



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:32 AM UTC

PDB ID : 9B2C / pdb_00009b2c
EMDB ID : EMD-44103
Title : Structure of the Porcine deltacoronavirus (PDCoV) receptor-binding domain bound to the PD33 antibody Fab fragment and the Kappa light chain nanobody
Authors : Park, Y.J.; Seattle Structural Genomics Center for Infectious Disease (SSG-CID); Veesler, D.
Deposited on : 2024-03-14
Resolution : 3.00 Å(reported)

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:

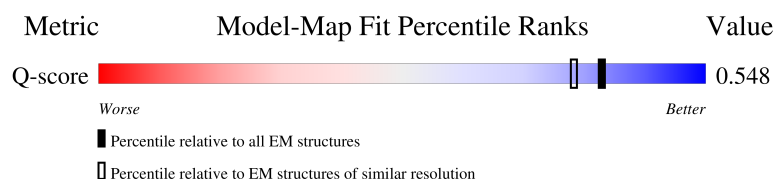
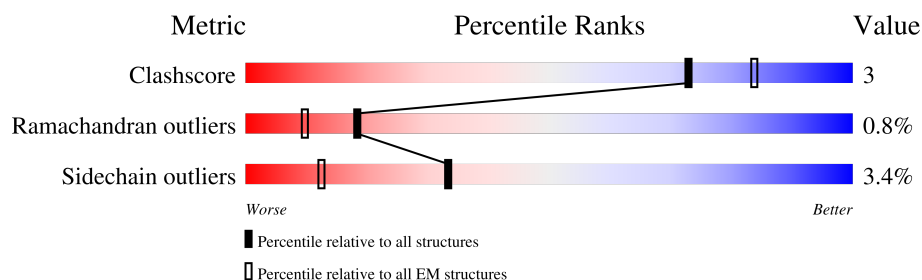
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.00 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	14081 (2.50 - 3.50)

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	163	28% 58% 8% 33%
2	L	219	5% 83% 14% ••
3	N	159	18% 69% 5% 25%
4	H	222	8% 85% 9% • 5%

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Mol	Chain	Length	Quality of chain
5	B	3	67% 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4596 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	110	Total	C	N	O	S	0	0
			761	490	135	126	10		

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	MET	-	expression tag	UNP A0A1S6L971
A	272	GLY	-	expression tag	UNP A0A1S6L971
A	273	ILE	-	expression tag	UNP A0A1S6L971
A	274	LEU	-	expression tag	UNP A0A1S6L971
A	275	PRO	-	expression tag	UNP A0A1S6L971
A	276	SER	-	expression tag	UNP A0A1S6L971
A	277	PRO	-	expression tag	UNP A0A1S6L971
A	278	GLY	-	expression tag	UNP A0A1S6L971
A	279	MET	-	expression tag	UNP A0A1S6L971
A	280	PRO	-	expression tag	UNP A0A1S6L971
A	281	ALA	-	expression tag	UNP A0A1S6L971
A	282	LEU	-	expression tag	UNP A0A1S6L971
A	283	LEU	-	expression tag	UNP A0A1S6L971
A	284	SER	-	expression tag	UNP A0A1S6L971
A	285	LEU	-	expression tag	UNP A0A1S6L971
A	286	VAL	-	expression tag	UNP A0A1S6L971
A	287	SER	-	expression tag	UNP A0A1S6L971
A	288	LEU	-	expression tag	UNP A0A1S6L971
A	289	LEU	-	expression tag	UNP A0A1S6L971
A	290	SER	-	expression tag	UNP A0A1S6L971
A	291	VAL	-	expression tag	UNP A0A1S6L971
A	292	LEU	-	expression tag	UNP A0A1S6L971
A	293	LEU	-	expression tag	UNP A0A1S6L971
A	294	MET	-	expression tag	UNP A0A1S6L971
A	295	GLY	-	expression tag	UNP A0A1S6L971
A	296	CYS	-	expression tag	UNP A0A1S6L971
A	297	VAL	-	expression tag	UNP A0A1S6L971
A	298	ALA	-	expression tag	UNP A0A1S6L971

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Chain	Residue	Modelled	Actual	Comment	Reference
A	299	GLU	-	expression tag	UNP A0A1S6L971
A	300	THR	-	expression tag	UNP A0A1S6L971
A	301	GLY	-	expression tag	UNP A0A1S6L971
A	302	THR	-	expression tag	UNP A0A1S6L971
A	417	LEU	-	expression tag	UNP A0A1S6L971
A	418	VAL	-	expression tag	UNP A0A1S6L971
A	419	PRO	-	expression tag	UNP A0A1S6L971
A	420	ARG	-	expression tag	UNP A0A1S6L971
A	421	GLY	-	expression tag	UNP A0A1S6L971
A	422	SER	-	expression tag	UNP A0A1S6L971
A	423	GLY	-	expression tag	UNP A0A1S6L971
A	424	GLY	-	expression tag	UNP A0A1S6L971
A	425	SER	-	expression tag	UNP A0A1S6L971
A	426	HIS	-	expression tag	UNP A0A1S6L971
A	427	HIS	-	expression tag	UNP A0A1S6L971
A	428	HIS	-	expression tag	UNP A0A1S6L971
A	429	HIS	-	expression tag	UNP A0A1S6L971
A	430	HIS	-	expression tag	UNP A0A1S6L971
A	431	HIS	-	expression tag	UNP A0A1S6L971
A	432	HIS	-	expression tag	UNP A0A1S6L971
A	433	HIS	-	expression tag	UNP A0A1S6L971

- Molecule 2 is a protein called PD33 Fab kappa light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	216	Total	C	N	O	S	0	0
			1535	988	275	266	6		

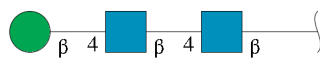
- Molecule 3 is a protein called Kappa light chain nanobody.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	119	Total	C	N	O	S	0	0
			759	490	139	126	4		

- Molecule 4 is a protein called PD33 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	212	Total	C	N	O	S	0	0
			1488	975	253	254	6		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
5	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

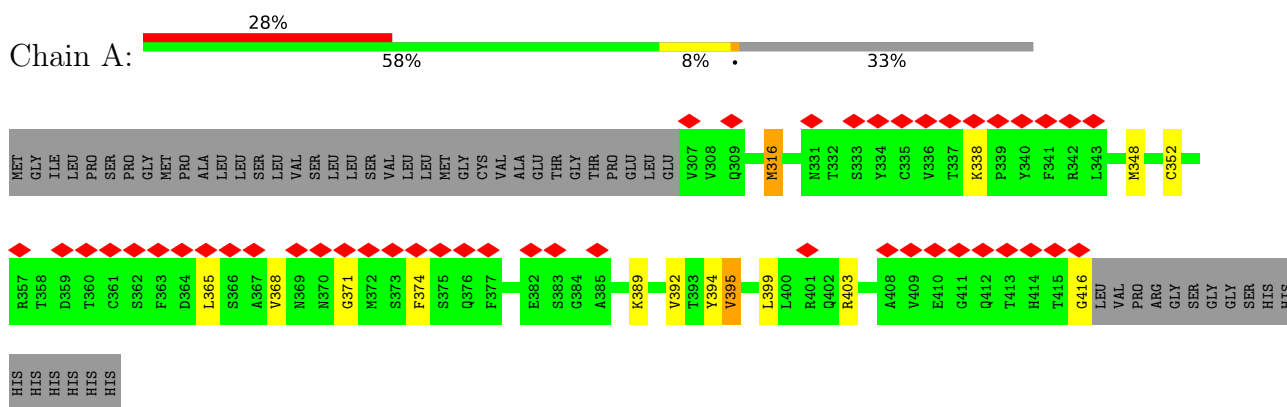


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	

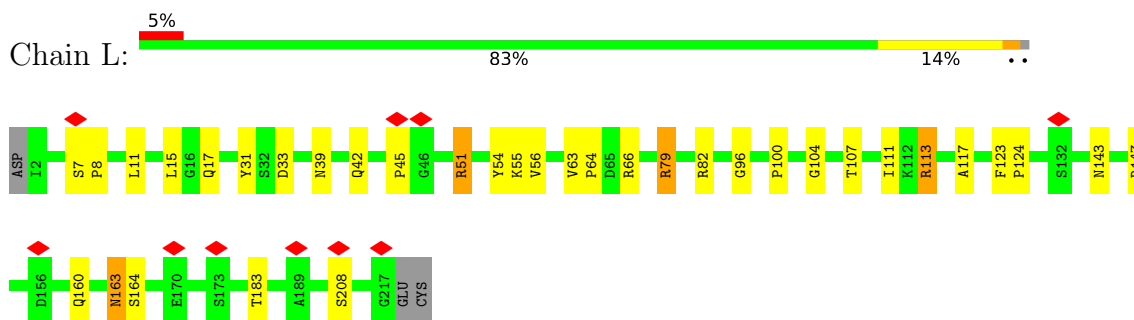
3 Residue-property plots

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.

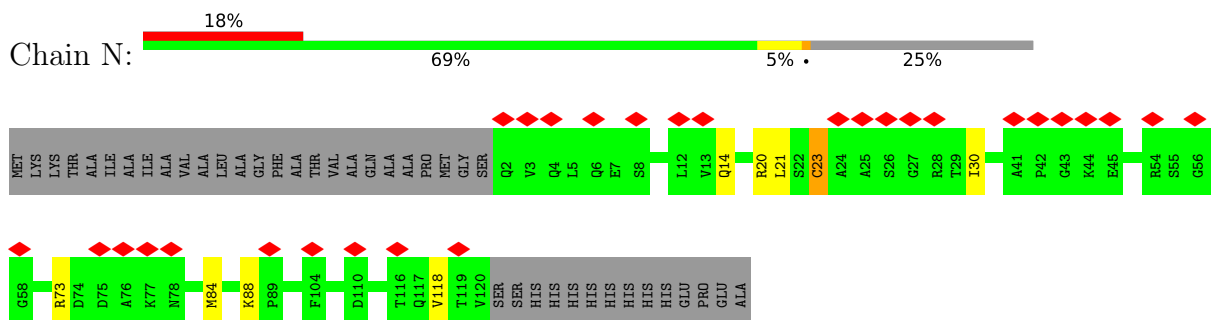
- Molecule 1: Spike glycoprotein



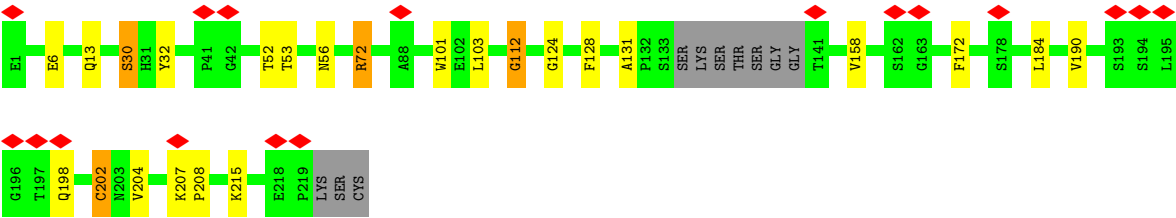
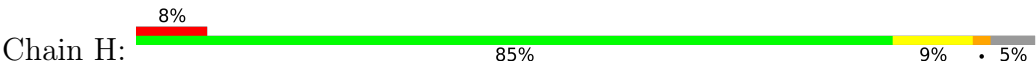
- Molecule 2: PD33 Fab kappa light chain



- Molecule 3: Kappa light chain nanobody



- Molecule 4: PD33 Fab heavy chain



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	564616	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 ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	8.376	Depositor
Minimum map value	-6.643	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.118	Depositor
Recommended contour level	1.4	Depositor
Map size (Å)	280.0, 280.0, 280.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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, 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	0.73	0/775	1.15	5/1056 (0.5%)
2	L	0.69	0/1575	1.19	21/2162 (1.0%)
3	N	0.75	0/776	1.17	5/1065 (0.5%)
4	H	0.71	1/1529 (0.1%)	1.18	19/2101 (0.9%)
All	All	0.72	1/4655 (0.0%)	1.18	50/6384 (0.8%)

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	L	0	3
3	N	0	1
4	H	0	2
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	208	PRO	N-CD	10.06	1.61	1.47

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	202	CYS	CB-CA-C	-8.71	96.49	111.30
4	H	124	GLY	CA-C-N	7.55	127.47	119.85
4	H	124	GLY	C-N-CA	7.55	127.47	119.85
2	L	104	GLY	CA-C-N	7.21	127.54	119.32
2	L	104	GLY	C-N-CA	7.21	127.54	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	17	GLN	CA-C-N	6.83	126.80	120.03
2	L	17	GLN	C-N-CA	6.83	126.80	120.03
1	A	338	LYS	CA-C-N	6.83	126.53	119.56
1	A	338	LYS	C-N-CA	6.83	126.53	119.56
2	L	63	VAL	CA-C-N	6.78	128.31	119.84
2	L	63	VAL	C-N-CA	6.78	128.31	119.84
4	H	172	PHE	CA-C-N	6.77	126.73	119.76
4	H	172	PHE	C-N-CA	6.77	126.73	119.76
2	L	147	ARG	CB-CA-C	-6.55	99.92	110.79
4	H	112	GLY	CA-C-O	-6.53	117.97	122.22
1	A	394	TYR	N-CA-CB	6.45	119.43	110.07
2	L	42	GLN	CB-CA-C	-6.39	98.02	109.71
2	L	100	PRO	CA-C-N	6.32	126.35	119.90
2	L	100	PRO	C-N-CA	6.32	126.35	119.90
4	H	207	LYS	CA-C-N	6.26	125.95	119.56
4	H	207	LYS	C-N-CA	6.26	125.95	119.56
2	L	124	PRO	CA-C-N	6.25	126.20	119.76
2	L	124	PRO	C-N-CA	6.25	126.20	119.76
2	L	117	ALA	CA-C-N	6.24	126.15	119.85
2	L	117	ALA	C-N-CA	6.24	126.15	119.85
2	L	208	SER	CA-C-N	6.07	126.01	119.76
2	L	208	SER	C-N-CA	6.07	126.01	119.76
3	N	14	GLN	CA-C-N	5.93	126.28	119.93
3	N	14	GLN	C-N-CA	5.93	126.28	119.93
4	H	56	ASN	N-CA-C	-5.92	105.89	113.23
4	H	128	PHE	CA-C-N	5.85	125.76	119.85
4	H	128	PHE	C-N-CA	5.85	125.76	119.85
2	L	11	LEU	CA-C-N	5.83	126.02	119.90
2	L	11	LEU	C-N-CA	5.83	126.02	119.90
4	H	190	VAL	CA-C-N	5.73	125.67	119.76
4	H	190	VAL	C-N-CA	5.73	125.67	119.76
3	N	88	LYS	CA-C-N	5.72	126.10	119.47
3	N	88	LYS	C-N-CA	5.72	126.10	119.47
4	H	131	ALA	CA-C-N	5.72	126.05	119.93
4	H	131	ALA	C-N-CA	5.72	126.05	119.93
1	A	394	TYR	CB-CA-C	-5.70	101.89	110.90
4	H	13	GLN	CA-C-N	5.64	125.57	119.76
4	H	13	GLN	C-N-CA	5.64	125.57	119.76
2	L	123	PHE	CA-C-N	5.40	125.94	120.38
2	L	123	PHE	C-N-CA	5.40	125.94	120.38
3	N	20	ARG	CB-CA-C	-5.09	102.93	110.62
1	A	348	MET	N-CA-C	5.08	117.83	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	215	LYS	CA-C-N	-5.03	113.90	120.95
4	H	215	LYS	C-N-CA	-5.03	113.90	120.95
2	L	45	PRO	CA-N-CD	5.02	119.03	112.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	30	SER	Mainchain
4	H	72	ARG	Sidechain
2	L	113	ARG	Sidechain
2	L	51	ARG	Sidechain
2	L	79	ARG	Sidechain
3	N	73	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	761	0	643	6	0
2	L	1535	0	1332	14	0
3	N	759	0	592	3	0
4	H	1488	0	1312	7	0
5	B	39	0	34	0	0
6	A	14	0	13	0	0
All	All	4596	0	3926	28	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 3.

All (28) 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:L:8:PRO:O	2:L:107:THR:HG23	1.64	0.97
2:L:15:LEU:HD11	2:L:111:ILE:HG12	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:8:PRO:O	2:L:107:THR:CG2	2.39	0.69
2:L:15:LEU:CD1	2:L:111:ILE:HG12	2.24	0.65
4:H:30:SER:O	4:H:53:THR:HG23	2.07	0.55
1:A:371:GLY:HA2	1:A:416:GLY:O	2.06	0.55
3:N:21:LEU:HD11	3:N:118:VAL:HG21	1.89	0.54
3:N:23:CYS:SG	3:N:23:CYS:O	2.67	0.53
2:L:51:ARG:NH2	4:H:103:LEU:O	2.44	0.51
2:L:54:TYR:O	2:L:56:VAL:N	2.44	0.51
1:A:368:VAL:HG13	1:A:374:PHE:HE1	1.76	0.50
1:A:389:LYS:HB3	1:A:399:LEU:HD11	1.93	0.49
1:A:368:VAL:HG13	1:A:374:PHE:CE1	2.47	0.49
2:L:15:LEU:HD11	2:L:111:ILE:CG1	2.39	0.48
1:A:316:MET:HE2	4:H:101:TRP:CZ2	2.49	0.47
4:H:6:GLU:OE1	4:H:112:GLY:N	2.47	0.47
4:H:158:VAL:HG22	4:H:204:VAL:HG13	1.97	0.47
4:H:52:THR:O	4:H:72:ARG:NH1	2.48	0.46
1:A:352:CYS:SG	1:A:392:VAL:HG13	2.56	0.46
2:L:66:ARG:HD2	2:L:82:ARG:O	2.16	0.46
2:L:7:SER:N	2:L:8:PRO:CD	2.80	0.44
2:L:160:GLN:HB3	2:L:163:ASN:OD1	2.18	0.43
2:L:164:SER:HA	2:L:183:THR:O	2.18	0.43
2:L:79:ARG:HE	2:L:79:ARG:HB3	1.74	0.43
4:H:32:TYR:CD2	4:H:103:LEU:HD11	2.55	0.42
2:L:7:SER:N	2:L:8:PRO:HD2	2.36	0.40
2:L:31:TYR:HB3	2:L:33:ASP:OD2	2.21	0.40
3:N:21:LEU:HG	3:N:84:MET:HE3	2.04	0.40

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	108/163 (66%)	102 (94%)	5 (5%)	1 (1%)	14	48
2	L	214/219 (98%)	202 (94%)	8 (4%)	4 (2%)	6	30
3	N	117/159 (74%)	115 (98%)	2 (2%)	0	100	100
4	H	208/222 (94%)	206 (99%)	2 (1%)	0	100	100
All	All	647/763 (85%)	625 (97%)	17 (3%)	5 (1%)	18	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	395	VAL
2	L	55	LYS
2	L	143	ASN
2	L	64	PRO
2	L	96	GLY

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	60/142 (42%)	56 (93%)	4 (7%)	15	46
2	L	128/195 (66%)	125 (98%)	3 (2%)	44	74
3	N	41/123 (33%)	39 (95%)	2 (5%)	22	56
4	H	123/188 (65%)	120 (98%)	3 (2%)	43	73
All	All	352/648 (54%)	340 (97%)	12 (3%)	33	66

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	MET
1	A	365	LEU
1	A	395	VAL
1	A	403	ARG
2	L	39	ASN
2	L	113	ARG

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Mol	Chain	Res	Type
2	L	163	ASN
3	N	23	CYS
3	N	30	ILE
4	H	184	LEU
4	H	198	GLN
4	H	202	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	17	GLN
4	H	56	ASN
4	H	198	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 ⓘ

3 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	B	1	5,1	14,14,15	0.37	0	17,19,21	0.51	0
5	NAG	B	2	5	14,14,15	0.38	0	17,19,21	0.51	0
5	BMA	B	3	5	11,11,12	0.25	0	15,15,17	0.57	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
5	NAG	B	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	B	2	5	-	0/6/23/26	0/1/1/1
5	BMA	B	3	5	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

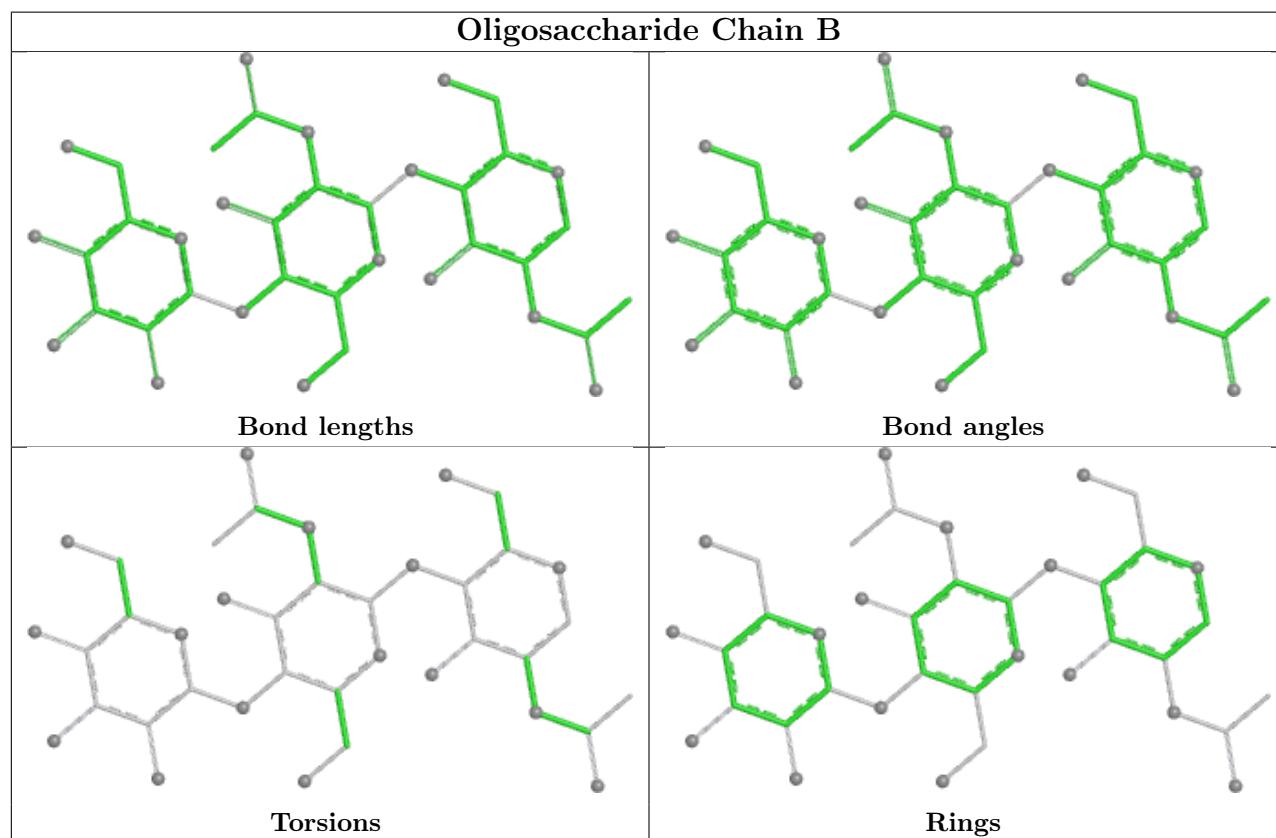
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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	$\# Z > 2$
6	NAG	A	501	1	14,14,15	0.38	0	17,19,21	0.66	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
6	NAG	A	501	1	-	0/6/23/26	0/1/1/1

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.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

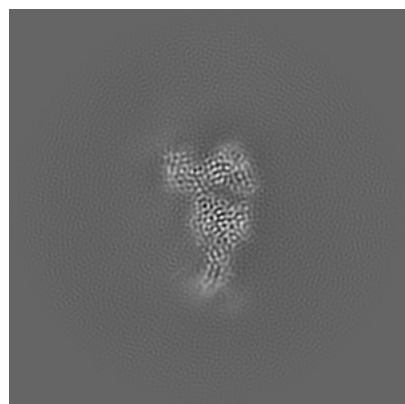
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44103. These allow visual inspection of the internal detail of the map and identification of artifacts.

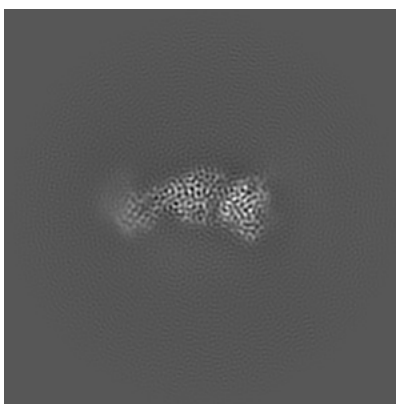
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

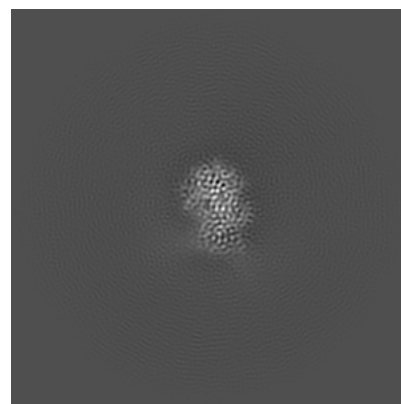
6.1.1 Primary map



X

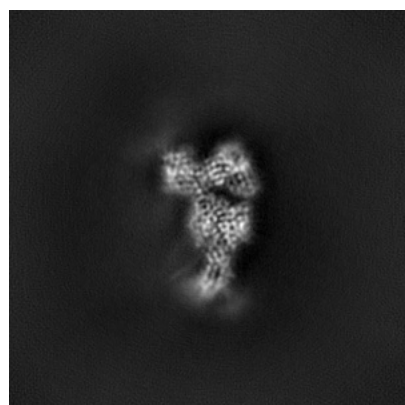


Y

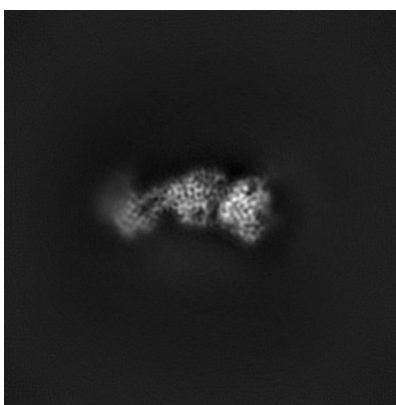


Z

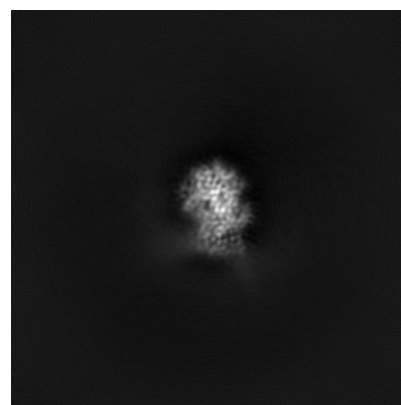
6.1.2 Raw map



X



Y

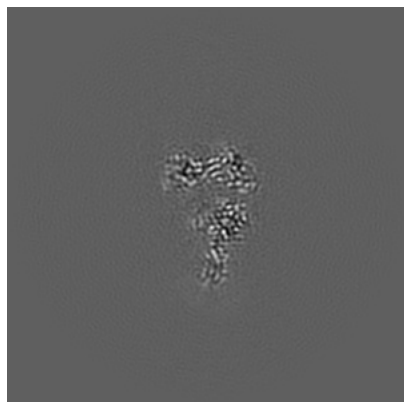


Z

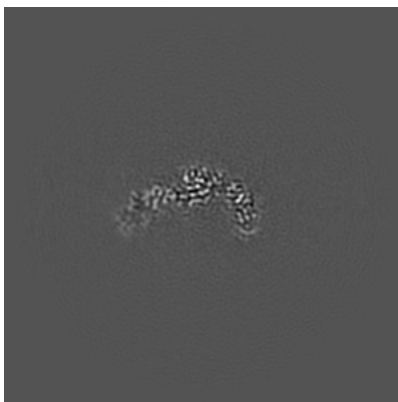
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

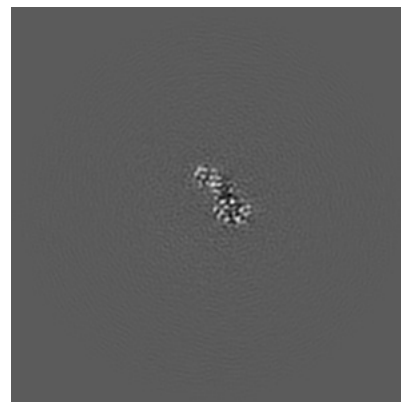
6.2.1 Primary map



X Index: 140

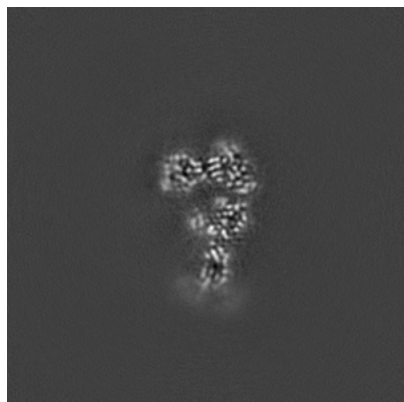


Y Index: 140

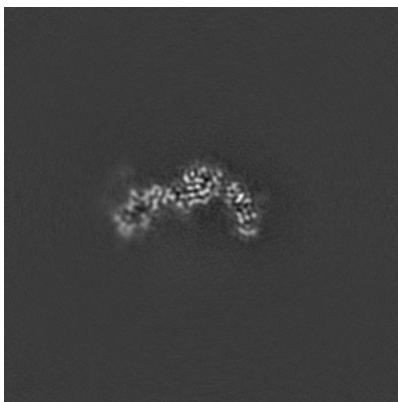


Z Index: 140

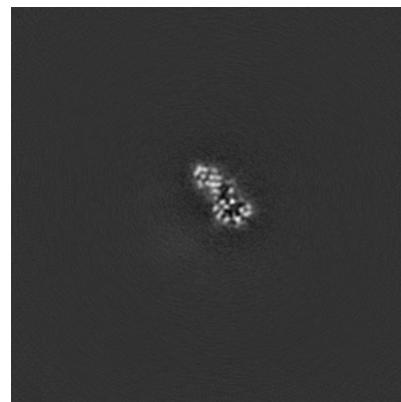
6.2.2 Raw map



X Index: 140



Y Index: 140

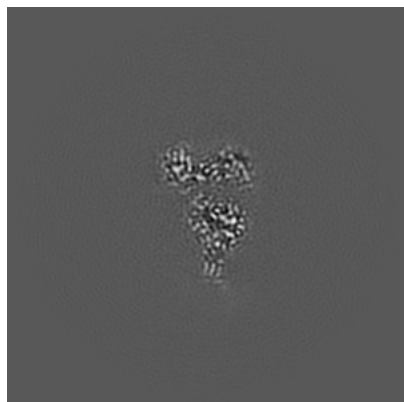


Z Index: 140

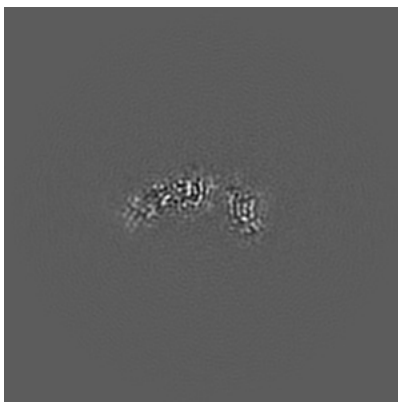
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

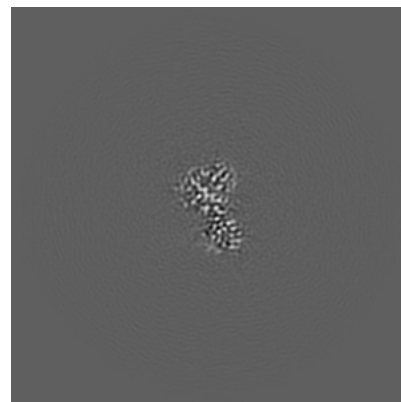
6.3.1 Primary map



X Index: 146

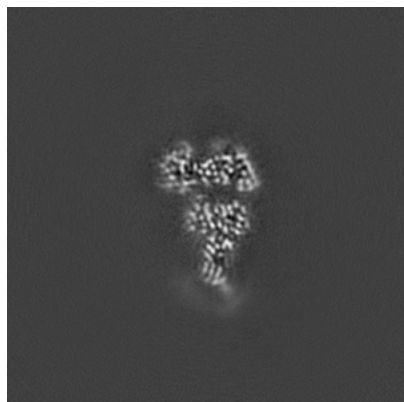


Y Index: 147

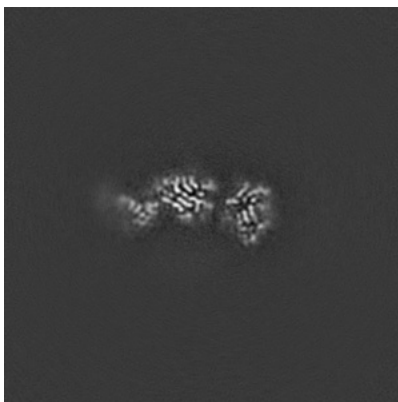


Z Index: 168

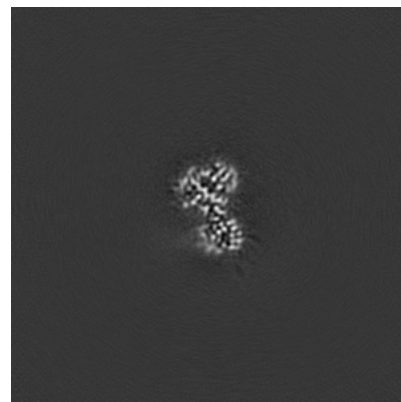
6.3.2 Raw map



X Index: 144



Y Index: 152



Z Index: 168

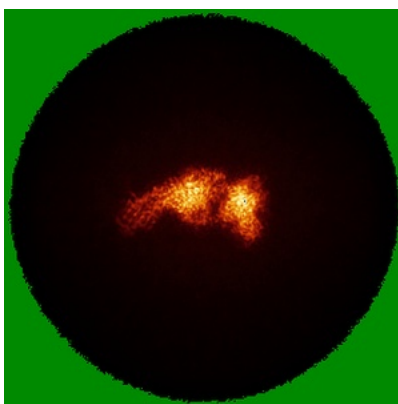
The images above show the largest variance slices of the map in three orthogonal directions.

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

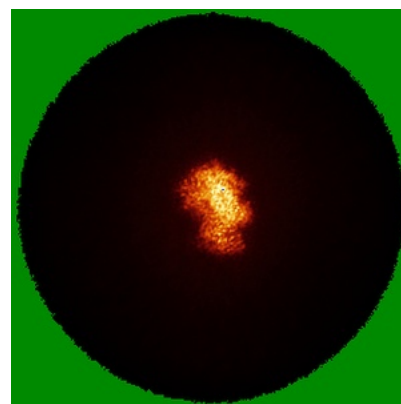
6.4.1 Primary map



X



Y

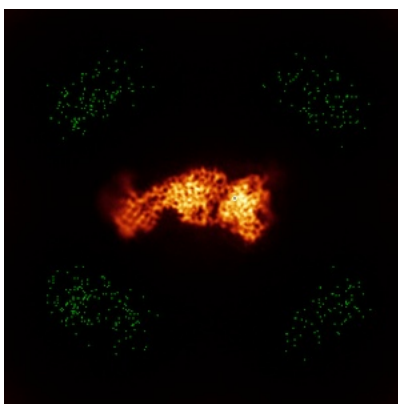


Z

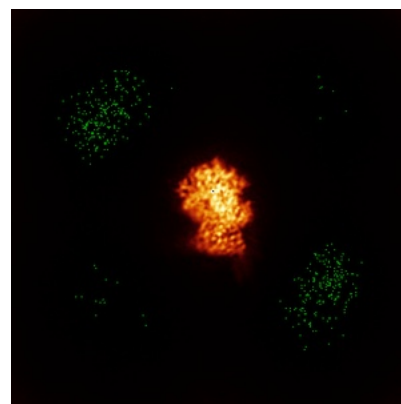
6.4.2 Raw map



X



Y

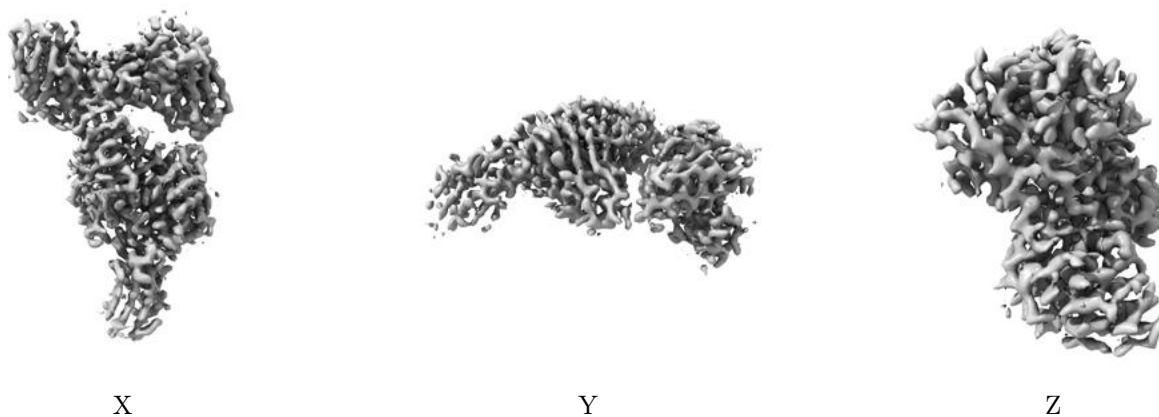


Z

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



The images above show the 3D surface view of the map at the recommended contour level 1.4. 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



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.

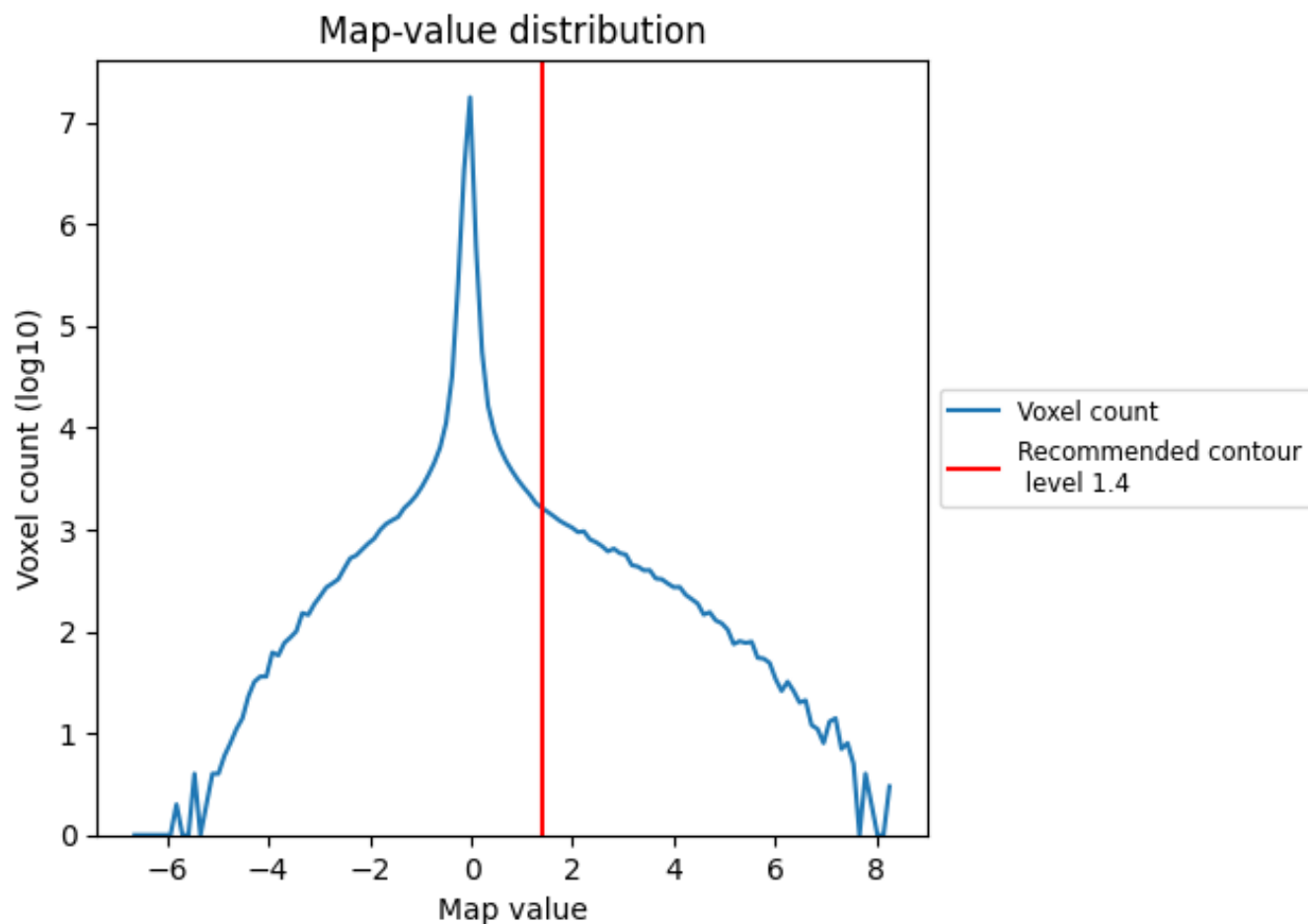
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

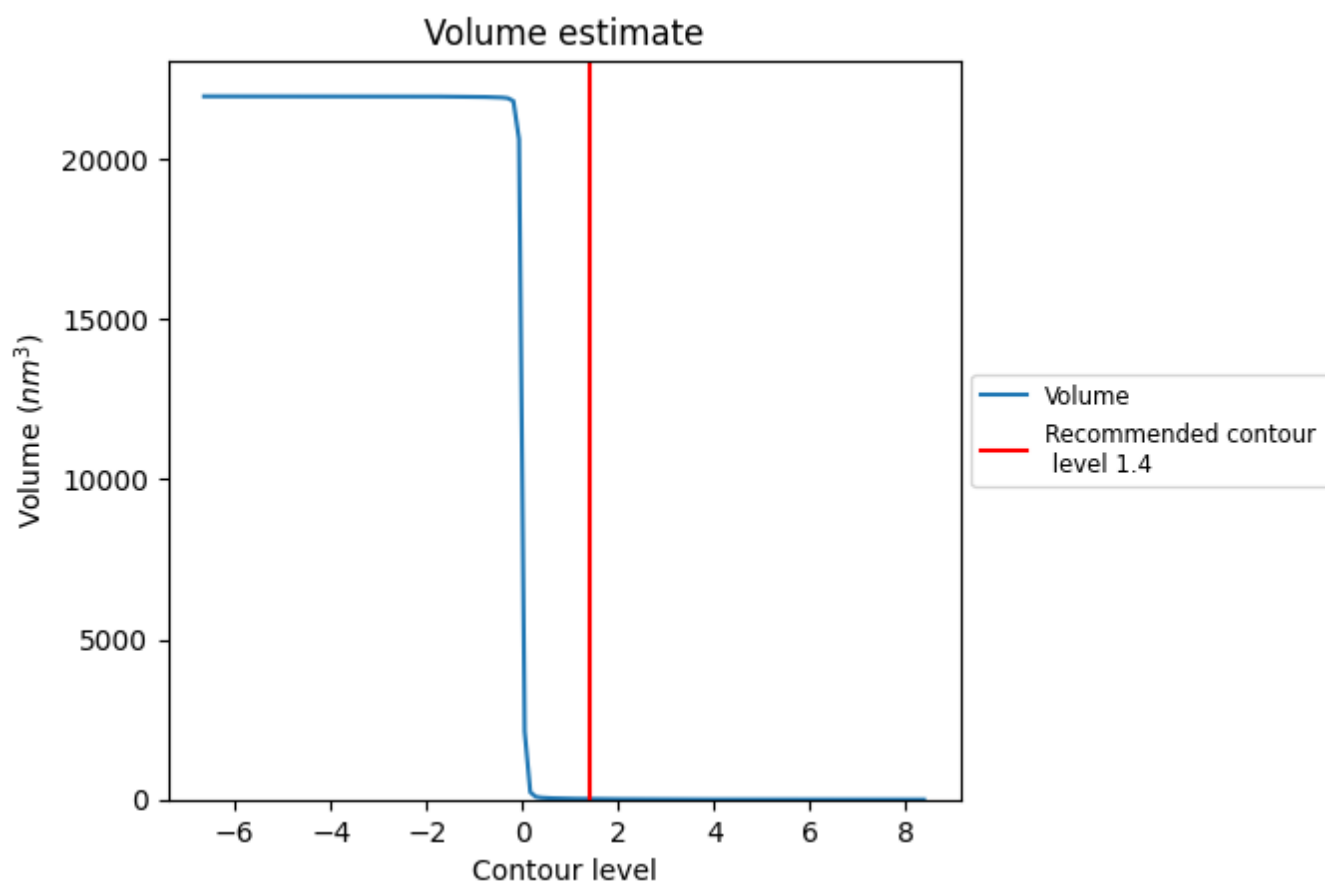
This section contains the results of statistical analysis of the map.

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.

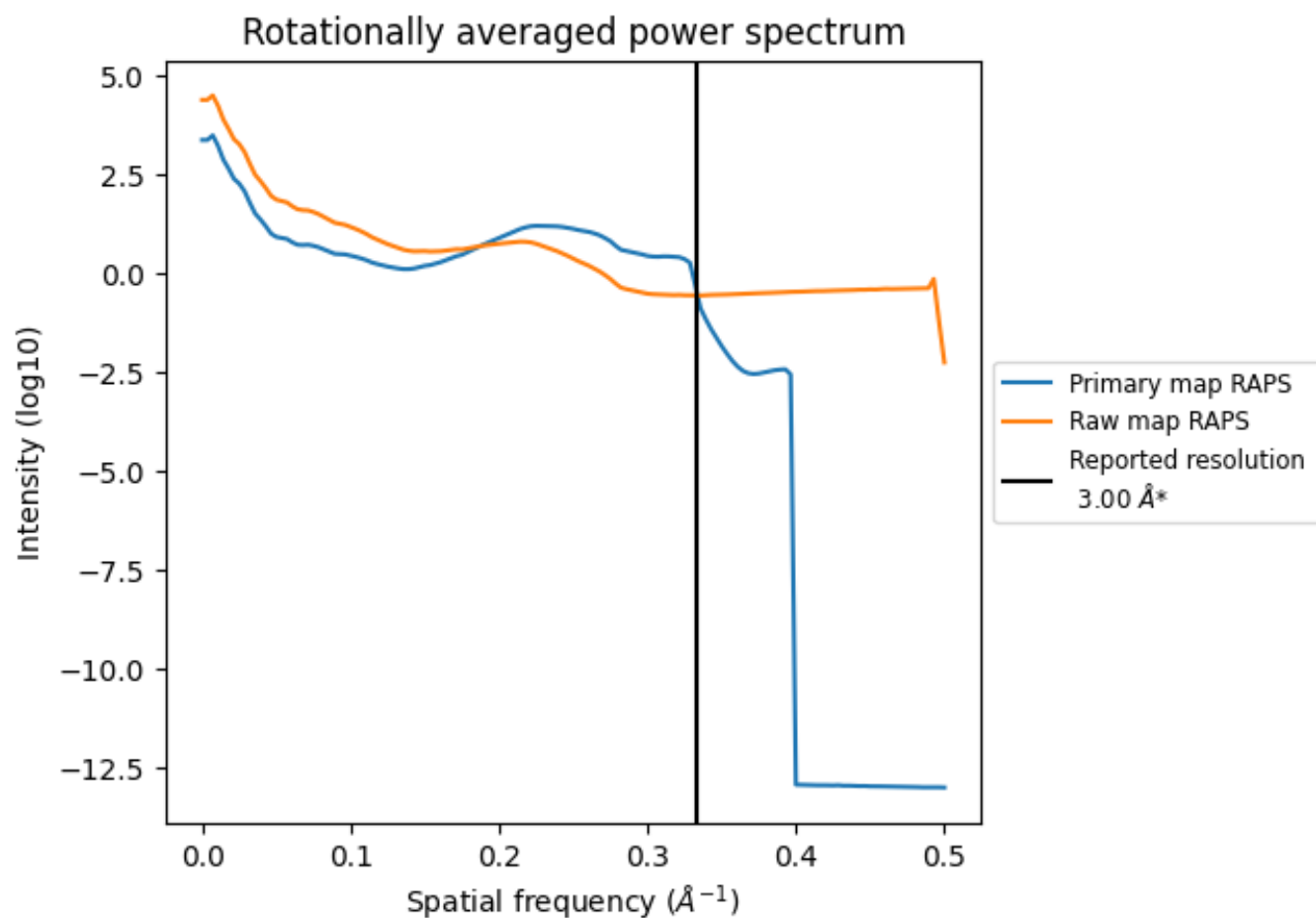
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 20 nm³; this corresponds to an approximate mass of 18 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 ⓘ

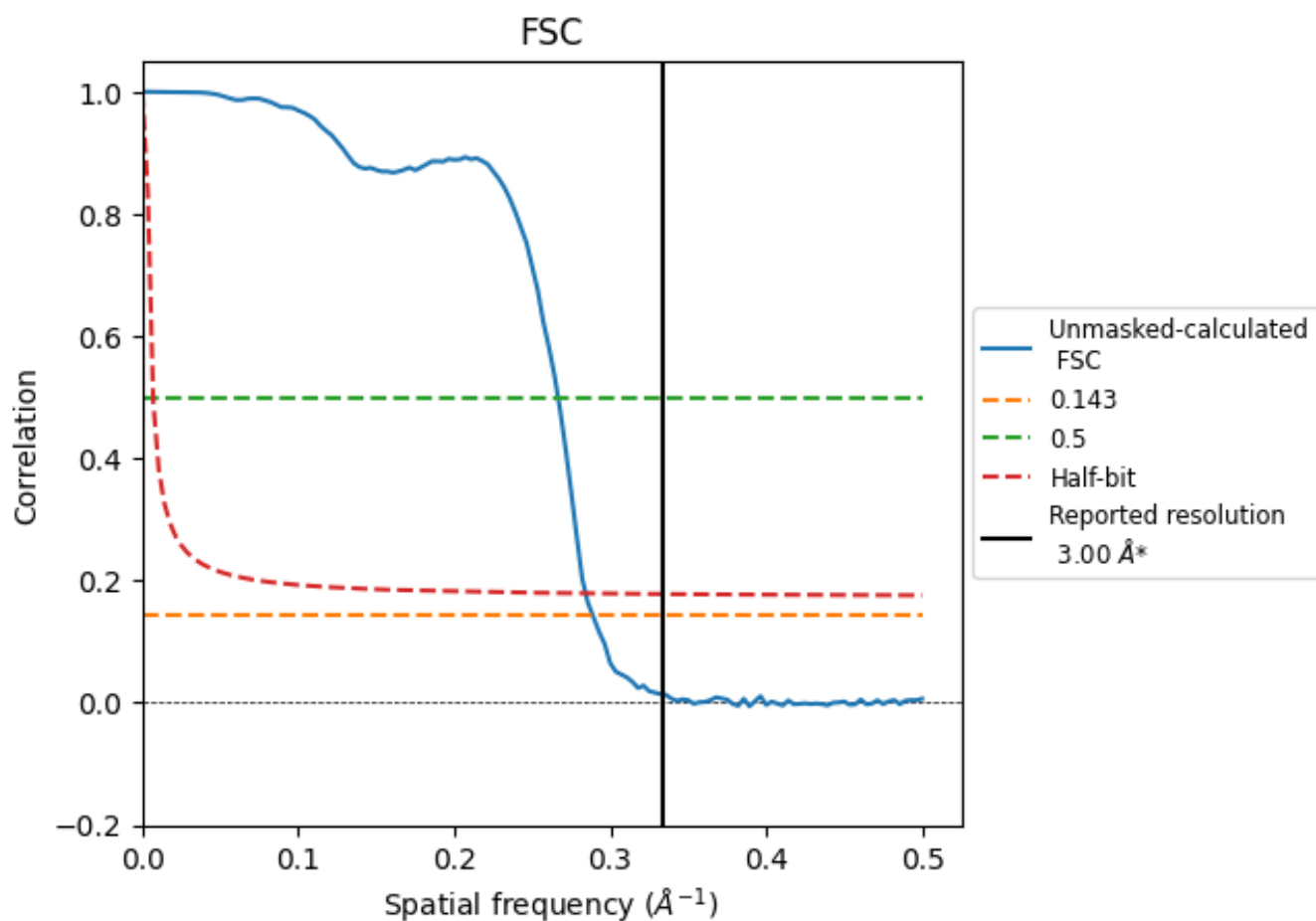


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.46	3.75	3.52

*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 3.46 differs from the reported value 3.0 by more than 10 %

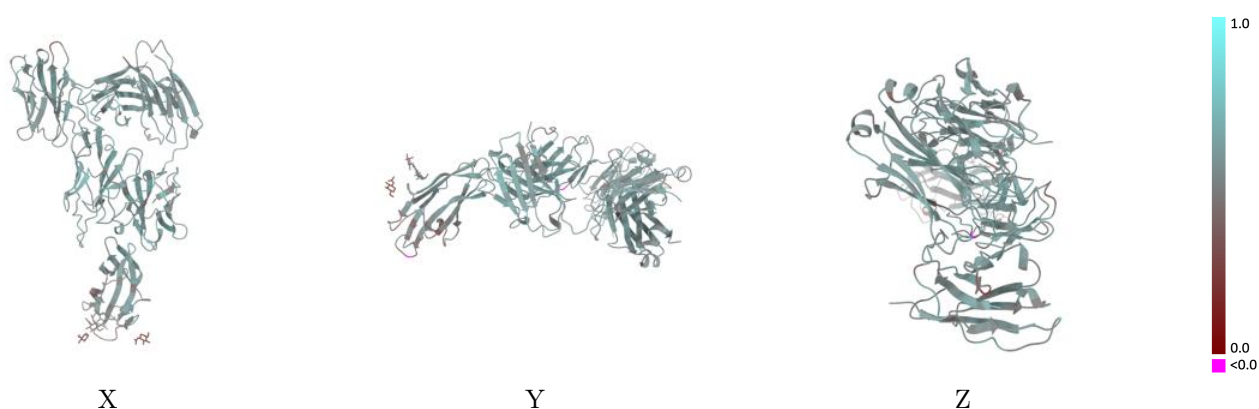
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44103 and PDB model 9B2C. 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](#)

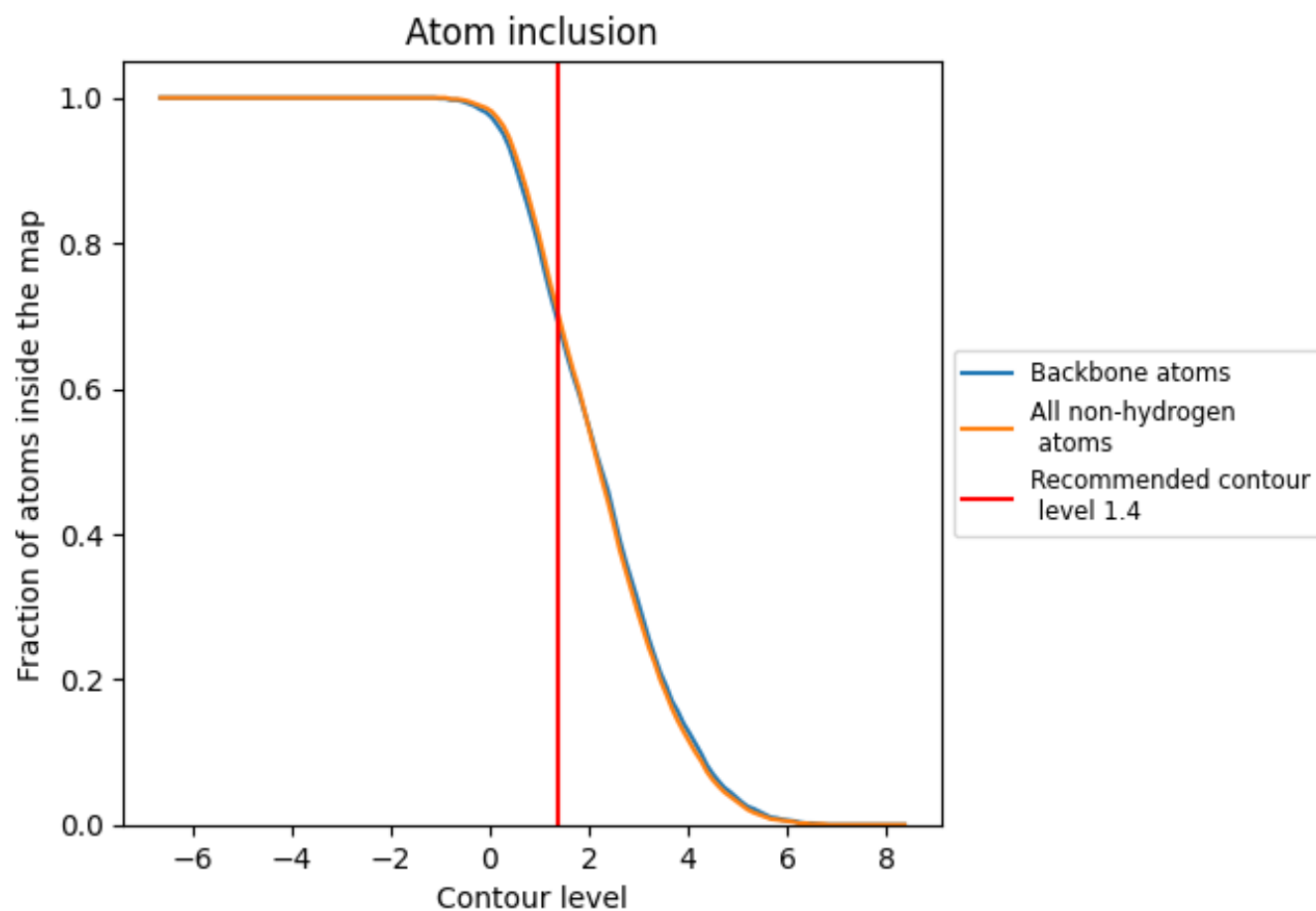


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 70% 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 (1.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6980	0.5480
A	0.4670	0.4960
B	0.1540	0.4460
H	0.7680	0.5650
L	0.7780	0.5650
N	0.6610	0.5410

