



Full wwPDB EM Validation Report ⓘ

Nov 12, 2024 – 01:06 AM EST

PDB ID : 8FXB
EMDB ID : EMD-29530
Title : SARS-CoV-2 XBB.1 spike RBD bound to the human ACE2 ectodomain and the S309 neutralizing antibody Fab fragment
Authors : Park, Y.J.; Seattle Structural Genomics Center for Infectious Disease (SSG-CID); Veesler, D.
Deposited on : 2023-01-24
Resolution : 3.10 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

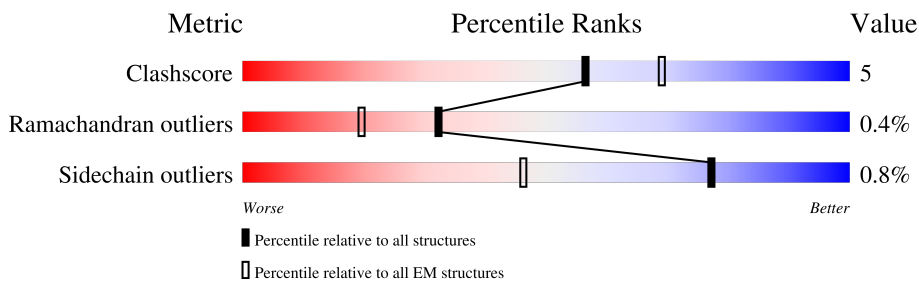
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	L	214	
2	H	457	
3	A	648	
4	E	249	
5	B	2	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 7912 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 S309 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	L	103	769	479	133	155	2	0	0

- Molecule 2 is a protein called S309 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	124	964	608	166	185	5	0	0

- Molecule 3 is a protein called Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	587	4789	3067	793	900	29	0	0

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	616	LEU	-	expression tag	UNP Q9BYF1
A	617	VAL	-	expression tag	UNP Q9BYF1
A	618	PRO	-	expression tag	UNP Q9BYF1
A	619	ARG	-	expression tag	UNP Q9BYF1
A	620	GLY	-	expression tag	UNP Q9BYF1
A	621	SER	-	expression tag	UNP Q9BYF1
A	622	SER	-	expression tag	UNP Q9BYF1
A	623	ALA	-	expression tag	UNP Q9BYF1
A	624	TRP	-	expression tag	UNP Q9BYF1
A	625	SER	-	expression tag	UNP Q9BYF1
A	626	HIS	-	expression tag	UNP Q9BYF1
A	627	PRO	-	expression tag	UNP Q9BYF1
A	628	GLN	-	expression tag	UNP Q9BYF1
A	629	PHE	-	expression tag	UNP Q9BYF1
A	630	GLU	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	631	LYS	-	expression tag	UNP Q9BYF1
A	632	GLY	-	expression tag	UNP Q9BYF1
A	633	GLY	-	expression tag	UNP Q9BYF1
A	634	GLY	-	expression tag	UNP Q9BYF1
A	635	SER	-	expression tag	UNP Q9BYF1
A	636	GLY	-	expression tag	UNP Q9BYF1
A	637	GLY	-	expression tag	UNP Q9BYF1
A	638	GLY	-	expression tag	UNP Q9BYF1
A	639	SER	-	expression tag	UNP Q9BYF1
A	640	GLY	-	expression tag	UNP Q9BYF1
A	641	GLY	-	expression tag	UNP Q9BYF1
A	642	SER	-	expression tag	UNP Q9BYF1
A	643	ALA	-	expression tag	UNP Q9BYF1
A	644	TRP	-	expression tag	UNP Q9BYF1
A	645	SER	-	expression tag	UNP Q9BYF1
A	646	HIS	-	expression tag	UNP Q9BYF1
A	647	PRO	-	expression tag	UNP Q9BYF1
A	648	GLN	-	expression tag	UNP Q9BYF1
A	649	PHE	-	expression tag	UNP Q9BYF1
A	650	GLU	-	expression tag	UNP Q9BYF1
A	651	LYS	-	expression tag	UNP Q9BYF1
A	652	GLY	-	expression tag	UNP Q9BYF1
A	653	SER	-	expression tag	UNP Q9BYF1
A	654	HIS	-	expression tag	UNP Q9BYF1
A	655	HIS	-	expression tag	UNP Q9BYF1
A	656	HIS	-	expression tag	UNP Q9BYF1
A	657	HIS	-	expression tag	UNP Q9BYF1
A	658	HIS	-	expression tag	UNP Q9BYF1
A	659	HIS	-	expression tag	UNP Q9BYF1
A	660	HIS	-	expression tag	UNP Q9BYF1
A	661	HIS	-	expression tag	UNP Q9BYF1
A	662	HIS	-	expression tag	UNP Q9BYF1
A	663	HIS	-	expression tag	UNP Q9BYF1
A	664	GLY	-	expression tag	UNP Q9BYF1
A	665	GLY	-	expression tag	UNP Q9BYF1
A	666	GLY	-	expression tag	UNP Q9BYF1

- Molecule 4 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	162	1296	833	220	237	6	0	0

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	310	MET	-	initiating methionine	UNP P0DTC2
E	311	ALA	-	expression tag	UNP P0DTC2
E	312	ARG	-	expression tag	UNP P0DTC2
E	313	ALA	-	expression tag	UNP P0DTC2
E	314	TRP	-	expression tag	UNP P0DTC2
E	315	ILE	-	expression tag	UNP P0DTC2
E	316	PHE	-	expression tag	UNP P0DTC2
E	317	PHE	-	expression tag	UNP P0DTC2
E	318	LEU	-	expression tag	UNP P0DTC2
E	319	LEU	-	expression tag	UNP P0DTC2
E	320	CYS	-	expression tag	UNP P0DTC2
E	321	LEU	-	expression tag	UNP P0DTC2
E	322	ALA	-	expression tag	UNP P0DTC2
E	323	GLY	-	expression tag	UNP P0DTC2
E	324	ARG	-	expression tag	UNP P0DTC2
E	325	ALA	-	expression tag	UNP P0DTC2
E	326	LEU	-	expression tag	UNP P0DTC2
E	327	ALA	-	expression tag	UNP P0DTC2
E	339	HIS	GLY	conflict	UNP P0DTC2
E	346	THR	ARG	conflict	UNP P0DTC2
E	368	ILE	LEU	conflict	UNP P0DTC2
E	371	PHE	SER	conflict	UNP P0DTC2
E	373	PRO	SER	conflict	UNP P0DTC2
E	375	PHE	SER	conflict	UNP P0DTC2
E	376	ALA	THR	conflict	UNP P0DTC2
E	405	ASN	ASP	conflict	UNP P0DTC2
E	408	SER	ARG	conflict	UNP P0DTC2
E	417	ASN	LYS	conflict	UNP P0DTC2
E	440	LYS	ASN	conflict	UNP P0DTC2
E	445	PRO	VAL	conflict	UNP P0DTC2
E	446	SER	GLY	conflict	UNP P0DTC2
E	460	LYS	ASN	conflict	UNP P0DTC2
E	477	ASN	SER	conflict	UNP P0DTC2
E	478	LYS	THR	conflict	UNP P0DTC2
E	484	ALA	GLU	conflict	UNP P0DTC2
E	486	SER	PHE	conflict	UNP P0DTC2
E	490	SER	PHE	conflict	UNP P0DTC2
E	498	ARG	GLN	conflict	UNP P0DTC2
E	501	TYR	ASN	conflict	UNP P0DTC2
E	505	HIS	TYR	conflict	UNP P0DTC2
E	529	LYS	-	expression tag	UNP P0DTC2
E	530	SER	-	expression tag	UNP P0DTC2

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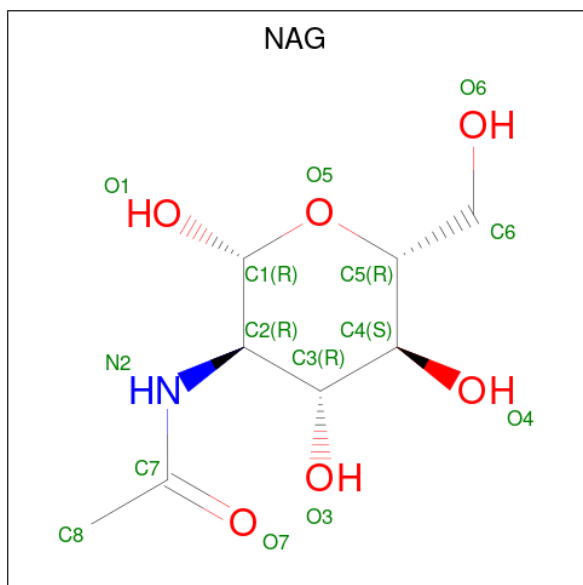
Chain	Residue	Modelled	Actual	Comment	Reference
E	531	THR	-	expression tag	UNP P0DTC2
E	532	GLY	-	expression tag	UNP P0DTC2
E	533	GLY	-	expression tag	UNP P0DTC2
E	534	LEU	-	expression tag	UNP P0DTC2
E	535	ASN	-	expression tag	UNP P0DTC2
E	536	ASP	-	expression tag	UNP P0DTC2
E	537	ILE	-	expression tag	UNP P0DTC2
E	538	PHE	-	expression tag	UNP P0DTC2
E	539	GLU	-	expression tag	UNP P0DTC2
E	540	ALA	-	expression tag	UNP P0DTC2
E	541	GLN	-	expression tag	UNP P0DTC2
E	542	LYS	-	expression tag	UNP P0DTC2
E	543	ILE	-	expression tag	UNP P0DTC2
E	544	GLU	-	expression tag	UNP P0DTC2
E	545	TRP	-	expression tag	UNP P0DTC2
E	546	HIS	-	expression tag	UNP P0DTC2
E	547	GLU	-	expression tag	UNP P0DTC2
E	548	GLY	-	expression tag	UNP P0DTC2
E	549	SER	-	expression tag	UNP P0DTC2
E	550	GLY	-	expression tag	UNP P0DTC2
E	551	HIS	-	expression tag	UNP P0DTC2
E	552	HIS	-	expression tag	UNP P0DTC2
E	553	HIS	-	expression tag	UNP P0DTC2
E	554	HIS	-	expression tag	UNP P0DTC2
E	555	HIS	-	expression tag	UNP P0DTC2
E	556	HIS	-	expression tag	UNP P0DTC2
E	557	HIS	-	expression tag	UNP P0DTC2
E	558	HIS	-	expression tag	UNP P0DTC2

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
5	B	2	24	14	1	9	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

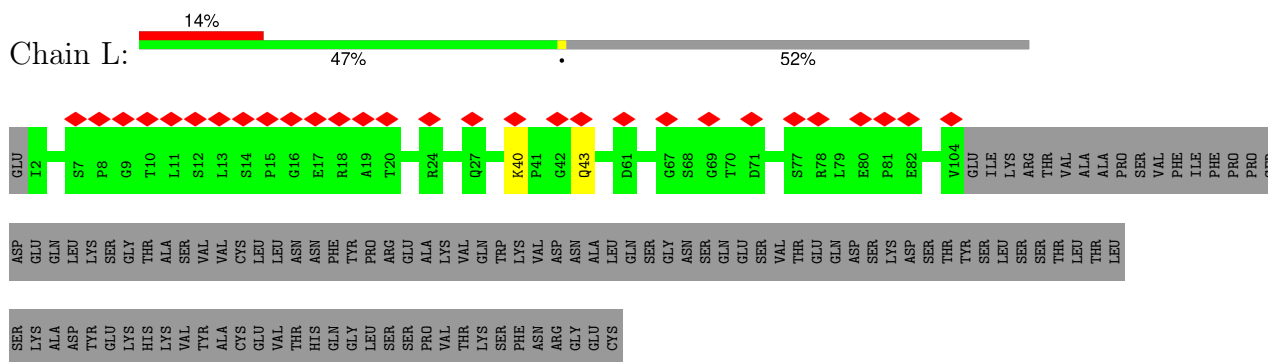


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	A	1	Total	C	N	O	0
			14	8	1	5	

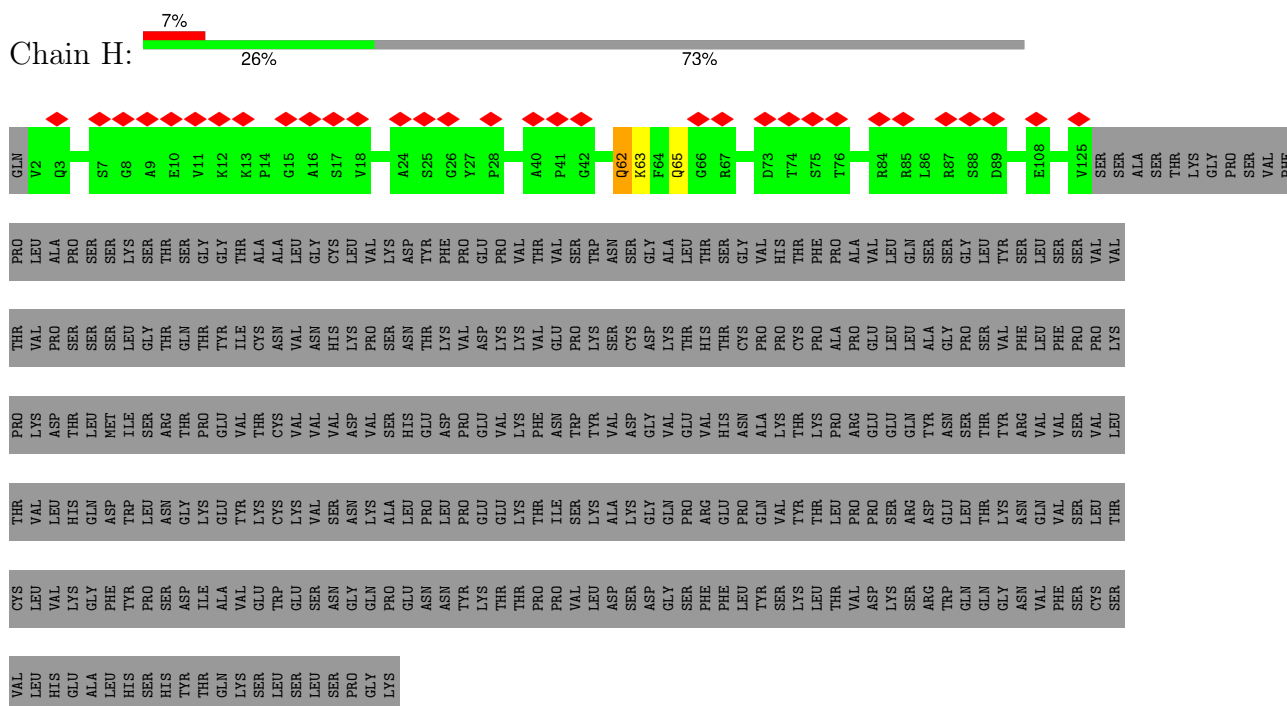
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: S309 Light chain



- Molecule 2: S309 Heavy chain



- Molecule 3: Processed angiotensin-converting enzyme 2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	281957	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	6.481	Depositor
Minimum map value	-4.367	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.107	Depositor
Recommended contour level	0.8	Depositor
Map size (\AA)	256.0, 256.0, 256.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0, 1.0, 1.0	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, 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	L	0.62	0/785	0.57	0/1067
2	H	0.63	0/988	0.56	0/1341
3	A	0.69	0/4922	0.54	0/6683
4	E	0.63	0/1333	0.63	1/1808 (0.1%)
All	All	0.66	0/8028	0.56	1/10899 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	449	TYR	CB-CA-C	-5.56	99.28	110.40

There are no chirality outliers.

There are no planarity outliers.

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	L	769	0	749	4	0
2	H	964	0	918	2	0
3	A	4789	0	4575	59	0
4	E	1296	0	1228	8	0
5	B	24	0	22	1	0
6	A	70	0	65	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7912	0	7557	73	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 5.

All (73) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:40:LYS:HB2	1:L:43:GLN:OE1	1.50	1.08
3:A:305:GLN:O	3:A:309:LYS:HG2	1.64	0.94
3:A:394:ASN:HB3	3:A:562:LYS:HE2	1.51	0.90
3:A:487:VAL:HG12	3:A:488:VAL:H	1.43	0.84
1:L:40:LYS:CB	1:L:43:GLN:OE1	2.31	0.79
3:A:471:ASP:O	3:A:495:GLU:OE1	2.02	0.77
3:A:305:GLN:HE21	3:A:309:LYS:HD3	1.50	0.76
3:A:203:TRP:CZ3	3:A:464:PHE:HE1	2.07	0.72
3:A:482:ARG:O	3:A:483:GLU:HG3	1.91	0.70
1:L:40:LYS:HD2	1:L:43:GLN:OE1	1.93	0.68
3:A:177:ARG:NH1	3:A:495:GLU:O	2.27	0.68
3:A:495:GLU:C	3:A:497:TYR:H	1.98	0.67
3:A:305:GLN:NE2	3:A:309:LYS:HD3	2.09	0.67
3:A:544:ILE:HD12	3:A:544:ILE:O	1.93	0.67
3:A:530:CYS:HA	3:A:544:ILE:HG22	1.76	0.65
3:A:394:ASN:CB	3:A:562:LYS:HE2	2.26	0.63
3:A:177:ARG:HB3	3:A:178:PRO:HD3	1.82	0.62
3:A:495:GLU:O	3:A:497:TYR:N	2.34	0.61
3:A:487:VAL:HG12	3:A:488:VAL:N	2.14	0.60
2:H:62:GLN:HA	2:H:65:GLN:CD	2.22	0.60
3:A:177:ARG:CZ	3:A:473:TRP:HE1	2.15	0.59
3:A:495:GLU:C	3:A:497:TYR:N	2.54	0.59
4:E:357:ARG:NH2	4:E:394:ASN:ND2	2.51	0.58
3:A:177:ARG:NE	3:A:473:TRP:HZ2	2.03	0.56
3:A:463:VAL:HG21	3:A:473:TRP:HE3	1.71	0.56
3:A:36:ALA:HB2	3:A:72:PHE:HE2	1.71	0.55
3:A:36:ALA:HB2	3:A:72:PHE:CE2	2.42	0.54
3:A:485:VAL:HG12	3:A:487:VAL:HG23	1.90	0.53
3:A:123:MET:HA	3:A:176:LEU:CD2	2.39	0.53
3:A:450:LEU:N	3:A:451:PRO:CD	2.71	0.53
4:E:454:ARG:HG3	4:E:491:PRO:O	2.08	0.53
4:E:357:ARG:NH2	4:E:394:ASN:HD21	2.06	0.52
3:A:589:GLU:N	3:A:590:PRO:CD	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:357:ARG:HH21	4:E:394:ASN:CG	2.12	0.51
3:A:126:ILE:HB	3:A:176:LEU:HD21	1.92	0.51
3:A:169:ARG:HG3	3:A:493:HIS:HE1	1.76	0.51
3:A:203:TRP:CH2	3:A:464:PHE:HE1	2.29	0.51
4:E:357:ARG:HH21	4:E:394:ASN:ND2	2.08	0.51
3:A:203:TRP:CZ3	3:A:464:PHE:CE1	2.95	0.51
3:A:488:VAL:O	3:A:490:PRO:HD3	2.11	0.50
3:A:582:ARG:N	3:A:583:PRO:CD	2.74	0.50
4:E:342:PHE:HB2	5:B:1:NAG:H82	1.92	0.50
3:A:473:TRP:HD1	3:A:474:MET:H	1.58	0.50
3:A:460:ARG:O	3:A:463:VAL:HG12	2.13	0.48
2:H:62:GLN:HG2	2:H:63:LYS:N	2.28	0.48
3:A:177:ARG:NH1	3:A:473:TRP:HE1	2.11	0.48
3:A:402:GLU:OE1	3:A:518:ARG:HD3	2.13	0.48
3:A:491:VAL:HB	3:A:492:PRO:HD2	1.96	0.47
3:A:123:MET:HA	3:A:176:LEU:HD21	1.97	0.47
3:A:544:ILE:O	3:A:544:ILE:CD1	2.63	0.46
3:A:487:VAL:CG1	3:A:488:VAL:H	2.21	0.46
3:A:459:TRP:HZ2	3:A:473:TRP:HB2	1.81	0.46
3:A:476:LYS:O	3:A:480:MET:HG2	2.16	0.45
3:A:165:TRP:CH2	3:A:490:PRO:HD2	2.51	0.45
4:E:420:ASP:OD1	4:E:460:LYS:HD3	2.15	0.45
3:A:494:ASP:CG	3:A:495:GLU:H	2.20	0.45
3:A:402:GLU:HB2	3:A:518:ARG:HD2	2.00	0.43
1:L:40:LYS:CD	1:L:43:GLN:OE1	2.63	0.43
3:A:165:TRP:CZ3	3:A:493:HIS:CE1	3.06	0.43
3:A:381:TYR:HE2	3:A:400:PHE:O	2.02	0.43
3:A:404:VAL:HG12	3:A:404:VAL:O	2.18	0.43
4:E:493:GLN:HE21	4:E:493:GLN:HB3	1.57	0.43
3:A:402:GLU:O	3:A:406:GLU:HG2	2.18	0.43
3:A:463:VAL:CG2	3:A:473:TRP:HE3	2.31	0.43
3:A:165:TRP:CH2	3:A:493:HIS:CE1	3.07	0.43
3:A:321:PRO:HA	6:A:704:NAG:H81	2.00	0.42
3:A:485:VAL:CG1	3:A:487:VAL:HG23	2.49	0.42
3:A:487:VAL:CG1	3:A:488:VAL:N	2.82	0.41
3:A:459:TRP:CZ2	3:A:473:TRP:HB2	2.54	0.41
3:A:500:PRO:O	3:A:506:VAL:HG21	2.20	0.41
3:A:544:ILE:O	3:A:544:ILE:CG1	2.68	0.41
3:A:40:PHE:O	3:A:41:TYR:C	2.59	0.41
3:A:263:PRO:HA	3:A:488:VAL:HG12	2.03	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	L	101/214 (47%)	99 (98%)	2 (2%)	0	100	100
2	H	122/457 (27%)	120 (98%)	2 (2%)	0	100	100
3	A	583/648 (90%)	559 (96%)	20 (3%)	4 (1%)	19	51
4	E	156/249 (63%)	149 (96%)	7 (4%)	0	100	100
All	All	962/1568 (61%)	927 (96%)	31 (3%)	4 (0%)	32	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	496	THR
3	A	322	ASN
3	A	483	GLU
3	A	146	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	85/185 (46%)	85 (100%)	0	100	100
2	H	100/403 (25%)	99 (99%)	1 (1%)	73	86
3	A	518/563 (92%)	513 (99%)	5 (1%)	73	86
4	E	140/211 (66%)	139 (99%)	1 (1%)	81	90
All	All	843/1362 (62%)	836 (99%)	7 (1%)	77	89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	62	GLN
3	A	381	TYR
3	A	385	TYR
3	A	401	HIS
3	A	473	TRP
3	A	489	GLU
4	E	456	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	305	GLN

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](#)

2 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	5,4	14,14,15	0.79	0	17,19,21	1.13	2 (11%)
5	FUC	B	2	5	10,10,11	0.95	0	14,14,16	0.63	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	5,4	-	0/6/23/26	0/1/1/1
5	FUC	B	2	5	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1	NAG	C8-C7-N2	2.39	120.08	116.12
5	B	1	NAG	C4-C3-C2	-2.20	107.79	111.02

There are no chirality outliers.

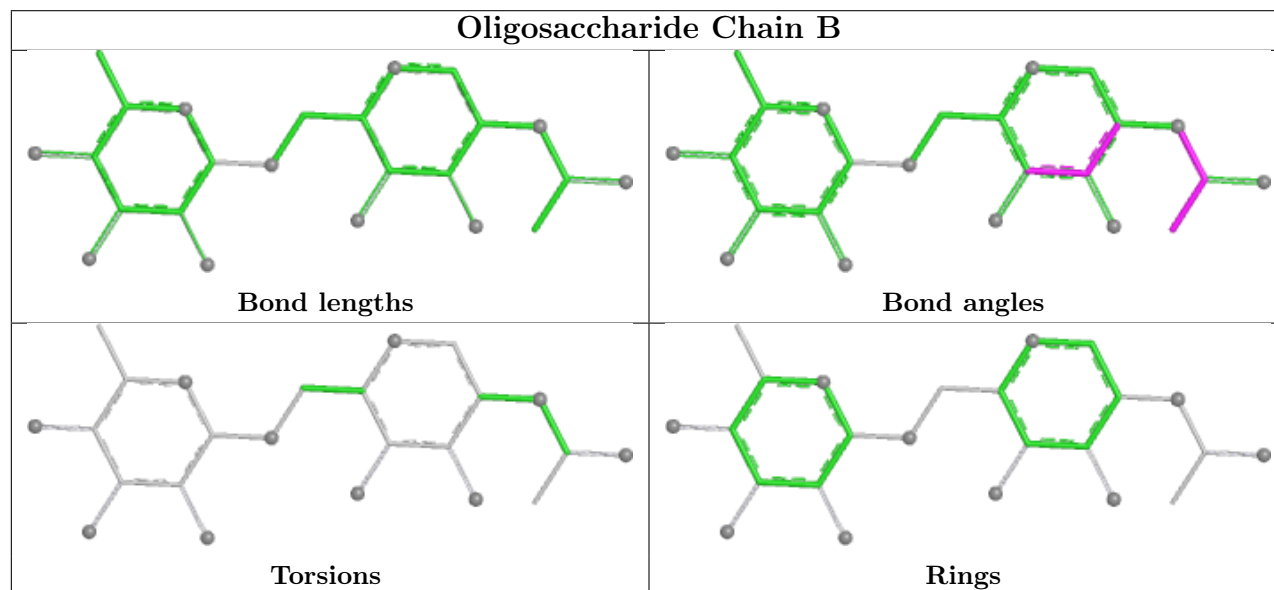
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	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

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	701	3	14,14,15	1.22	1 (7%)	17,19,21	1.05	1 (5%)
6	NAG	A	704	3	14,14,15	0.29	0	17,19,21	0.68	0
6	NAG	A	703	3	14,14,15	1.24	1 (7%)	17,19,21	1.08	2 (11%)
6	NAG	A	702	3	14,14,15	1.28	1 (7%)	17,19,21	1.18	1 (5%)
6	NAG	A	705	3	14,14,15	0.39	0	17,19,21	0.76	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	701	3	-	0/6/23/26	0/1/1/1
6	NAG	A	704	3	-	0/6/23/26	0/1/1/1
6	NAG	A	703	3	-	0/6/23/26	0/1/1/1
6	NAG	A	702	3	-	0/6/23/26	0/1/1/1
6	NAG	A	705	3	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	702	NAG	C1-C2	3.97	1.57	1.52
6	A	703	NAG	C1-C2	3.79	1.57	1.52
6	A	701	NAG	C1-C2	3.69	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	702	NAG	C8-C7-N2	2.59	120.41	116.12
6	A	701	NAG	C8-C7-N2	2.44	120.16	116.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	703	NAG	C8-C7-N2	2.31	119.94	116.12
6	A	703	NAG	C2-N2-C7	-2.02	120.19	122.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	705	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	704	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

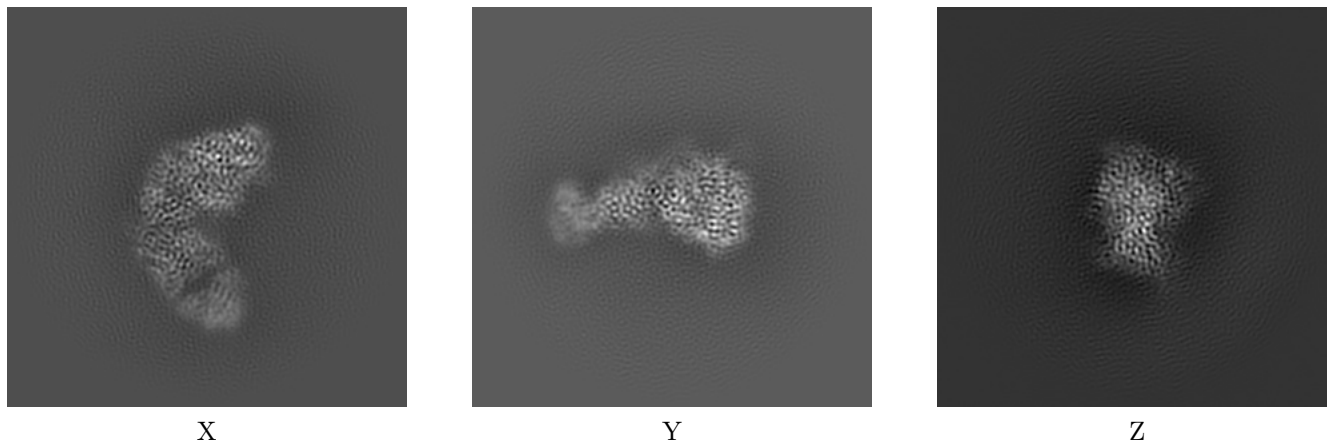
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29530. These allow visual inspection of the internal detail of the map and identification of artifacts.

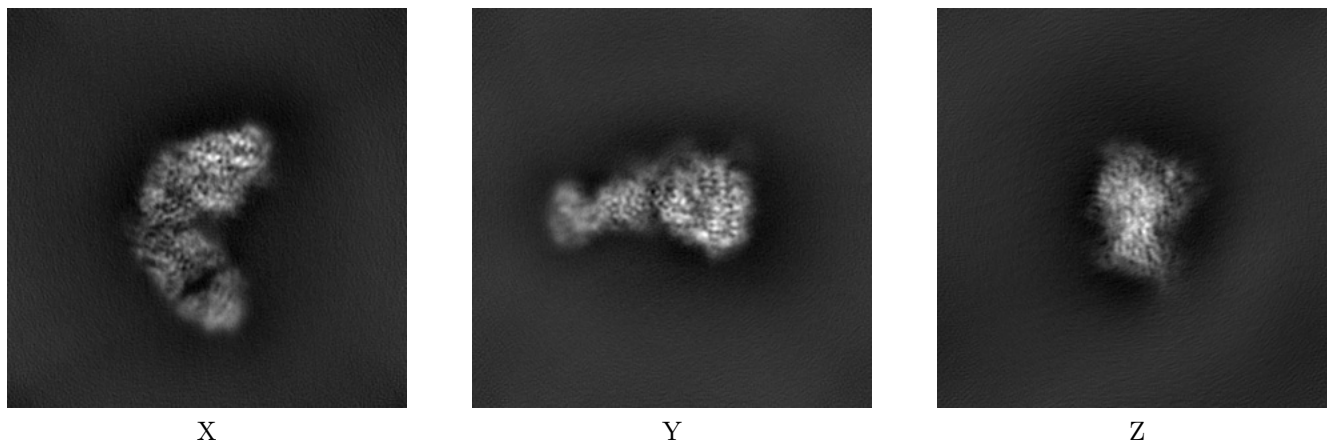
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



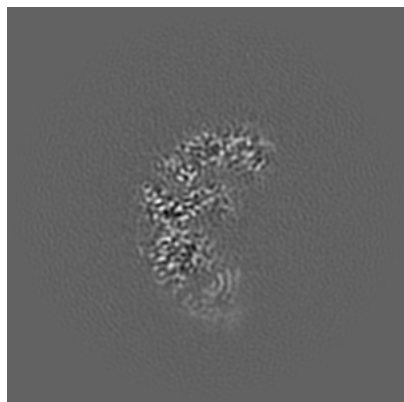
6.1.2 Raw map



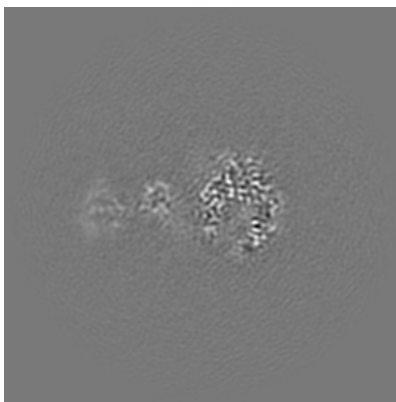
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

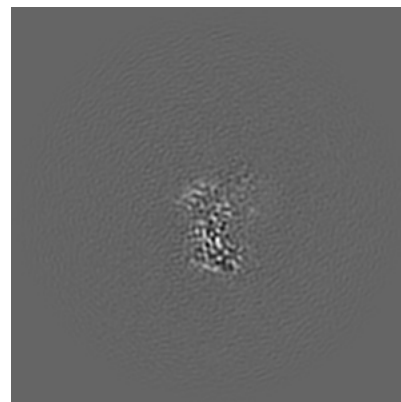
6.2.1 Primary map



X Index: 128

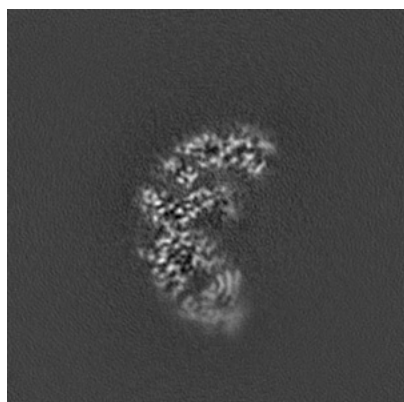


Y Index: 128

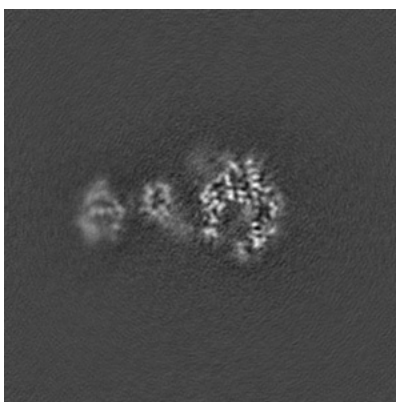


Z Index: 128

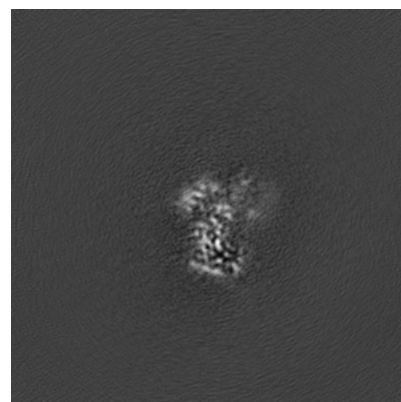
6.2.2 Raw map



X Index: 128



Y Index: 128

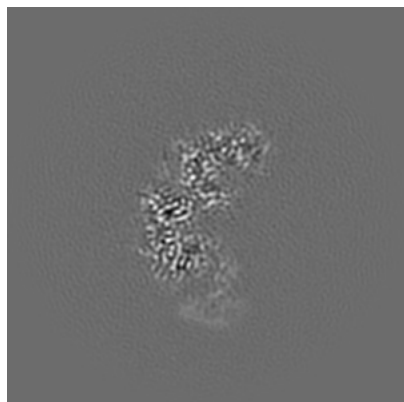


Z Index: 128

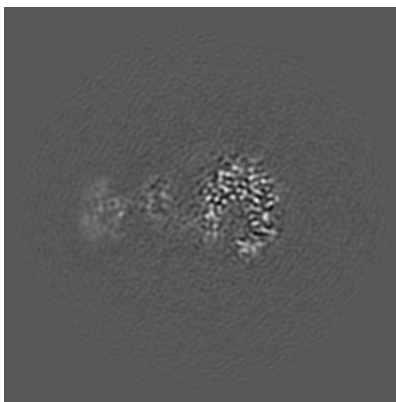
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

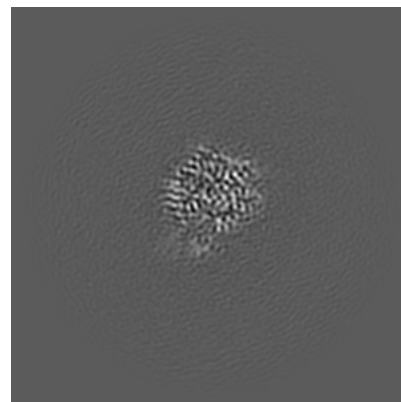
6.3.1 Primary map



X Index: 133

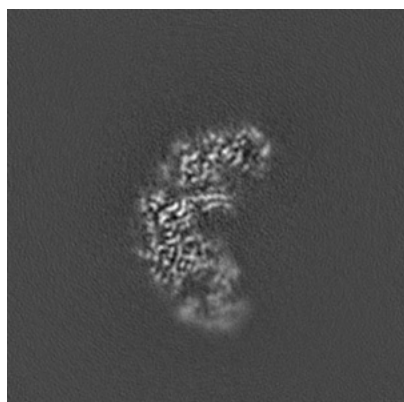


Y Index: 130

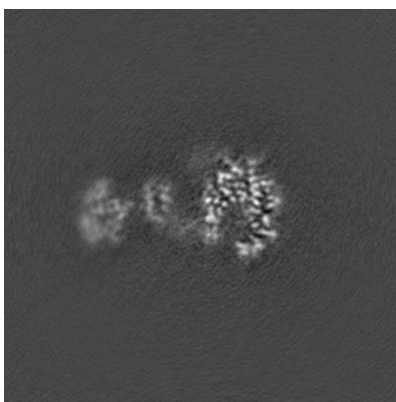


Z Index: 160

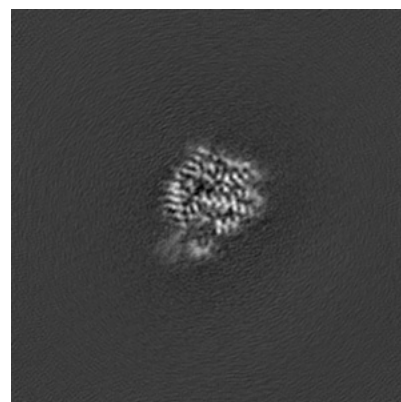
6.3.2 Raw map



X Index: 132



Y Index: 130

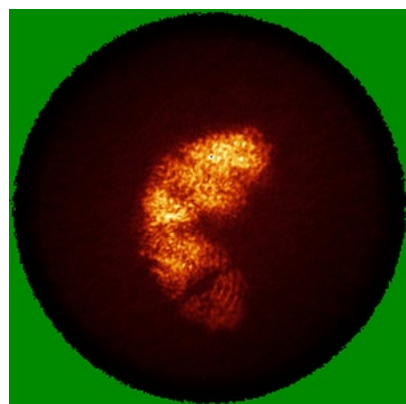


Z Index: 160

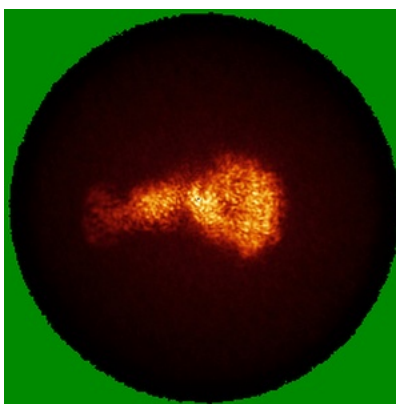
The images above show the largest variance slices of the map in three orthogonal directions.

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

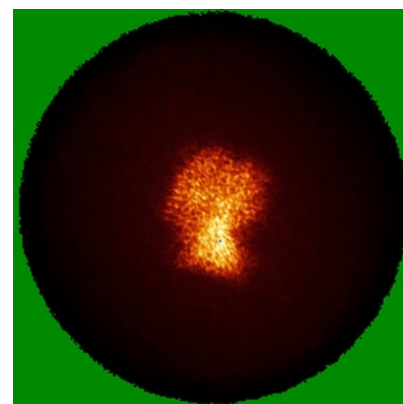
6.4.1 Primary map



X

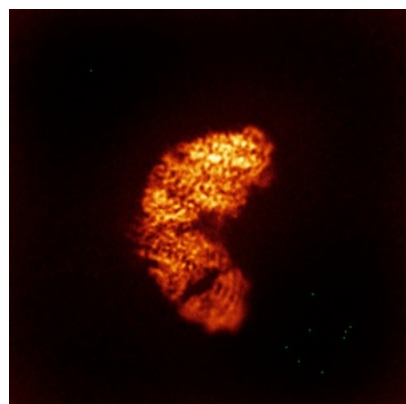


Y

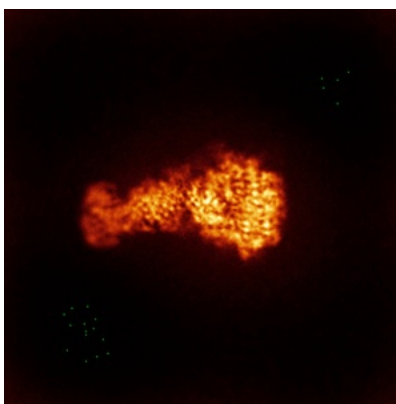


Z

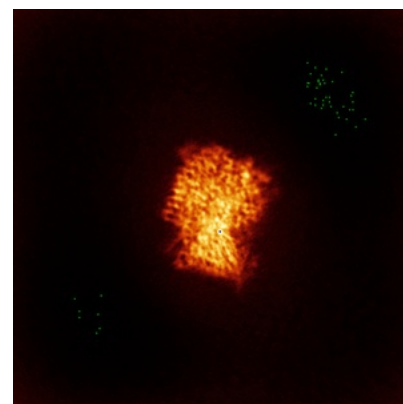
6.4.2 Raw map



X



Y

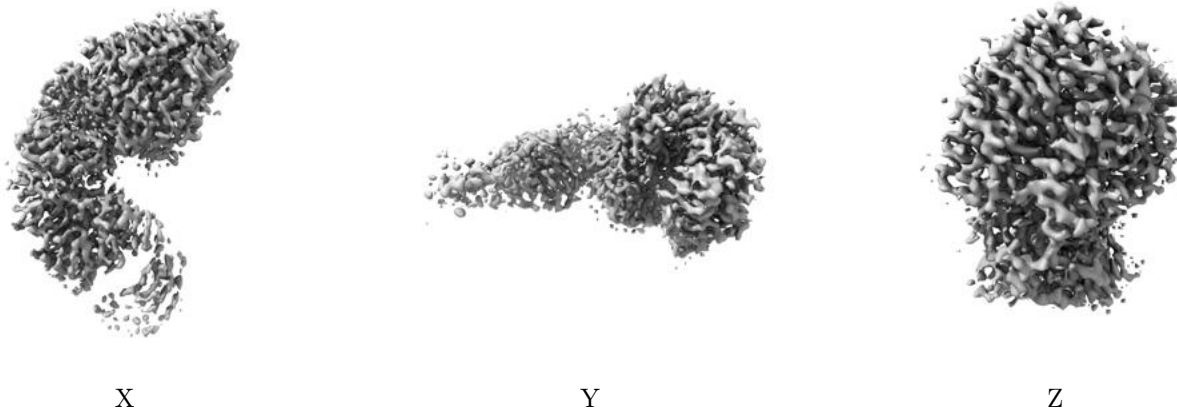


Z

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.

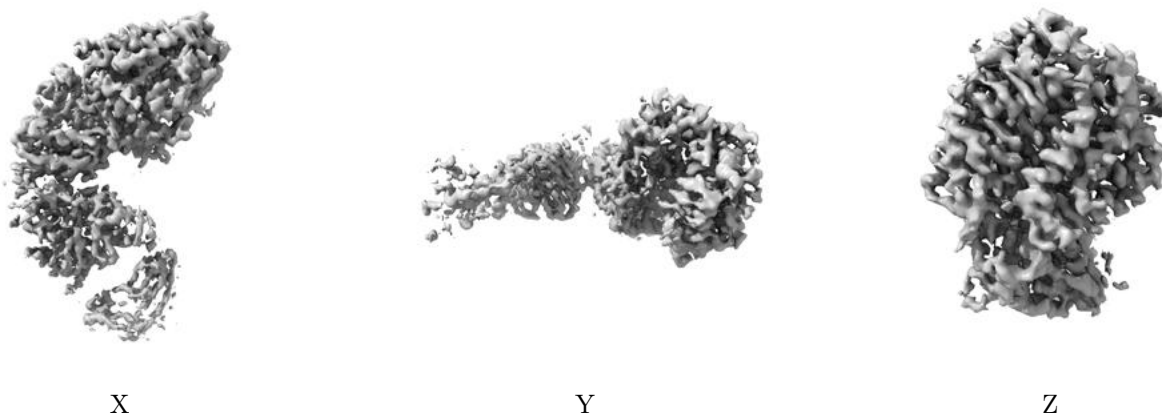
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.8. 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.

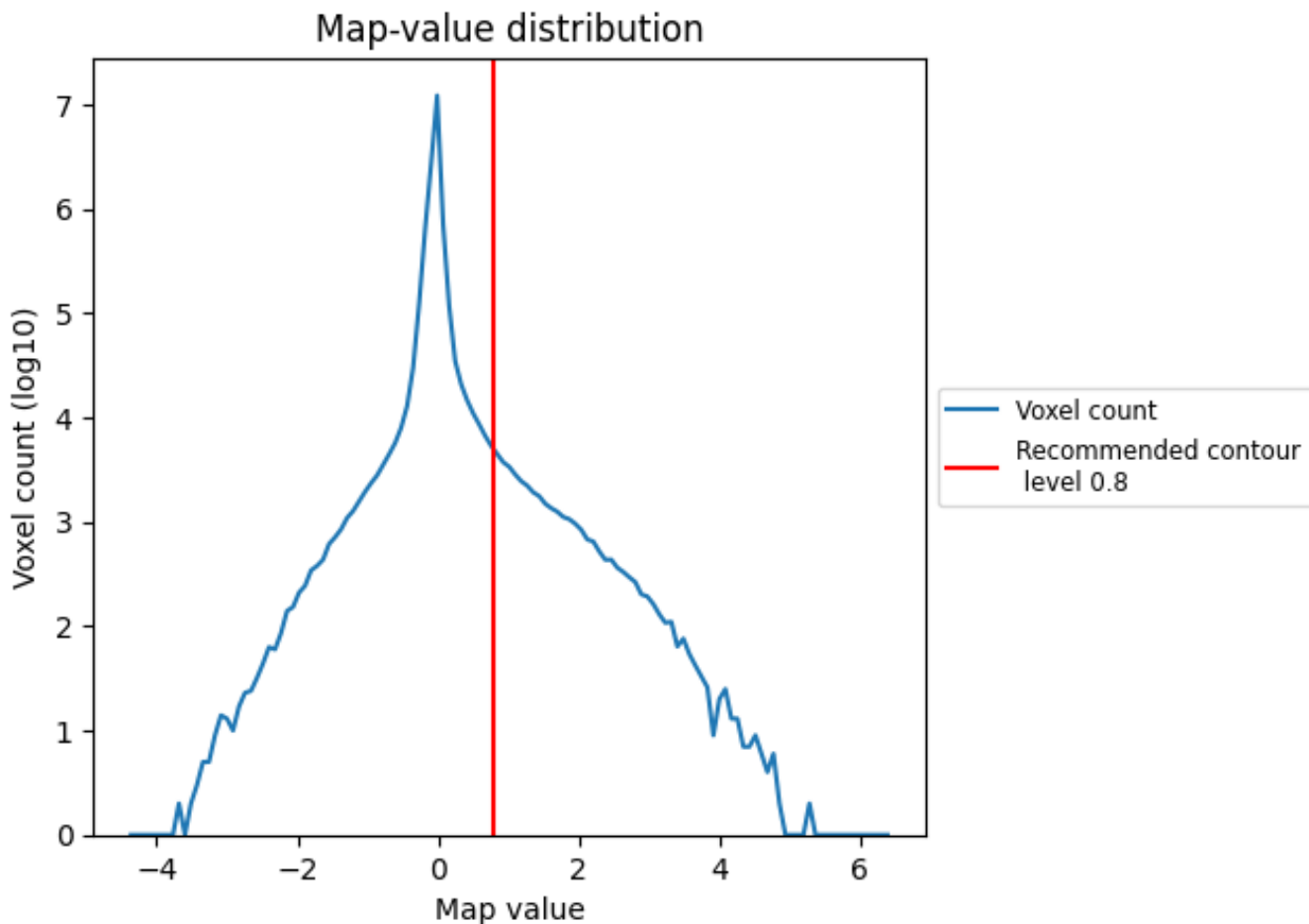
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

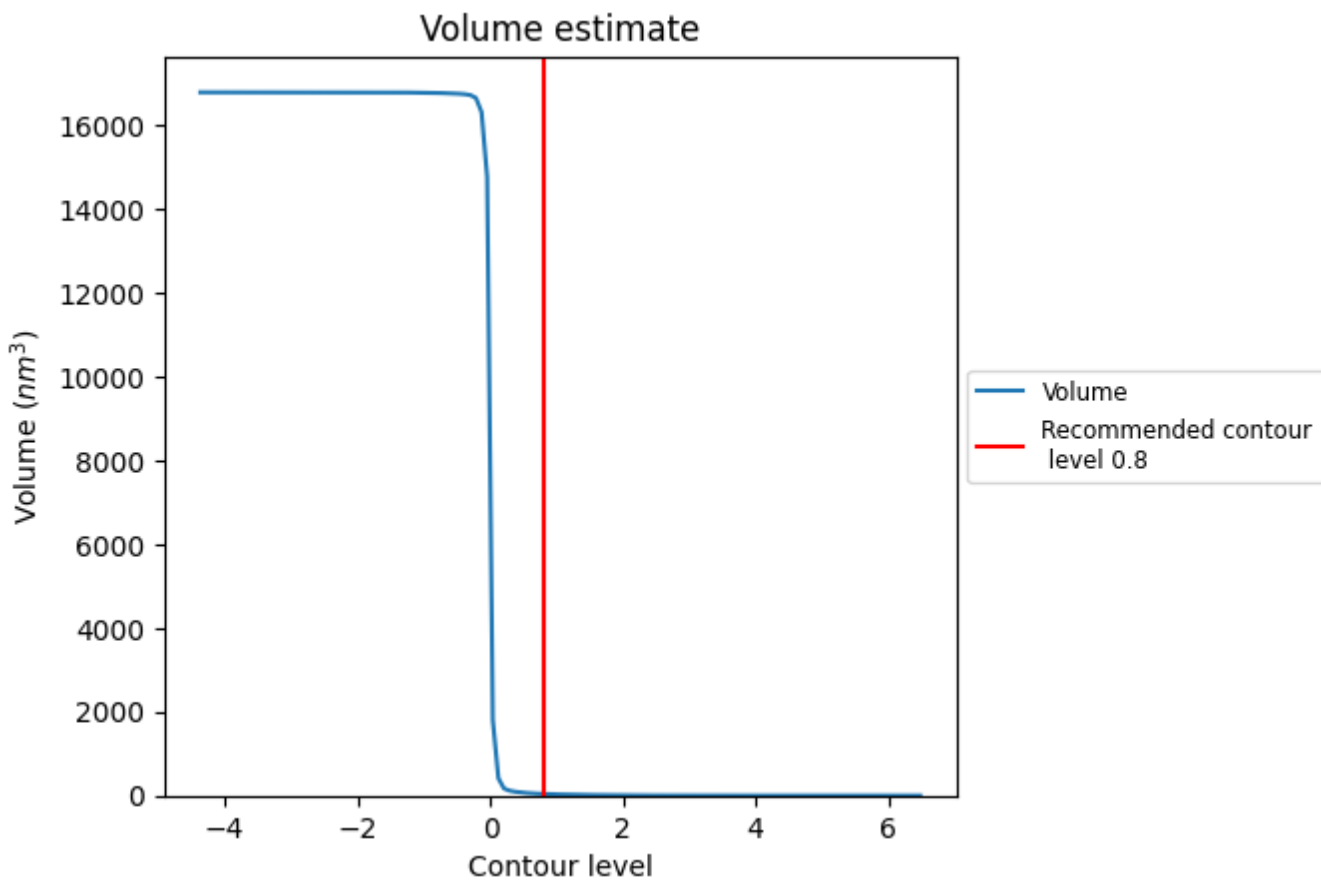
This section contains the results of statistical analysis of the map.

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.

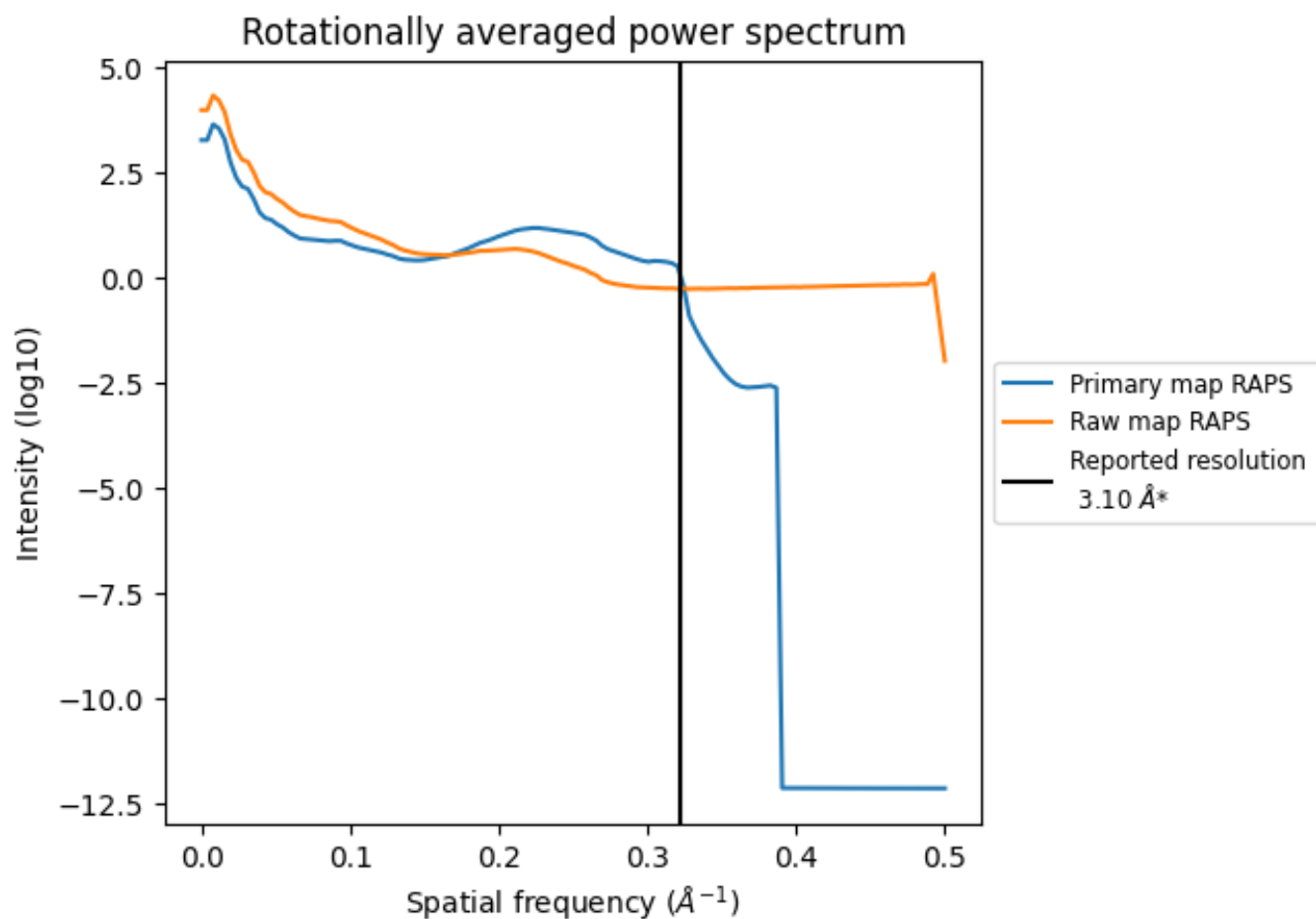
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 39 nm³; this corresponds to an approximate mass of 35 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](#)

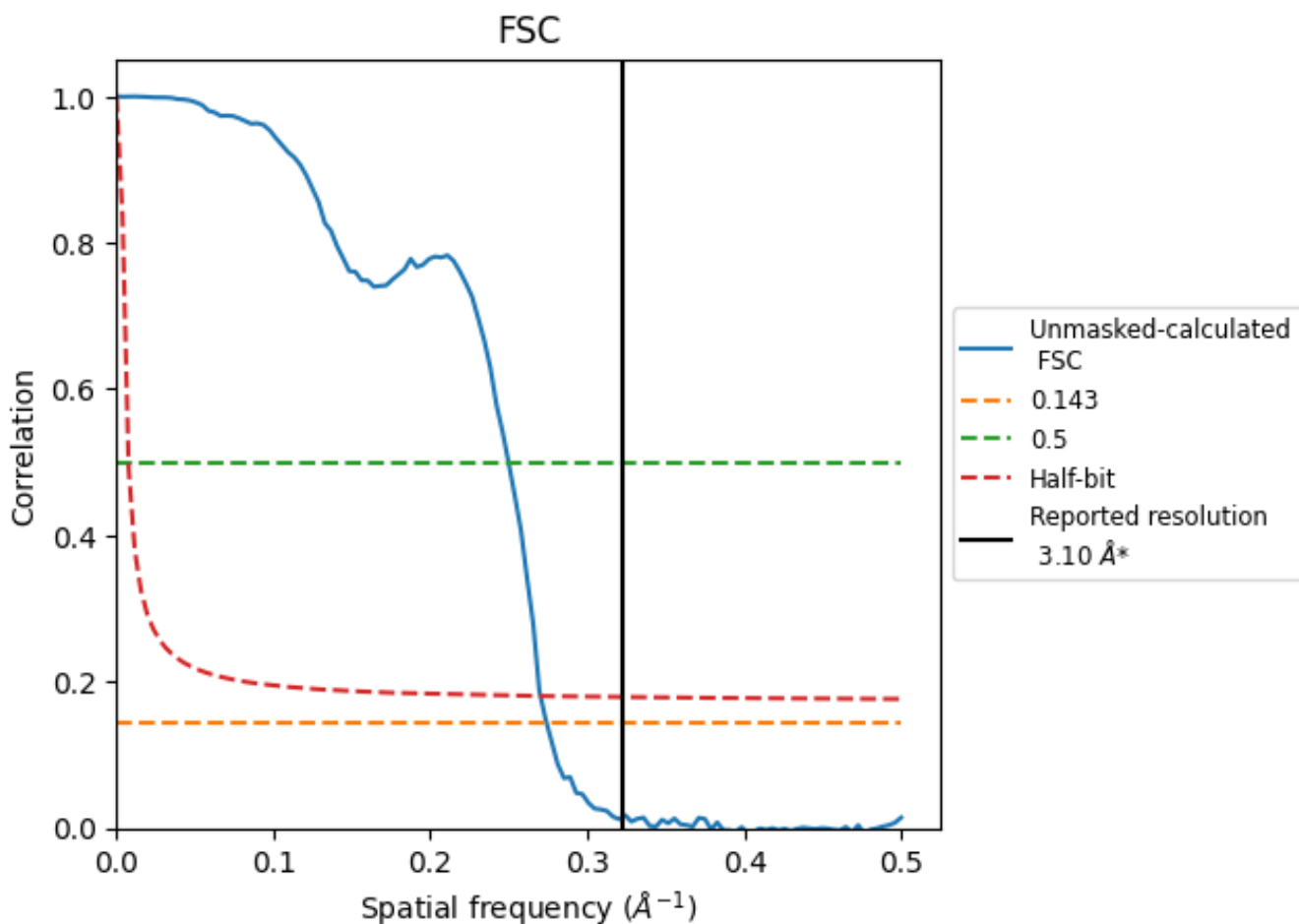


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

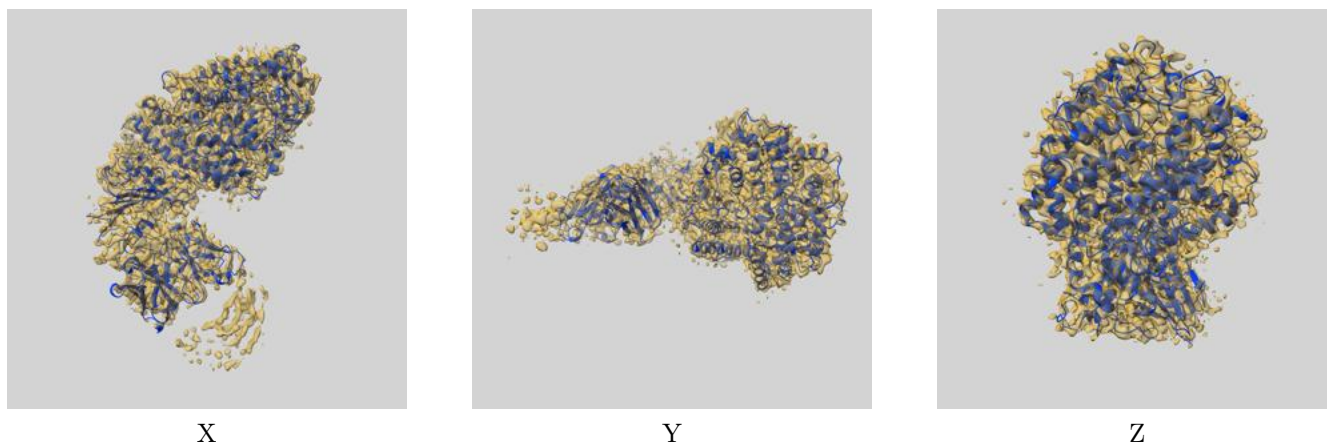
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.65	4.00	3.70

*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 3.65 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

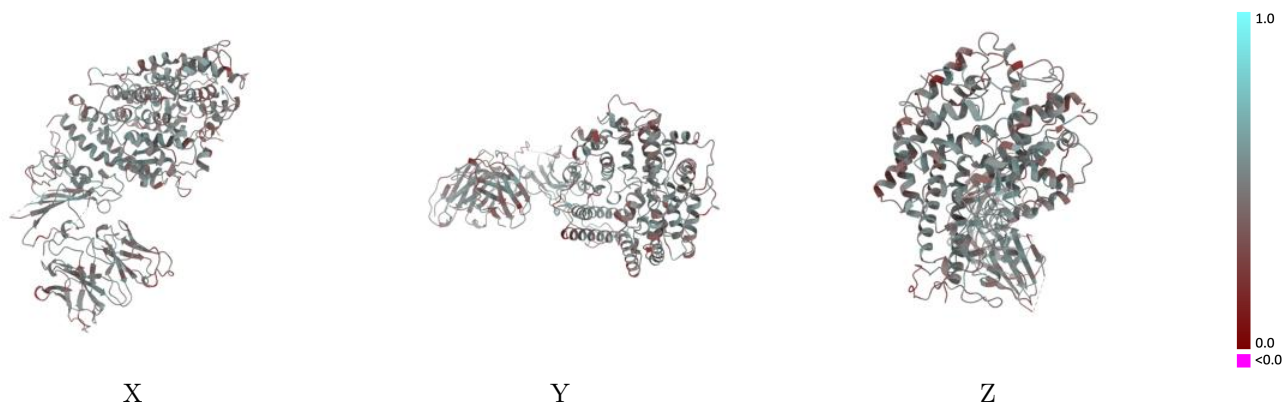
This section contains information regarding the fit between EMDB map EMD-29530 and PDB model 8FXB. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



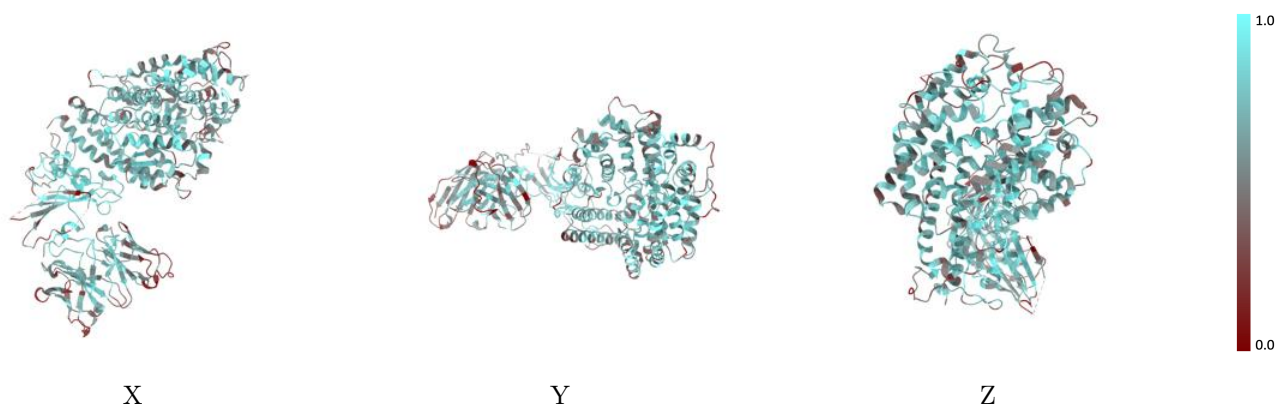
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



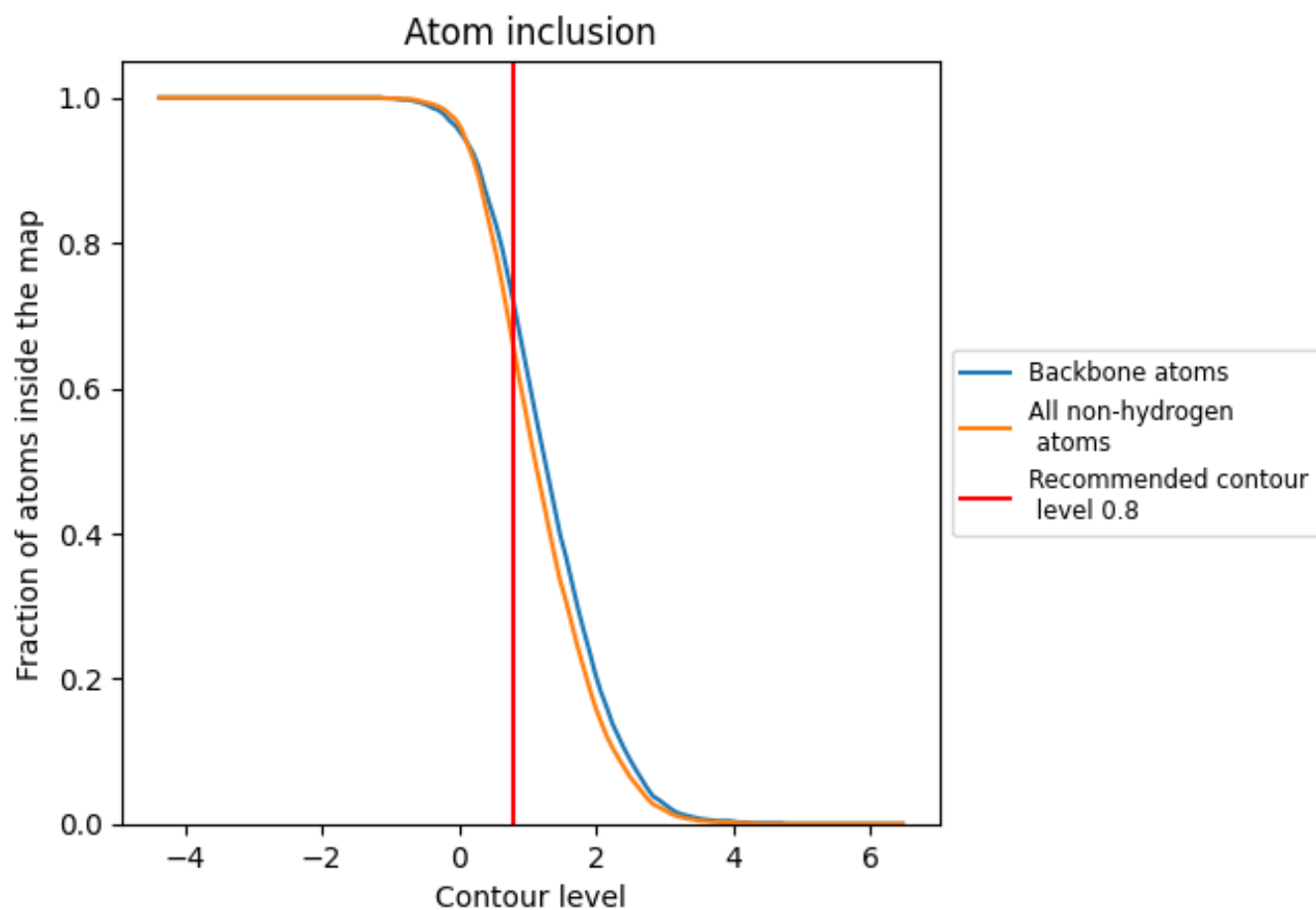
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).













9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6560	 0.4690
A	 0.6770	 0.4690
B	 0.7080	 0.5030
E	 0.6940	 0.4740
H	 0.5750	 0.4730
L	 0.5610	 0.4460

