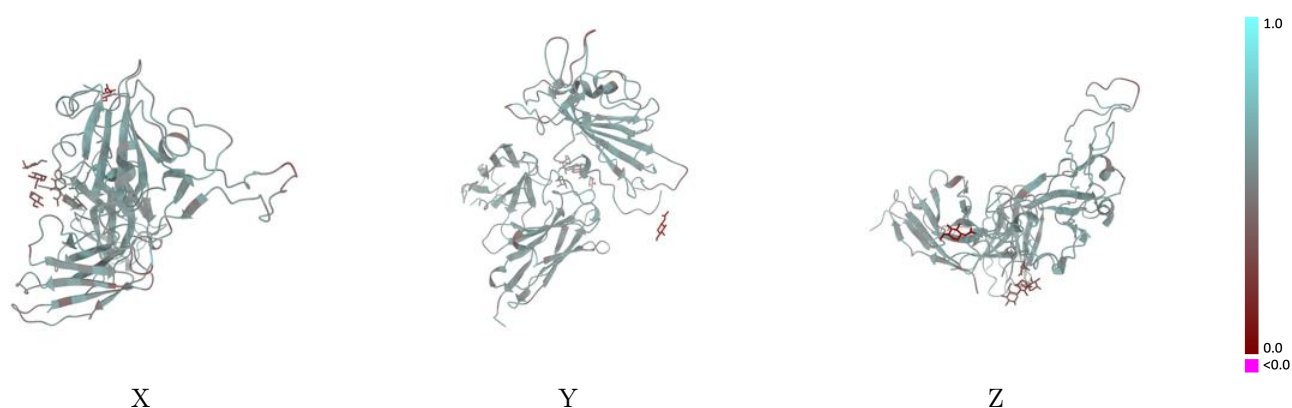
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-25266 and PDB model 7SOC. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

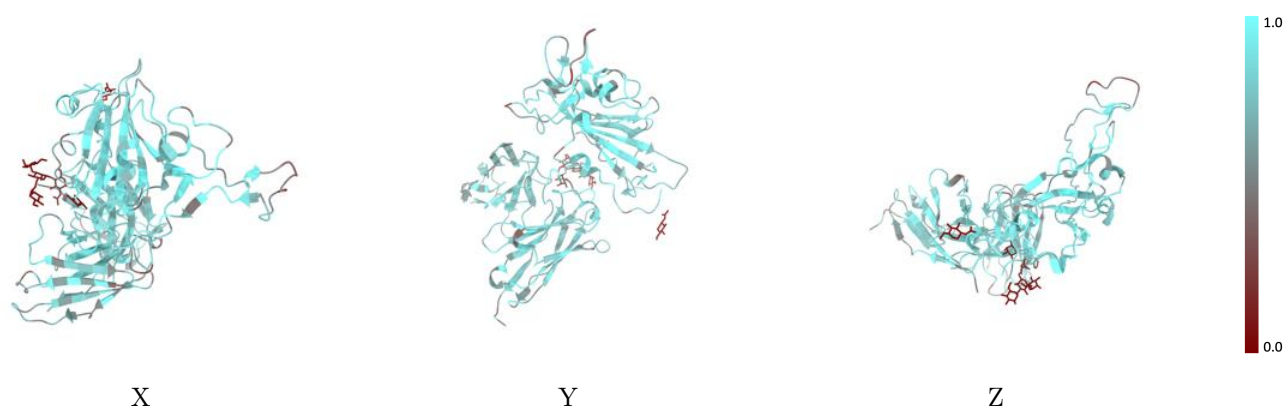
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



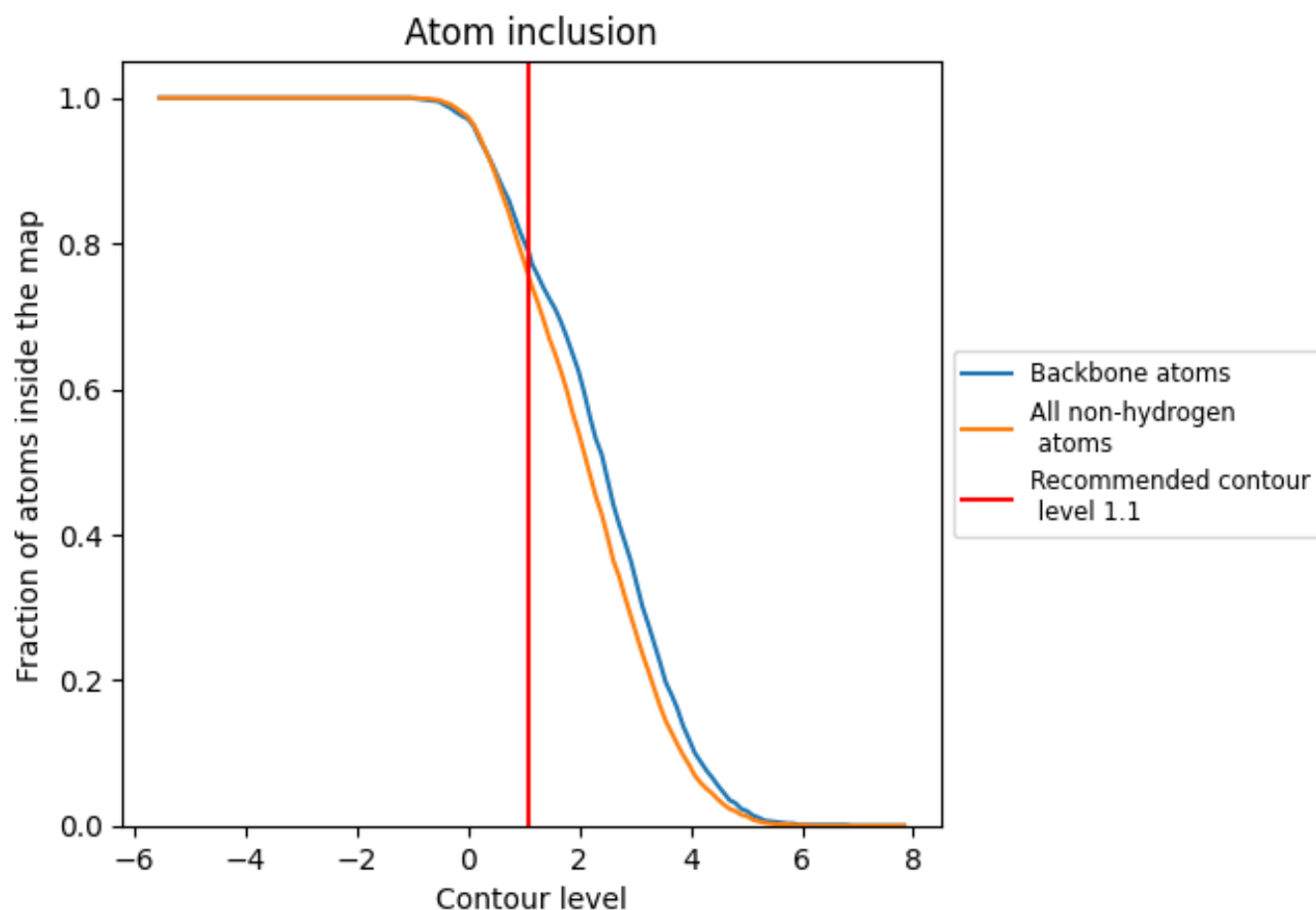
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (1.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 75% 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 (1.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7540	0.5410
A	0.7730	0.5440
B	0.2680	0.3870
H	0.7750	0.5490
L	0.7330	0.5370

