



Full wwPDB EM Validation Report ⓘ

Mar 24, 2025 – 11:05 AM EDT

PDB ID : 9E0I
EMDB ID : EMD-47358
Title : Structure of the HKU5-19s RBD bound to the Bos taurus ACE2 receptor
Authors : Park, Y.J.; Seattle Structural Genomics Center for Infectious Disease (SSG-CID); Veesler, D.
Deposited on : 2024-10-18
Resolution : 2.40 Å(reported)

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

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
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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.dev117
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) : 2.41.4

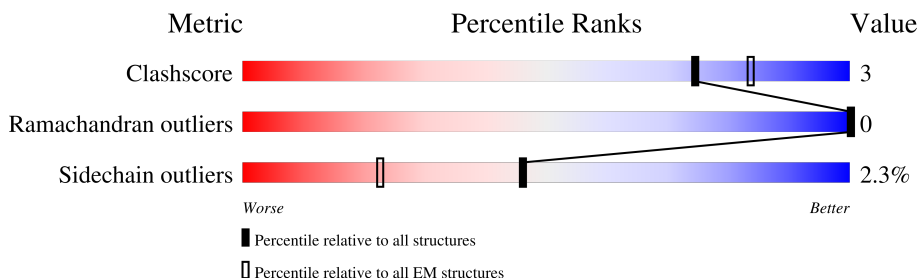
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	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	A	766	
2	B	267	
3	C	2	
4	D	4	
4	E	4	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6423 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	592	Total	C	N	O	S	0	0
			4740	3050	803	857	30		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	740	HIS	-	expression tag	UNP Q58DD0
A	741	HIS	-	expression tag	UNP Q58DD0
A	742	HIS	-	expression tag	UNP Q58DD0
A	743	HIS	-	expression tag	UNP Q58DD0
A	744	HIS	-	expression tag	UNP Q58DD0
A	745	HIS	-	expression tag	UNP Q58DD0
A	746	HIS	-	expression tag	UNP Q58DD0
A	747	HIS	-	expression tag	UNP Q58DD0
A	748	GLY	-	expression tag	UNP Q58DD0
A	749	GLY	-	expression tag	UNP Q58DD0
A	750	SER	-	expression tag	UNP Q58DD0
A	751	SER	-	expression tag	UNP Q58DD0
A	752	GLY	-	expression tag	UNP Q58DD0
A	753	LEU	-	expression tag	UNP Q58DD0
A	754	ASN	-	expression tag	UNP Q58DD0
A	755	ASP	-	expression tag	UNP Q58DD0
A	756	ILE	-	expression tag	UNP Q58DD0
A	757	PHE	-	expression tag	UNP Q58DD0
A	758	GLU	-	expression tag	UNP Q58DD0
A	759	ALA	-	expression tag	UNP Q58DD0
A	760	GLN	-	expression tag	UNP Q58DD0
A	761	LYS	-	expression tag	UNP Q58DD0
A	762	ILE	-	expression tag	UNP Q58DD0
A	763	GLU	-	expression tag	UNP Q58DD0
A	764	TRP	-	expression tag	UNP Q58DD0
A	765	HIS	-	expression tag	UNP Q58DD0
A	766	GLU	-	expression tag	UNP Q58DD0

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	194	Total	C	N	O	S	0	0
			1423	932	227	253	11		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	358	MET	-	expression tag	UNP S4WZQ4
B	359	GLY	-	expression tag	UNP S4WZQ4
B	360	ILE	-	expression tag	UNP S4WZQ4
B	361	LEU	-	expression tag	UNP S4WZQ4
B	362	PRO	-	expression tag	UNP S4WZQ4
B	363	SER	-	expression tag	UNP S4WZQ4
B	364	PRO	-	expression tag	UNP S4WZQ4
B	365	GLY	-	expression tag	UNP S4WZQ4
B	366	MET	-	expression tag	UNP S4WZQ4
B	367	PRO	-	expression tag	UNP S4WZQ4
B	368	ALA	-	expression tag	UNP S4WZQ4
B	369	LEU	-	expression tag	UNP S4WZQ4
B	370	LEU	-	expression tag	UNP S4WZQ4
B	371	SER	-	expression tag	UNP S4WZQ4
B	372	LEU	-	expression tag	UNP S4WZQ4
B	373	VAL	-	expression tag	UNP S4WZQ4
B	374	SER	-	expression tag	UNP S4WZQ4
B	375	LEU	-	expression tag	UNP S4WZQ4
B	376	LEU	-	expression tag	UNP S4WZQ4
B	377	SER	-	expression tag	UNP S4WZQ4
B	378	VAL	-	expression tag	UNP S4WZQ4
B	379	LEU	-	expression tag	UNP S4WZQ4
B	380	LEU	-	expression tag	UNP S4WZQ4
B	381	MET	-	expression tag	UNP S4WZQ4
B	382	GLY	-	expression tag	UNP S4WZQ4
B	383	CYS	-	expression tag	UNP S4WZQ4
B	384	VAL	-	expression tag	UNP S4WZQ4
B	385	ALA	-	expression tag	UNP S4WZQ4
B	386	GLU	-	expression tag	UNP S4WZQ4
B	387	THR	-	expression tag	UNP S4WZQ4
B	388	GLY	-	expression tag	UNP S4WZQ4
B	588	LEU	-	expression tag	UNP S4WZQ4
B	589	VAL	-	expression tag	UNP S4WZQ4
B	590	PRO	-	expression tag	UNP S4WZQ4
B	591	ARG	-	expression tag	UNP S4WZQ4
B	592	GLY	-	expression tag	UNP S4WZQ4

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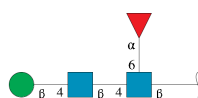
Chain	Residue	Modelled	Actual	Comment	Reference
B	593	SER	-	expression tag	UNP S4WZQ4
B	594	SER	-	expression tag	UNP S4WZQ4
B	595	SER	-	expression tag	UNP S4WZQ4
B	596	GLY	-	expression tag	UNP S4WZQ4
B	597	GLY	-	expression tag	UNP S4WZQ4
B	598	SER	-	expression tag	UNP S4WZQ4
B	599	GLY	-	expression tag	UNP S4WZQ4
B	600	LEU	-	expression tag	UNP S4WZQ4
B	601	ASN	-	expression tag	UNP S4WZQ4
B	602	ASP	-	expression tag	UNP S4WZQ4
B	603	ILE	-	expression tag	UNP S4WZQ4
B	604	PHE	-	expression tag	UNP S4WZQ4
B	605	GLU	-	expression tag	UNP S4WZQ4
B	606	ALA	-	expression tag	UNP S4WZQ4
B	607	GLN	-	expression tag	UNP S4WZQ4
B	608	LYS	-	expression tag	UNP S4WZQ4
B	609	ILE	-	expression tag	UNP S4WZQ4
B	610	GLU	-	expression tag	UNP S4WZQ4
B	611	TRP	-	expression tag	UNP S4WZQ4
B	612	HIS	-	expression tag	UNP S4WZQ4
B	613	GLU	-	expression tag	UNP S4WZQ4
B	614	GLY	-	expression tag	UNP S4WZQ4
B	615	GLY	-	expression tag	UNP S4WZQ4
B	616	SER	-	expression tag	UNP S4WZQ4
B	617	HIS	-	expression tag	UNP S4WZQ4
B	618	HIS	-	expression tag	UNP S4WZQ4
B	619	HIS	-	expression tag	UNP S4WZQ4
B	620	HIS	-	expression tag	UNP S4WZQ4
B	621	HIS	-	expression tag	UNP S4WZQ4
B	622	HIS	-	expression tag	UNP S4WZQ4
B	623	HIS	-	expression tag	UNP S4WZQ4
B	624	HIS	-	expression tag	UNP S4WZQ4

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



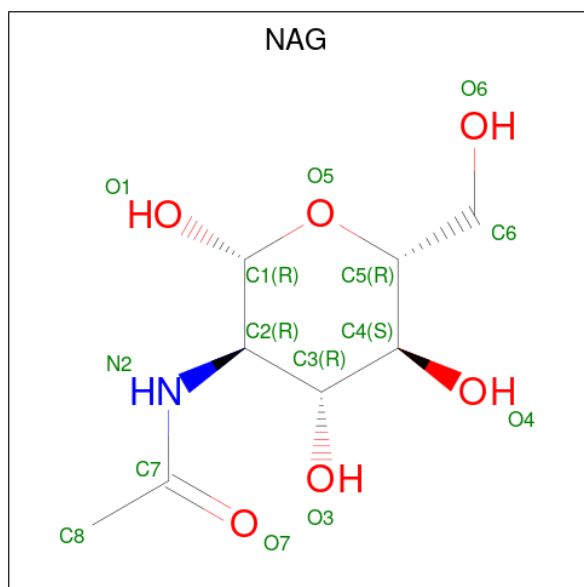
Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	4	Total	C	N	O	0	0
			49	28	2	19		
4	E	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total 1	Zn 1	0

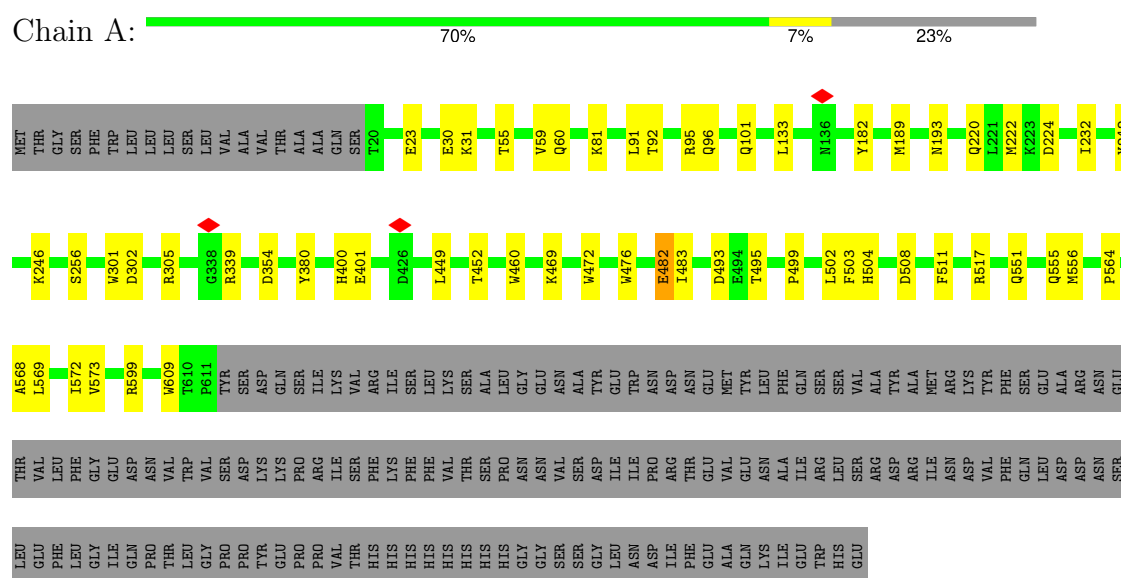
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	81	Total 81	O 81	0
7	B	10	Total 10	O 10	0

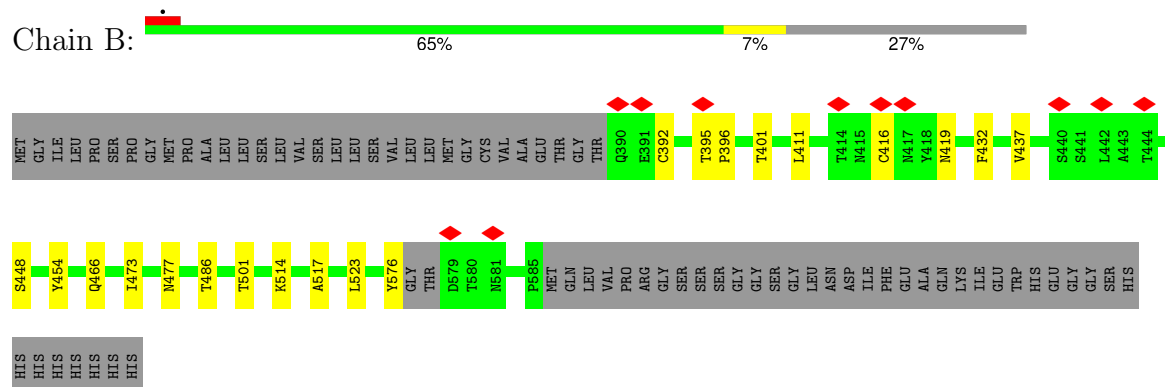
3 Residue-property plots

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

• Molecule 1: Angiotensin-converting enzyme 2



• Molecule 2: Spike glycoprotein



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

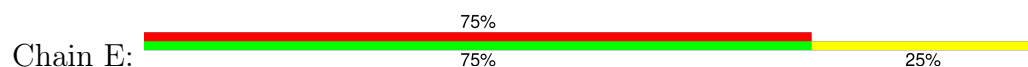




- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT, POINT, POINT	Depositor
Number of particles used	1598132, 1598132, 1598132, 1598132	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.00	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.259	Depositor
Minimum map value	-3.403	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.5	Depositor
Map size (\AA)	320.3392, 320.3392, 320.3392	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.00106, 1.00106, 1.00106	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: BMA, NAG, FUC, ZN

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	0.28	0/4876	0.48	0/6627
2	B	0.28	0/1464	0.48	0/2008
All	All	0.28	0/6340	0.48	0/8635

There are no bond length outliers.

There are no bond angle outliers.

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	A	4740	0	4463	30	0
2	B	1423	0	1263	7	0
3	C	28	0	25	1	0
4	D	49	0	43	0	0
4	E	49	0	43	0	0
5	A	14	0	13	1	0
5	B	28	0	26	0	0
6	A	1	0	0	0	0
7	A	81	0	0	1	0
7	B	10	0	0	0	0
All	All	6423	0	5876	36	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 (36) 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:514:LYS:HE2	2:B:523:LEU:HD21	1.74	0.69
1:A:572:ILE:HG23	1:A:573:VAL:HG13	1.74	0.67
1:A:401:GLU:HB3	1:A:517:ARG:HG3	1.85	0.57
1:A:482:GLU:HG3	1:A:483:ILE:HG13	1.88	0.55
1:A:469:LYS:HA	1:A:472:TRP:CD1	2.43	0.54
2:B:448:SER:H	2:B:576:TYR:HB3	1.73	0.53
1:A:502:LEU:HD22	1:A:503:PHE:H	1.75	0.52
1:A:220:GLN:NE2	1:A:224:ASP:OD1	2.41	0.52
2:B:473:ILE:HA	2:B:477:ASN:HD22	1.75	0.52
1:A:92:THR:HG22	1:A:96:GLN:HE21	1.78	0.49
1:A:189:MET:O	1:A:193:ASN:ND2	2.45	0.49
1:A:476:TRP:CE3	1:A:499:PRO:HG3	2.48	0.49
1:A:81:LYS:HA	1:A:101:GLN:HG2	1.95	0.48
1:A:242:TYR:O	1:A:246:LYS:HG2	2.13	0.48
1:A:339:ARG:HD2	3:C:1:NAG:H82	1.95	0.48
1:A:222:MET:HG2	1:A:460:TRP:CZ3	2.49	0.48
1:A:301:TRP:CD2	1:A:305:ARG:HD3	2.50	0.47
1:A:31:LYS:HE3	1:A:31:LYS:HB2	1.71	0.46
1:A:502:LEU:HD13	1:A:504:HIS:H	1.81	0.46
1:A:493:ASP:OD1	1:A:495:THR:OG1	2.27	0.45
1:A:302:ASP:N	1:A:302:ASP:OD1	2.49	0.44
1:A:556:MET:HG2	1:A:568:ALA:HB1	1.99	0.44
2:B:411:LEU:HD13	2:B:454:TYR:HE1	1.82	0.44
1:A:182:TYR:OH	1:A:508:ASP:OD1	2.30	0.44
2:B:401:THR:OG1	2:B:501:THR:OG1	2.30	0.43
1:A:232:ILE:HD13	1:A:449:LEU:HD13	2.00	0.43
1:A:551:GLN:O	1:A:555:GLN:HG2	2.19	0.43
1:A:91:LEU:H	5:A:801:NAG:H82	1.84	0.43
1:A:30:GLU:HG3	2:B:517:ALA:HB2	2.01	0.42
1:A:452:THR:HG23	1:A:511:PHE:CD2	2.54	0.42
1:A:95:ARG:NH2	1:A:564:PRO:HD3	2.35	0.42
1:A:354:ASP:OD1	7:A:901:HOH:O	2.22	0.41
1:A:256:SER:HB2	1:A:609:TRP:CE2	2.56	0.41
2:B:395:THR:N	2:B:396:PRO:HD2	2.36	0.41
1:A:569:LEU:O	1:A:573:VAL:HG22	2.21	0.40
1:A:55:THR:O	1:A:59:VAL:HG23	2.21	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	590/766 (77%)	586 (99%)	4 (1%)	0	100	100
2	B	190/267 (71%)	188 (99%)	2 (1%)	0	100	100
All	All	780/1033 (76%)	774 (99%)	6 (1%)	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	478/677 (71%)	471 (98%)	7 (2%)	60	77
2	B	132/233 (57%)	125 (95%)	7 (5%)	19	33
All	All	610/910 (67%)	596 (98%)	14 (2%)	46	66

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	60	GLN
1	A	133	LEU
1	A	380	TYR
1	A	400	HIS
1	A	482	GLU
1	A	599	ARG
2	B	392	CYS

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Mol	Chain	Res	Type
2	B	416	CYS
2	B	419	ASN
2	B	432	PHE
2	B	437	VAL
2	B	466	GLN
2	B	486	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
2	B	567	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 ⓘ

10 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	$\# Z > 2$
3	NAG	C	1	3,1	14,14,15	0.73	0	17,19,21	0.93	1 (5%)
3	NAG	C	2	3	14,14,15	0.73	0	17,19,21	0.83	0
4	NAG	D	1	4,1	14,14,15	0.76	0	17,19,21	0.98	1 (5%)
4	NAG	D	2	4	14,14,15	0.73	0	17,19,21	0.77	0
4	BMA	D	3	4	11,11,12	0.88	0	15,15,17	1.69	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUC	D	4	4	10,10,11	0.82	0	14,14,16	0.89	0
4	NAG	E	1	4,1	14,14,15	0.76	0	17,19,21	0.95	0
4	NAG	E	2	4	14,14,15	0.73	0	17,19,21	0.84	0
4	BMA	E	3	4	11,11,12	0.80	0	15,15,17	1.74	1 (6%)
4	FUC	E	4	4	10,10,11	0.79	0	14,14,16	0.88	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
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	1/2/19/22	0/1/1/1
4	FUC	D	4	4	-	-	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	1/2/19/22	0/1/1/1
4	FUC	E	4	4	-	-	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(°)
4	E	3	BMA	C1-O5-C5	5.13	119.06	112.19
4	D	3	BMA	C1-O5-C5	5.07	118.98	112.19
4	D	1	NAG	C1-O5-C5	2.35	115.33	112.19
3	C	1	NAG	C1-O5-C5	2.10	115.00	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6

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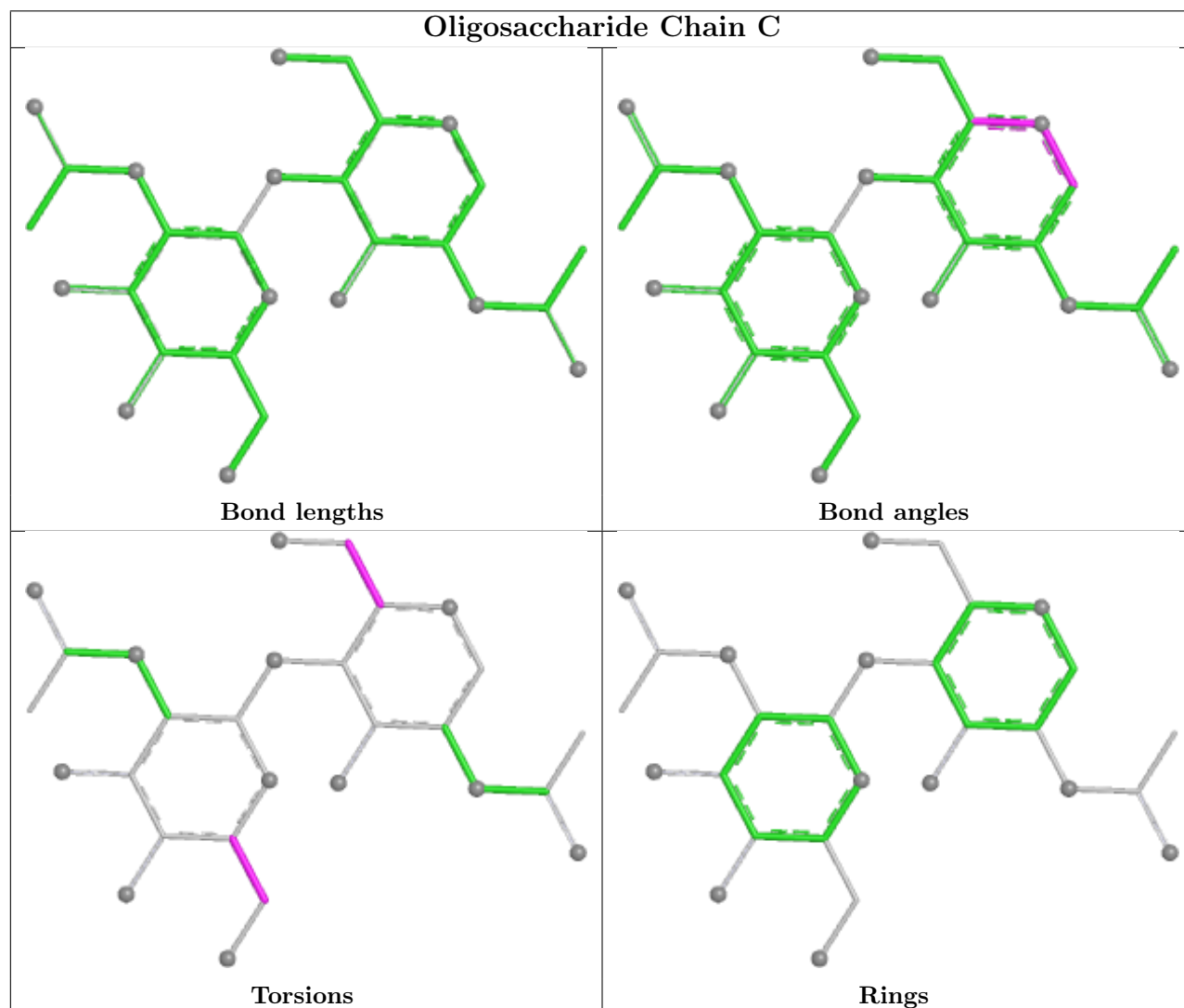
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
4	D	3	BMA	C4-C5-C6-O6

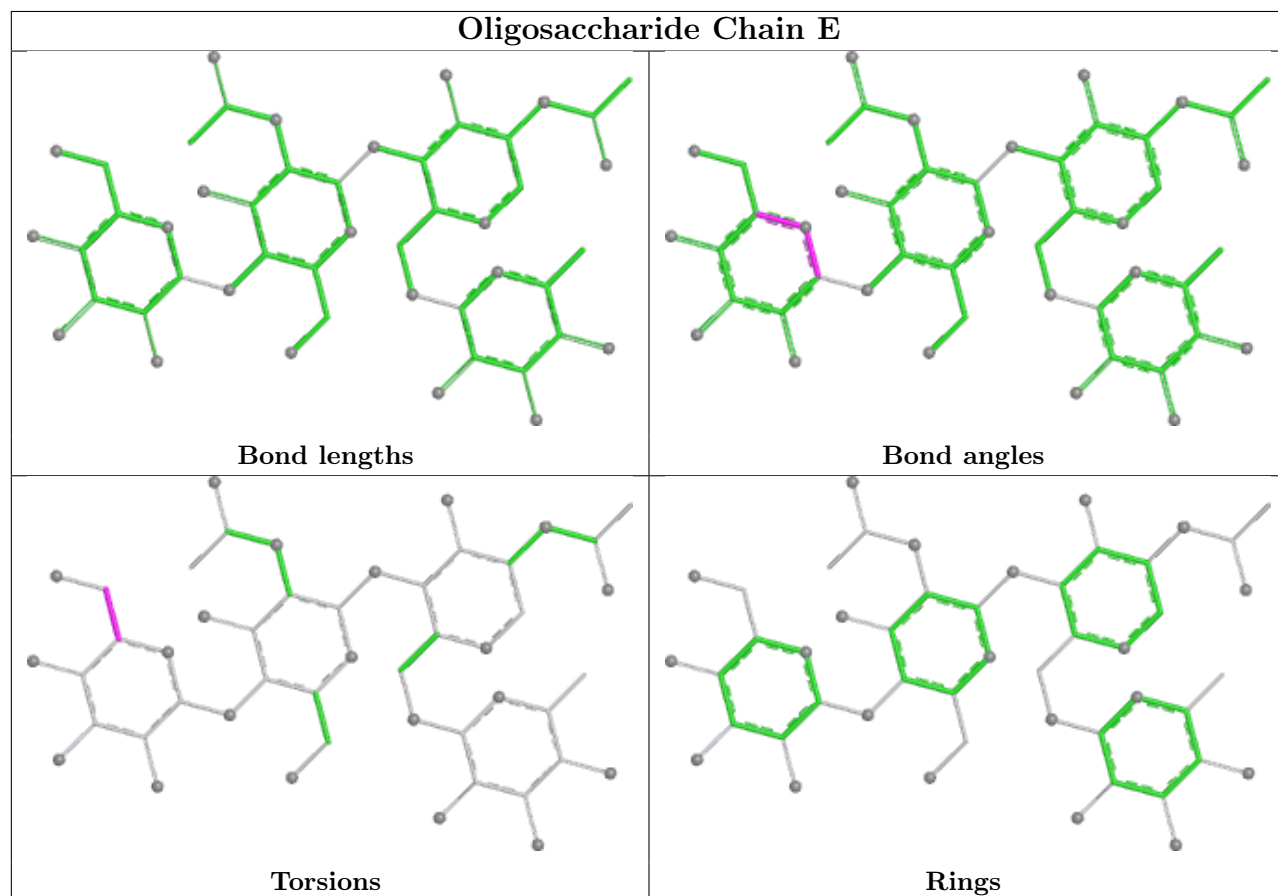
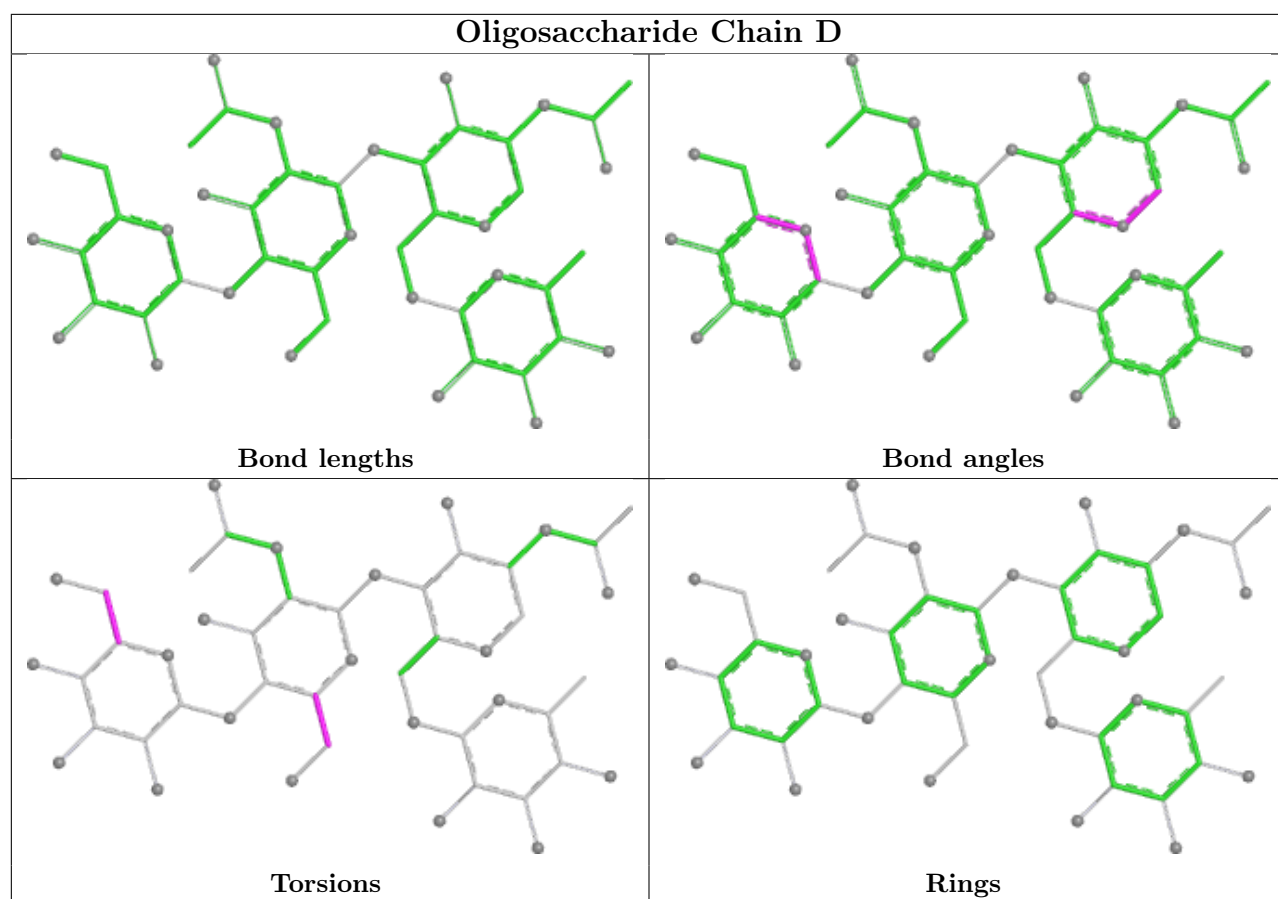
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	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

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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
5	NAG	B	702	2	14,14,15	0.75	0	17,19,21	0.92	1 (5%)
5	NAG	A	801	1	14,14,15	0.73	0	17,19,21	0.78	0
5	NAG	B	701	2	14,14,15	0.72	0	17,19,21	1.04	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	702	2	-	2/6/23/26	0/1/1/1
5	NAG	A	801	1	-	2/6/23/26	0/1/1/1
5	NAG	B	701	2	-	4/6/23/26	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	702	NAG	O5-C1-C2	-2.34	107.67	111.29
5	B	701	NAG	C1-O5-C5	2.23	115.18	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	701	NAG	O5-C5-C6-O6
5	B	702	NAG	C4-C5-C6-O6
5	B	701	NAG	C4-C5-C6-O6
5	A	801	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	702	NAG	O5-C5-C6-O6
5	A	801	NAG	C4-C5-C6-O6
5	B	701	NAG	C8-C7-N2-C2
5	B	701	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	801	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.

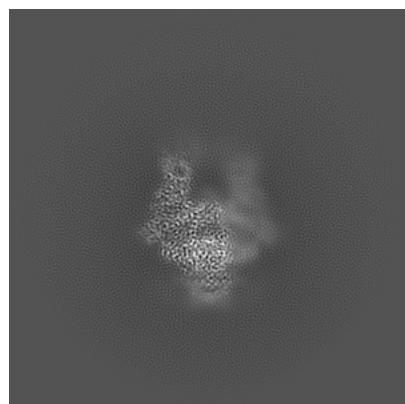
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47358. These allow visual inspection of the internal detail of the map and identification of artifacts.

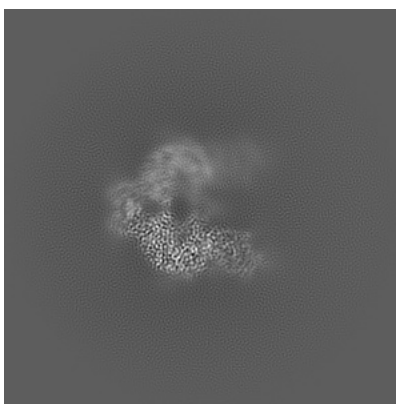
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

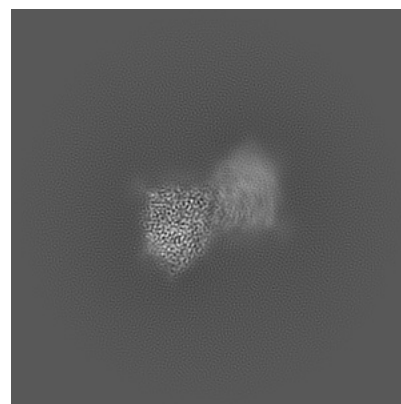
6.1.1 Primary map



X

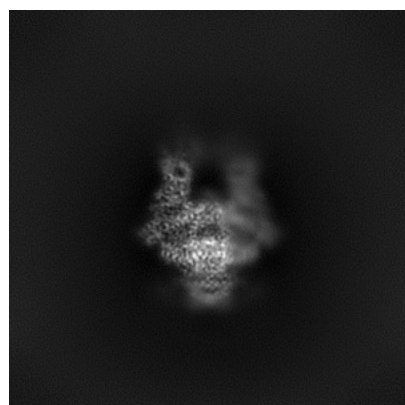


Y

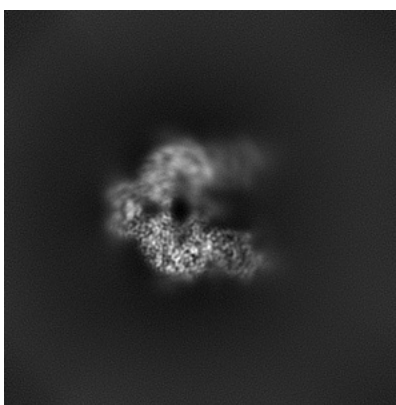


Z

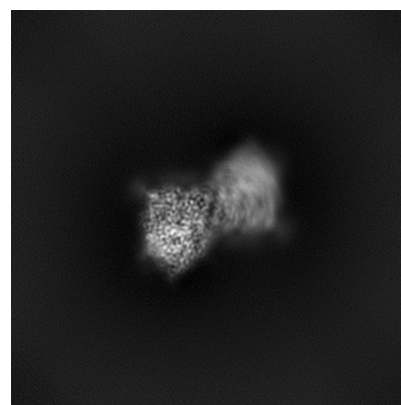
6.1.2 Raw map



X



Y

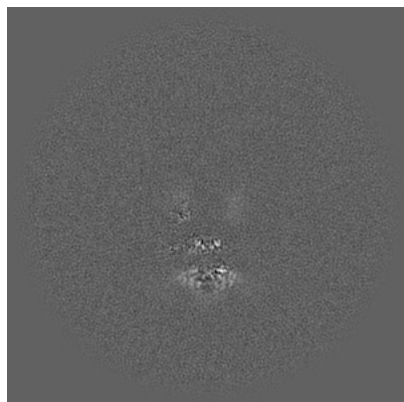


Z

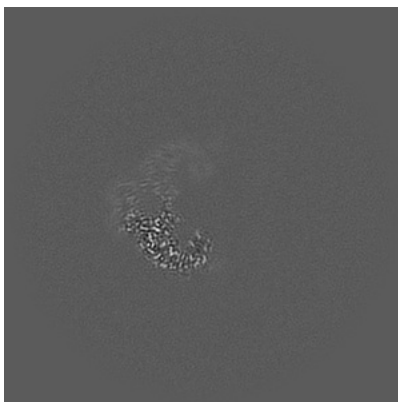
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

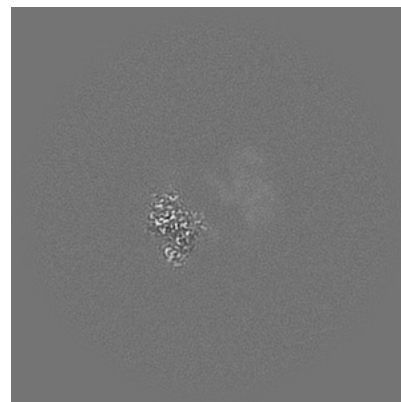
6.2.1 Primary map



X Index: 160



Y Index: 160

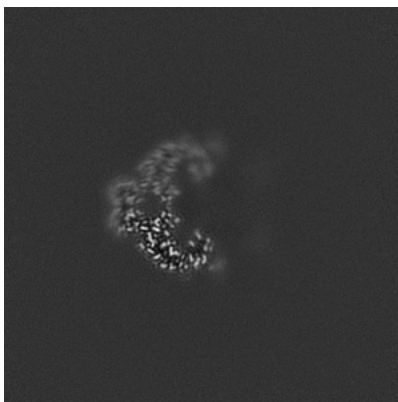


Z Index: 160

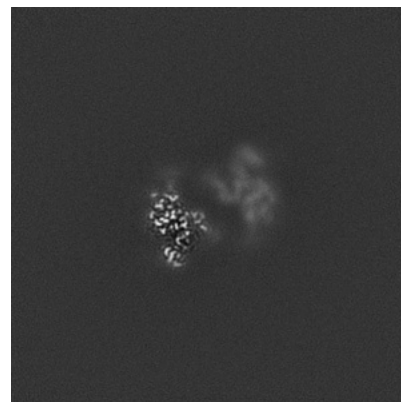
6.2.2 Raw map



X Index: 160



Y Index: 160

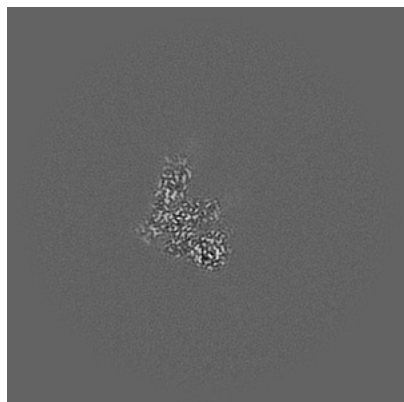


Z Index: 160

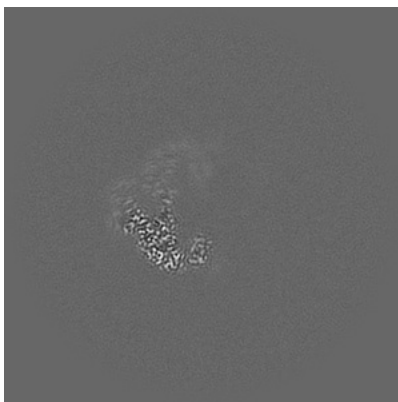
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

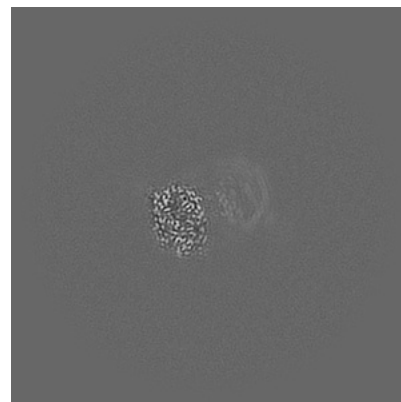
6.3.1 Primary map



X Index: 126

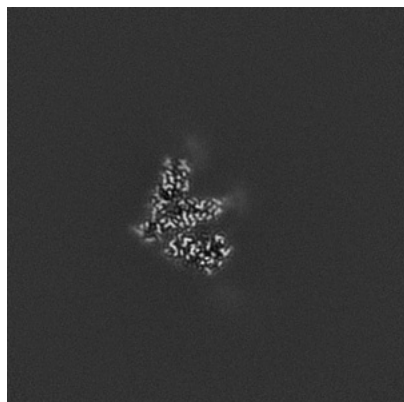


Y Index: 163

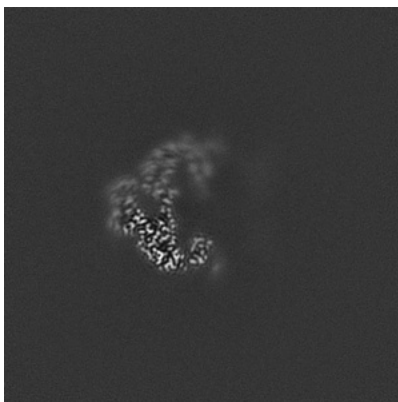


Z Index: 123

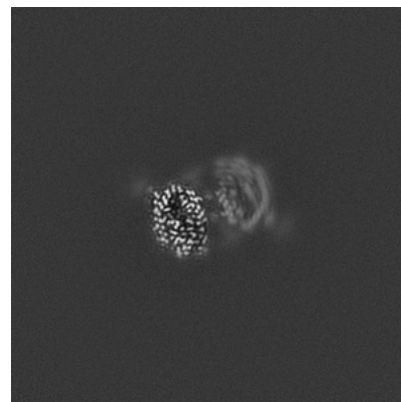
6.3.2 Raw map



X Index: 129



Y Index: 163

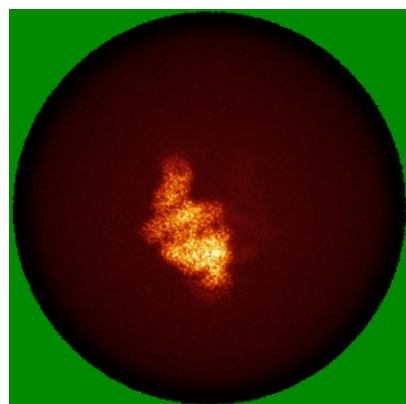


Z Index: 123

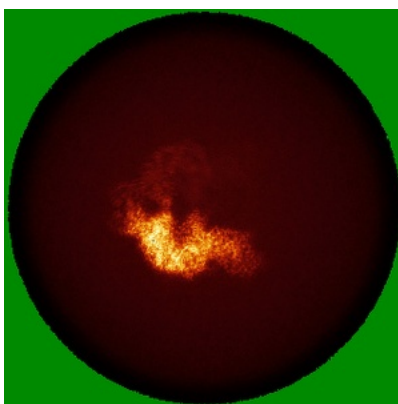
The images above show the largest variance slices of the map in three orthogonal directions.

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

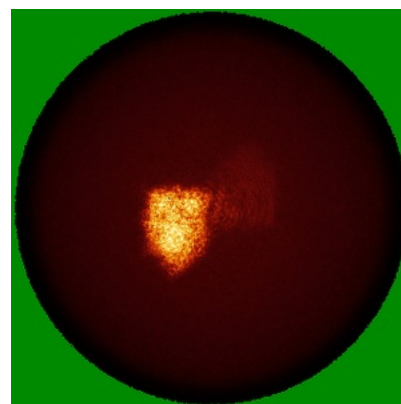
6.4.1 Primary map



X

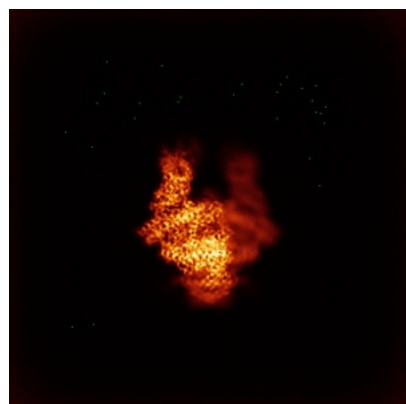


Y

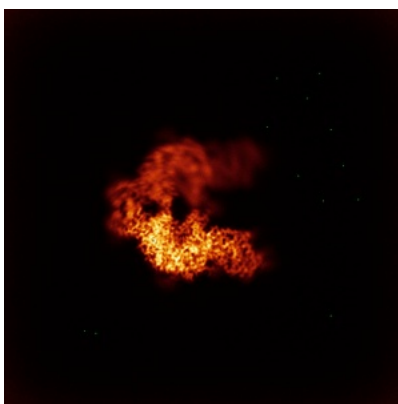


Z

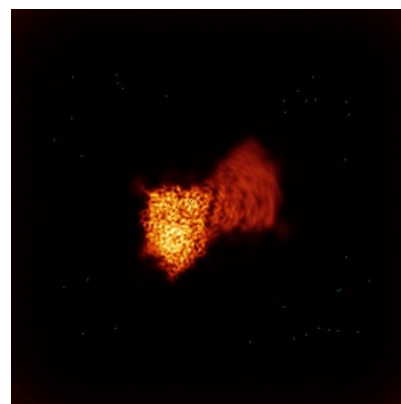
6.4.2 Raw map



X



Y

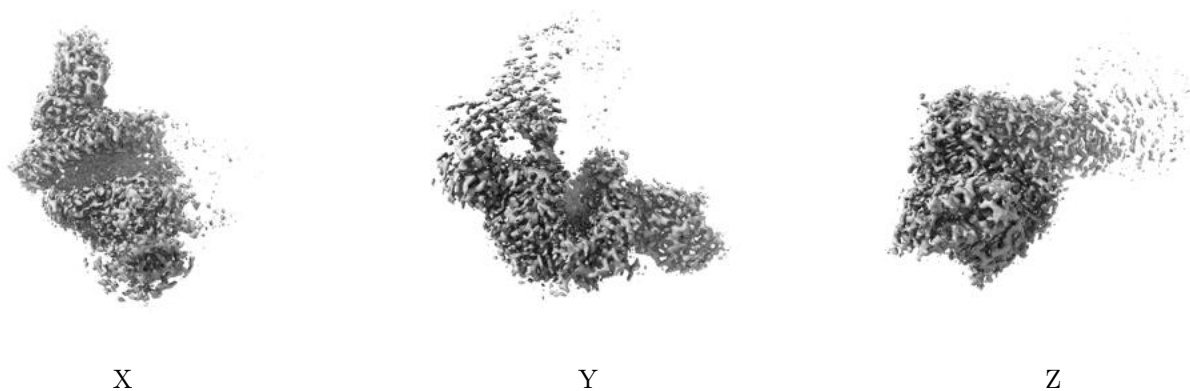


Z

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.

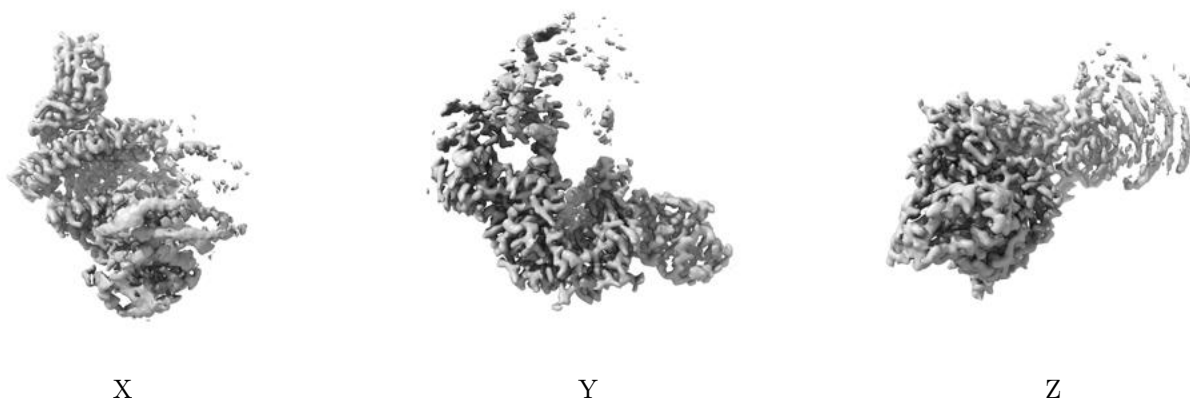
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

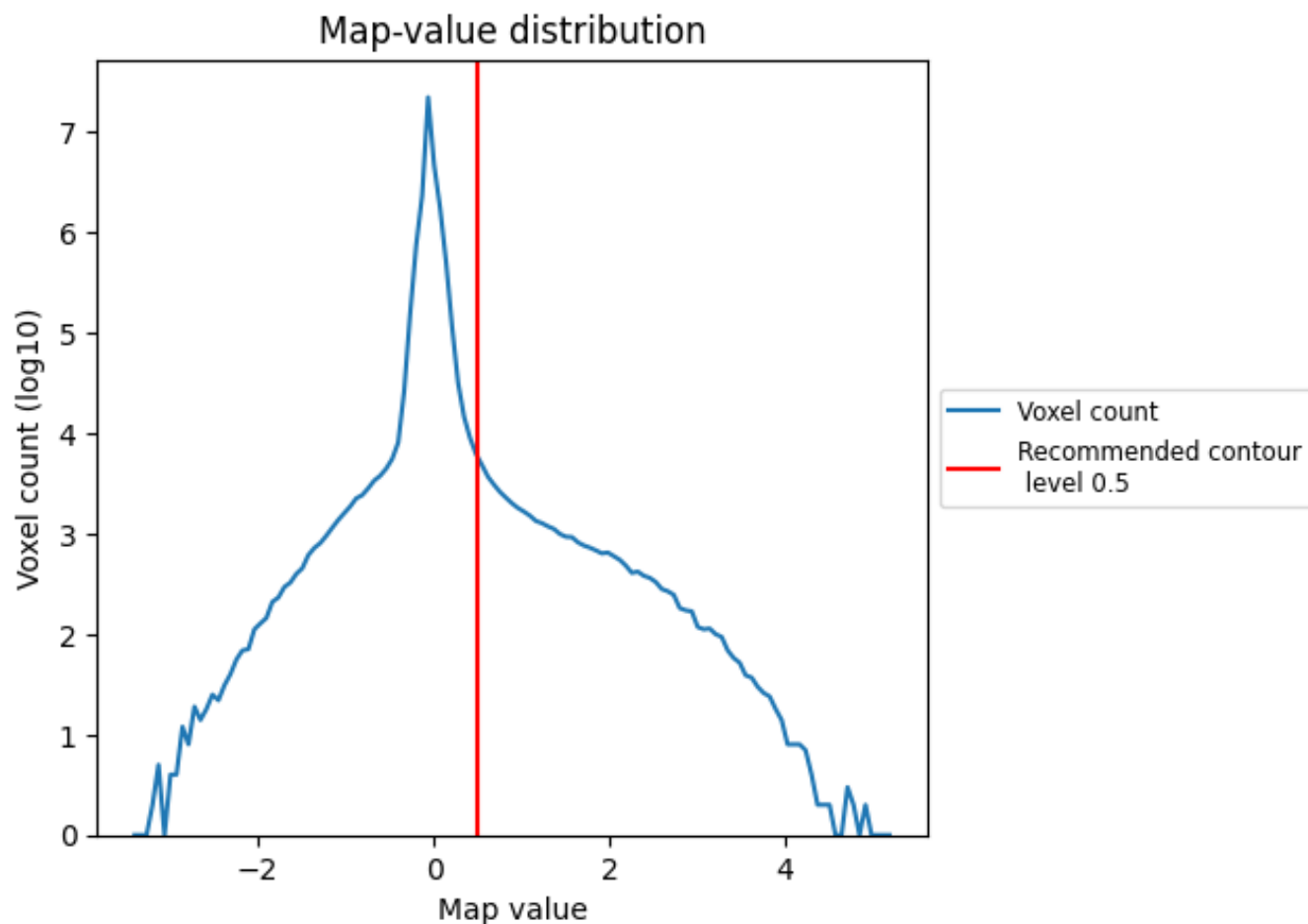
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

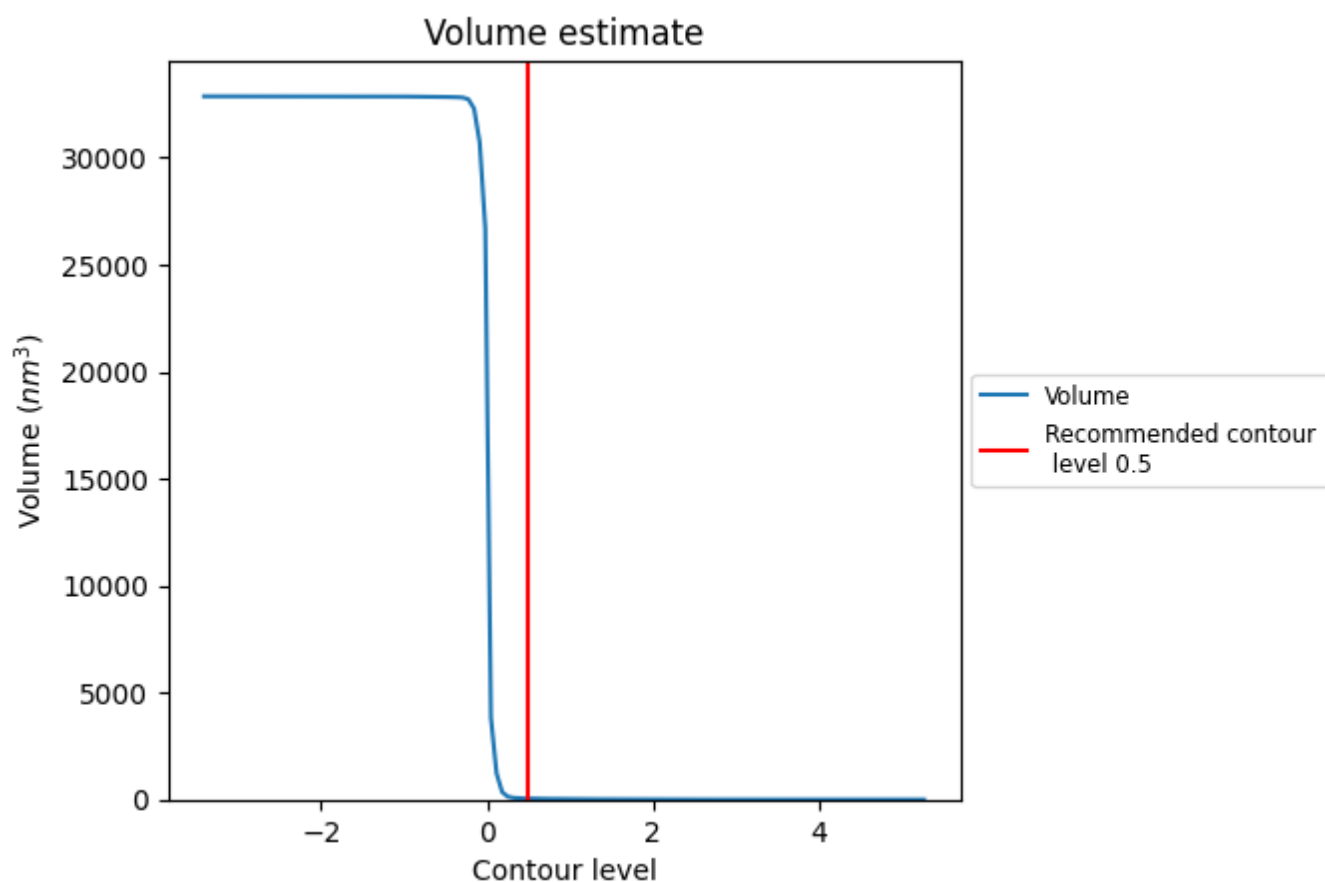
This section contains the results of statistical analysis of the map.

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.

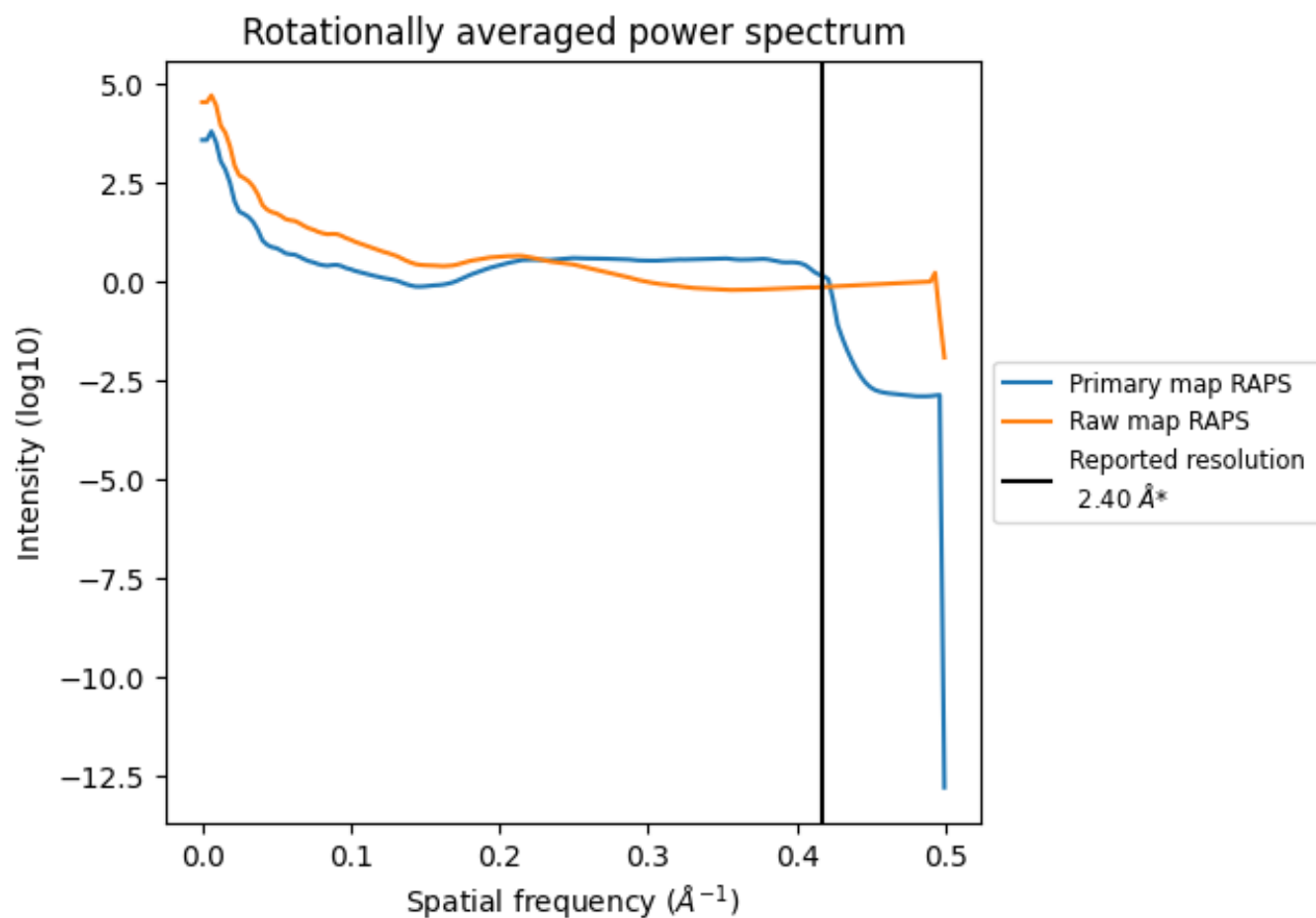
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46 nm³; this corresponds to an approximate mass of 42 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 ⓘ

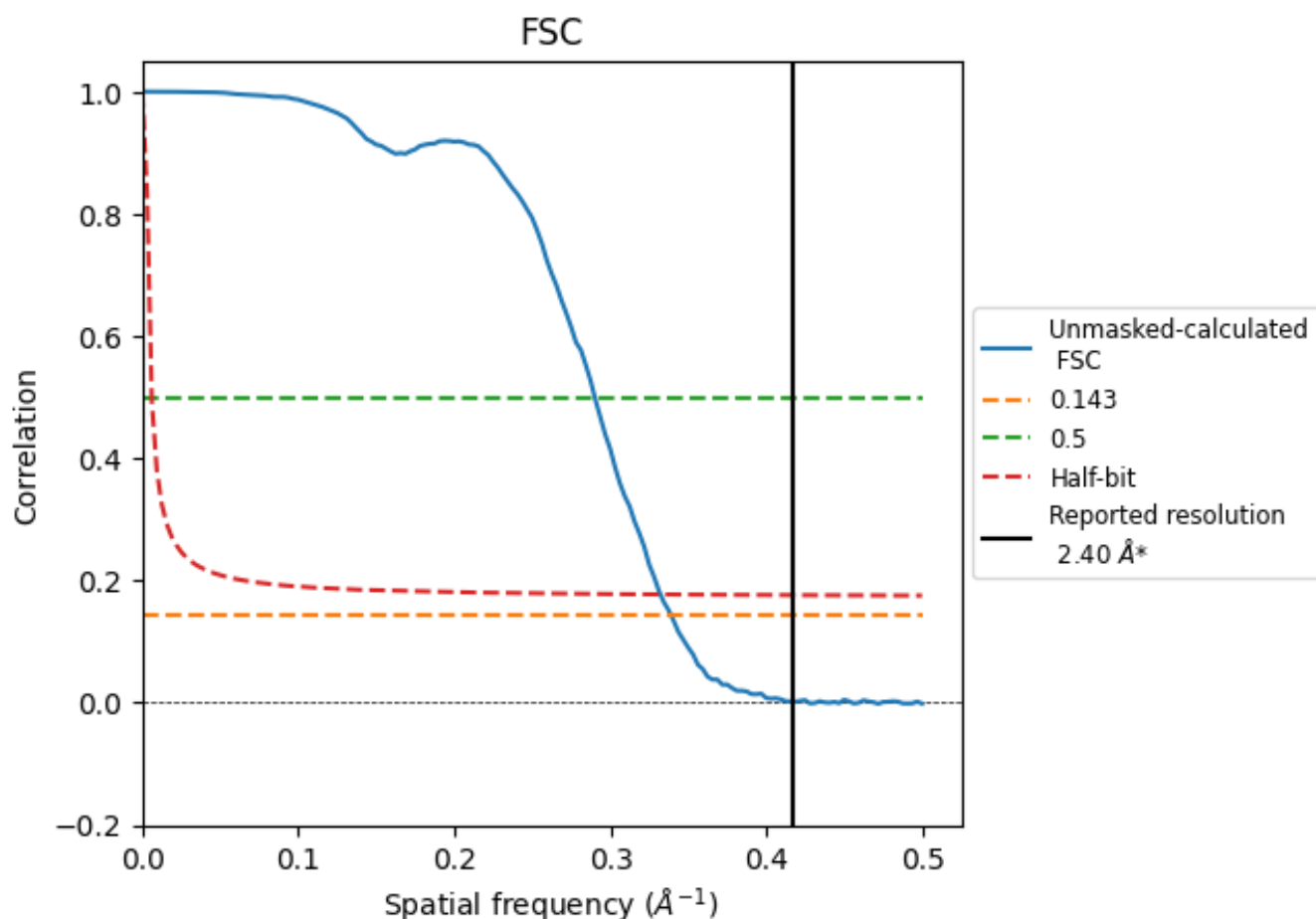


*Reported resolution corresponds to spatial frequency of 0.417 \AA^{-1}

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 0.417 \AA^{-1}

8.2 Resolution estimates [i](#)

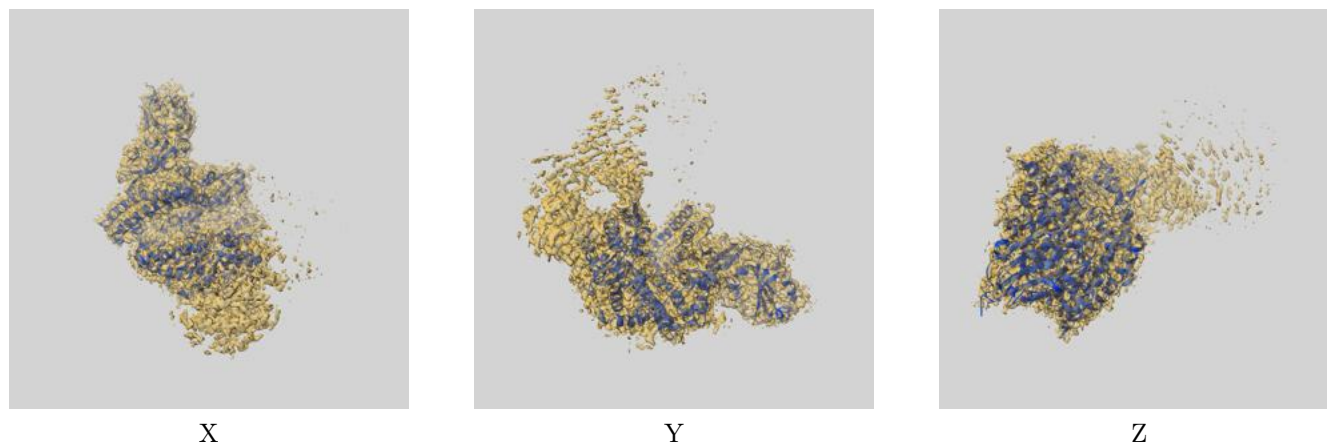
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.95	3.45	3.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47358 and PDB model 9E0I. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



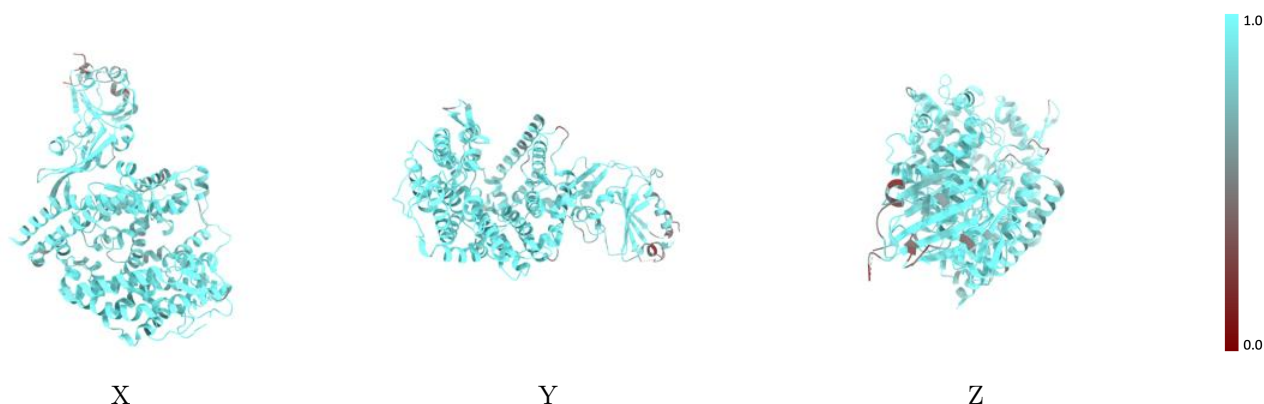
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



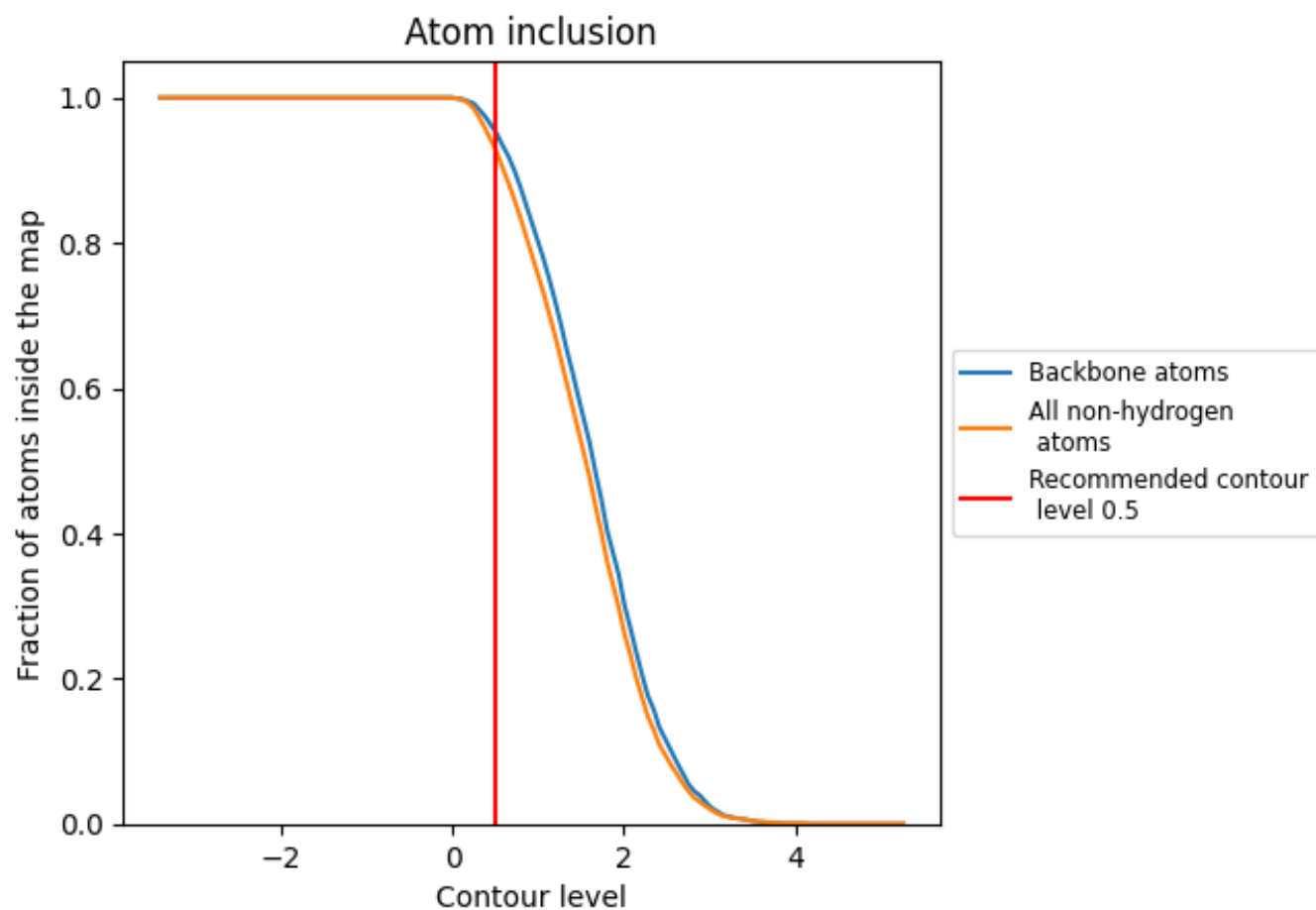
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9300	<div></div> 0.6760
A	<div></div> 0.9600	<div></div> 0.6910
B	<div></div> 0.8770	<div></div> 0.6390
C	<div></div> 0.4640	<div></div> 0.5460
D	<div></div> 0.5100	<div></div> 0.5500
E	<div></div> 0.3060	<div></div> 0.4760

