



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 03:11 AM JST

PDB ID : 22HG / pdb_000022hg
EMDB ID : EMD-68270
Title : SARS-CoV-2 BA.3.2.2(RE.2.2) RBD in complex with human ACE2 and monoclonal antibody S2H97
Authors : Li, L.J.; Qu, H.; Wu, Q.L.; Gao, G.F.
Deposited on : 2026-01-10
Resolution : 2.61 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:

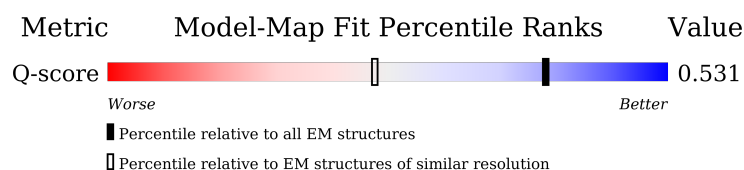
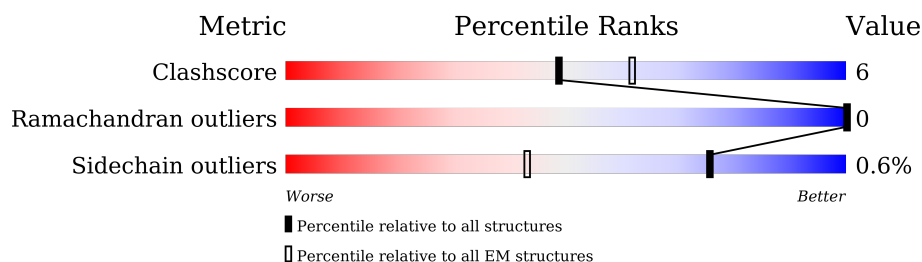
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.61 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	8735 (2.11 - 3.11)

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	186	
2	B	588	
3	I	119	
4	M	112	

Continued on next page...

Mol	Chain	Length	Quality of chain
5	C	3	67% 67% 33%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8224 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 protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	186	Total	C	N	O	S	0	0
			1519	987	249	276	7		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	339	TYR	GLY	conflict	UNP P0DTC2
A	348	PRO	ALA	conflict	UNP P0DTC2
A	356	THR	LYS	conflict	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	403	LYS	ARG	conflict	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	435	SER	ALA	conflict	UNP P0DTC2
A	440	ARG	ASN	conflict	UNP P0DTC2
A	445	ALA	VAL	conflict	UNP P0DTC2
A	446	ASP	GLY	conflict	UNP P0DTC2
A	452	TRP	LEU	conflict	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	ASN	THR	conflict	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2

- Molecule 2 is a protein called Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	588	Total	C	N	O	S	0	0
			4797	3069	796	903	29		

- Molecule 3 is a protein called Heavy chain of monoclonal antibody S2H97.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	119	Total	C	N	O	S	0	0
			953	613	153	182	5		

- Molecule 4 is a protein called Light chain of monoclonal antibody S2H97.

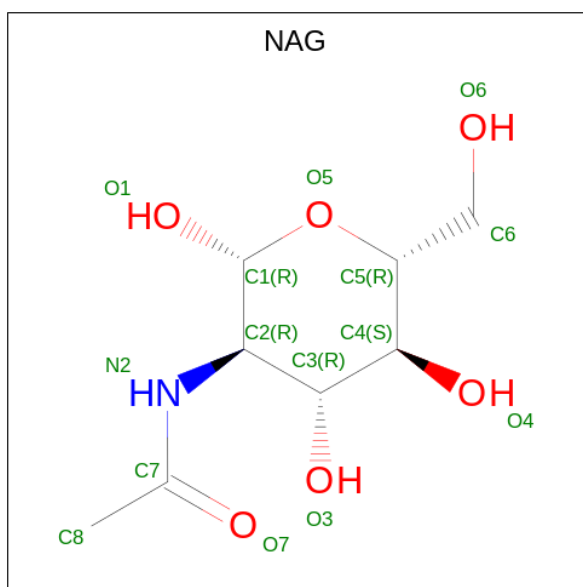
Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	112	Total	C	N	O	S	0	0
			817	505	135	174	3		

- 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	C	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: C₈H₁₅NO₆).



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

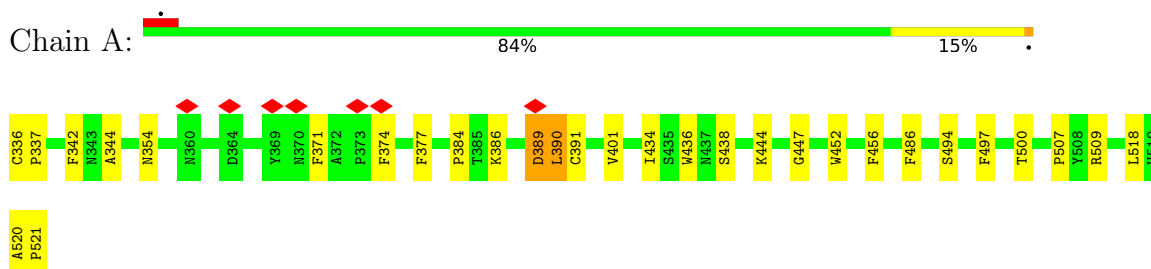
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	B	1	Total	Zn	0
			1	1	

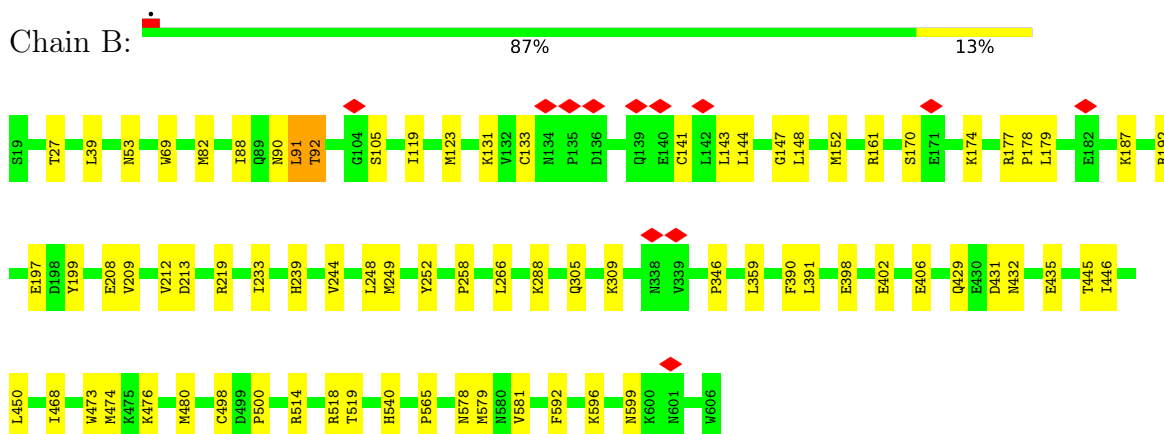
3 Residue-property plots

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.

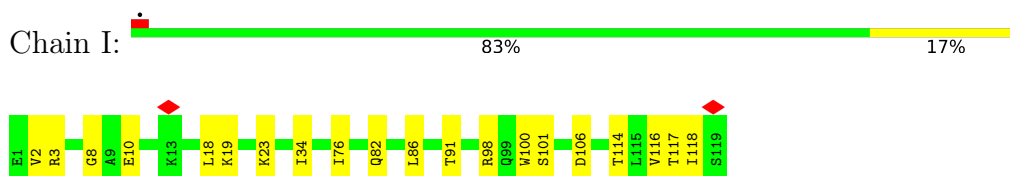
- Molecule 1: Spike protein S1



- Molecule 2: Processed angiotensin-converting enzyme 2

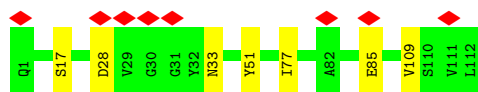


- Molecule 3: Heavy chain of monoclonal antibody S2H97



- Molecule 4: Light chain of monoclonal antibody S2H97





- 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	400633	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.243	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	334.4, 334.4, 334.4	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.76, 0.76, 0.76	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, ZN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/1570	0.72	3/2139 (0.1%)
2	B	0.26	0/4930	0.49	6/6695 (0.1%)
3	I	0.14	0/982	0.35	0/1332
4	M	0.13	0/835	0.35	0/1138
All	All	0.27	0/8317	0.52	9/11304 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	92	THR	N-CA-C	-13.42	93.74	112.13
2	B	213	ASP	N-CA-C	-8.47	99.61	110.53
1	A	390	LEU	N-CA-CB	-8.14	97.09	110.52
2	B	53	ASN	CA-CB-CG	7.34	119.94	112.60
1	A	390	LEU	N-CA-C	6.32	120.12	109.76
2	B	91	LEU	CB-CA-C	-6.29	97.04	110.76
2	B	147	GLY	CA-C-O	-6.21	116.61	122.39
1	A	389	ASP	N-CA-C	-5.86	100.47	108.38
2	B	212	VAL	N-CA-C	-5.38	100.00	107.80

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	1519	0	1426	29	0
2	B	4797	0	4581	52	0
3	I	953	0	907	13	0
4	M	817	0	781	6	0
5	C	39	0	34	0	0
6	A	28	0	26	5	0
6	B	70	0	65	0	0
7	B	1	0	0	0	0
All	All	8224	0	7820	93	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 6.

All (93) 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:B:144:LEU:HD12	2:B:148:LEU:CD2	1.64	1.26
2:B:144:LEU:CD1	2:B:148:LEU:HD23	1.66	1.23
1:A:486:PHE:CE1	2:B:82:MET:SD	2.60	0.95
1:A:436:TRP:CZ2	6:A:602:NAG:H83	2.04	0.92
2:B:144:LEU:HD12	2:B:148:LEU:HD23	0.91	0.91
2:B:144:LEU:CD1	2:B:148:LEU:CD2	2.39	0.85
1:A:436:TRP:HZ2	6:A:602:NAG:H83	1.42	0.82
1:A:342:PHE:HB3	6:A:602:NAG:H2	1.61	0.82
1:A:390:LEU:HD12	1:A:390:LEU:O	1.80	0.81
2:B:133:CYS:HA	2:B:141:CYS:HB2	1.68	0.76
1:A:486:PHE:CD1	2:B:82:MET:SD	2.87	0.68
1:A:456:PHE:CE1	2:B:27:THR:HG23	2.29	0.67
2:B:305:GLN:O	2:B:309:LYS:HG2	1.94	0.66
1:A:389:ASP:OD1	1:A:389:ASP:C	2.39	0.66
2:B:474:MET:HE1	2:B:500:PRO:HD2	1.78	0.65
2:B:402:GLU:HB3	2:B:518:ARG:HD3	1.77	0.65
4:M:28:ASP:H	4:M:33:ASN:HD21	1.46	0.63
1:A:518:LEU:HD21	3:I:101:SER:HB3	1.82	0.62
3:I:8:GLY:HA2	3:I:114:THR:HG23	1.83	0.61
2:B:208:GLU:OE1	2:B:219:ARG:NH2	2.34	0.60
2:B:406:GLU:HG3	2:B:518:ARG:HH11	1.66	0.59
1:A:444:LYS:HG3	1:A:447:GLY:H	1.68	0.59
2:B:192:ARG:NH1	2:B:197:GLU:O	2.34	0.59
3:I:23:LYS:NZ	3:I:76:ILE:O	2.37	0.58
2:B:239:HIS:HD2	2:B:599:ASN:HD21	1.52	0.58
1:A:374:PHE:HD2	1:A:436:TRP:HA	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:435:GLU:OE2	2:B:540:HIS:NE2	2.36	0.57
2:B:144:LEU:HA	2:B:148:LEU:HB3	1.87	0.56
2:B:131:LYS:HG2	2:B:143:LEU:HG	1.87	0.55
2:B:233:ILE:HD11	2:B:581:VAL:HG21	1.89	0.54
2:B:592:PHE:O	2:B:596:LYS:HG2	2.10	0.52
1:A:497:PHE:CG	1:A:507:PRO:HG3	2.45	0.52
3:I:10:GLU:HG2	3:I:18:LEU:HD21	1.92	0.52
2:B:144:LEU:HD13	2:B:148:LEU:CD2	2.38	0.51
1:A:371:PHE:CD2	6:A:602:NAG:H3	2.45	0.51
1:A:438:SER:OG	1:A:507:PRO:O	2.26	0.51
2:B:578:ASN:OD1	2:B:579:MET:N	2.40	0.51
2:B:239:HIS:CD2	2:B:599:ASN:HD21	2.28	0.50
2:B:288:LYS:NZ	2:B:429:GLN:HE22	2.09	0.50
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.94	0.50
2:B:123:MET:HE3	2:B:179:LEU:HG	1.93	0.50
4:M:17:SER:HA	4:M:77:ILE:O	2.13	0.49
1:A:436:TRP:CZ2	6:A:602:NAG:C8	2.89	0.49
3:I:91:THR:HG23	3:I:117:THR:HA	1.94	0.49
2:B:431:ASP:OD1	2:B:432:ASN:N	2.41	0.49
1:A:390:LEU:HD12	1:A:390:LEU:C	2.39	0.48
2:B:90:ASN:O	2:B:91:LEU:HB2	2.13	0.48
2:B:249:MET:HE1	2:B:258:PRO:HA	1.94	0.48
2:B:445:THR:HG23	2:B:446:ILE:HG13	1.95	0.48
2:B:119:ILE:HG23	2:B:179:LEU:HG	1.97	0.47
2:B:152:MET:O	2:B:161:ARG:NH2	2.47	0.47
4:M:28:ASP:N	4:M:33:ASN:HD21	2.11	0.46
2:B:209:VAL:HG21	2:B:565:PRO:HB3	1.98	0.46
3:I:2:VAL:O	3:I:3:ARG:NE	2.47	0.46
2:B:144:LEU:CD1	2:B:148:LEU:HD21	2.37	0.46
3:I:91:THR:HA	3:I:116:VAL:O	2.16	0.46
3:I:34:ILE:HD13	3:I:98:ARG:HG3	1.99	0.45
1:A:377:PHE:HD1	1:A:434:ILE:HG12	1.81	0.45
1:A:518:LEU:HD22	3:I:100:TRP:CD1	2.52	0.45
1:A:520:ALA:O	1:A:521:PRO:C	2.58	0.45
2:B:170:SER:HA	2:B:174:LYS:NZ	2.32	0.44
1:A:452:TRP:CZ3	1:A:494:SER:HB3	2.52	0.44
1:A:344:ALA:O	1:A:509:ARG:NH2	2.44	0.44
2:B:177:ARG:HB2	2:B:498:CYS:HB2	2.00	0.44
2:B:244:VAL:HG13	2:B:248:LEU:HD13	2.00	0.44
3:I:19:LYS:HZ1	3:I:82:GLN:CD	2.19	0.43
1:A:374:PHE:O	1:A:374:PHE:CG	2.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:106:ASP:OD2	4:M:51:TYR:HB2	2.19	0.43
2:B:346:PRO:HA	2:B:359:LEU:O	2.19	0.43
2:B:474:MET:HE3	2:B:498:CYS:HA	2.00	0.43
1:A:384:PRO:HA	1:A:386:LYS:HZ2	1.82	0.43
3:I:86:LEU:HD13	3:I:118:ILE:HD11	2.00	0.43
3:I:19:LYS:NZ	3:I:82:GLN:OE1	2.25	0.43
2:B:177:ARG:HB3	2:B:178:PRO:HD3	2.00	0.42
2:B:39:LEU:HB3	2:B:69:TRP:HE3	1.85	0.42
4:M:85:GLU:HA	4:M:109:VAL:HG13	2.02	0.42
1:A:336:CYS:HB3	1:A:337:PRO:CD	2.50	0.42
1:A:486:PHE:CZ	2:B:82:MET:SD	3.09	0.42
2:B:233:ILE:HD11	2:B:581:VAL:CG2	2.48	0.41
2:B:119:ILE:HA	2:B:179:LEU:HD11	2.01	0.41
2:B:450:LEU:HD21	2:B:519:THR:HG21	2.02	0.41
1:A:336:CYS:HB3	1:A:337:PRO:HD3	2.02	0.41
2:B:252:TYR:CE2	2:B:266:LEU:HD22	2.55	0.41
2:B:390:PHE:HD2	2:B:391:LEU:HD22	1.85	0.41
2:B:406:GLU:HG3	2:B:518:ARG:HD2	2.02	0.41
2:B:398:GLU:HG3	2:B:514:ARG:HG2	2.02	0.41
4:M:85:GLU:O	4:M:85:GLU:HG2	2.22	0.40
1:A:390:LEU:H	1:A:390:LEU:HG	1.68	0.40
2:B:187:LYS:HD2	2:B:199:TYR:CE1	2.56	0.40
1:A:384:PRO:HA	1:A:386:LYS:NZ	2.36	0.40
2:B:105:SER:O	2:B:105:SER:OG	2.34	0.40
2:B:476:LYS:HB3	2:B:480:MET:HE3	2.04	0.40
2:B:468:ILE:HG22	2:B:473:TRP:HD1	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/186 (99%)	165 (90%)	19 (10%)	0	100	100
2	B	586/588 (100%)	564 (96%)	22 (4%)	0	100	100
3	I	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
4	M	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
All	All	997/1005 (99%)	950 (95%)	47 (5%)	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	165/165 (100%)	162 (98%)	3 (2%)	51	75
2	B	519/519 (100%)	517 (100%)	2 (0%)	84	92
3	I	102/102 (100%)	102 (100%)	0	100	100
4	M	95/95 (100%)	95 (100%)	0	100	100
All	All	881/881 (100%)	876 (99%)	5 (1%)	76	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	354	ASN
1	A	391	CYS
1	A	500	THR
2	B	88	ILE
2	B	92	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	388	ASN
1	A	394	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	477	ASN
2	B	51	ASN
2	B	325	GLN
2	B	340	GLN
2	B	429	GLN
2	B	599	ASN
3	I	67	GLN
4	M	33	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

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	C	1	2,5	14,14,15	0.41	0	17,19,21	0.83	1 (5%)
5	NAG	C	2	5	14,14,15	0.38	0	17,19,21	0.48	0
5	BMA	C	3	5	11,11,12	0.32	0	15,15,17	0.47	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	C	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
5	BMA	C	3	5	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	NAG	C1-O5-C5	2.26	115.26	112.19

There are no chirality outliers.

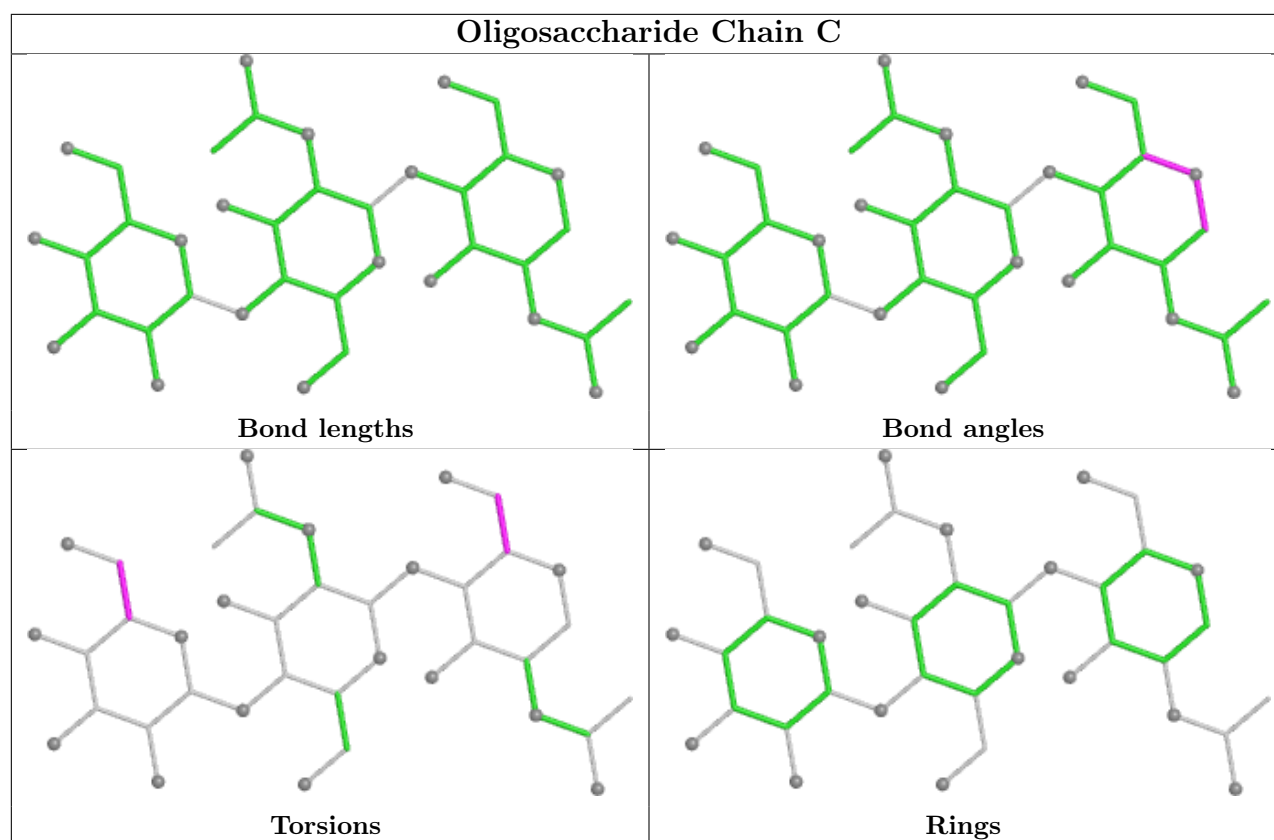
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1	NAG	C4-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6
5	C	3	BMA	O5-C5-C6-O6

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 [i](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

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	601	1	14,14,15	0.41	0	17,19,21	0.60	0
6	NAG	B	703	2	14,14,15	0.39	0	17,19,21	0.62	0
6	NAG	A	602	1	14,14,15	0.37	0	17,19,21	1.52	3 (17%)
6	NAG	B	705	2	14,14,15	0.37	0	17,19,21	0.43	0
6	NAG	B	701	2	14,14,15	0.40	0	17,19,21	0.51	0
6	NAG	B	702	2	14,14,15	0.38	0	17,19,21	0.99	1 (5%)
6	NAG	B	704	2	14,14,15	0.40	0	17,19,21	0.65	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	601	1	-	3/6/23/26	0/1/1/1
6	NAG	B	703	2	-	4/6/23/26	0/1/1/1
6	NAG	A	602	1	-	4/6/23/26	0/1/1/1
6	NAG	B	705	2	-	3/6/23/26	0/1/1/1
6	NAG	B	701	2	-	2/6/23/26	0/1/1/1
6	NAG	B	702	2	-	3/6/23/26	0/1/1/1
6	NAG	B	704	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	602	NAG	C2-N2-C7	4.63	129.50	122.90
6	B	702	NAG	C2-N2-C7	3.58	128.00	122.90
6	A	602	NAG	C1-C2-N2	3.02	115.65	110.49
6	A	602	NAG	C1-O5-C5	2.57	115.68	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	601	NAG	C3-C2-N2-C7
6	A	601	NAG	C8-C7-N2-C2
6	A	601	NAG	O7-C7-N2-C2
6	A	602	NAG	C3-C2-N2-C7
6	A	602	NAG	C8-C7-N2-C2
6	A	602	NAG	O7-C7-N2-C2
6	B	705	NAG	C8-C7-N2-C2
6	B	705	NAG	O7-C7-N2-C2
6	B	701	NAG	C8-C7-N2-C2
6	B	701	NAG	O7-C7-N2-C2
6	B	703	NAG	C1-C2-N2-C7
6	B	705	NAG	O5-C5-C6-O6
6	A	602	NAG	C1-C2-N2-C7
6	B	702	NAG	C3-C2-N2-C7
6	B	702	NAG	C8-C7-N2-C2
6	B	703	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B	703	NAG	O7-C7-N2-C2
6	B	703	NAG	C3-C2-N2-C7
6	B	702	NAG	O7-C7-N2-C2
6	B	704	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	602	NAG	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

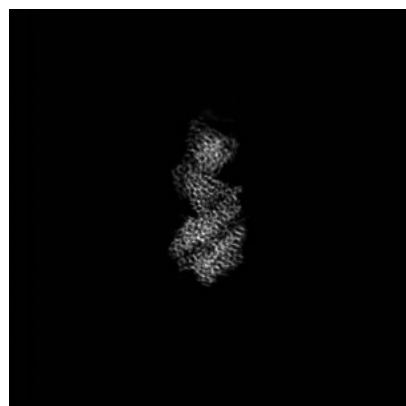
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68270. These allow visual inspection of the internal detail of the map and identification of artifacts.

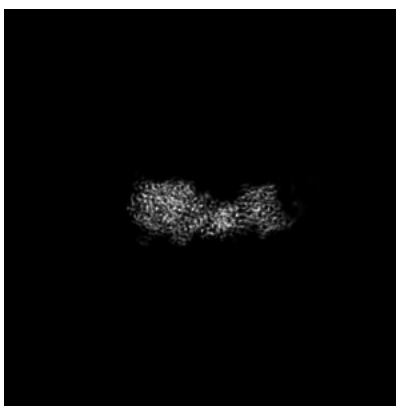
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

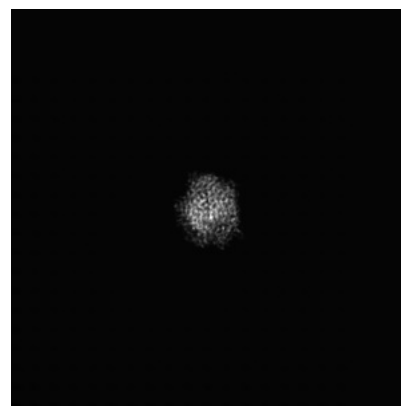
6.1.1 Primary map



X

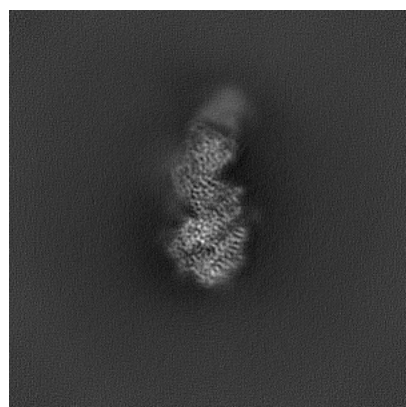


Y

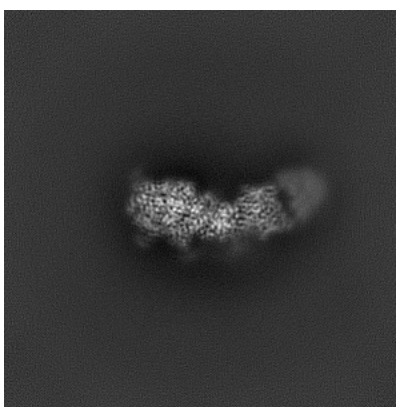


Z

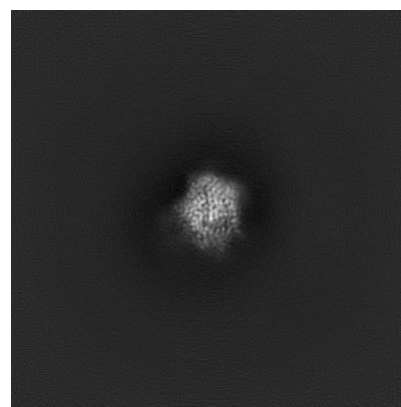
6.1.2 Raw map



X



Y

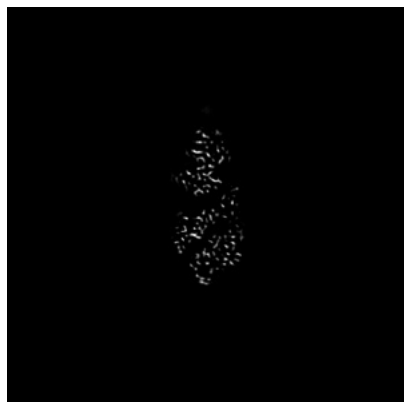


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 220

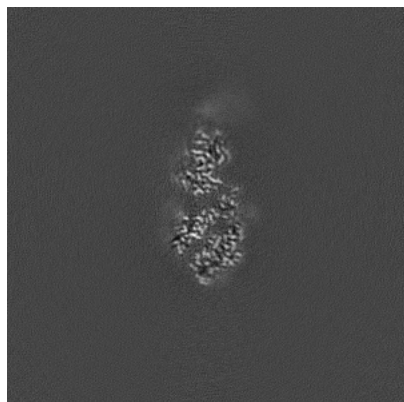


Y Index: 220

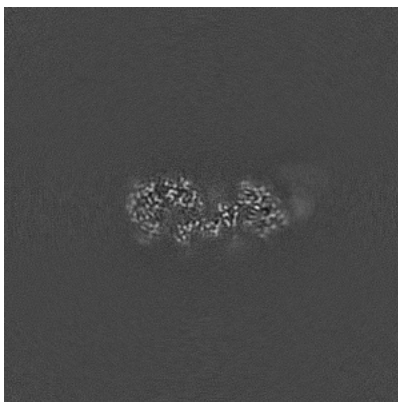


Z Index: 220

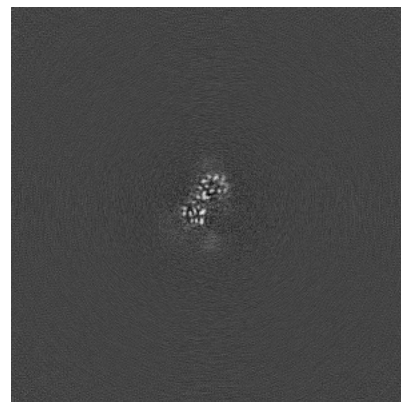
6.2.2 Raw map



X Index: 220



Y Index: 220



Z Index: 220

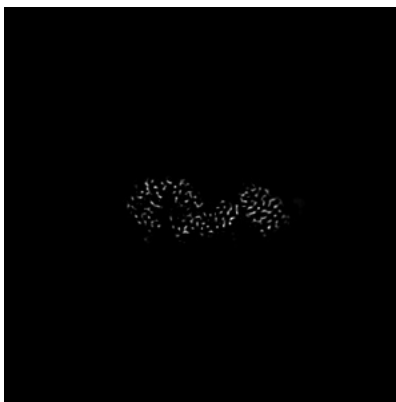
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

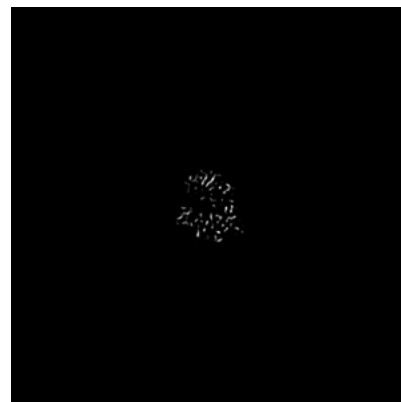
6.3.1 Primary map



X Index: 219

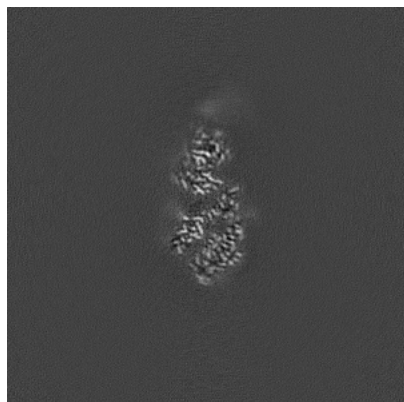


Y Index: 216

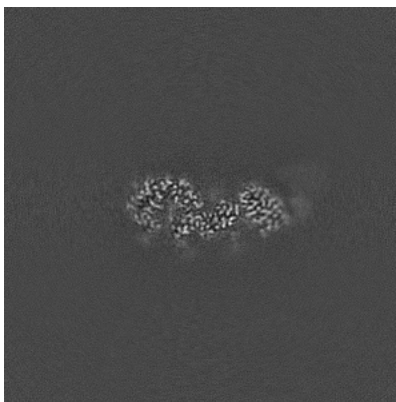


Z Index: 187

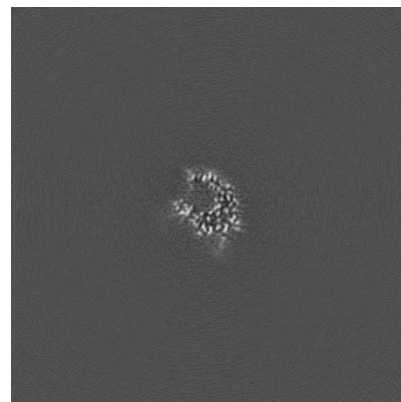
6.3.2 Raw map



X Index: 219



Y Index: 216

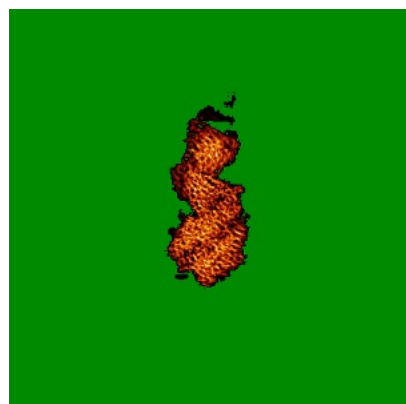


Z Index: 193

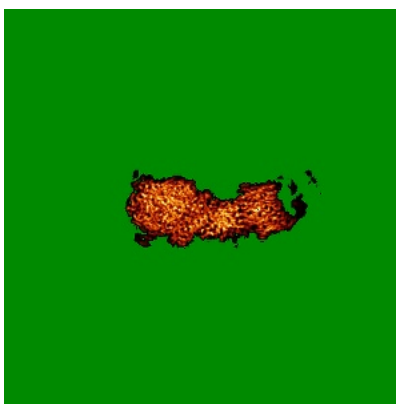
The images above show the largest variance slices of the map in three orthogonal directions.

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

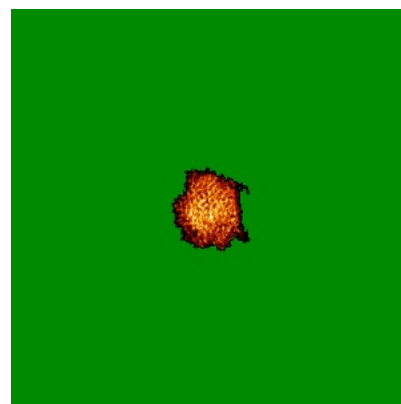
6.4.1 Primary map



X

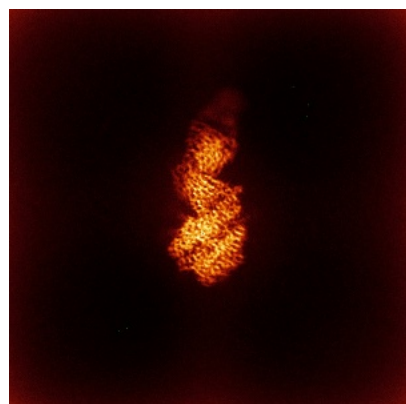


Y

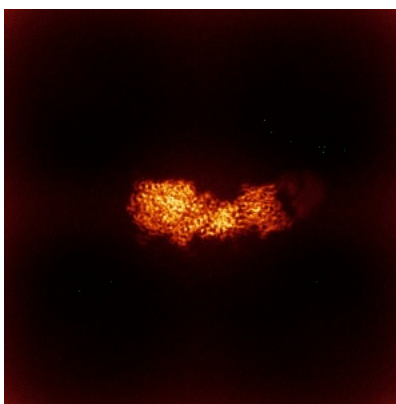


Z

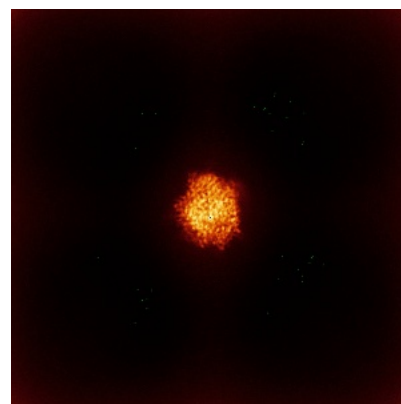
6.4.2 Raw map



X



Y

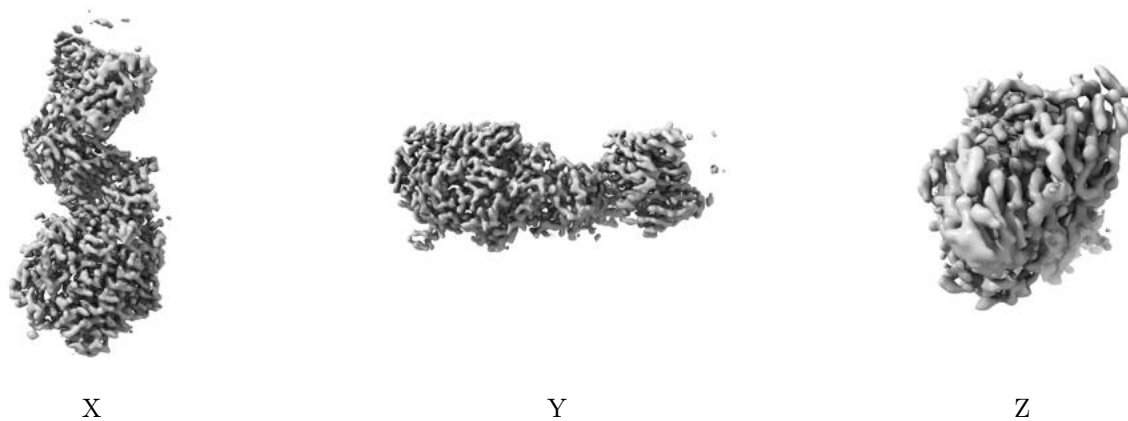


Z

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.

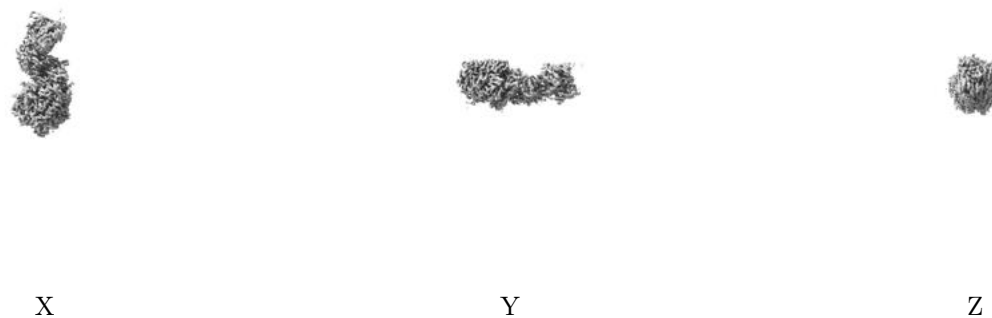
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

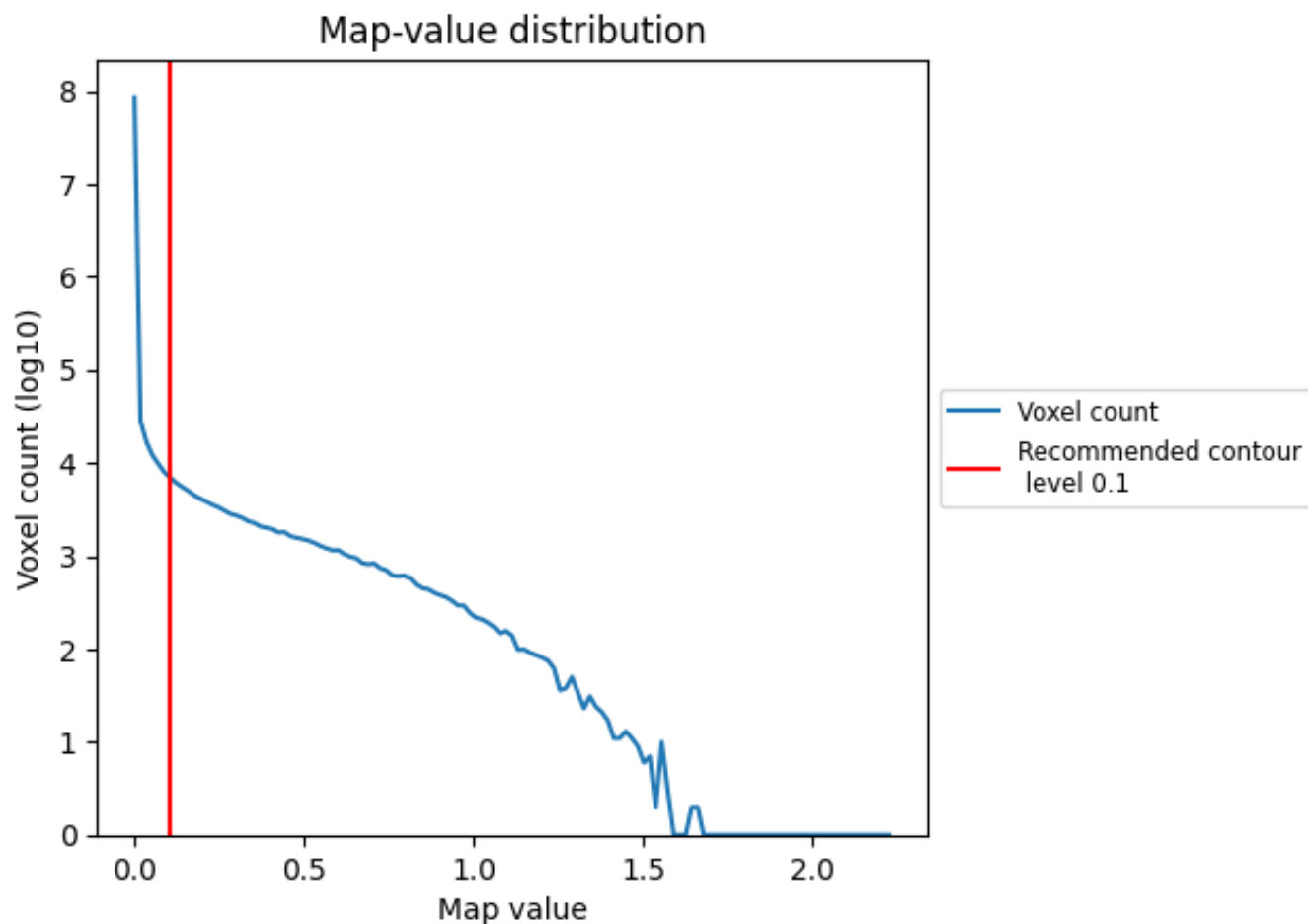
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

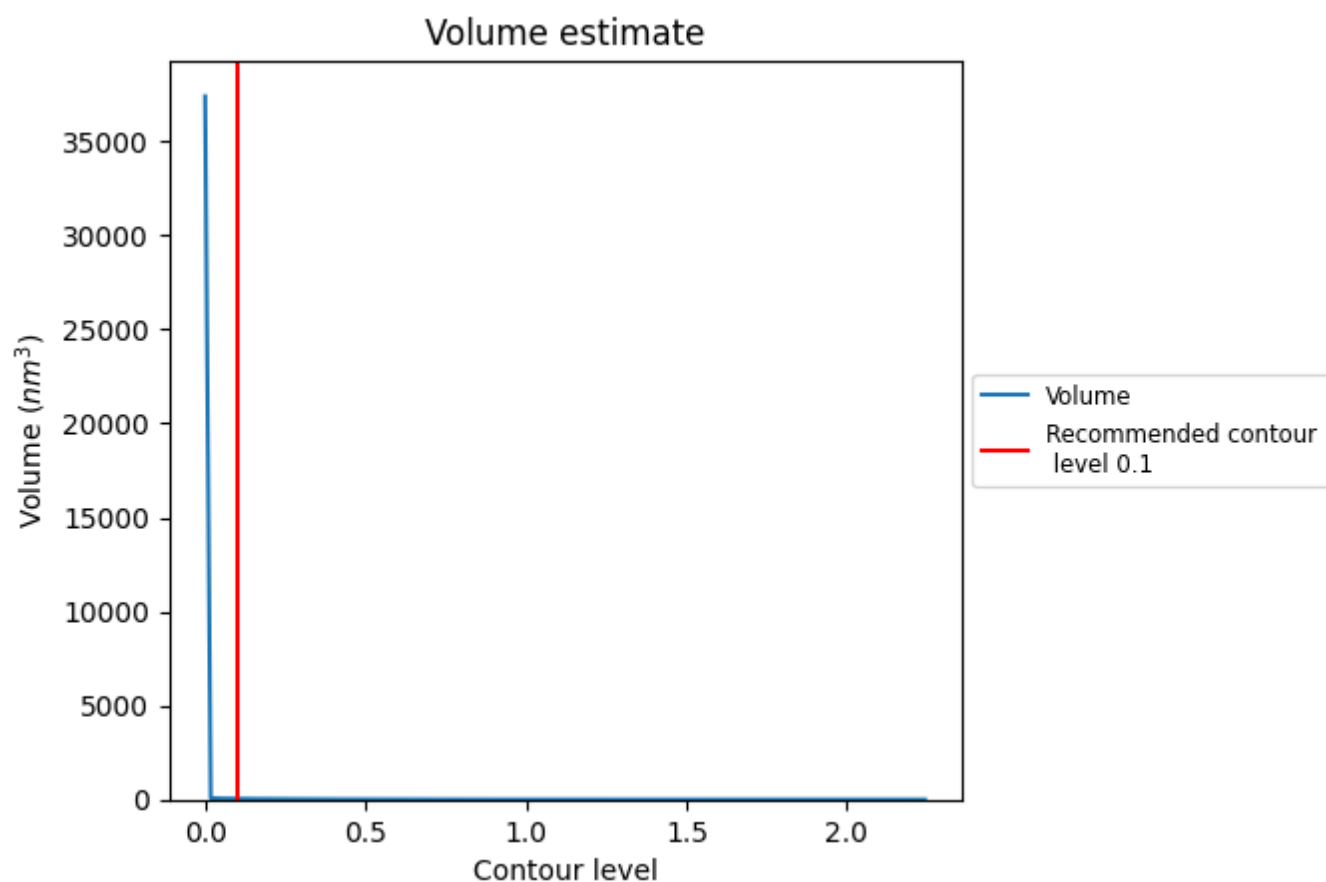
This section contains the results of statistical analysis of the map.

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.

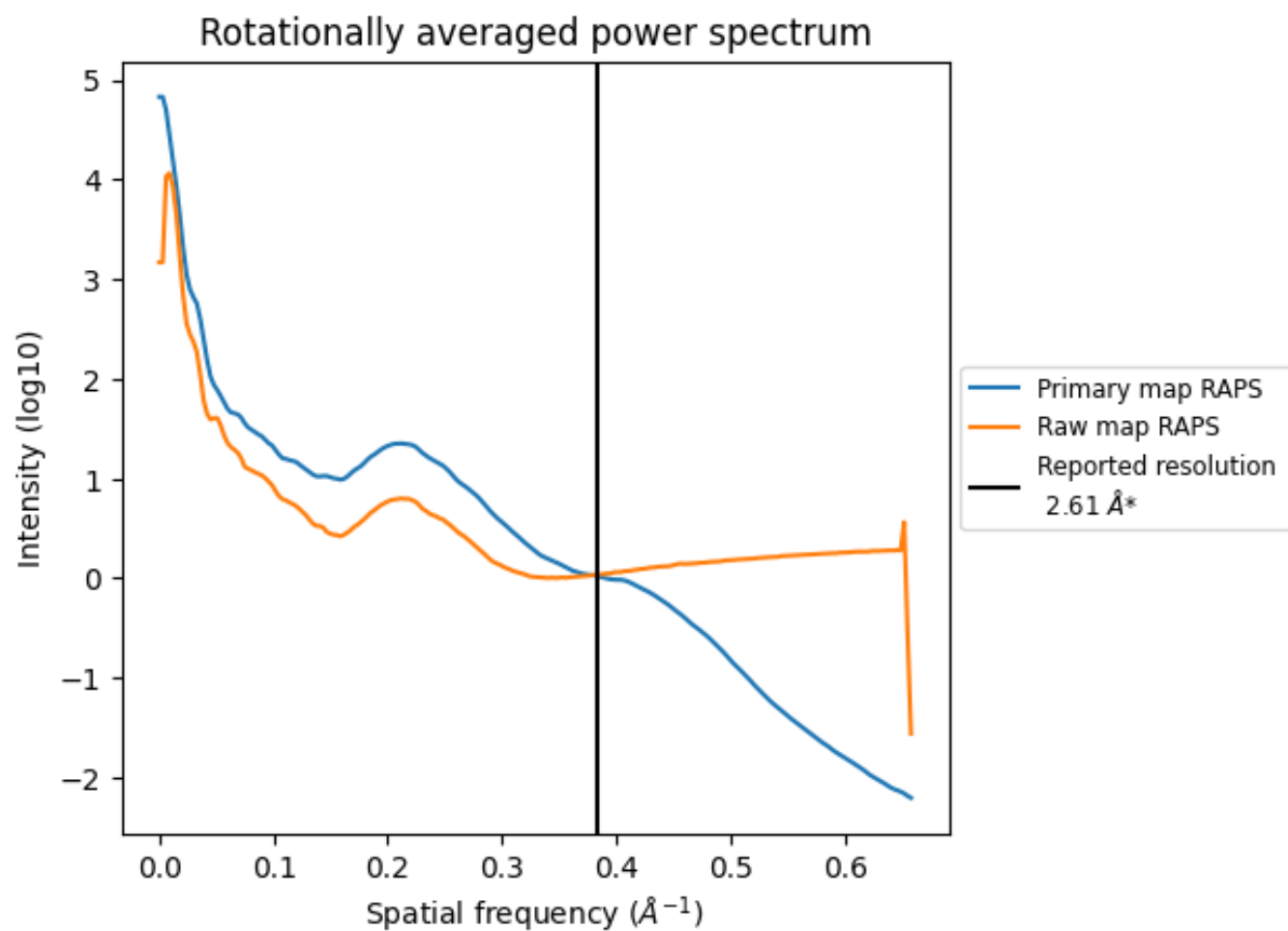
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 43 nm^3 ; this corresponds to an approximate mass of 39 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

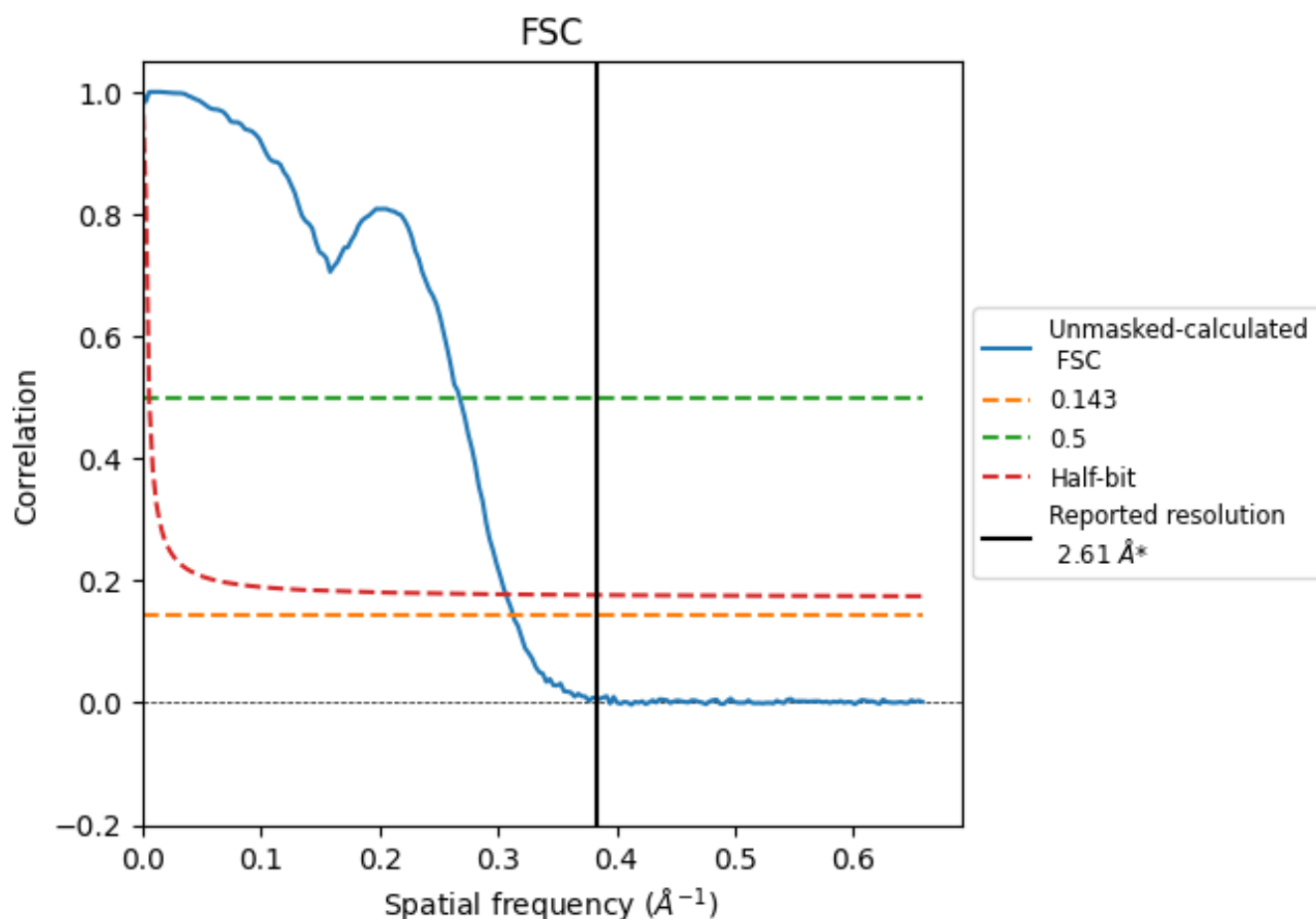


*Reported resolution corresponds to spatial frequency of $0.383 \text{ \AA}^{-1}$

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 0.383 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

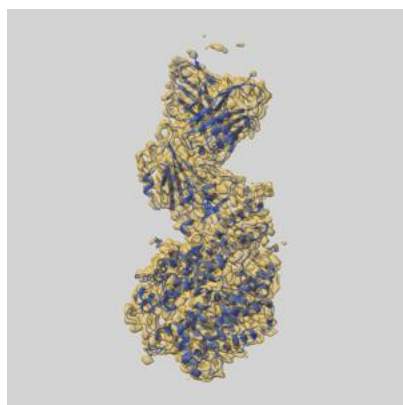
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.61	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.20	3.74	3.26

*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 3.20 differs from the reported value 2.61 by more than 10 %

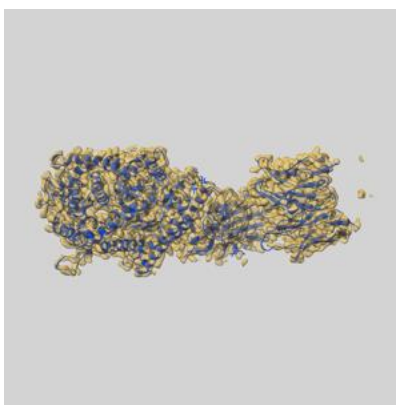
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-68270 and PDB model 22HG. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

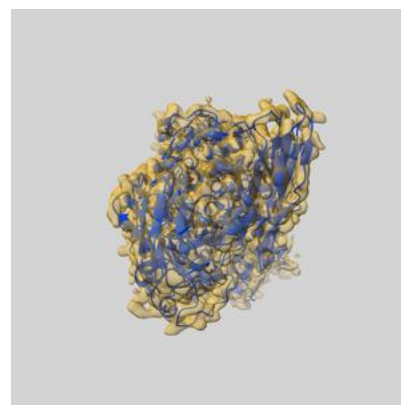
9.1 Map-model overlay [i](#)



X



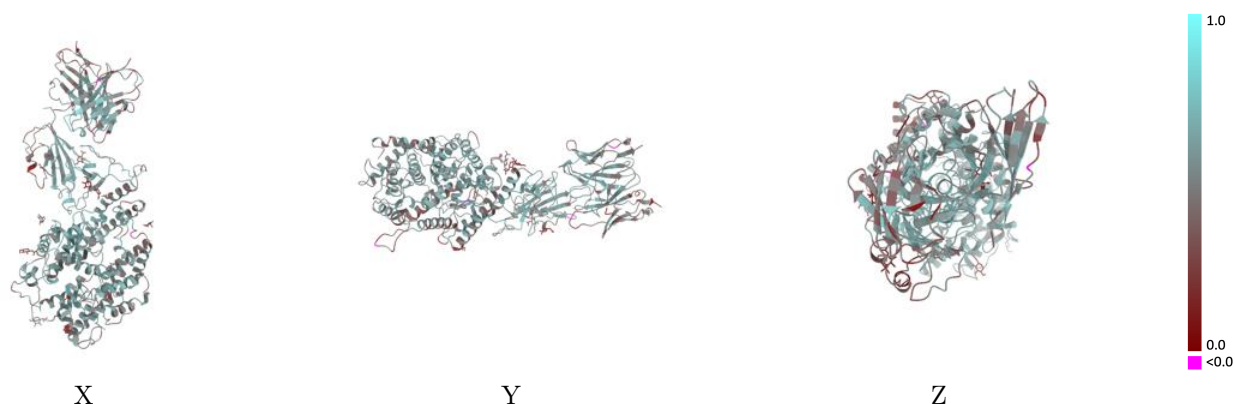
Y



Z

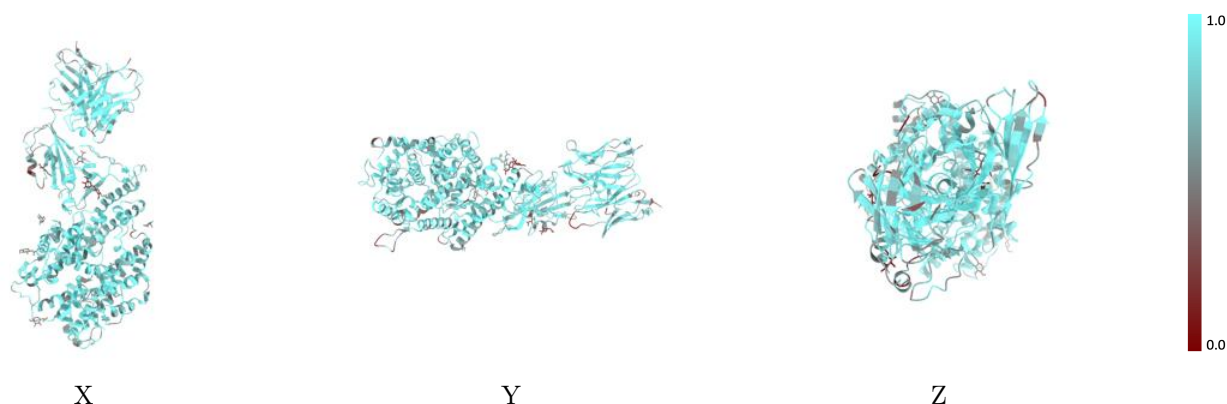
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



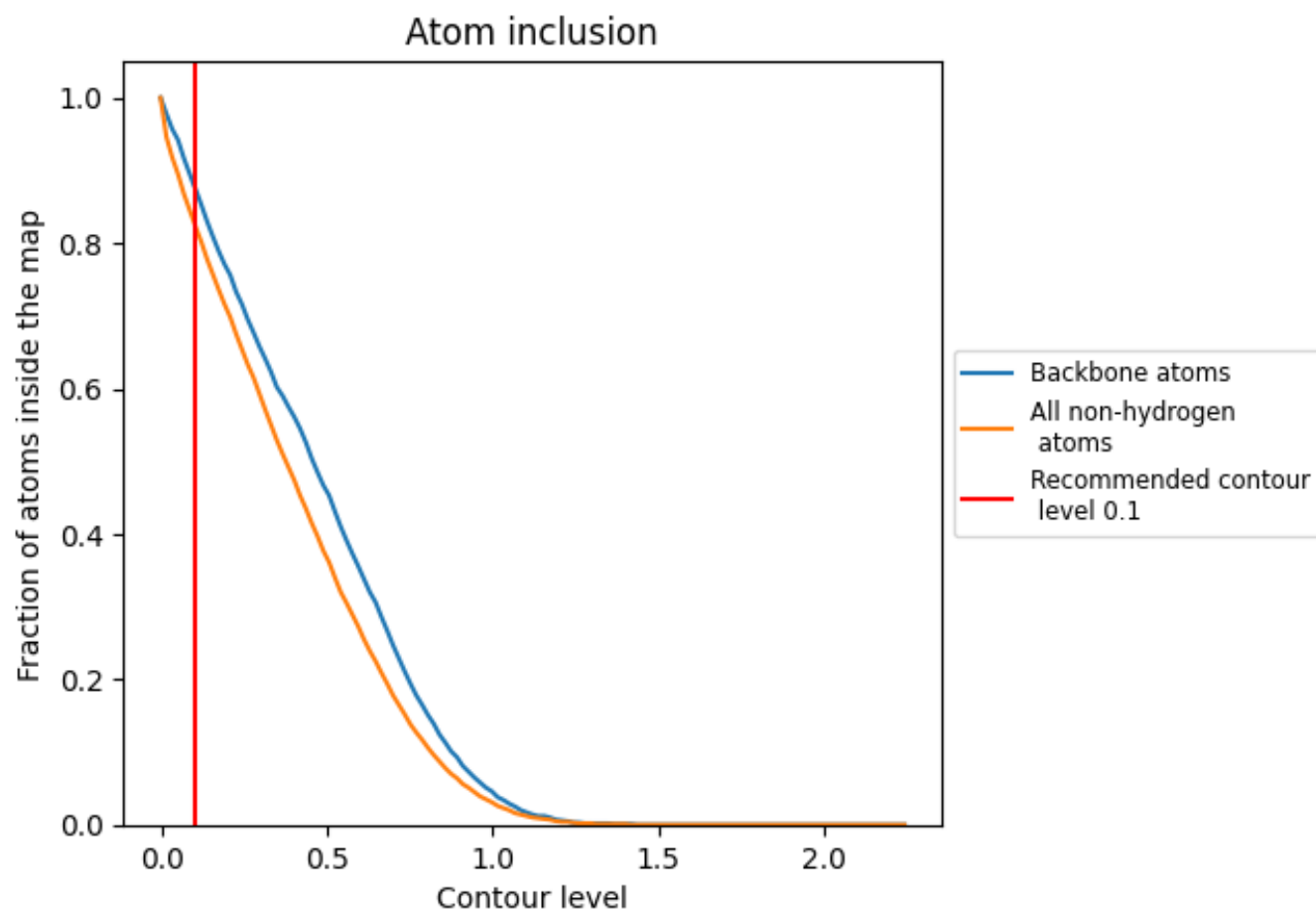
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8270	0.5310
A	0.8140	0.5400
B	0.8410	0.5430
C	0.2820	0.2040
I	0.8600	0.5360
M	0.7550	0.4580

