



Full wwPDB EM Validation Report ⓘ

Aug 18, 2025 – 11:08 AM EDT

PDB ID : 9N7D / pdb_00009n7d
EMDB ID : EMD-49092
Title : Structure of the Rattus norvegicus ACE2 receptor bound HsItaly2011 RBD complex
Authors : Park, Y.J.; Seattle Structural Genomics Center for Infectious Disease (SSG-CID); Veessler, D.
Deposited on : 2025-02-05
Resolution : 2.50 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>
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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.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.45.1

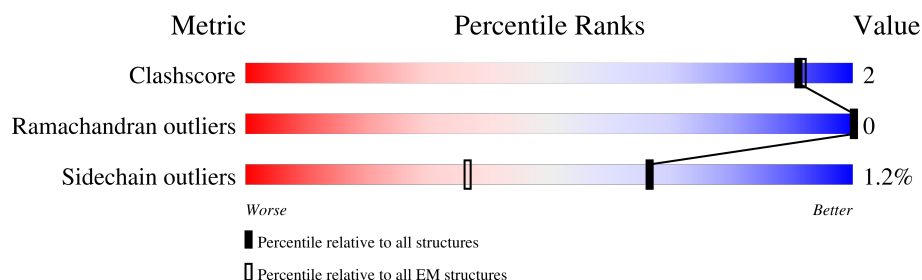
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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	767	
2	B	271	
3	C	2	
3	D	2	
3	E	2	
3	F	2	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7246 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	704	Total	C	N	O	S	0	0
			5502	3540	939	993	30		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	742	GLY	TRP	conflict	UNP Q5EGZ1
A	744	ASN	-	expression tag	UNP Q5EGZ1
A	745	ASP	-	expression tag	UNP Q5EGZ1
A	746	ILE	-	expression tag	UNP Q5EGZ1
A	747	PHE	-	expression tag	UNP Q5EGZ1
A	748	GLU	-	expression tag	UNP Q5EGZ1
A	749	ALA	-	expression tag	UNP Q5EGZ1
A	750	GLN	-	expression tag	UNP Q5EGZ1
A	751	LYS	-	expression tag	UNP Q5EGZ1
A	752	ILE	-	expression tag	UNP Q5EGZ1
A	753	GLU	-	expression tag	UNP Q5EGZ1
A	754	TRP	-	expression tag	UNP Q5EGZ1
A	755	HIS	-	expression tag	UNP Q5EGZ1
A	756	GLU	-	expression tag	UNP Q5EGZ1
A	757	GLY	-	expression tag	UNP Q5EGZ1
A	758	GLY	-	expression tag	UNP Q5EGZ1
A	759	SER	-	expression tag	UNP Q5EGZ1
A	760	HIS	-	expression tag	UNP Q5EGZ1
A	761	HIS	-	expression tag	UNP Q5EGZ1
A	762	HIS	-	expression tag	UNP Q5EGZ1
A	763	HIS	-	expression tag	UNP Q5EGZ1
A	764	HIS	-	expression tag	UNP Q5EGZ1
A	765	HIS	-	expression tag	UNP Q5EGZ1
A	766	HIS	-	expression tag	UNP Q5EGZ1
A	767	HIS	-	expression tag	UNP Q5EGZ1

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	193	Total	C	N	O	S	0	0
			1451	952	232	256	11		

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	356	MET	-	expression tag	UNP A0A2I6PIW5
B	357	GLY	-	expression tag	UNP A0A2I6PIW5
B	358	ILE	-	expression tag	UNP A0A2I6PIW5
B	359	LEU	-	expression tag	UNP A0A2I6PIW5
B	360	PRO	-	expression tag	UNP A0A2I6PIW5
B	361	SER	-	expression tag	UNP A0A2I6PIW5
B	362	PRO	-	expression tag	UNP A0A2I6PIW5
B	363	GLY	-	expression tag	UNP A0A2I6PIW5
B	364	MET	-	expression tag	UNP A0A2I6PIW5
B	365	PRO	-	expression tag	UNP A0A2I6PIW5
B	366	ALA	-	expression tag	UNP A0A2I6PIW5
B	367	LEU	-	expression tag	UNP A0A2I6PIW5
B	368	LEU	-	expression tag	UNP A0A2I6PIW5
B	369	SER	-	expression tag	UNP A0A2I6PIW5
B	370	LEU	-	expression tag	UNP A0A2I6PIW5
B	371	VAL	-	expression tag	UNP A0A2I6PIW5
B	372	SER	-	expression tag	UNP A0A2I6PIW5
B	373	LEU	-	expression tag	UNP A0A2I6PIW5
B	374	LEU	-	expression tag	UNP A0A2I6PIW5
B	375	SER	-	expression tag	UNP A0A2I6PIW5
B	376	VAL	-	expression tag	UNP A0A2I6PIW5
B	377	LEU	-	expression tag	UNP A0A2I6PIW5
B	378	LEU	-	expression tag	UNP A0A2I6PIW5
B	379	MET	-	expression tag	UNP A0A2I6PIW5
B	380	GLY	-	expression tag	UNP A0A2I6PIW5
B	381	CYS	-	expression tag	UNP A0A2I6PIW5
B	382	VAL	-	expression tag	UNP A0A2I6PIW5
B	383	ALA	-	expression tag	UNP A0A2I6PIW5
B	384	GLU	-	expression tag	UNP A0A2I6PIW5
B	385	THR	-	expression tag	UNP A0A2I6PIW5
B	386	GLY	-	expression tag	UNP A0A2I6PIW5
B	387	THR	-	expression tag	UNP A0A2I6PIW5
B	590	LEU	-	expression tag	UNP A0A2I6PIW5
B	591	VAL	-	expression tag	UNP A0A2I6PIW5
B	592	PRO	-	expression tag	UNP A0A2I6PIW5
B	593	ARG	-	expression tag	UNP A0A2I6PIW5
B	594	GLY	-	expression tag	UNP A0A2I6PIW5

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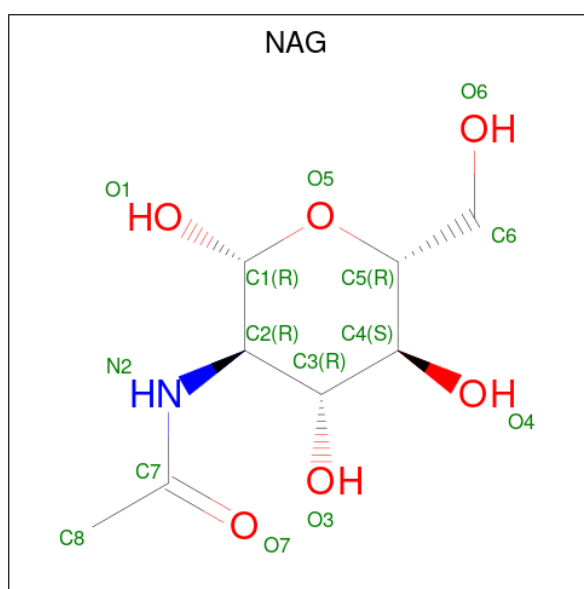
Chain	Residue	Modelled	Actual	Comment	Reference
B	595	SER	-	expression tag	UNP A0A2I6PIW5
B	596	SER	-	expression tag	UNP A0A2I6PIW5
B	597	SER	-	expression tag	UNP A0A2I6PIW5
B	598	GLY	-	expression tag	UNP A0A2I6PIW5
B	599	GLY	-	expression tag	UNP A0A2I6PIW5
B	600	SER	-	expression tag	UNP A0A2I6PIW5
B	601	GLY	-	expression tag	UNP A0A2I6PIW5
B	602	LEU	-	expression tag	UNP A0A2I6PIW5
B	603	ASN	-	expression tag	UNP A0A2I6PIW5
B	604	ASP	-	expression tag	UNP A0A2I6PIW5
B	605	ILE	-	expression tag	UNP A0A2I6PIW5
B	606	PHE	-	expression tag	UNP A0A2I6PIW5
B	607	GLU	-	expression tag	UNP A0A2I6PIW5
B	608	ALA	-	expression tag	UNP A0A2I6PIW5
B	609	GLN	-	expression tag	UNP A0A2I6PIW5
B	610	LYS	-	expression tag	UNP A0A2I6PIW5
B	611	ILE	-	expression tag	UNP A0A2I6PIW5
B	612	GLU	-	expression tag	UNP A0A2I6PIW5
B	613	TRP	-	expression tag	UNP A0A2I6PIW5
B	614	HIS	-	expression tag	UNP A0A2I6PIW5
B	615	GLU	-	expression tag	UNP A0A2I6PIW5
B	616	GLY	-	expression tag	UNP A0A2I6PIW5
B	617	GLY	-	expression tag	UNP A0A2I6PIW5
B	618	SER	-	expression tag	UNP A0A2I6PIW5
B	619	HIS	-	expression tag	UNP A0A2I6PIW5
B	620	HIS	-	expression tag	UNP A0A2I6PIW5
B	621	HIS	-	expression tag	UNP A0A2I6PIW5
B	622	HIS	-	expression tag	UNP A0A2I6PIW5
B	623	HIS	-	expression tag	UNP A0A2I6PIW5
B	624	HIS	-	expression tag	UNP A0A2I6PIW5
B	625	HIS	-	expression tag	UNP A0A2I6PIW5
B	626	HIS	-	expression tag	UNP A0A2I6PIW5

- 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		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

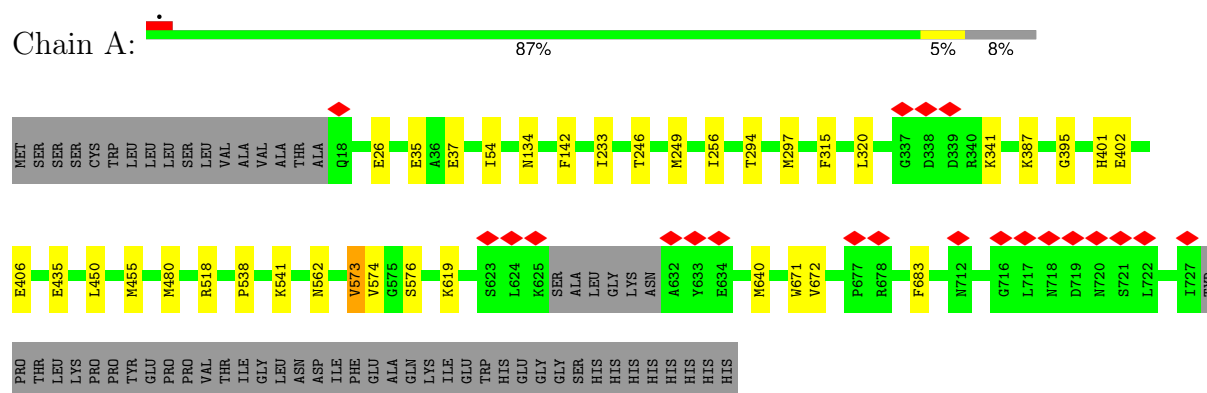
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	95	Total 95	O 95	0
6	B	15	Total 15	O 15	0

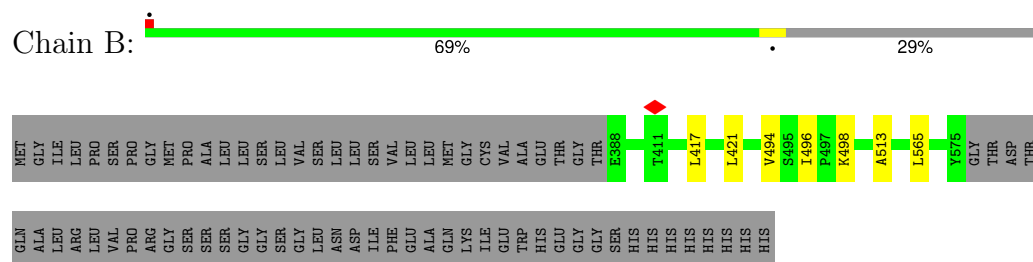
3 Residue-property plots

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.

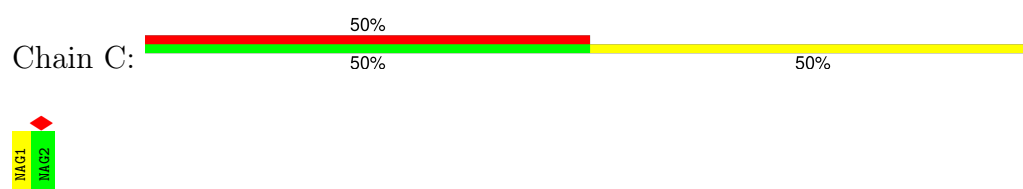
• Molecule 1: Angiotensin-converting enzyme 2



• Molecule 2: Spike glycoprotein



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



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





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



- Molecule 3: 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	831432	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 ($e^-/\text{\AA}^2$)	60.00	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.901	Depositor
Minimum map value	-3.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.45	Depositor
Map size (\AA)	320.352, 320.352, 320.352	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0011, 1.0011, 1.0011	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 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	0.17	0/5655	0.30	0/7708
2	B	0.11	0/1495	0.27	0/2049
All	All	0.16	0/7150	0.29	0/9757

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 ⓘ

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	5502	0	5109	19	0
2	B	1451	0	1297	3	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	A	42	0	39	0	0
4	B	28	0	26	0	0
5	A	1	0	0	0	0
6	A	95	0	0	0	0
6	B	15	0	0	0	0
All	All	7246	0	6571	21	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 2.

All (21) 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:A:233:ILE:HD13	1:A:450:LEU:HD13	1.80	0.64
1:A:134:ASN:HD21	1:A:142:PHE:HE1	1.47	0.62
1:A:54:ILE:HB	1:A:341:LYS:HG3	1.85	0.59
1:A:402:GLU:O	1:A:406:GLU:HG2	2.10	0.51
1:A:640:MET:HE2	1:A:672:VAL:HG21	1.92	0.51
1:A:249:MET:HG2	1:A:256:ILE:HB	1.94	0.49
1:A:402:GLU:HB2	1:A:518:ARG:HG3	1.95	0.48
1:A:315:PHE:HD1	1:A:320:LEU:HD12	1.79	0.46
1:A:246:THR:HA	1:A:249:MET:HE3	1.98	0.46
1:A:573:VAL:HG13	1:A:574:VAL:HG13	1.99	0.44
1:A:619:LYS:N	1:A:619:LYS:HD2	2.32	0.43
1:A:26:GLU:HG2	2:B:513:ALA:HB3	2.00	0.43
2:B:494:VAL:HG12	2:B:496:ILE:HG13	2.01	0.42
1:A:395:GLY:O	1:A:562:ASN:HB3	2.20	0.42
1:A:574:VAL:HG23	1:A:576:SER:H	1.84	0.42
1:A:455:MET:HE3	1:A:480:MET:HB2	2.00	0.42
1:A:671:TRP:O	1:A:683:PHE:HA	2.19	0.41
2:B:498:LYS:HB2	2:B:565:LEU:HD13	2.02	0.41
1:A:134:ASN:H	1:A:134:ASN:HD22	1.68	0.41
1:A:294:THR:HA	1:A:297:MET:HE3	2.04	0.40
1:A:538:PRO:HG2	1:A:541:LYS:HD2	2.04	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	700/767 (91%)	694 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	189/271 (70%)	185 (98%)	4 (2%)	0	100	100
All	All	889/1038 (86%)	879 (99%)	10 (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	546/680 (80%)	540 (99%)	6 (1%)	70	87
2	B	139/236 (59%)	137 (99%)	2 (1%)	62	83
All	All	685/916 (75%)	677 (99%)	8 (1%)	66	86

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	37	GLU
1	A	387	LYS
1	A	401	HIS
1	A	435	GLU
1	A	573	VAL
2	B	417	LEU
2	B	421	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	134	ASN
1	A	159	ASN
1	A	239	GLN
1	A	522	GLN

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Mol	Chain	Res	Type
1	A	531	GLN
1	A	599	ASN

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 ⓘ

8 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	1,3	14,14,15	0.72	0	17,19,21	0.95	1 (5%)
3	NAG	C	2	3	14,14,15	0.71	0	17,19,21	0.88	0
3	NAG	D	1	1,3	14,14,15	0.75	0	17,19,21	0.97	1 (5%)
3	NAG	D	2	3	14,14,15	0.74	0	17,19,21	0.79	0
3	NAG	E	1	1,3	14,14,15	0.72	0	17,19,21	0.82	0
3	NAG	E	2	3	14,14,15	0.72	0	17,19,21	0.83	0
3	NAG	F	1	2,3	14,14,15	0.76	0	17,19,21	0.96	0
3	NAG	F	2	3	14,14,15	0.71	0	17,19,21	0.82	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	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	NAG	F	1	2,3	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	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(°)
3	C	1	NAG	C1-O5-C5	2.51	115.55	112.19
3	D	1	NAG	C2-N2-C7	2.18	125.82	122.90

There are no chirality outliers.

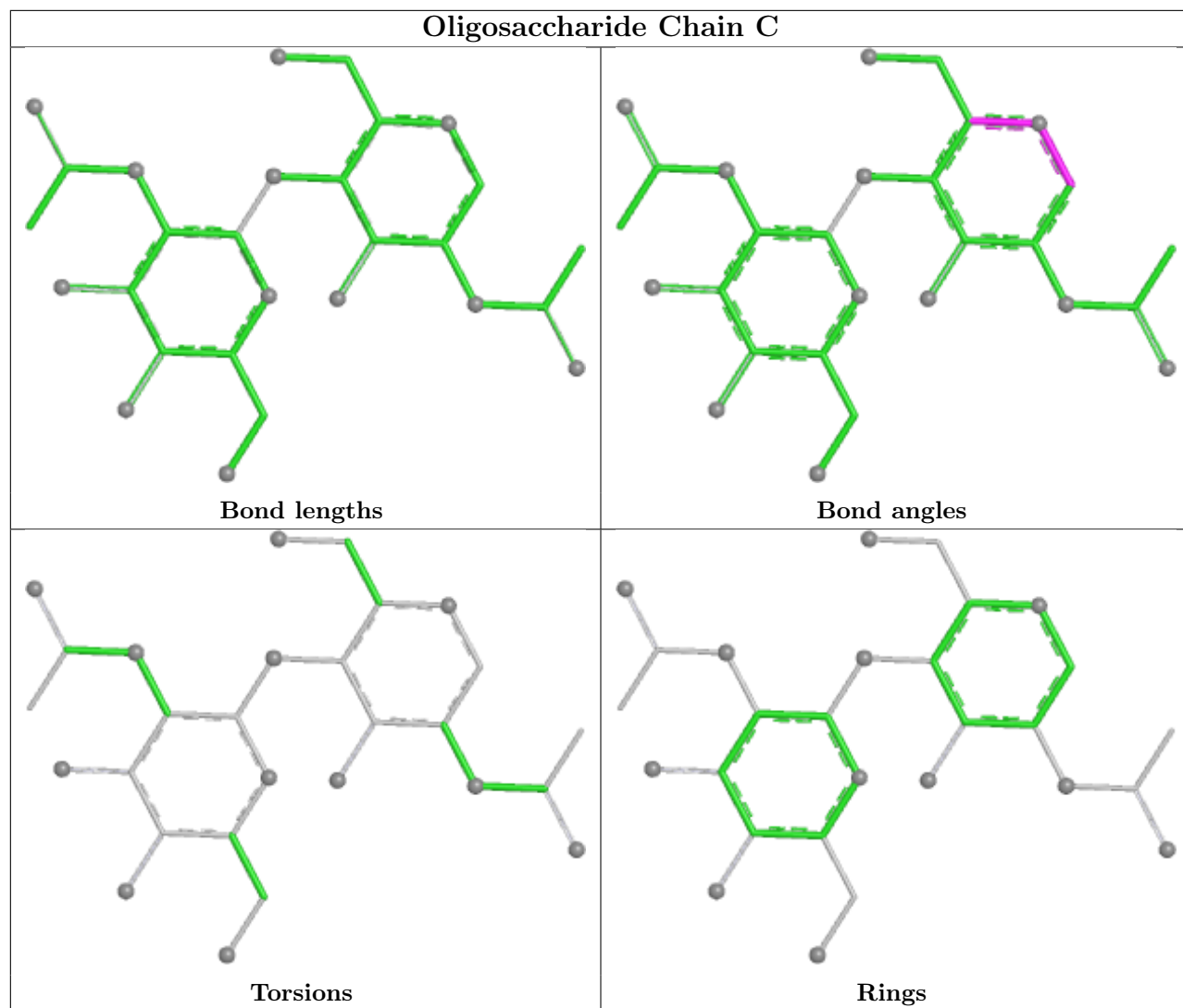
All (4) torsion outliers are listed below:

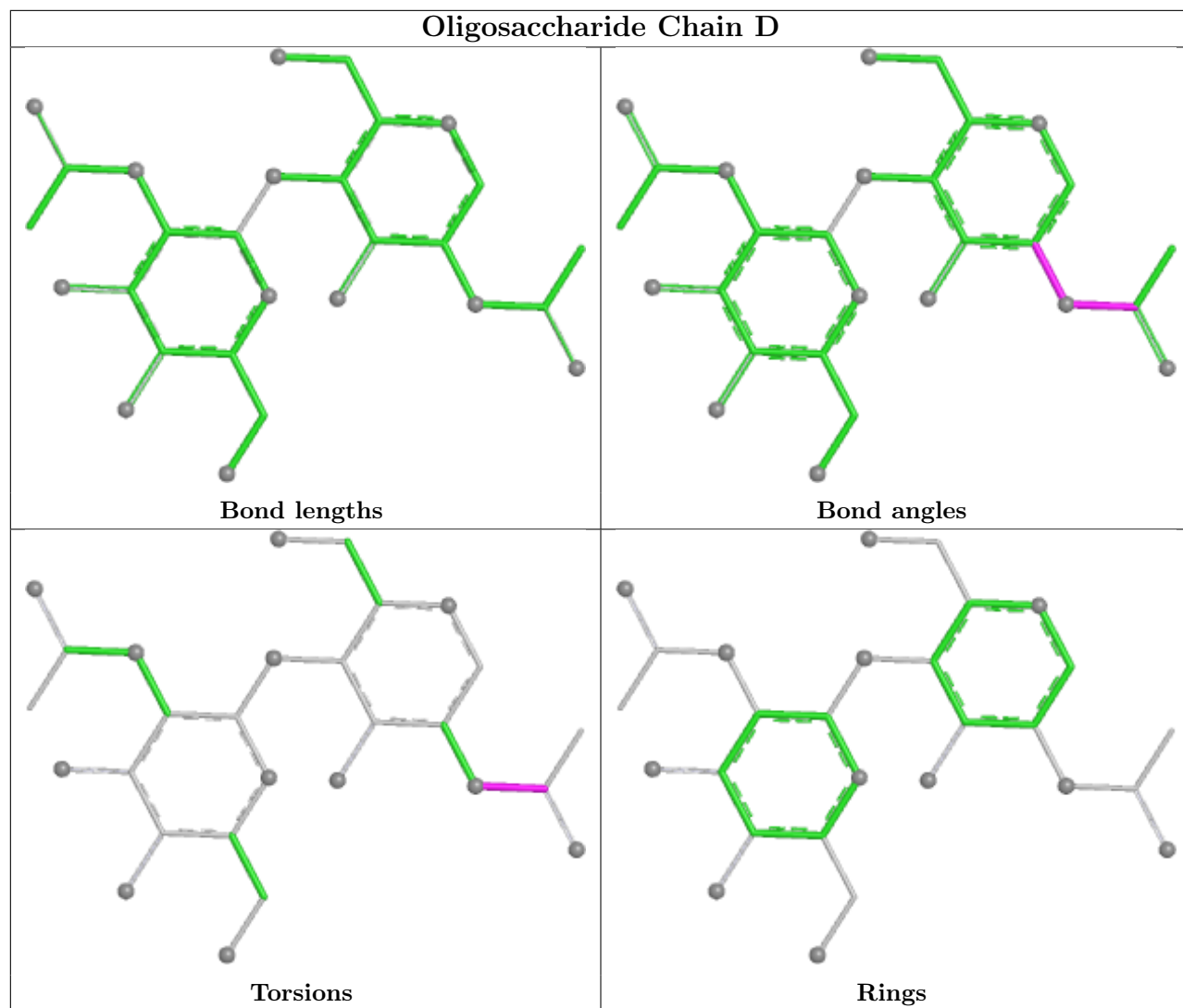
Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	F	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6

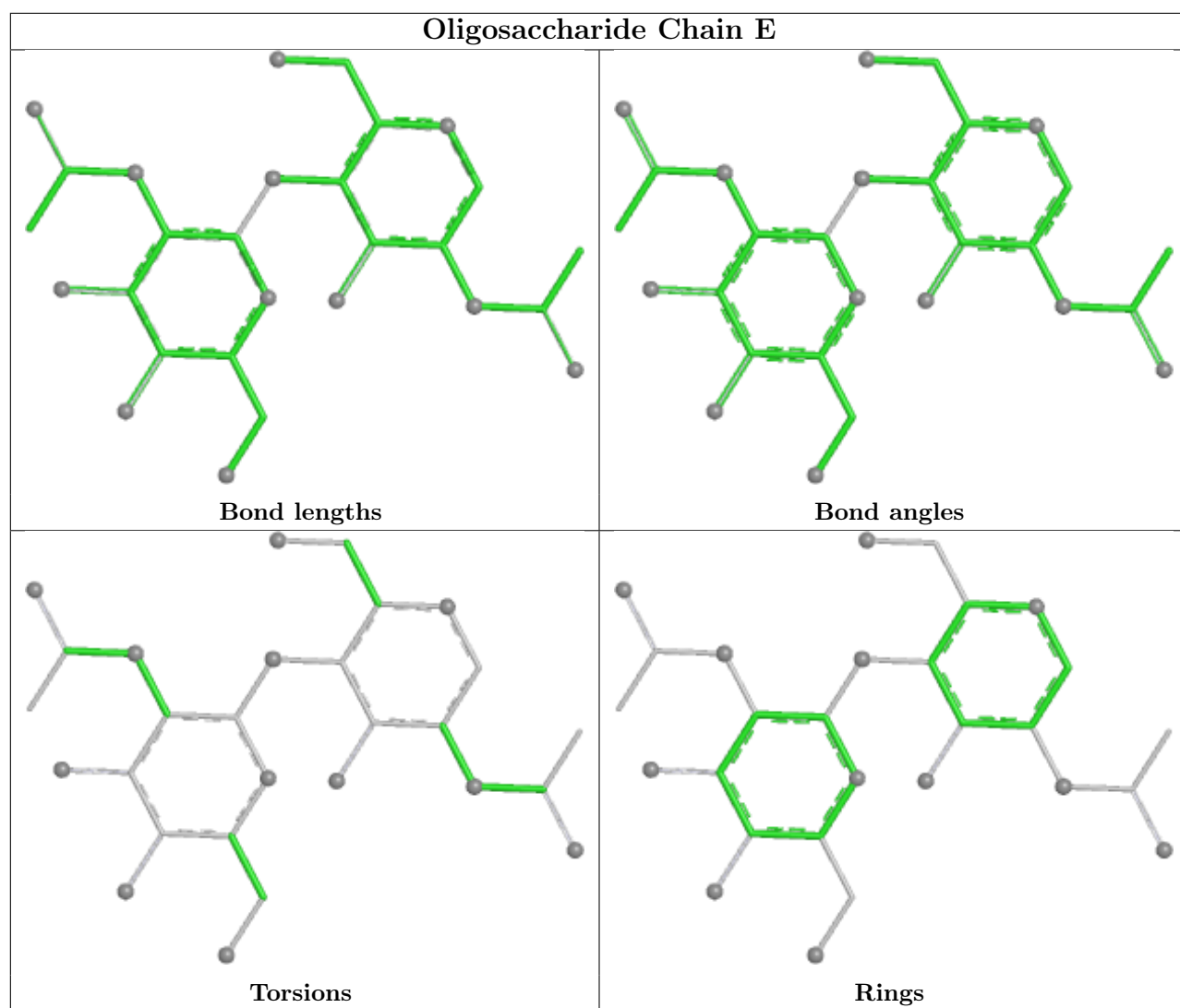
There are no ring outliers.

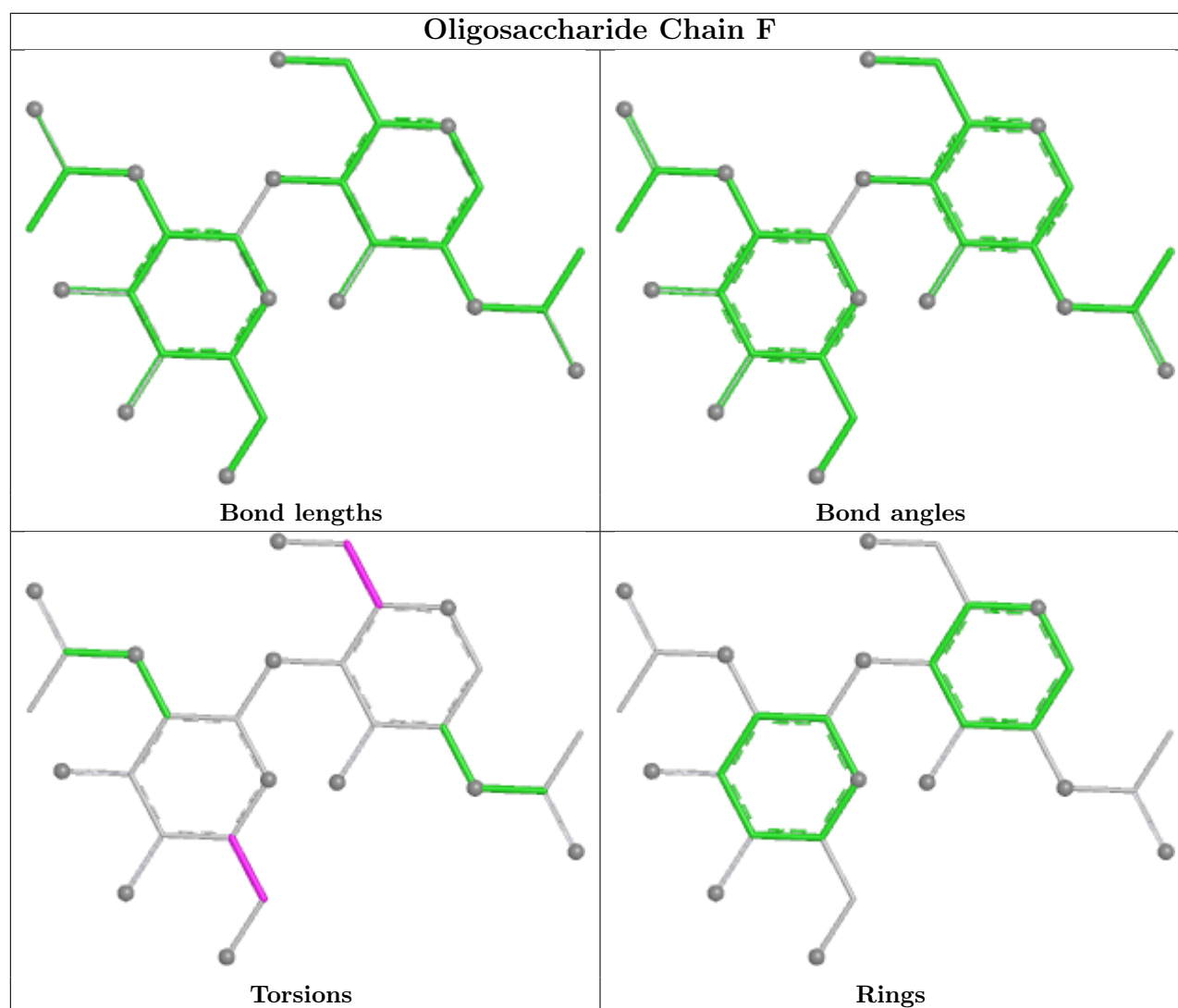
No monomer is involved in short contacts.

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 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
4	NAG	A	803	1	14,14,15	0.41	0	17,19,21	0.76	0
4	NAG	A	802	1	14,14,15	0.72	0	17,19,21	0.87	0
4	NAG	B	702	2	14,14,15	0.71	0	17,19,21	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	701	2	14,14,15	0.69	0	17,19,21	0.86	0
4	NAG	A	801	1	14,14,15	0.75	0	17,19,21	0.93	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	803	1	-	1/6/23/26	0/1/1/1
4	NAG	A	802	1	-	1/6/23/26	0/1/1/1
4	NAG	B	702	2	-	0/6/23/26	0/1/1/1
4	NAG	B	701	2	-	1/6/23/26	0/1/1/1
4	NAG	A	801	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	701	NAG	O5-C5-C6-O6
4	A	803	NAG	C1-C2-N2-C7
4	A	802	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

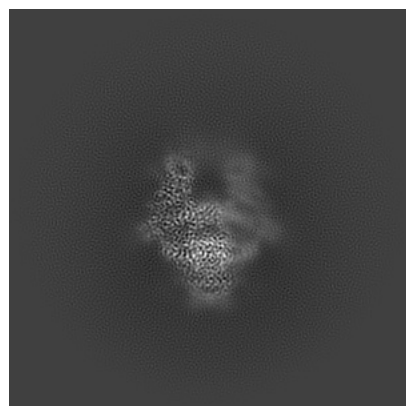
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49092. These allow visual inspection of the internal detail of the map and identification of artifacts.

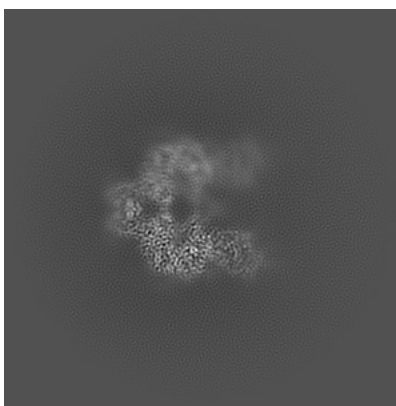
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

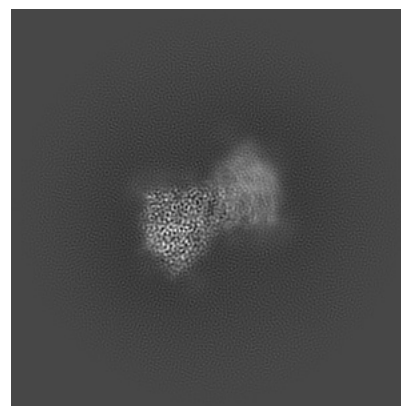
6.1.1 Primary map



X

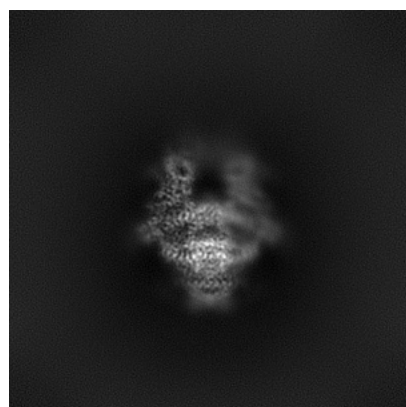


Y

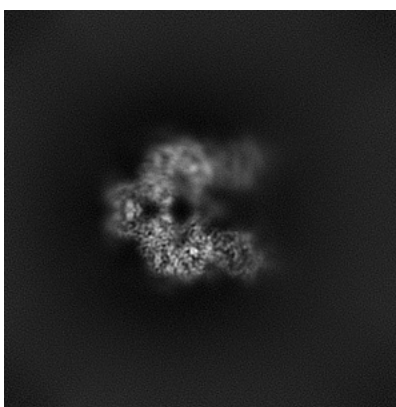


Z

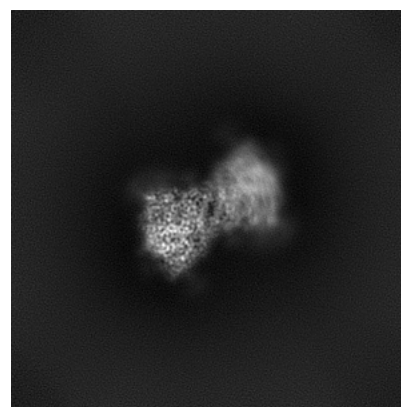
6.1.2 Raw map



X



Y

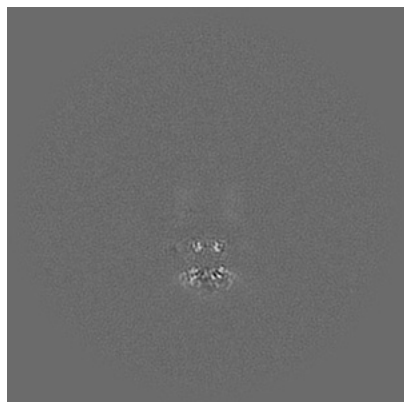


Z

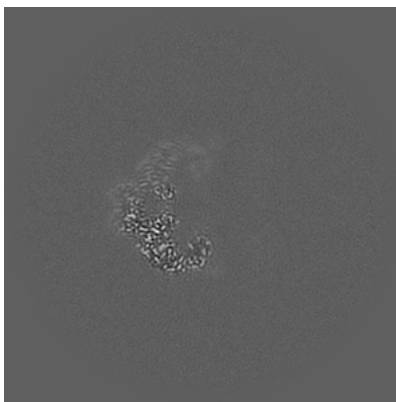
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

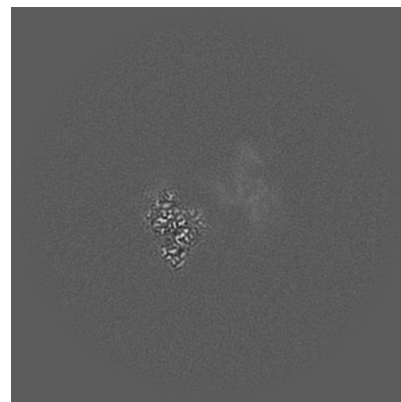
6.2.1 Primary map



X Index: 160

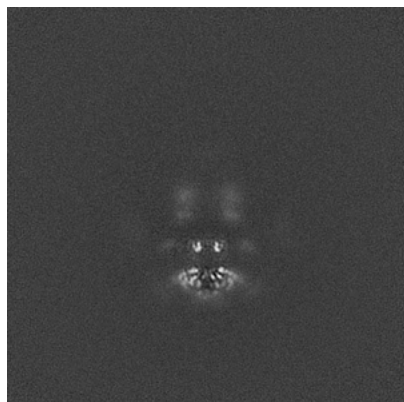


Y Index: 160

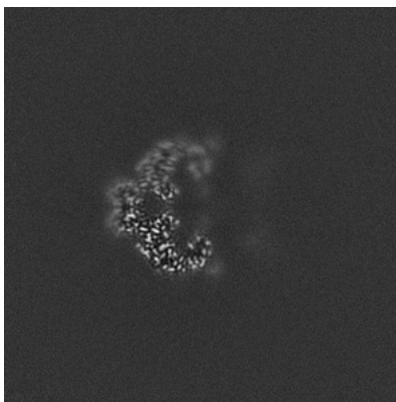


Z Index: 160

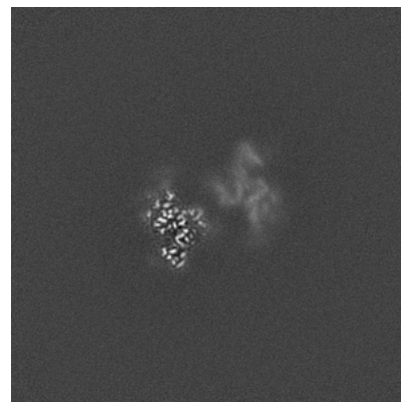
6.2.2 Raw map



X Index: 160



Y Index: 160

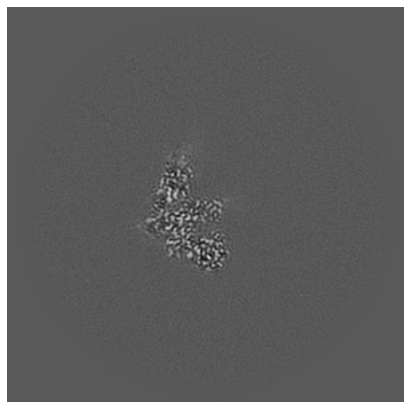


Z Index: 160

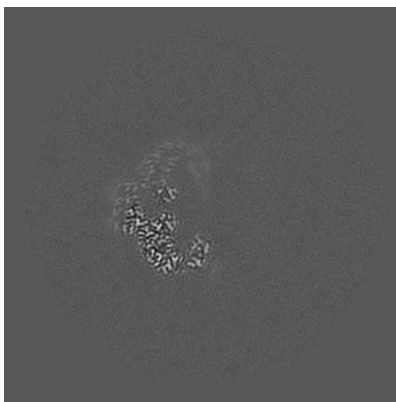
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

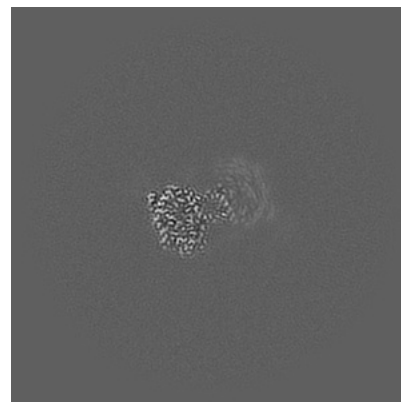
6.3.1 Primary map



X Index: 125

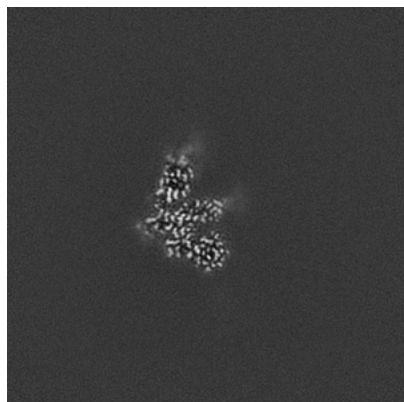


Y Index: 162

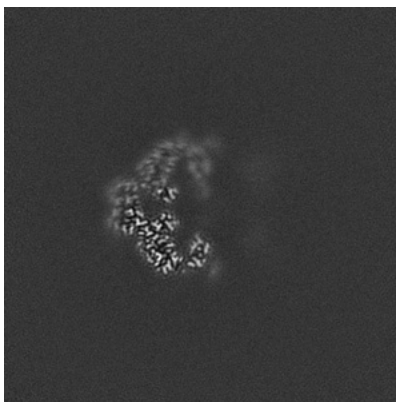


Z Index: 124

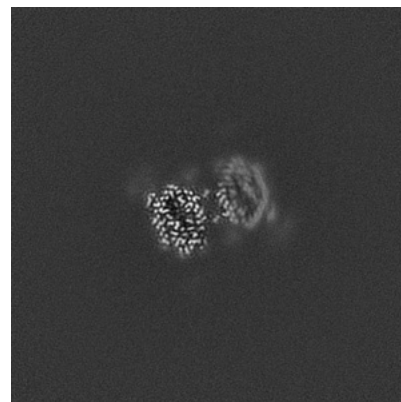
6.3.2 Raw map



X Index: 125



Y Index: 162

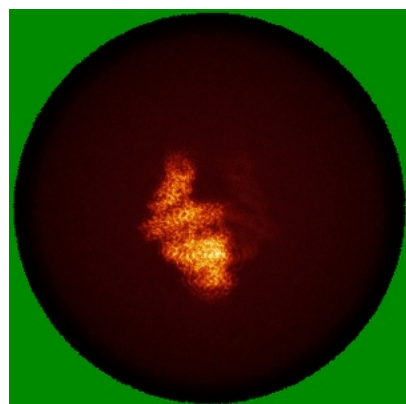


Z Index: 123

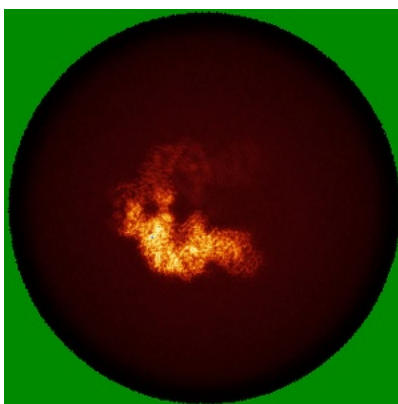
The images above show the largest variance slices of the map in three orthogonal directions.

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

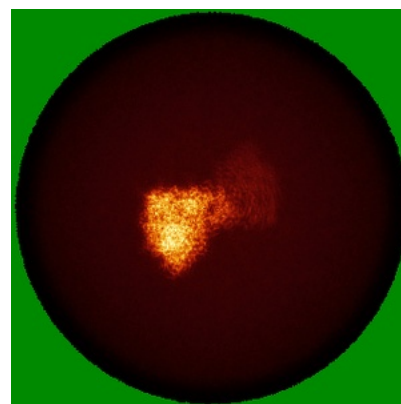
6.4.1 Primary map



X

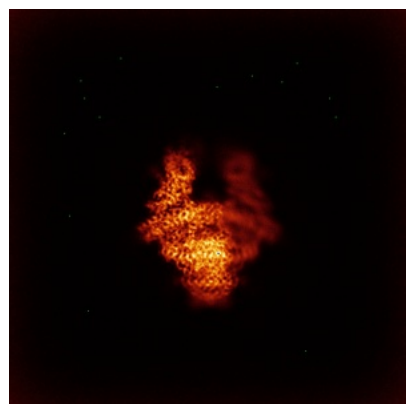


Y

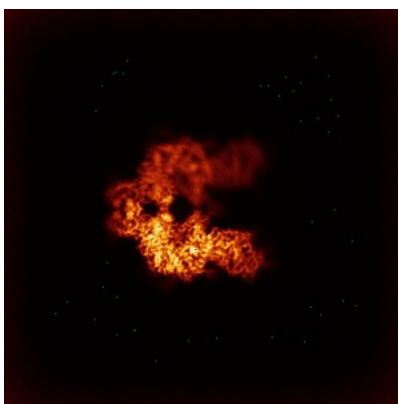


Z

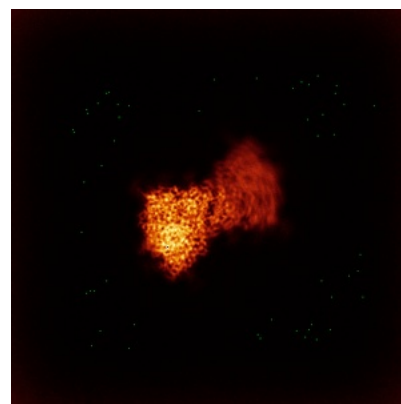
6.4.2 Raw map



X



Y

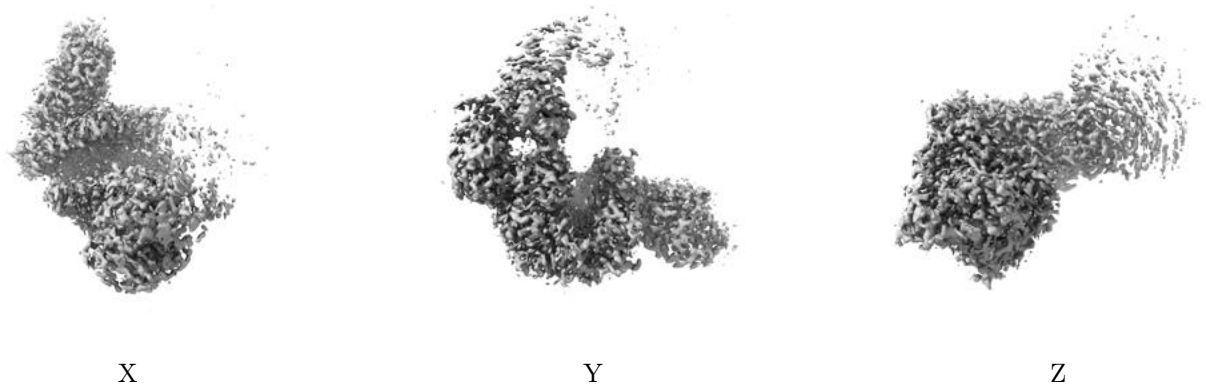


Z

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 0.45. 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.

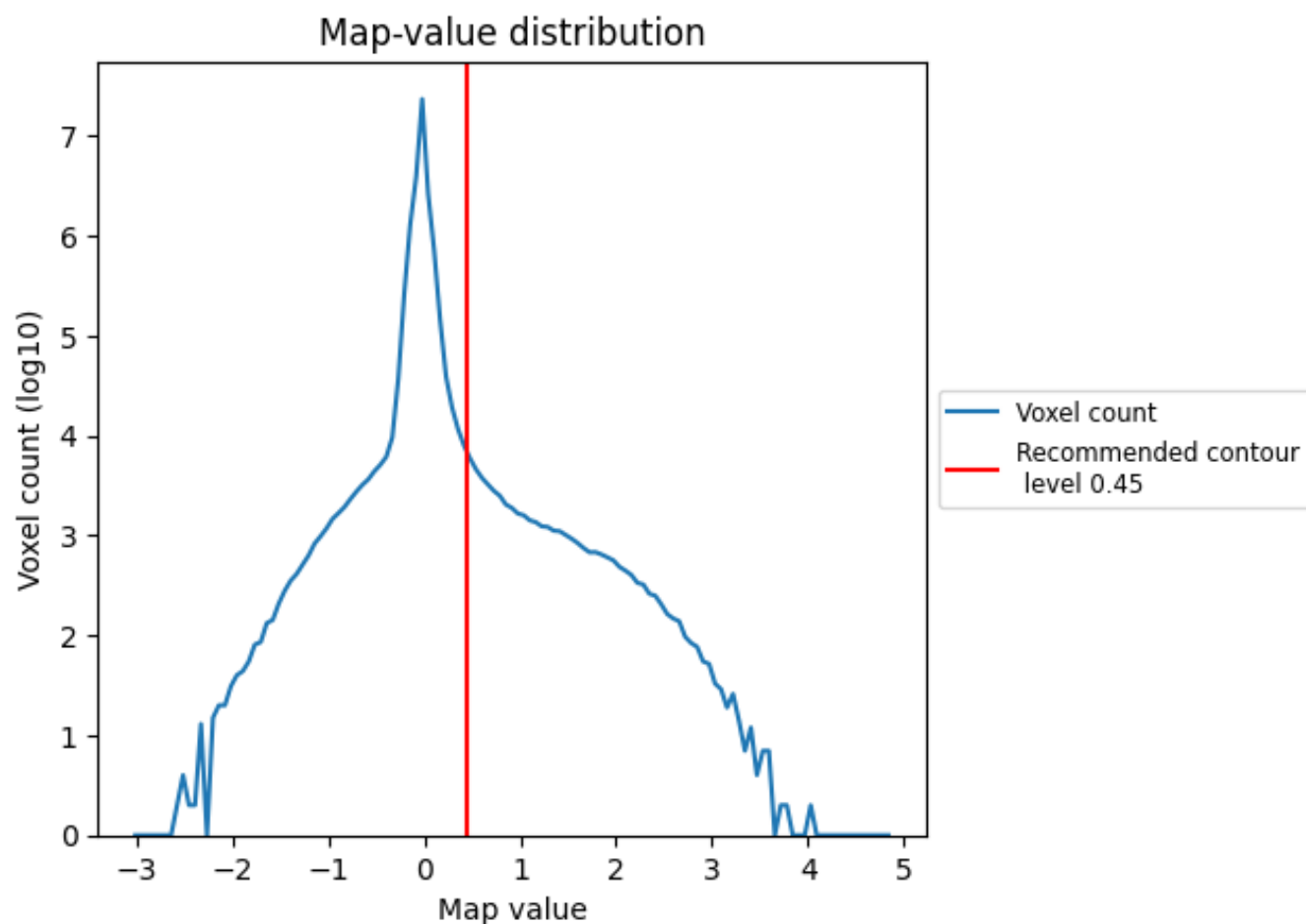
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

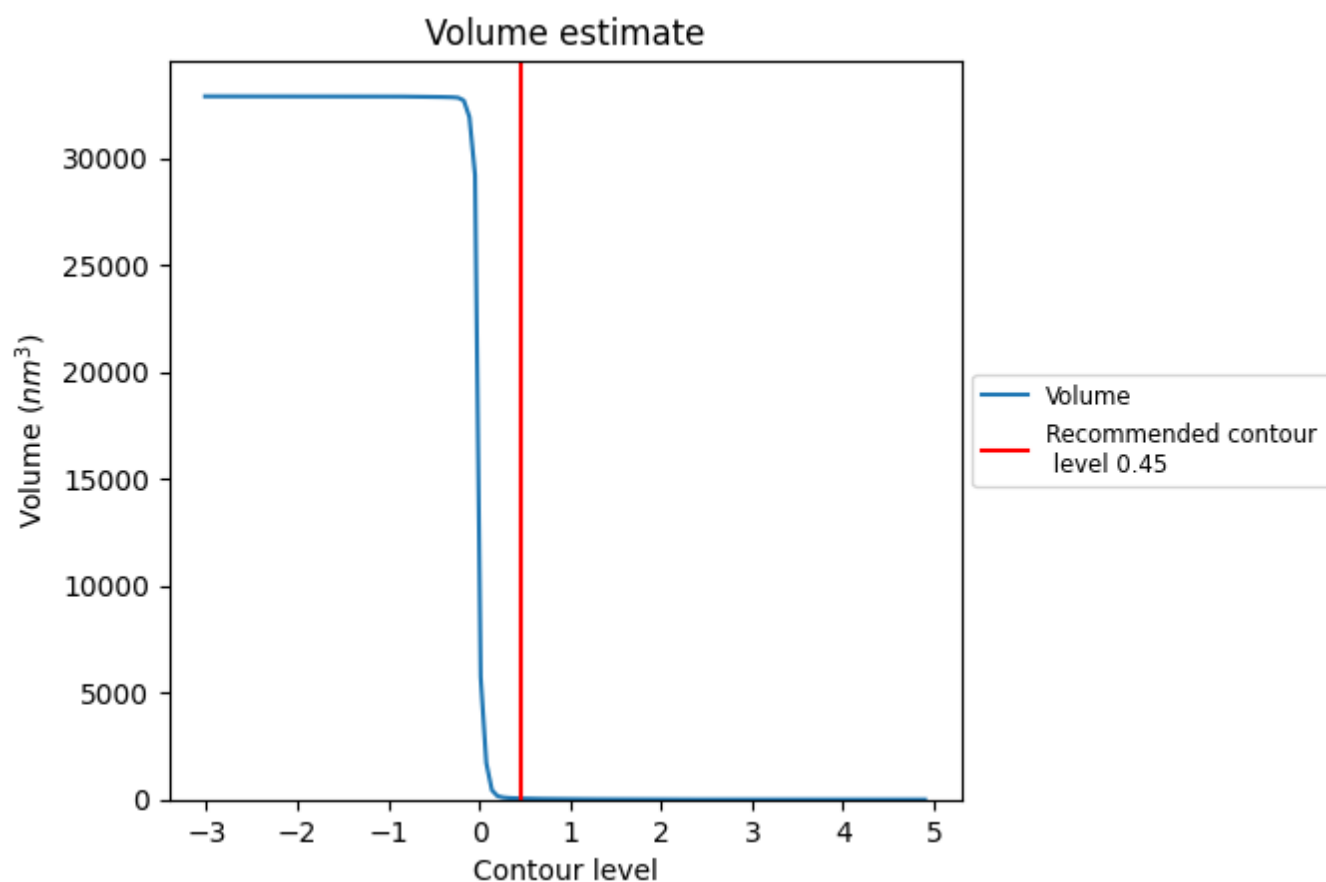
This section contains the results of statistical analysis of the map.

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.

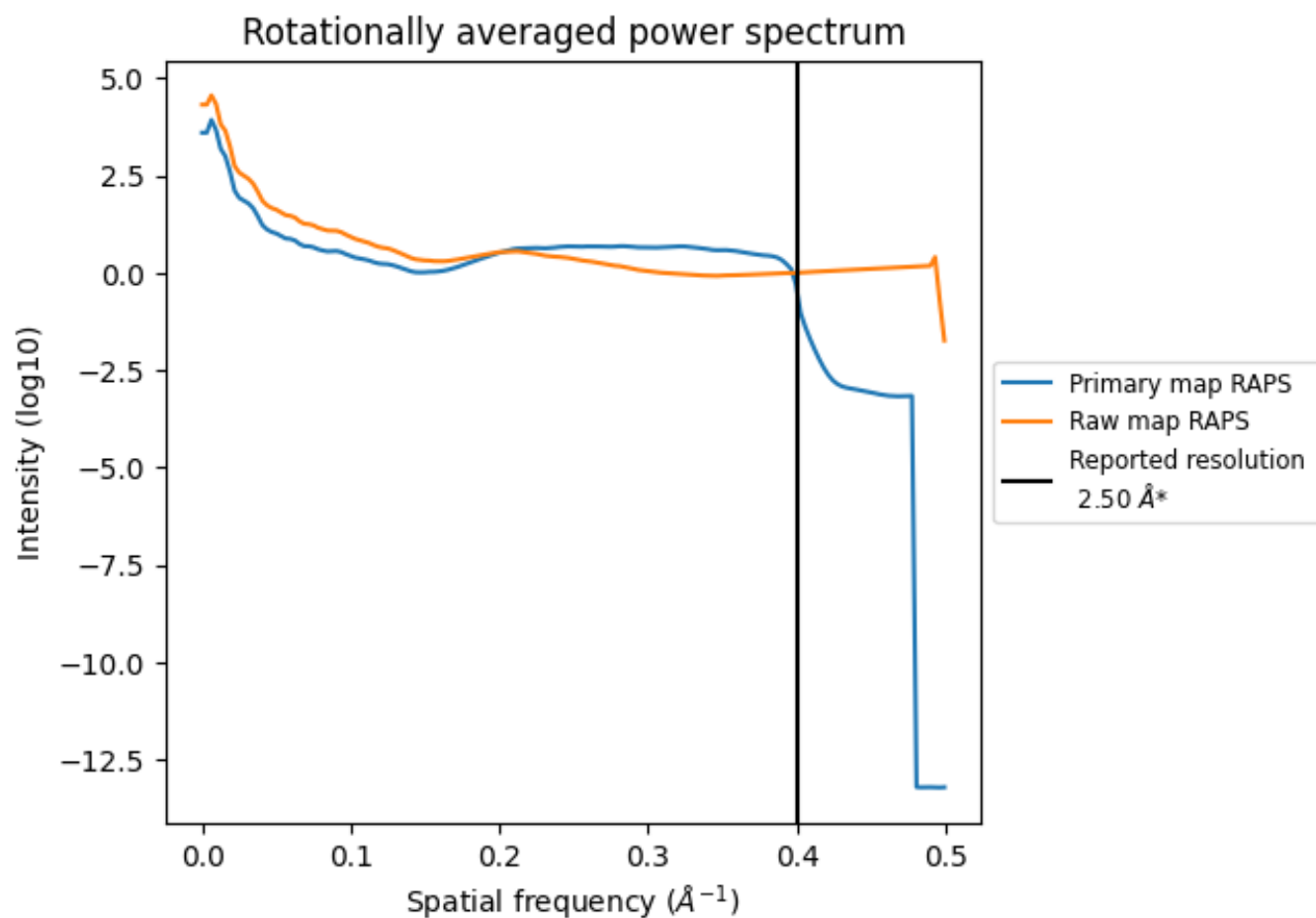
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 51 nm³; this corresponds to an approximate mass of 46 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 ⓘ

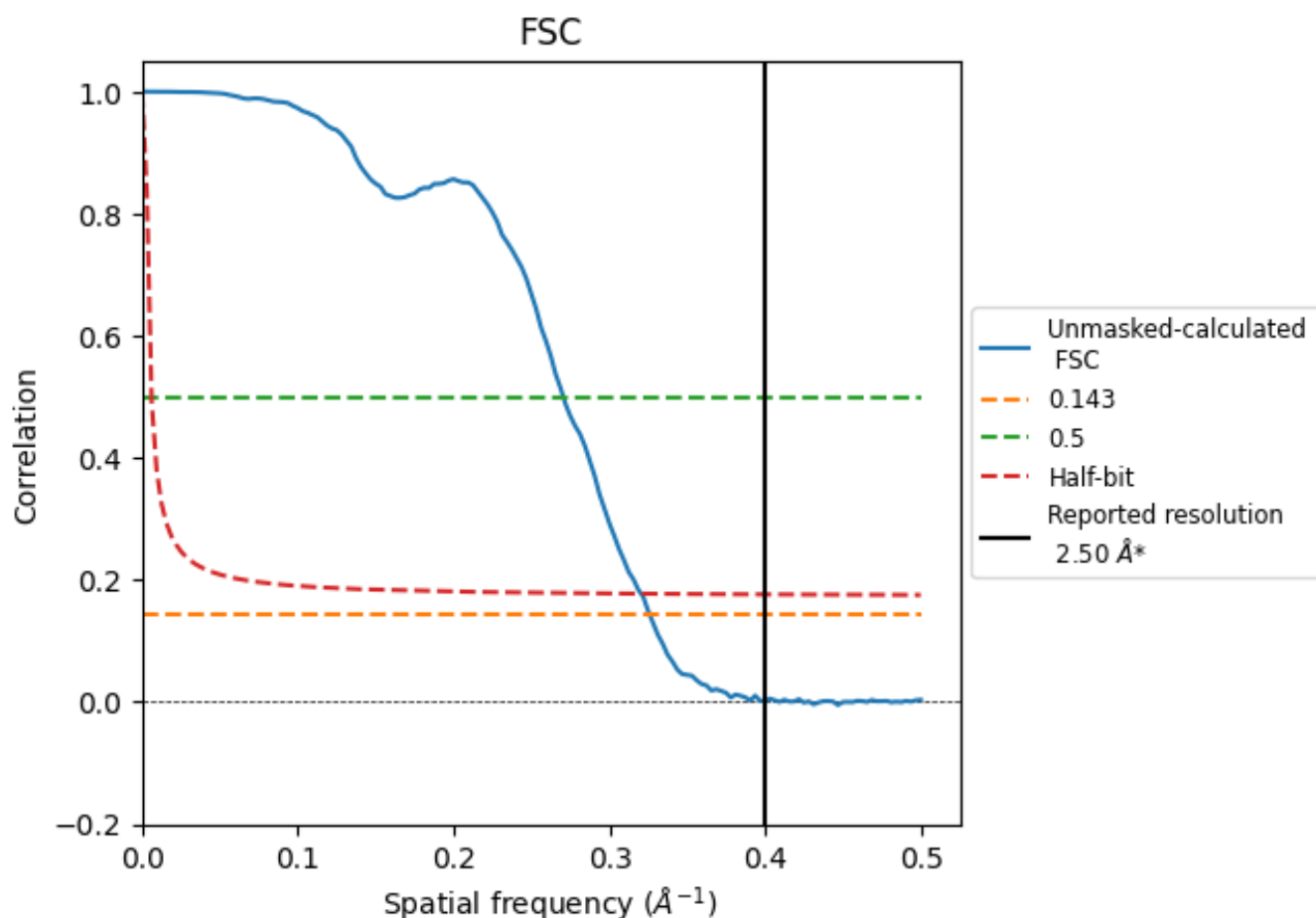


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 \AA^{-1}

8.2 Resolution estimates [i](#)

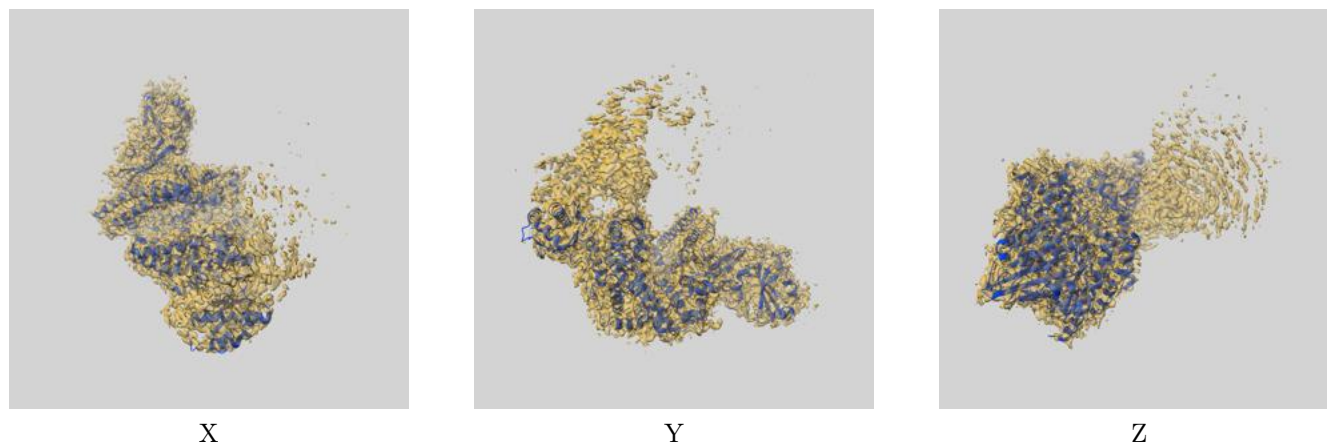
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.07	3.70	3.12

*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 3.07 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

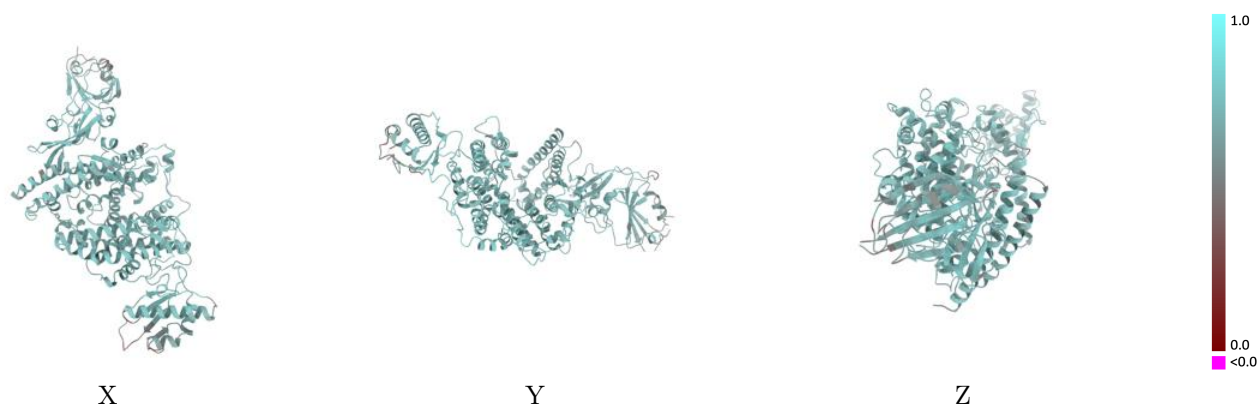
This section contains information regarding the fit between EMDB map EMD-49092 and PDB model 9N7D. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



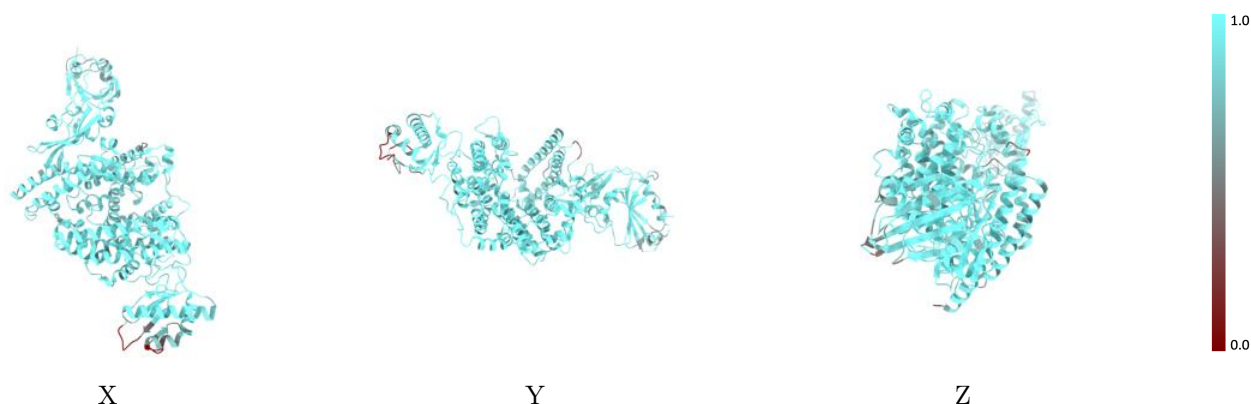
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



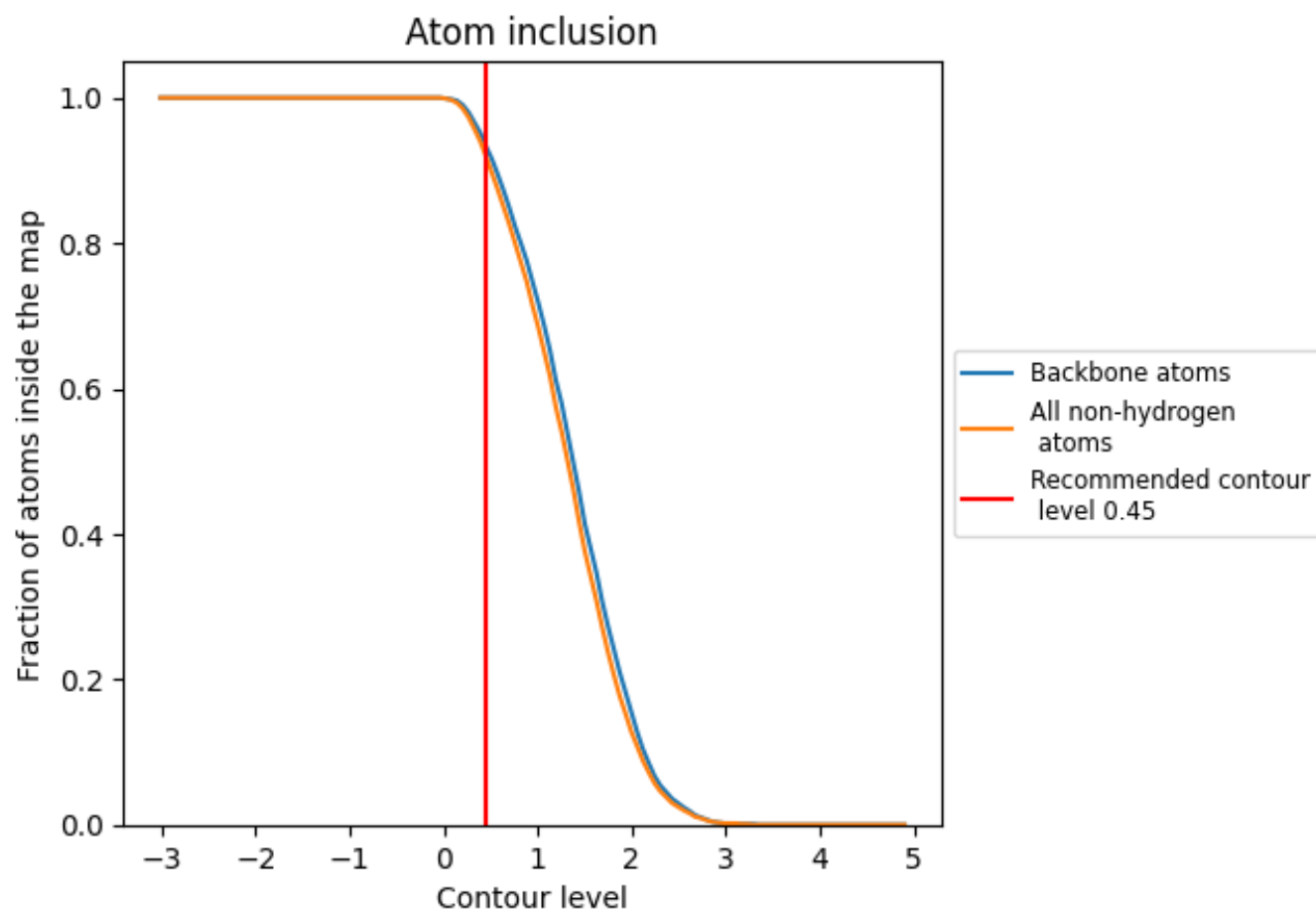
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9190</div>	<div><div></div>0.6590</div>
A	<div><div></div>0.9330</div>	<div><div></div>0.6690</div>
B	<div><div></div>0.9040</div>	<div><div></div>0.6350</div>
C	<div><div></div>0.4640</div>	<div><div></div>0.3950</div>
D	<div><div></div>0.5710</div>	<div><div></div>0.5460</div>
E	<div><div></div>0.3210</div>	<div><div></div>0.4820</div>
F	<div><div></div>0.3930</div>	<div><div></div>0.4230</div>

1.0

0.0

<0.0