



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2026 – 02:56 PM UTC

PDB ID : 6U02 / pdb_00006u02
EMDB ID : EMD-20594
Title : CryoEM-derived model of NA-63 Fab in complex with N9 Shanghai2
Authors : Ward, A.B.; Turner, H.L.; Zhu, X.
Deposited on : 2019-08-13
Resolution : 3.05 Å(reported)
Based on initial model : 5L14

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

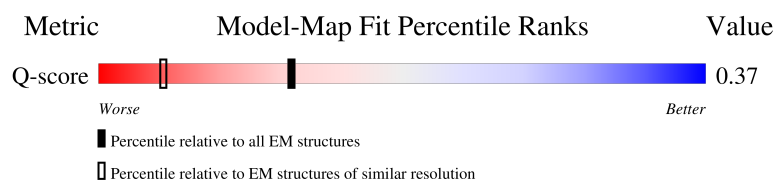
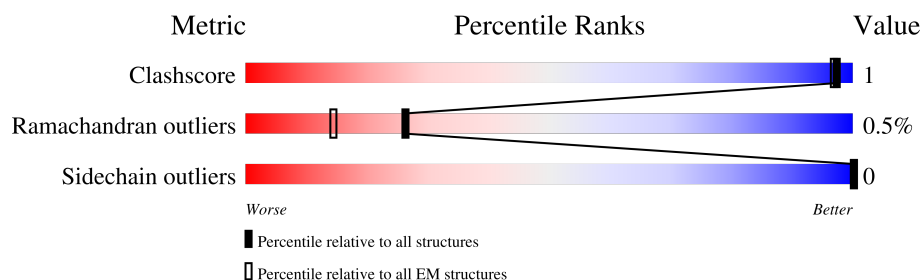
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13971 (2.55 - 3.55)

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	429	
1	B	429	
1	E	429	
1	J	429	

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Mol	Chain	Length	Quality of chain
2	C	215	
2	F	215	
2	I	215	
2	L	215	
3	D	221	
3	G	221	
3	H	221	
3	K	221	
4	M	9	
4	N	9	
4	O	9	
4	P	9	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19672 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 Neuraminidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	388	Total	C	N	O	S	0	0
			3054	1902	541	588	23		
1	B	388	Total	C	N	O	S	0	0
			3054	1902	541	588	23		
1	E	388	Total	C	N	O	S	0	0
			3054	1902	541	588	23		
1	J	388	Total	C	N	O	S	0	0
			3054	1902	541	588	23		

- Molecule 2 is a protein called Fab-63 Light Chain.

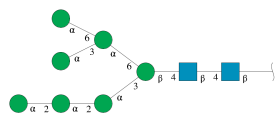
Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	109	Total	C	N	O	S	0	0
			831	524	137	167	3		
2	C	109	Total	C	N	O	S	0	0
			831	524	137	167	3		
2	F	109	Total	C	N	O	S	0	0
			831	524	137	167	3		
2	I	109	Total	C	N	O	S	0	0
			831	524	137	167	3		

- Molecule 3 is a protein called Fab-63 Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	116	Total	C	N	O	S	0	0
			900	571	152	173	4		
3	D	116	Total	C	N	O	S	0	0
			900	571	152	173	4		
3	G	116	Total	C	N	O	S	0	0
			900	571	152	173	4		
3	K	116	Total	C	N	O	S	0	0
			900	571	152	173	4		

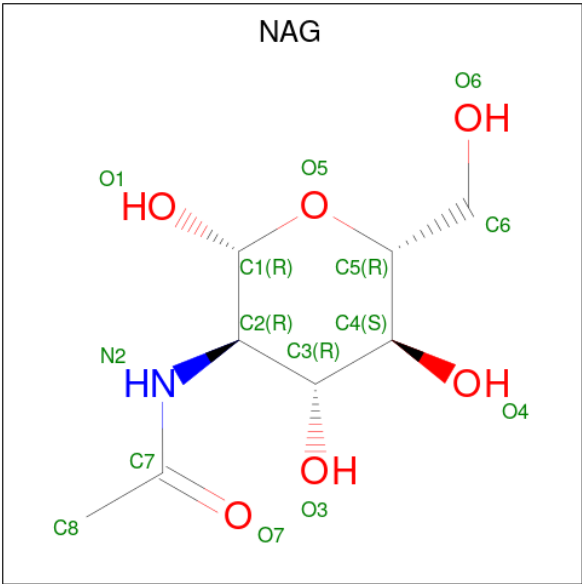
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran

ose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	M	9	Total	C	N	O	0	0
			105	58	2	45		
4	N	9	Total	C	N	O	0	0
			105	58	2	45		
4	O	9	Total	C	N	O	0	0
			105	58	2	45		
4	P	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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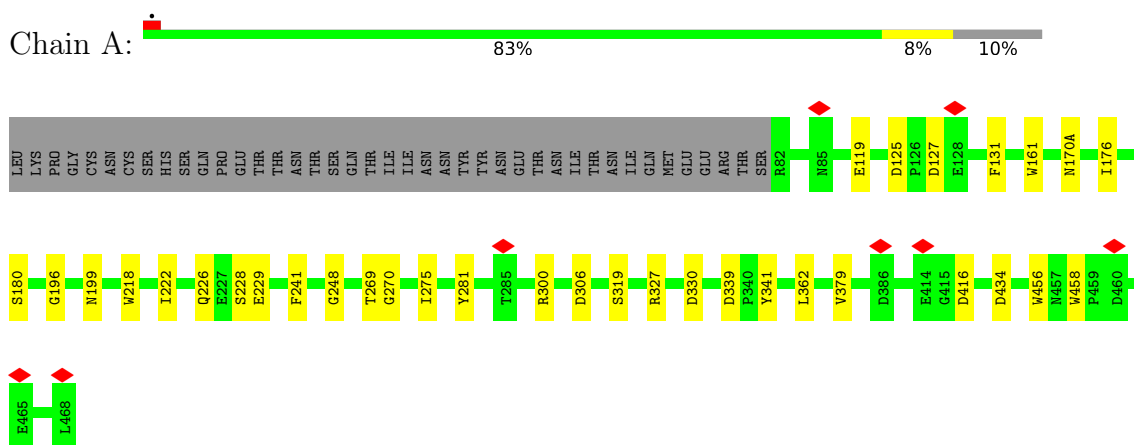
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Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	

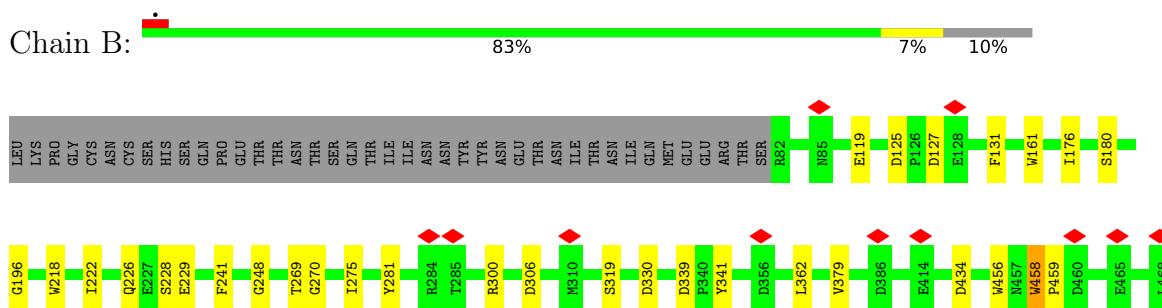
3 Residue-property plots

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

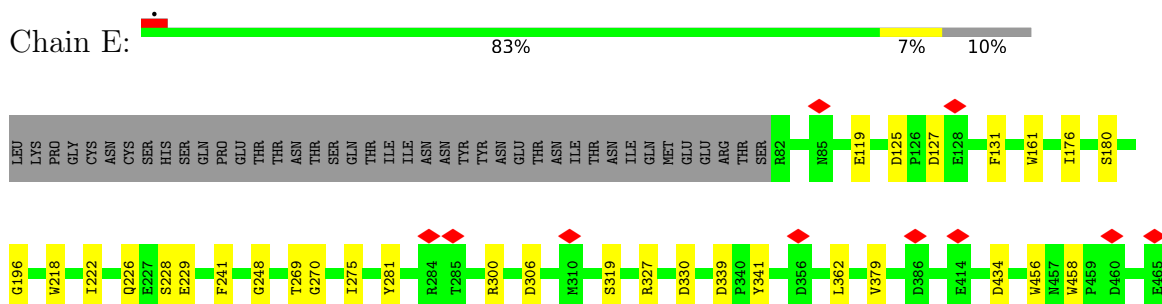
• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase

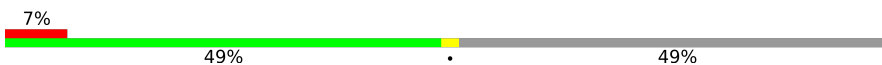


• Molecule 1: Neuraminidase



ALA ASP TYR GLU LYS HIS LYS VAL TYR TYR ALA CYS GLU VAL THR HIS GLN GLY LEU SER SER PRO VAL THR LYS SER PHE ASN ARG GLY GLU CYS

• Molecule 2: Fab-63 Light Chain

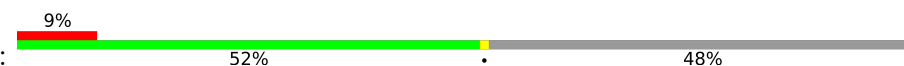
Chain I: 

D1 M4 S7 P8 S9 S12 V15 G16 D17 Q27 G41 K42 A43 S52 D70 Q79 D82 F98 G99 Q100 E105 I106 K107 R108 THR VAL ALA SER PRO SER THR VAL PHE THR PHE LYS PRO ASP SER ASP GLN LEU LYS HIS VAL SER GLY THR ALA VAL

VAL CYS LEU LEU ASN ASN PHE TYR PRO ARG SER GLU ALA LYS VAL GLN TRP LYS VAL ASP ASN ALA LEU GLN SER GLY ASN SER GLN GLU VAL THR GLU ASP LYS ASP SER THR TYR THR LEU SER SER THR LEU THR THR LEU SER LYS ALA PRO ASP TYR GLU HIS LYS VAL SER GLY THR ALA VAL

ALA CYS GLU VAL THR HIS LYS GLN LEU SER SER PRO VAL THR LYS SER PHE ASN ARG GLY CYS

• Molecule 3: Fab-63 Heavy Chain

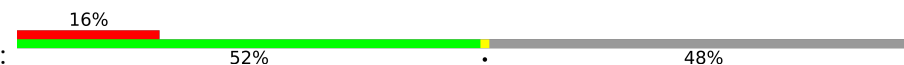
Chain H: 

E1 E6 G10 L11 V12 Q13 G16 A23 S31 P41 K52 G54 S55 E56 H72 K75 L80 A84 E85 D86 T87 D101 Q105 T110 SER SER ALA SER THR THR LYS PRO SER VAL PHE PRO ALA PRO SER SER LYS THR

SER GLY THR THR ALA ALA LEU GLY CYS LEU VAL LYS ASP TYR PHE PRO GLU VAL THR VAL SER TRP LYS ASN SER GLY ALA THR THR PHE THR ALA VAL LEU SER SER GLY THR TTR SER LEU SER SER VAL THR VAL PRO SER SER PHE LEU GLY THR

GLN THR TYR ILE CYS ASN VAL ASN HIS LYS PRO LYS SER ASN THR LYS VAL ASP ARG VAL GLU PRO LYS SER CYS

• Molecule 3: Fab-63 Heavy Chain

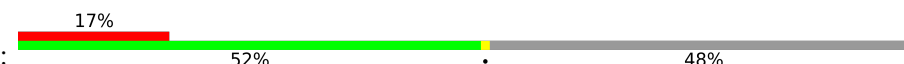
Chain D: 

E1 L4 V5 G9 G10 L11 V12 Q13 G16 S17 S18 C22 A23 S31 S35 P41 K42 G43 G44 K52 G54 S55 E56 S62 H72 N73 A74 K75 L78 Y79 Q81 M82 A84 E85 D86 T87 C92 T96 A97 A98 E99

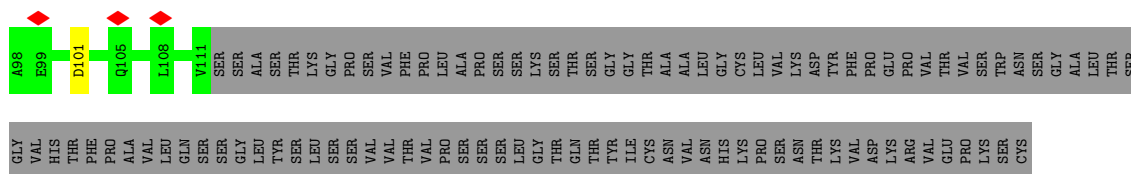
D101 Q105 L108 V109 T110 V111 SER SER ALA THR LYS GLY SER PRO VAL PHE PRO LEU ALA PRO SER SER SER LYS THR VAL THR PHE THR ASP THR TYR PHE PRO GLU PRO ARG VAL VAL THR TRP ASN SER GLY ALA LEU THR SER VAL

HIS THR PHE PRO VAL VAL GLN SER GLY LEU SER TYR SER LEU SER SER VAL THR VAL VAL SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS ARG VAL GLU PRO LYS CYS

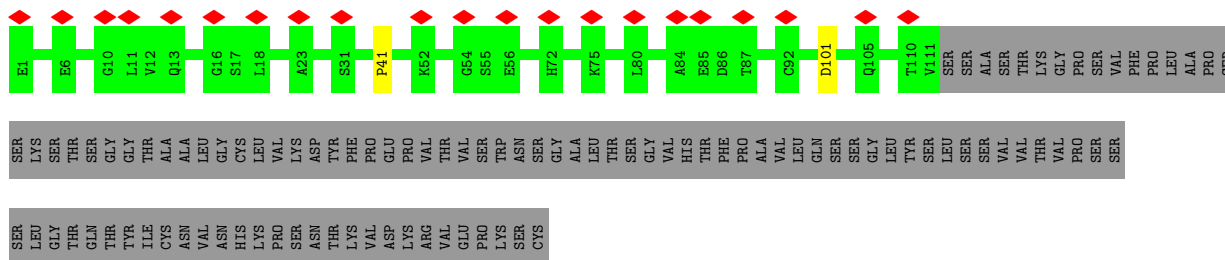
• Molecule 3: Fab-63 Heavy Chain

Chain G: 

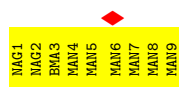
E1 L4 V5 G9 G10 L11 V12 Q13 G16 S17 S18 C22 A23 S31 S35 P41 K42 G43 G44 A49 K52 G54 S55 E56 S62 H72 N73 A74 K75 M76 S77 L78 Y79 Q81 M82 A84 E85 D86 T87 C92 T96 A97



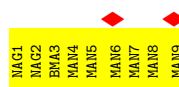
• Molecule 3: Fab-63 Heavy Chain



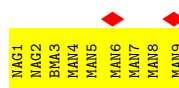
• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

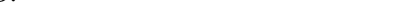


• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Chain P:  22% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	91117	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.970	Depositor
Minimum map value	-3.982	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.160	Depositor
Recommended contour level	1.01	Depositor
Map size (Å)	329.59998, 329.59998, 329.59998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	1.19	2/3136 (0.1%)	1.29	36/4271 (0.8%)
1	B	1.19	2/3136 (0.1%)	1.29	34/4271 (0.8%)
1	E	1.19	2/3136 (0.1%)	1.29	36/4271 (0.8%)
1	J	1.19	2/3136 (0.1%)	1.29	34/4271 (0.8%)
2	C	0.98	0/849	1.22	5/1152 (0.4%)
2	F	0.98	0/849	1.22	5/1152 (0.4%)
2	I	0.98	0/849	1.22	5/1152 (0.4%)
2	L	0.98	0/849	1.22	5/1152 (0.4%)
3	D	1.03	0/922	1.21	1/1249 (0.1%)
3	G	1.03	0/922	1.21	1/1249 (0.1%)
3	H	1.03	0/922	1.21	1/1249 (0.1%)
3	K	1.03	0/922	1.21	1/1249 (0.1%)
All	All	1.13	8/19628 (0.0%)	1.27	164/26688 (0.6%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	161	TRP	NE1-CE2	-5.57	1.31	1.37
1	E	161	TRP	NE1-CE2	-5.54	1.31	1.37
1	A	161	TRP	NE1-CE2	-5.52	1.31	1.37
1	J	161	TRP	NE1-CE2	-5.50	1.31	1.37
1	B	218	TRP	NE1-CE2	-5.38	1.31	1.37

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	TYR	CA-C-N	9.32	129.26	120.03
1	A	341	TYR	C-N-CA	9.32	129.26	120.03
1	J	341	TYR	CA-C-N	9.31	129.25	120.03
1	J	341	TYR	C-N-CA	9.31	129.25	120.03
1	B	341	TYR	CA-C-N	9.30	129.24	120.03

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	3054	0	2877	7	0
1	B	3054	0	2877	5	0
1	E	3054	0	2877	4	0
1	J	3054	0	2877	5	0
2	C	831	0	818	0	0
2	F	831	0	818	0	0
2	I	831	0	818	0	0
2	L	831	0	818	0	0
3	D	900	0	858	0	0
3	G	900	0	858	0	0
3	H	900	0	858	0	0
3	K	900	0	858	0	0
4	M	105	0	83	0	0
4	N	105	0	83	0	0
4	O	105	0	83	0	0
4	P	105	0	83	0	0
5	A	28	0	26	0	0
5	B	28	0	26	0	0
5	E	28	0	26	0	0
5	J	28	0	26	0	0
All	All	19672	0	18648	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 1.

The worst 5 of 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:J:127:ASP:OD1	1:J:127:ASP:N	2.46	0.47
1:B:127:ASP:N	1:B:127:ASP:OD1	2.46	0.46
1:A:127:ASP:N	1:A:127:ASP:OD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:ASP:OD1	1:E:127:ASP:N	2.46	0.45
1:B:434:ASP:OD1	1:B:434:ASP:N	2.45	0.45

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	386/429 (90%)	376 (97%)	9 (2%)	1 (0%)	36	63
1	B	386/429 (90%)	376 (97%)	9 (2%)	1 (0%)	36	63
1	E	386/429 (90%)	376 (97%)	9 (2%)	1 (0%)	36	63
1	J	386/429 (90%)	376 (97%)	9 (2%)	1 (0%)	36	63
2	C	107/215 (50%)	102 (95%)	4 (4%)	1 (1%)	14	39
2	F	107/215 (50%)	102 (95%)	4 (4%)	1 (1%)	14	39
2	I	107/215 (50%)	102 (95%)	4 (4%)	1 (1%)	14	39
2	L	107/215 (50%)	102 (95%)	4 (4%)	1 (1%)	14	39
3	D	114/221 (52%)	112 (98%)	1 (1%)	1 (1%)	14	39
3	G	114/221 (52%)	112 (98%)	1 (1%)	1 (1%)	14	39
3	H	114/221 (52%)	112 (98%)	1 (1%)	1 (1%)	14	39
3	K	114/221 (52%)	112 (98%)	1 (1%)	1 (1%)	14	39
All	All	2428/3460 (70%)	2360 (97%)	56 (2%)	12 (0%)	26	52

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	52	SER
3	H	41	PRO
2	C	52	SER

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Mol	Chain	Res	Type
3	D	41	PRO
2	F	52	SER

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	339/379 (89%)	339 (100%)	0	100	100
1	B	339/379 (89%)	339 (100%)	0	100	100
1	E	339/379 (89%)	339 (100%)	0	100	100
1	J	339/379 (89%)	339 (100%)	0	100	100
2	C	94/189 (50%)	94 (100%)	0	100	100
2	F	94/189 (50%)	94 (100%)	0	100	100
2	I	94/189 (50%)	94 (100%)	0	100	100
2	L	94/189 (50%)	94 (100%)	0	100	100
3	D	94/185 (51%)	94 (100%)	0	100	100
3	G	94/185 (51%)	94 (100%)	0	100	100
3	H	94/185 (51%)	94 (100%)	0	100	100
3	K	94/185 (51%)	94 (100%)	0	100	100
All	All	2108/3012 (70%)	2108 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	37	GLN
3	K	50	ASN
2	C	37	GLN
2	F	37	GLN
3	G	50	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 ⓘ

36 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
4	NAG	M	1	1,4	14,14,15	1.86	2 (14%)	17,19,21	0.99	1 (5%)
4	NAG	M	2	4	14,14,15	2.01	2 (14%)	17,19,21	1.41	2 (11%)
4	BMA	M	3	4	11,11,12	1.85	2 (18%)	15,15,17	1.03	1 (6%)
4	MAN	M	4	4	11,11,12	1.41	1 (9%)	15,15,17	1.28	1 (6%)
4	MAN	M	5	4	11,11,12	1.54	2 (18%)	15,15,17	0.89	0
4	MAN	M	6	4	11,11,12	1.87	2 (18%)	15,15,17	1.07	0
4	MAN	M	7	4	11,11,12	1.82	2 (18%)	15,15,17	0.96	1 (6%)
4	MAN	M	8	4	11,11,12	1.80	2 (18%)	15,15,17	0.88	0
4	MAN	M	9	4	11,11,12	1.79	2 (18%)	15,15,17	0.85	0
4	NAG	N	1	1,4	14,14,15	1.87	2 (14%)	17,19,21	0.98	1 (5%)
4	NAG	N	2	4	14,14,15	2.00	2 (14%)	17,19,21	1.40	2 (11%)
4	BMA	N	3	4	11,11,12	1.85	2 (18%)	15,15,17	1.04	1 (6%)
4	MAN	N	4	4	11,11,12	1.39	1 (9%)	15,15,17	1.28	1 (6%)
4	MAN	N	5	4	11,11,12	1.53	2 (18%)	15,15,17	0.88	0
4	MAN	N	6	4	11,11,12	1.87	2 (18%)	15,15,17	1.08	0
4	MAN	N	7	4	11,11,12	1.82	2 (18%)	15,15,17	0.96	1 (6%)
4	MAN	N	8	4	11,11,12	1.79	2 (18%)	15,15,17	0.88	0
4	MAN	N	9	4	11,11,12	1.81	2 (18%)	15,15,17	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	O	1	1,4	14,14,15	1.87	2 (14%)	17,19,21	0.98	1 (5%)
4	NAG	O	2	4	14,14,15	2.00	2 (14%)	17,19,21	1.39	2 (11%)
4	BMA	O	3	4	11,11,12	1.87	2 (18%)	15,15,17	1.04	1 (6%)
4	MAN	O	4	4	11,11,12	1.41	1 (9%)	15,15,17	1.28	1 (6%)
4	MAN	O	5	4	11,11,12	1.53	2 (18%)	15,15,17	0.88	0
4	MAN	O	6	4	11,11,12	1.87	2 (18%)	15,15,17	1.08	0
4	MAN	O	7	4	11,11,12	1.81	2 (18%)	15,15,17	0.96	1 (6%)
4	MAN	O	8	4	11,11,12	1.79	2 (18%)	15,15,17	0.88	0
4	MAN	O	9	4	11,11,12	1.80	2 (18%)	15,15,17	0.84	0
4	NAG	P	1	1,4	14,14,15	1.88	2 (14%)	17,19,21	0.98	1 (5%)
4	NAG	P	2	4	14,14,15	2.00	2 (14%)	17,19,21	1.40	2 (11%)
4	BMA	P	3	4	11,11,12	1.85	2 (18%)	15,15,17	1.03	1 (6%)
4	MAN	P	4	4	11,11,12	1.40	1 (9%)	15,15,17	1.28	1 (6%)
4	MAN	P	5	4	11,11,12	1.52	2 (18%)	15,15,17	0.88	0
4	MAN	P	6	4	11,11,12	1.86	2 (18%)	15,15,17	1.08	0
4	MAN	P	7	4	11,11,12	1.82	2 (18%)	15,15,17	0.96	1 (6%)
4	MAN	P	8	4	11,11,12	1.79	2 (18%)	15,15,17	0.89	0
4	MAN	P	9	4	11,11,12	1.80	2 (18%)	15,15,17	0.85	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	M	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
4	BMA	M	3	4	-	0/2/19/22	0/1/1/1
4	MAN	M	4	4	-	2/2/19/22	0/1/1/1
4	MAN	M	5	4	-	1/2/19/22	0/1/1/1
4	MAN	M	6	4	-	0/2/19/22	0/1/1/1
4	MAN	M	7	4	-	0/2/19/22	0/1/1/1
4	MAN	M	8	4	-	2/2/19/22	0/1/1/1
4	MAN	M	9	4	-	1/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	N	2	4	-	1/6/23/26	0/1/1/1
4	BMA	N	3	4	-	0/2/19/22	0/1/1/1
4	MAN	N	4	4	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	N	5	4	-	1/2/19/22	0/1/1/1
4	MAN	N	6	4	-	0/2/19/22	0/1/1/1
4	MAN	N	7	4	-	0/2/19/22	0/1/1/1
4	MAN	N	8	4	-	2/2/19/22	0/1/1/1
4	MAN	N	9	4	-	1/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	O	2	4	-	1/6/23/26	0/1/1/1
4	BMA	O	3	4	-	0/2/19/22	0/1/1/1
4	MAN	O	4	4	-	2/2/19/22	0/1/1/1
4	MAN	O	5	4	-	1/2/19/22	0/1/1/1
4	MAN	O	6	4	-	0/2/19/22	0/1/1/1
4	MAN	O	7	4	-	0/2/19/22	0/1/1/1
4	MAN	O	8	4	-	2/2/19/22	0/1/1/1
4	MAN	O	9	4	-	1/2/19/22	0/1/1/1
4	NAG	P	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	P	2	4	-	1/6/23/26	0/1/1/1
4	BMA	P	3	4	-	0/2/19/22	0/1/1/1
4	MAN	P	4	4	-	2/2/19/22	0/1/1/1
4	MAN	P	5	4	-	1/2/19/22	0/1/1/1
4	MAN	P	6	4	-	0/2/19/22	0/1/1/1
4	MAN	P	7	4	-	0/2/19/22	0/1/1/1
4	MAN	P	8	4	-	2/2/19/22	0/1/1/1
4	MAN	P	9	4	-	1/2/19/22	0/1/1/1

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	2	NAG	O5-C1	6.53	1.54	1.43
4	O	2	NAG	O5-C1	6.49	1.54	1.43
4	P	2	NAG	O5-C1	6.48	1.54	1.43
4	N	2	NAG	O5-C1	6.46	1.54	1.43
4	P	1	NAG	O5-C1	5.75	1.53	1.43

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	4	MAN	O2-C2-C1	-3.43	101.38	109.22
4	N	4	MAN	O2-C2-C1	-3.41	101.42	109.22
4	O	4	MAN	O2-C2-C1	-3.41	101.42	109.22
4	M	4	MAN	O2-C2-C1	-3.40	101.43	109.22
4	M	2	NAG	C3-C4-C5	-3.37	104.13	110.23

There are no chirality outliers.

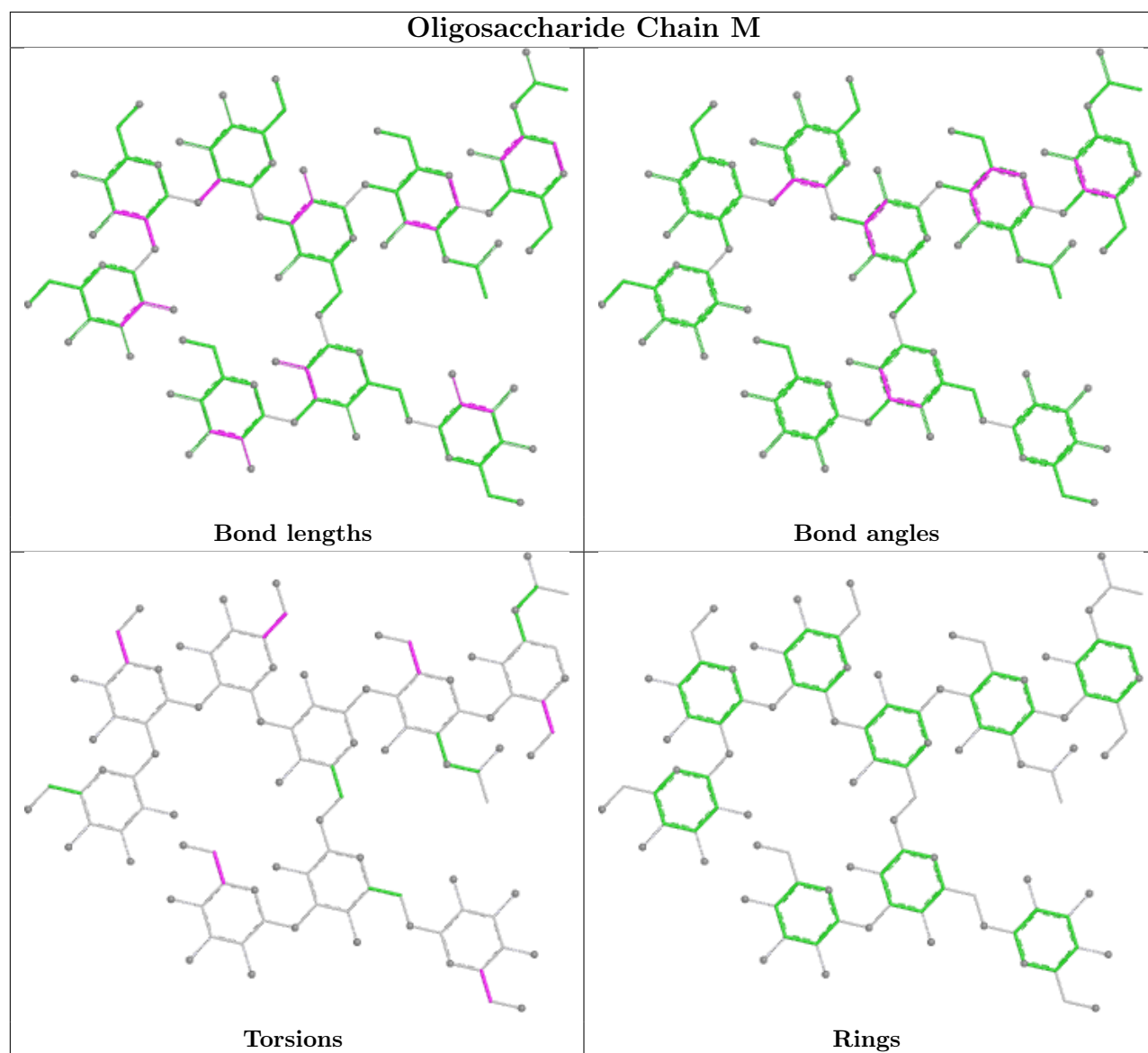
5 of 32 torsion outliers are listed below:

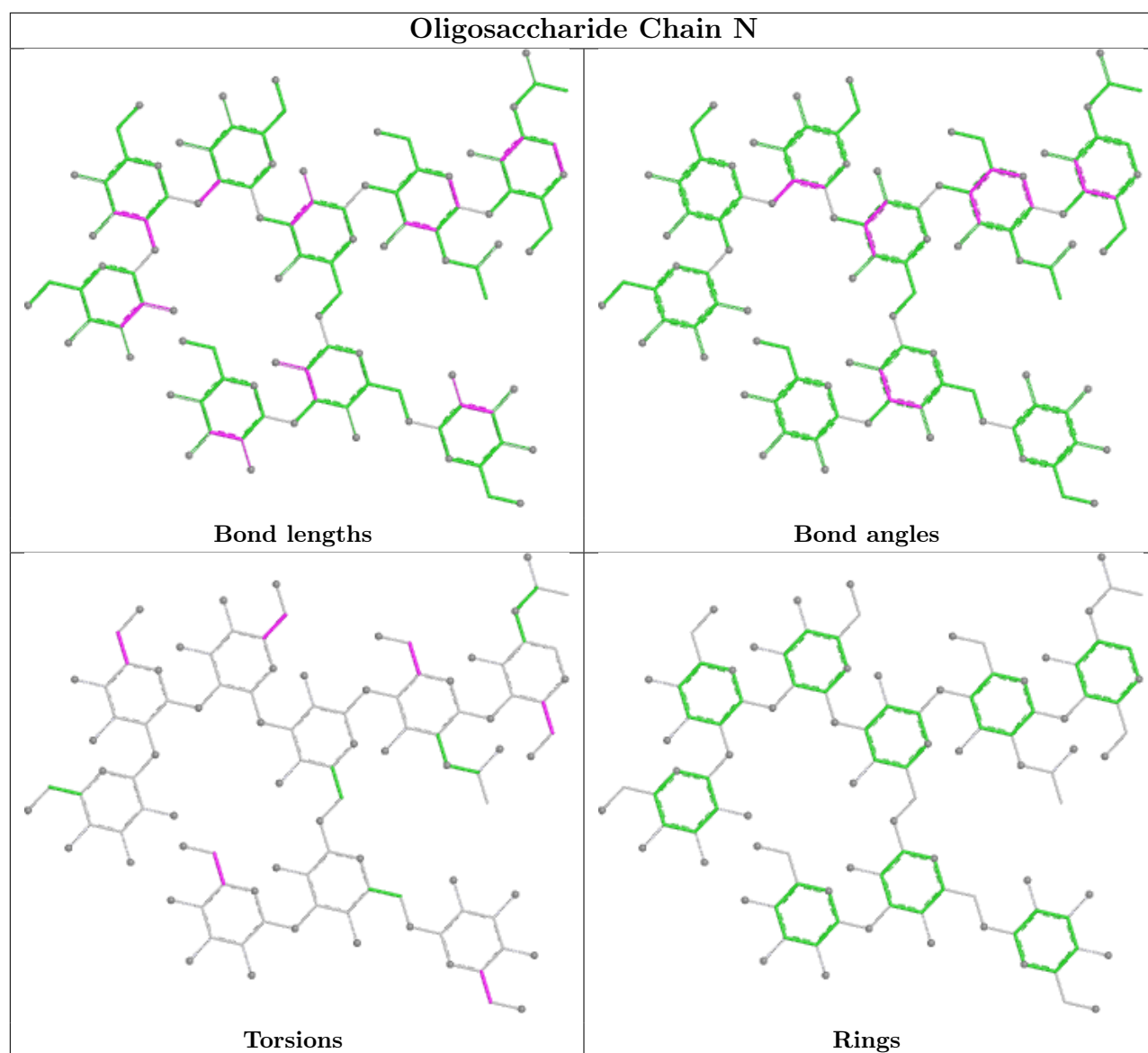
Mol	Chain	Res	Type	Atoms
4	M	8	MAN	C4-C5-C6-O6
4	N	8	MAN	C4-C5-C6-O6
4	O	8	MAN	C4-C5-C6-O6
4	P	8	MAN	C4-C5-C6-O6
4	M	4	MAN	O5-C5-C6-O6

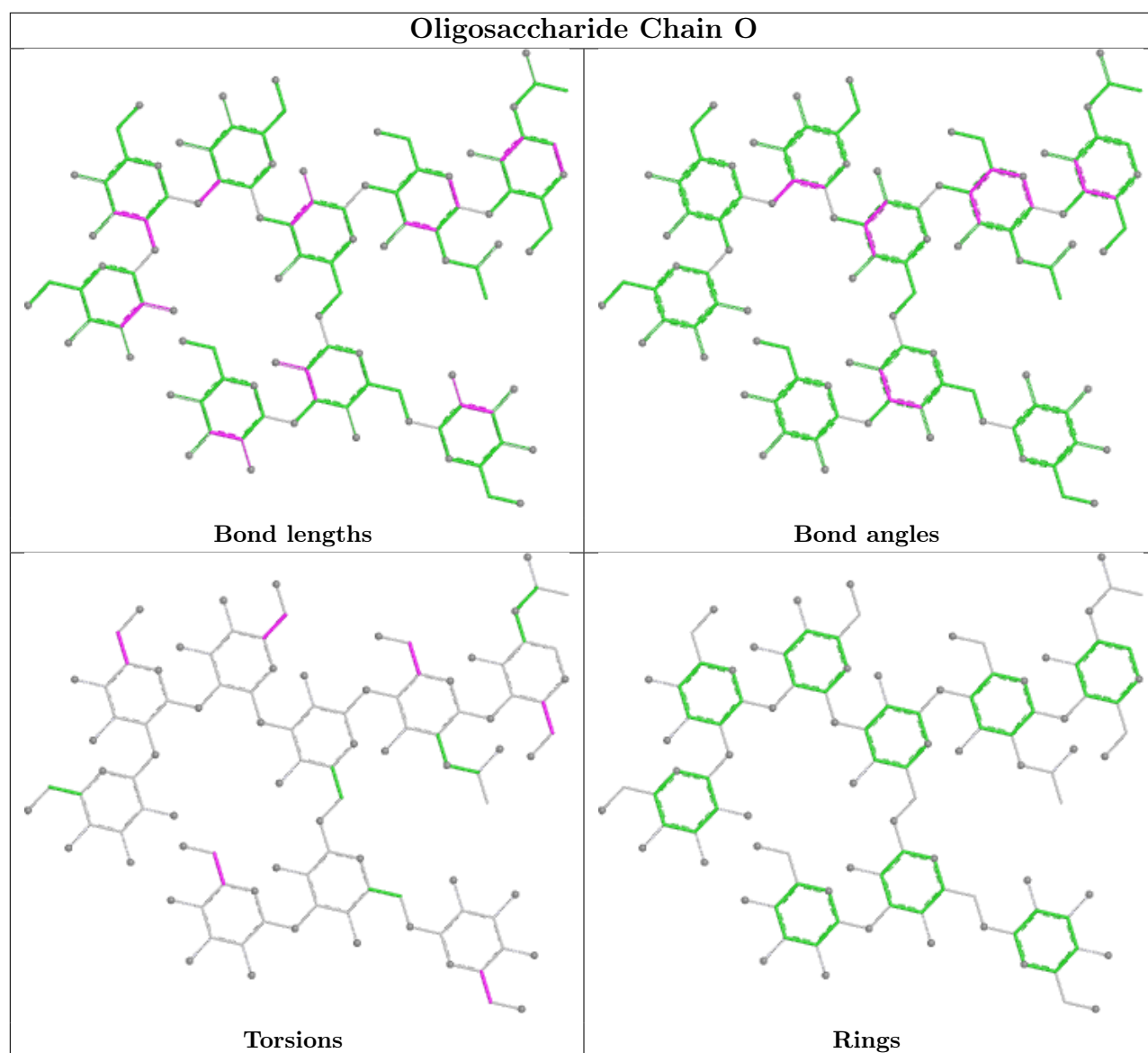
There are no ring outliers.

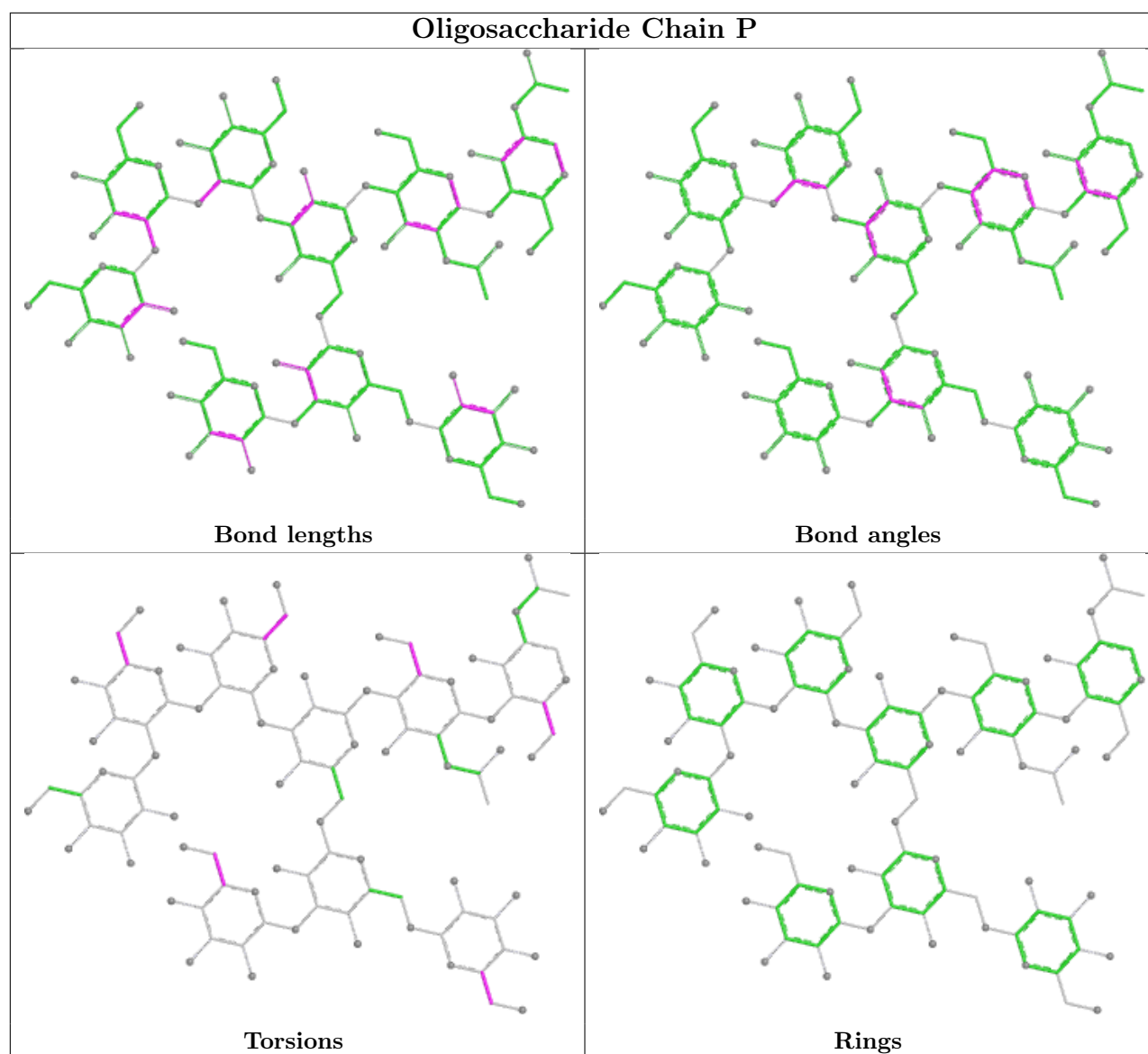
No monomer is involved in short contacts.

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](#)

8 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	$\# Z > 2$
5	NAG	E	510	1	14,14,15	2.06	2 (14%)	17,19,21	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	J	510	1	14,14,15	2.07	2 (14%)	17,19,21	0.80	0
5	NAG	A	511	1	14,14,15	2.03	2 (14%)	17,19,21	0.76	1 (5%)
5	NAG	B	510	1	14,14,15	2.06	2 (14%)	17,19,21	0.81	0
5	NAG	A	510	1	14,14,15	2.06	2 (14%)	17,19,21	0.81	0
5	NAG	B	511	1	14,14,15	2.03	2 (14%)	17,19,21	0.77	1 (5%)
5	NAG	E	511	1	14,14,15	2.03	2 (14%)	17,19,21	0.75	1 (5%)
5	NAG	J	511	1	14,14,15	2.04	2 (14%)	17,19,21	0.77	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	E	510	1	-	1/6/23/26	0/1/1/1
5	NAG	J	510	1	-	1/6/23/26	0/1/1/1
5	NAG	A	511	1	-	1/6/23/26	0/1/1/1
5	NAG	B	510	1	-	1/6/23/26	0/1/1/1
5	NAG	A	510	1	-	1/6/23/26	0/1/1/1
5	NAG	B	511	1	-	1/6/23/26	0/1/1/1
5	NAG	E	511	1	-	1/6/23/26	0/1/1/1
5	NAG	J	511	1	-	1/6/23/26	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	510	NAG	O5-C1	6.64	1.54	1.43
5	J	510	NAG	O5-C1	6.64	1.54	1.43
5	B	510	NAG	O5-C1	6.61	1.54	1.43
5	E	510	NAG	O5-C1	6.60	1.54	1.43
5	J	511	NAG	O5-C1	6.24	1.54	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	511	NAG	C1-O5-C5	-2.13	109.34	112.19
5	J	511	NAG	C1-O5-C5	-2.10	109.37	112.19
5	A	511	NAG	C1-O5-C5	-2.09	109.39	112.19
5	E	511	NAG	C1-O5-C5	-2.06	109.43	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	510	NAG	O5-C5-C6-O6
5	A	511	NAG	O5-C5-C6-O6
5	B	510	NAG	O5-C5-C6-O6
5	B	511	NAG	O5-C5-C6-O6
5	E	510	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.

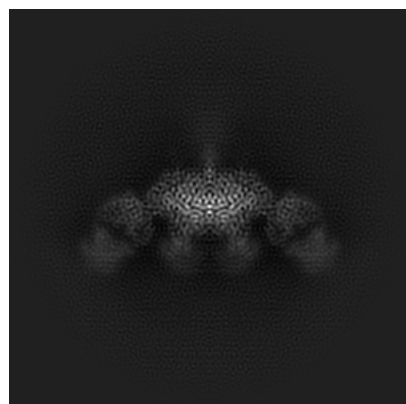
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20594. These allow visual inspection of the internal detail of the map and identification of artifacts.

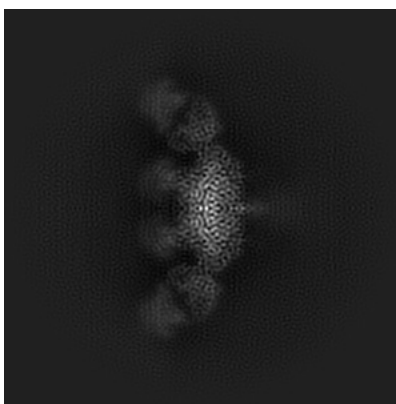
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

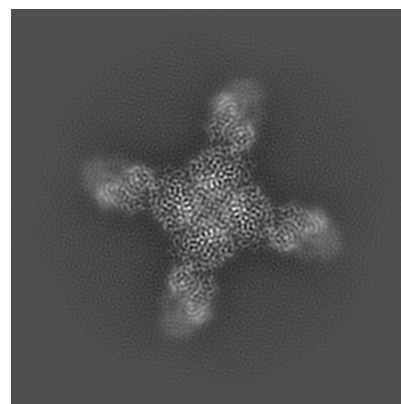
6.1.1 Primary map



X

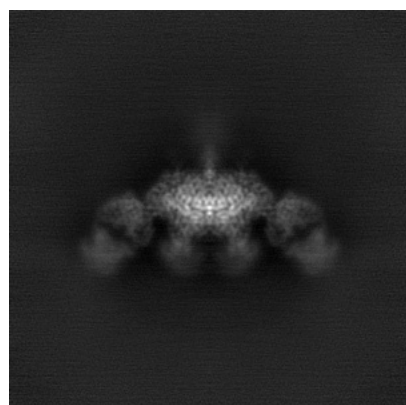


Y

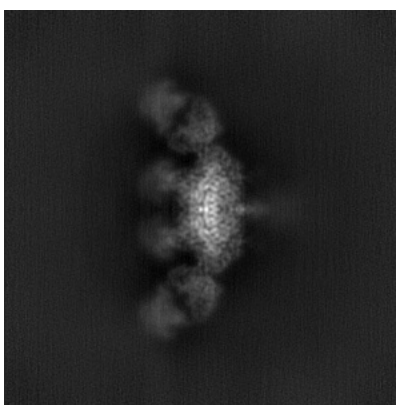


Z

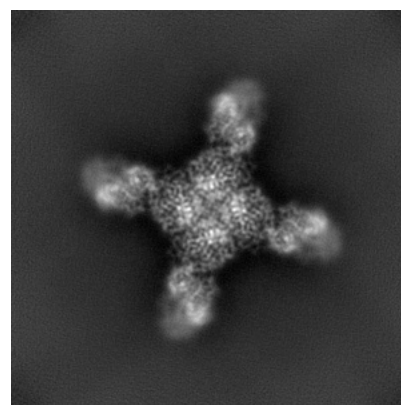
6.1.2 Raw map



X



Y

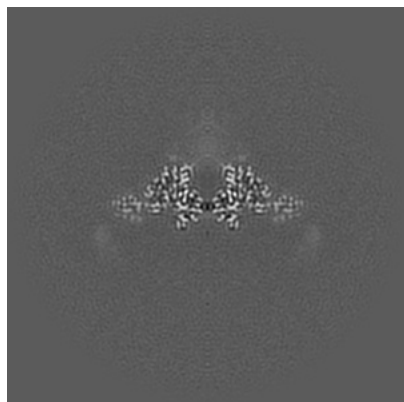


Z

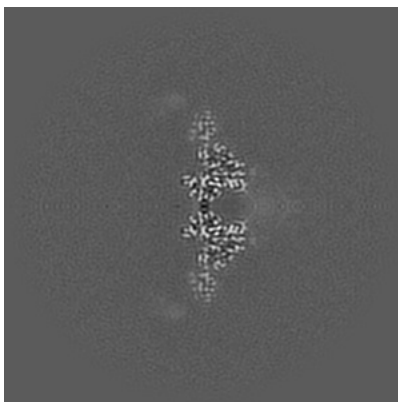
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

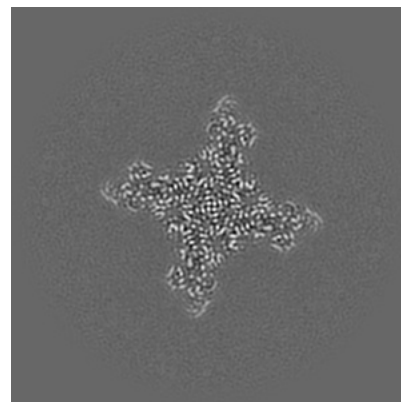
6.2.1 Primary map



X Index: 160

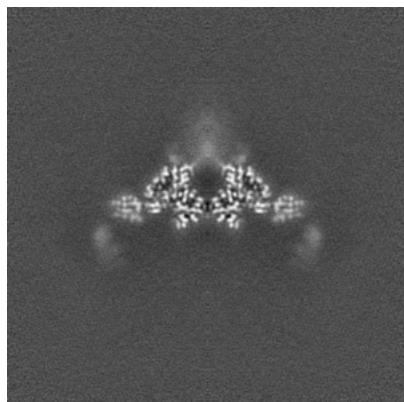


Y Index: 160

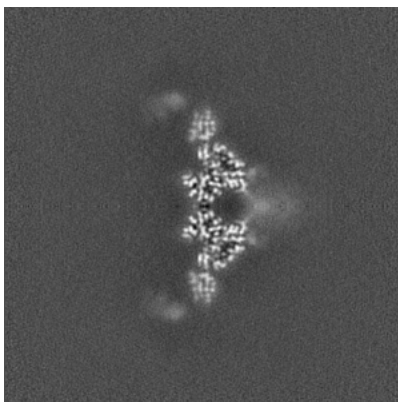


Z Index: 160

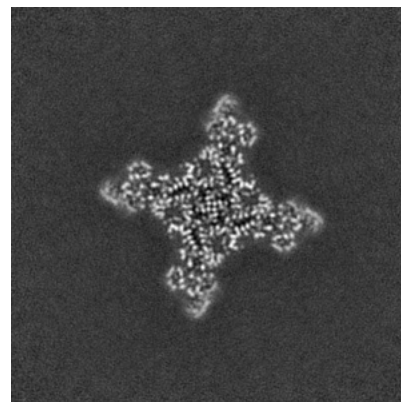
6.2.2 Raw map



X Index: 160



Y Index: 160

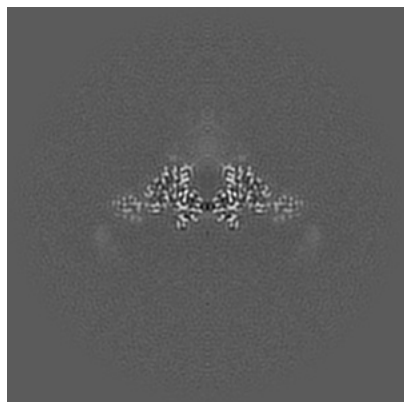


Z Index: 160

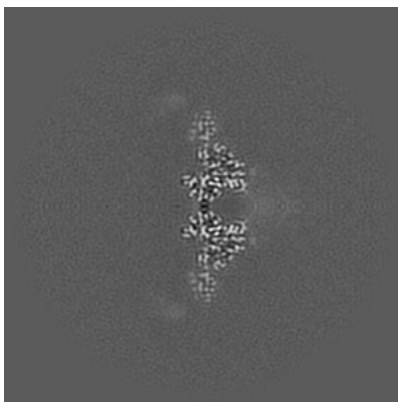
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

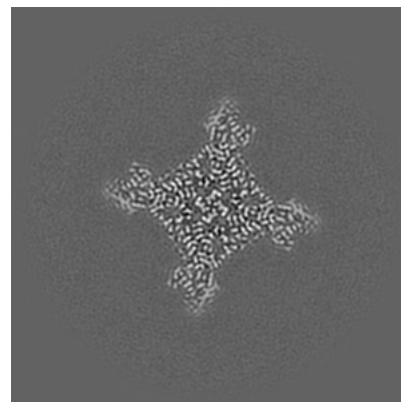
6.3.1 Primary map



X Index: 160

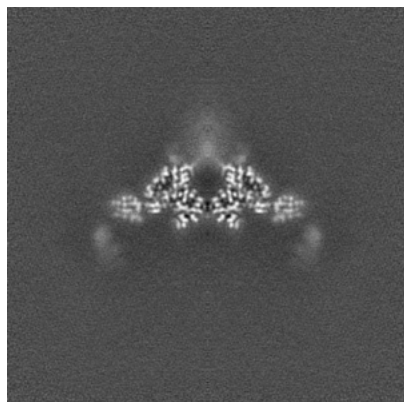


Y Index: 160

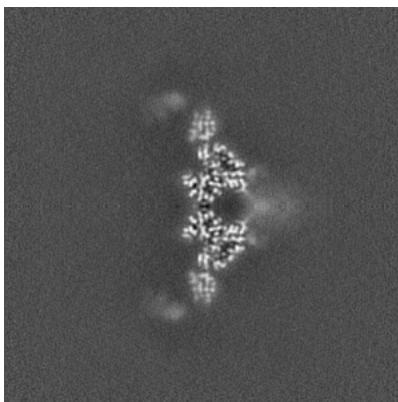


Z Index: 162

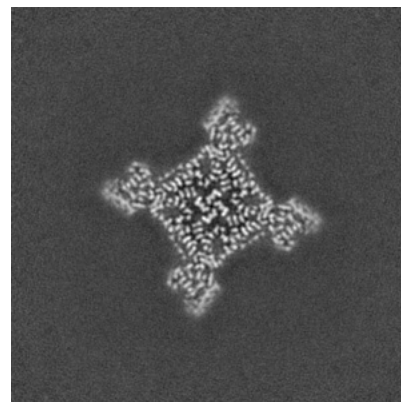
6.3.2 Raw map



X Index: 160



Y Index: 160

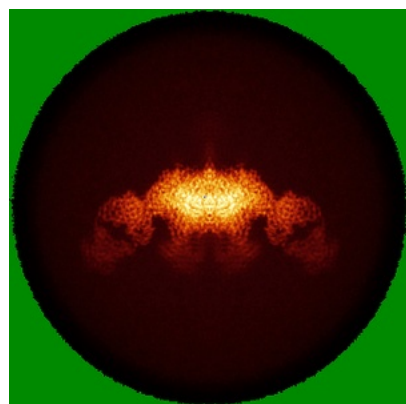


Z Index: 162

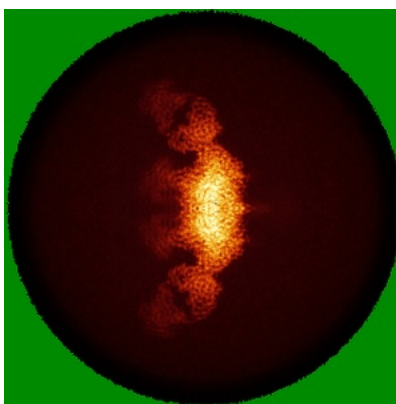
The images above show the largest variance slices of the map in three orthogonal directions.

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

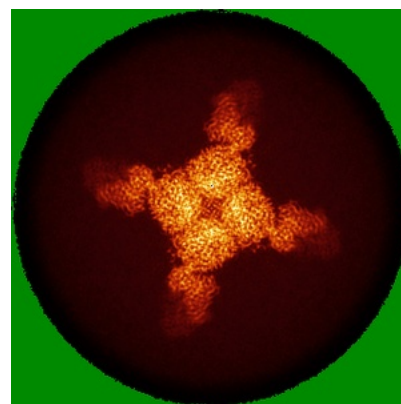
6.4.1 Primary map



X

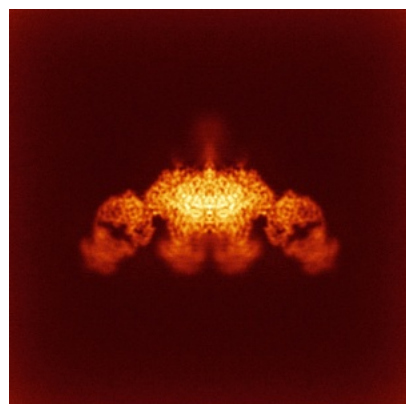


Y

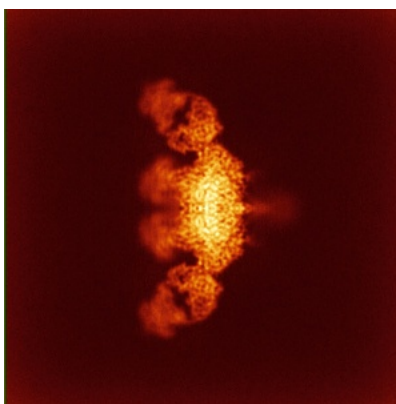


Z

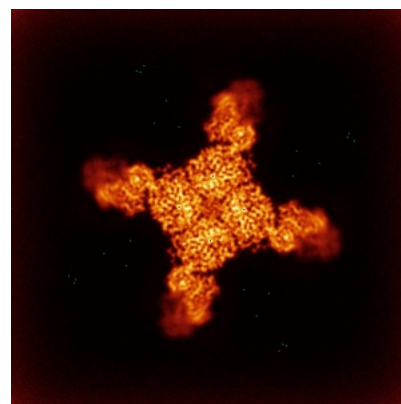
6.4.2 Raw map



X



Y

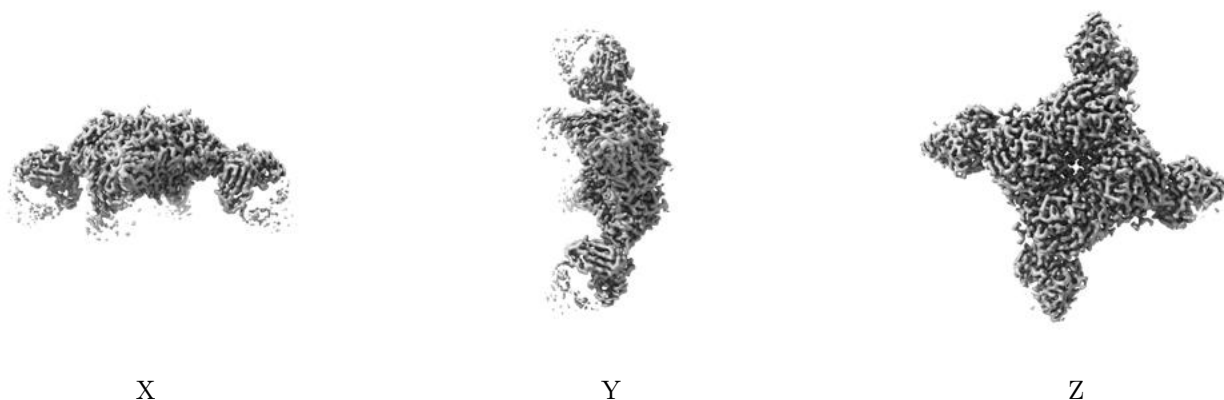


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

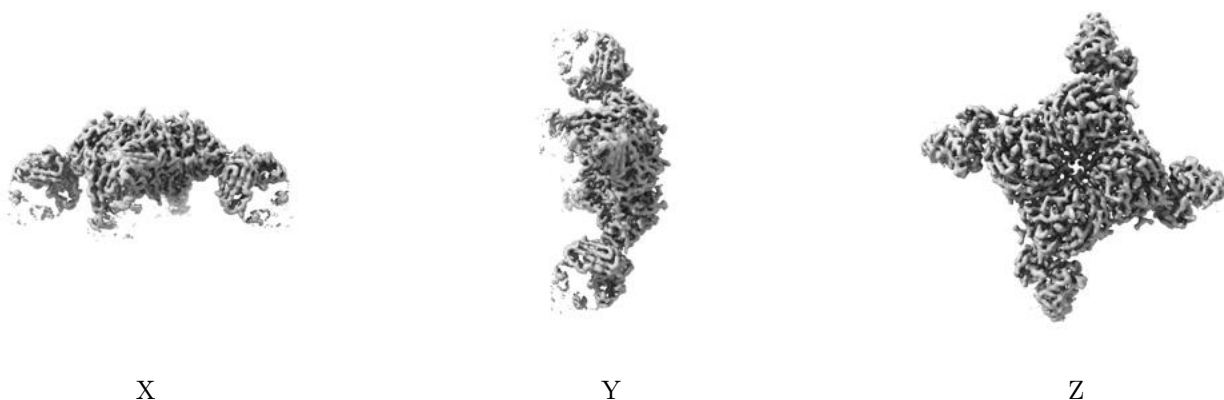
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.01. 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.

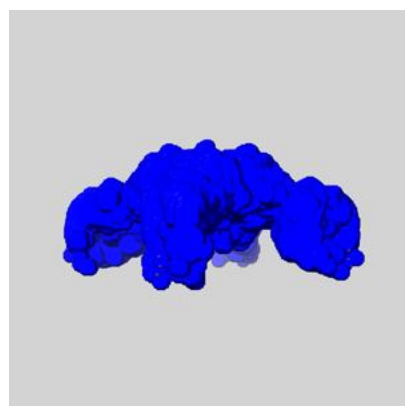
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

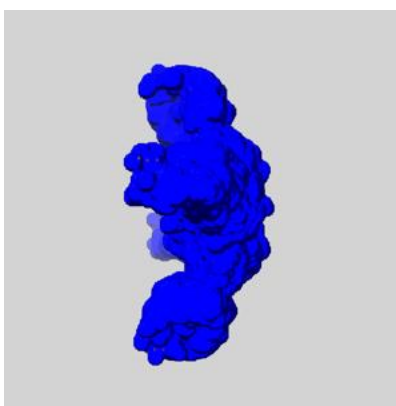
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

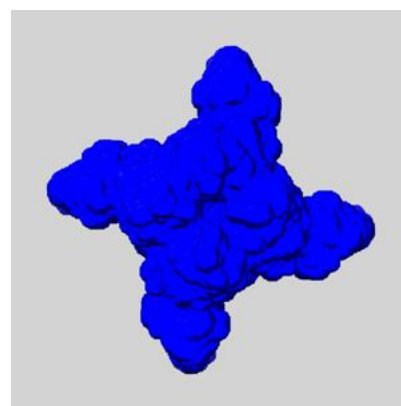
6.6.1 emd_20594_msk_1.map [i](#)



X



Y

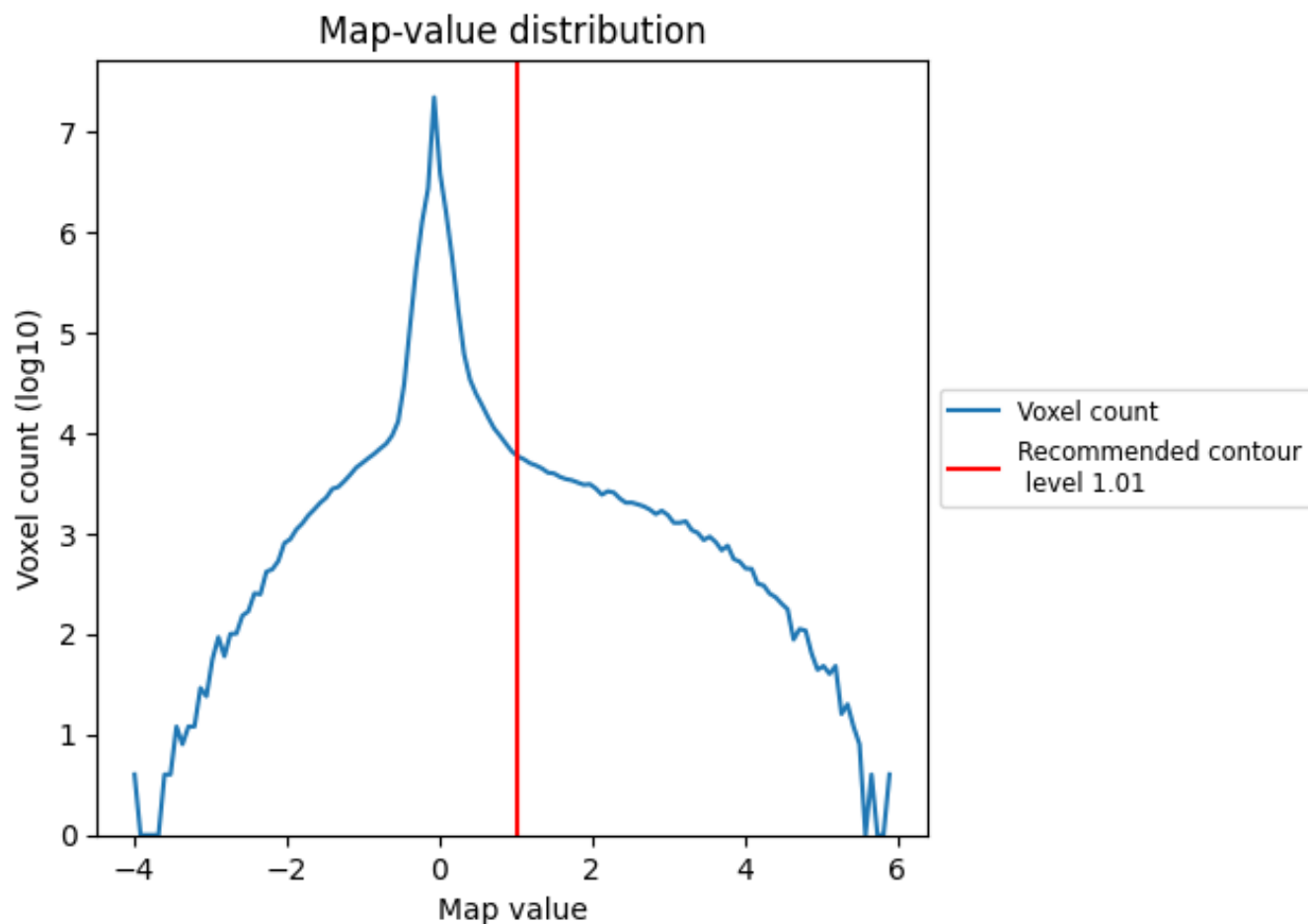


Z

7 Map analysis [i](#)

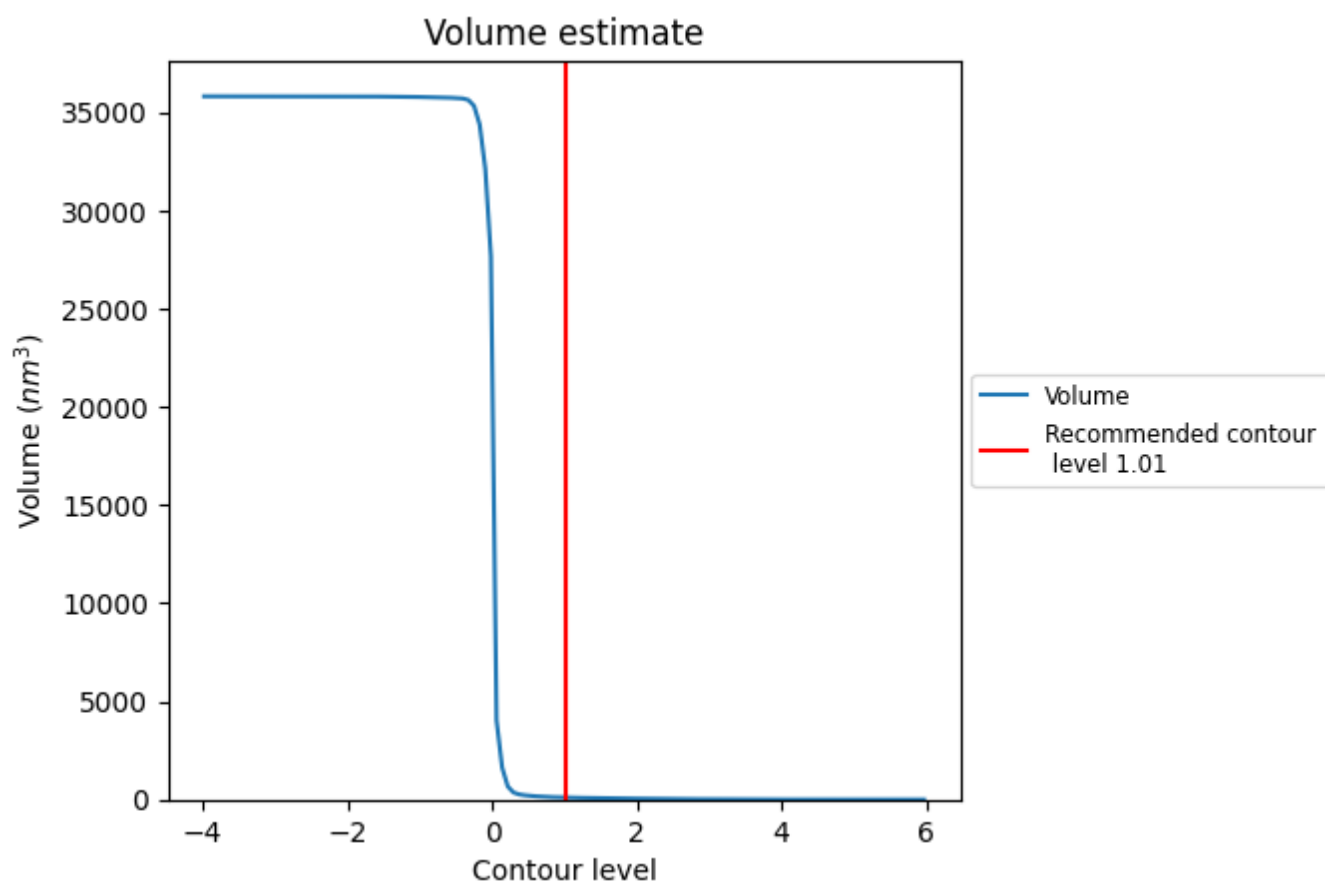
This section contains the results of statistical analysis of the map.

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.

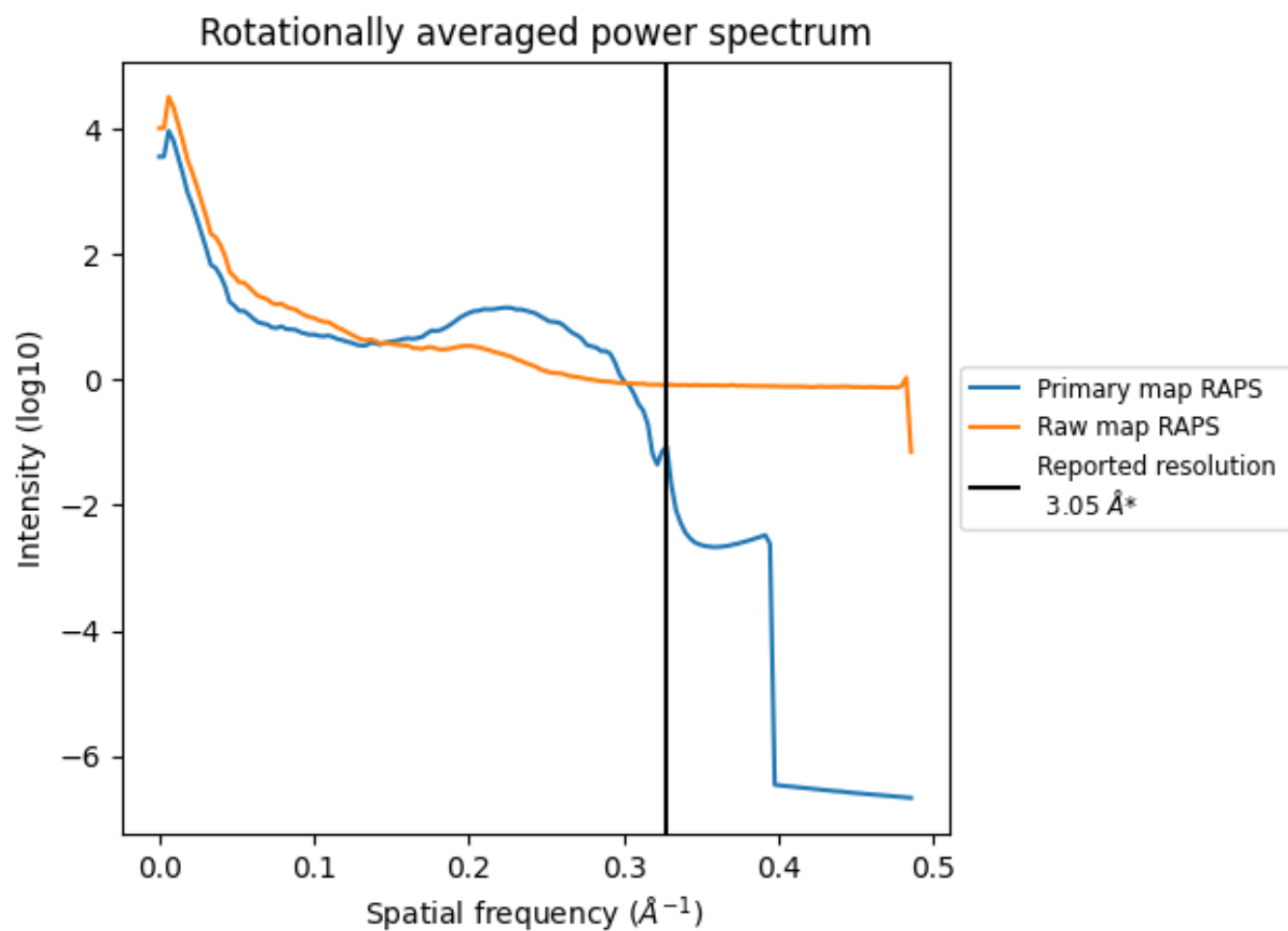
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm³; this corresponds to an approximate mass of 95 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 ⓘ

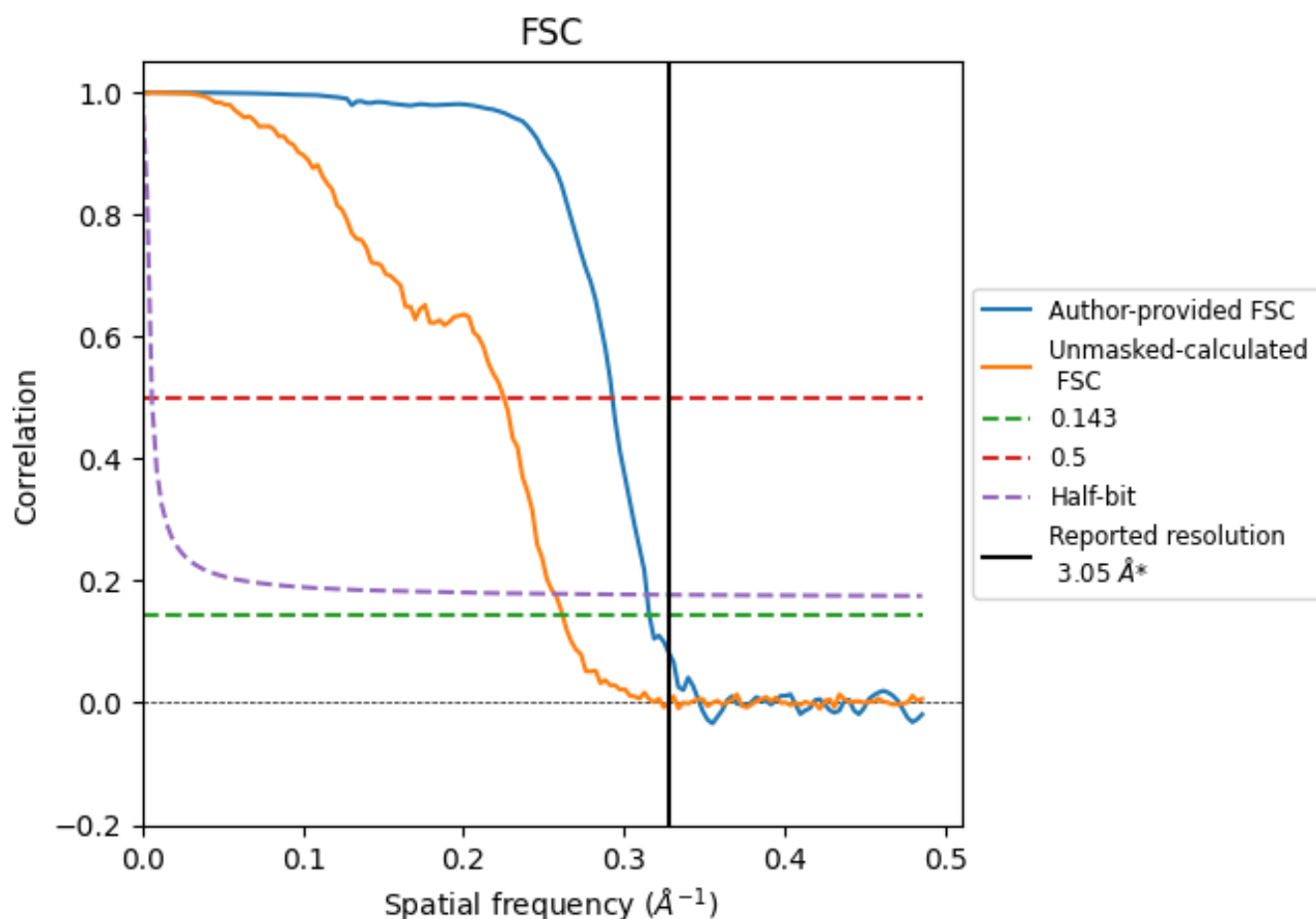


*Reported resolution corresponds to spatial frequency of 0.328 Å⁻¹

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 0.328 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

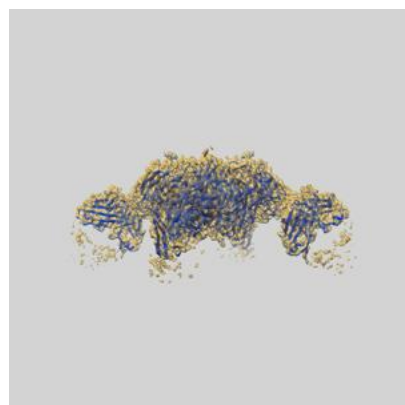
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	3.17	3.42	3.18
Unmasked-calculated*	3.82	4.44	3.90

*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 3.82 differs from the reported value 3.05 by more than 10 %

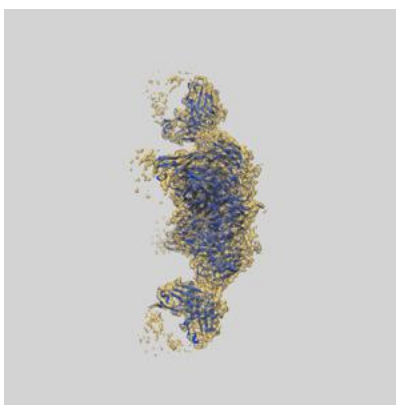
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20594 and PDB model 6U02. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

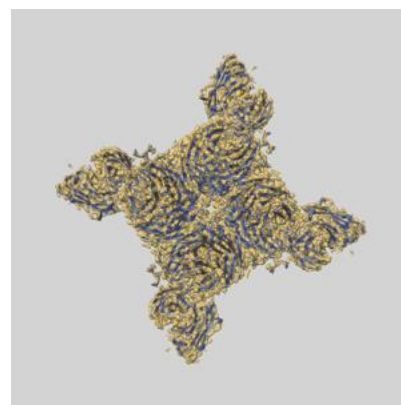
9.1 Map-model overlay [i](#)



X



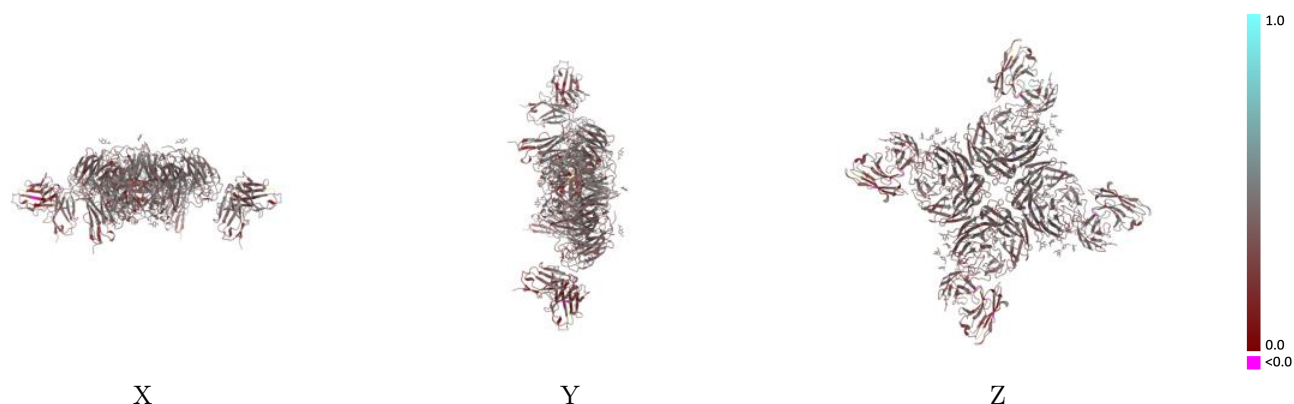
Y



Z

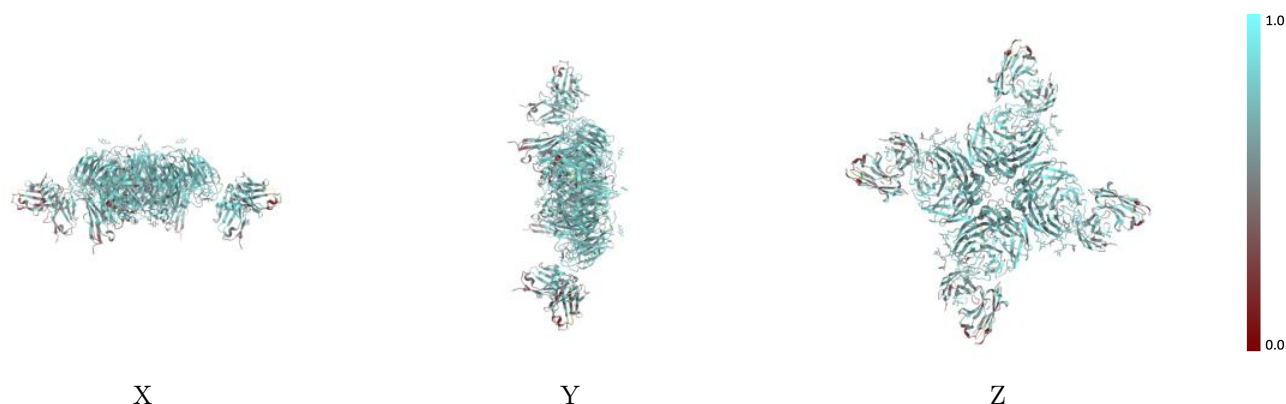
The images above show the 3D surface view of the map at the recommended contour level 1.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



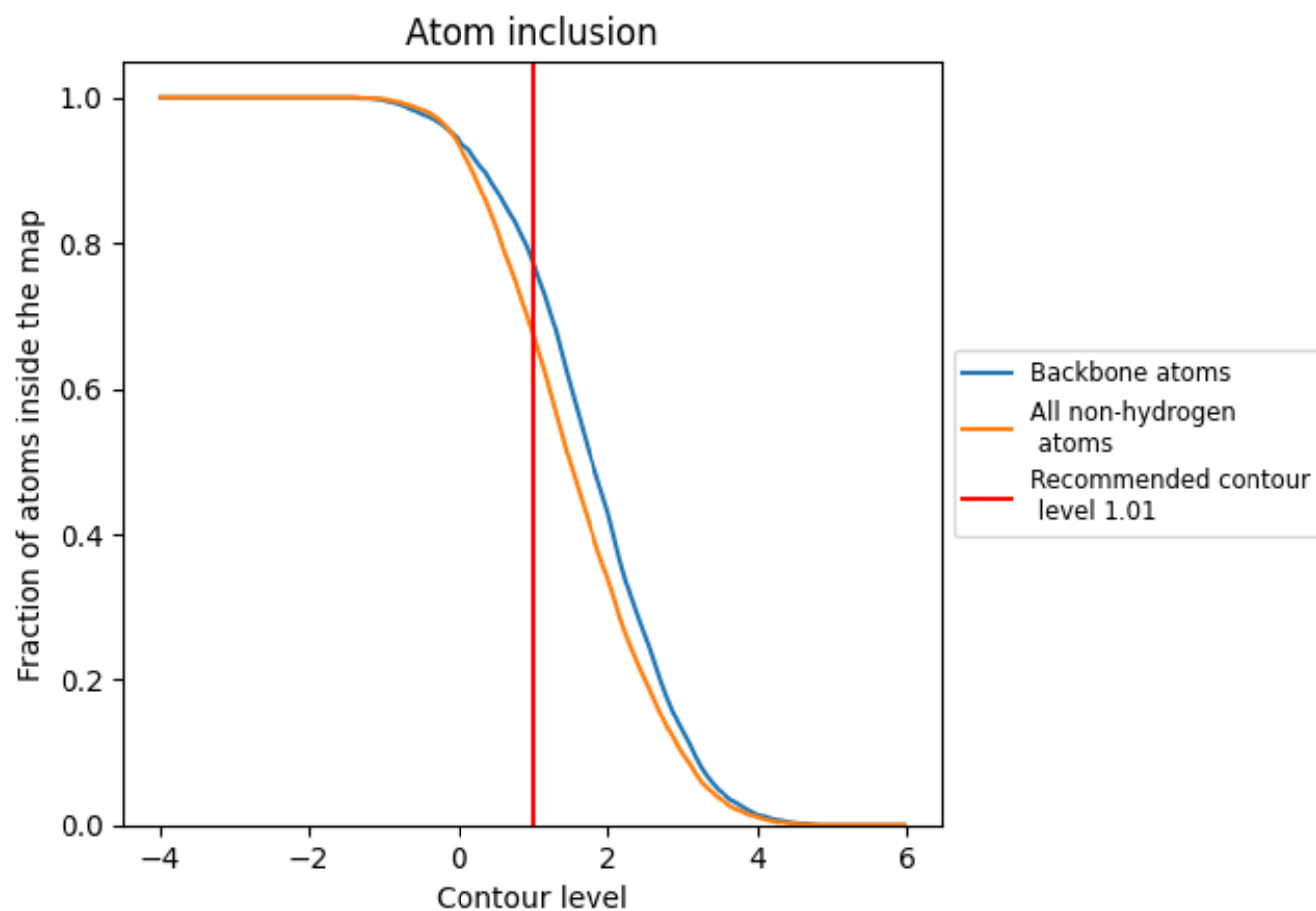
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6710	 0.3700
A	 0.7310	 0.4010
B	 0.7100	 0.3730
C	 0.5790	 0.3160
D	 0.5400	 0.3020
E	 0.7050	 0.3690
F	 0.5890	 0.3260
G	 0.5320	 0.2980
H	 0.6200	 0.3720
I	 0.6360	 0.3840
J	 0.7290	 0.3980
K	 0.6160	 0.3680
L	 0.6280	 0.3760
M	 0.6380	 0.3910
N	 0.6100	 0.3770
O	 0.5520	 0.3370
P	 0.5810	 0.3550

