



Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 01:38 PM EST

PDB ID : 6X9U
EMDB ID : EMD-22111
Title : HIV-1 Envelope Glycoprotein BG505 SOSIP.664, expressed in HEK293S cells and partially deglycosylated by endoglycosidase H, in complex with RM20A3 Fab
Authors : Berndsen, Z.T.; Ward, A.B.
Deposited on : 2020-06-03
Resolution : 3.20 Å(reported)

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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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

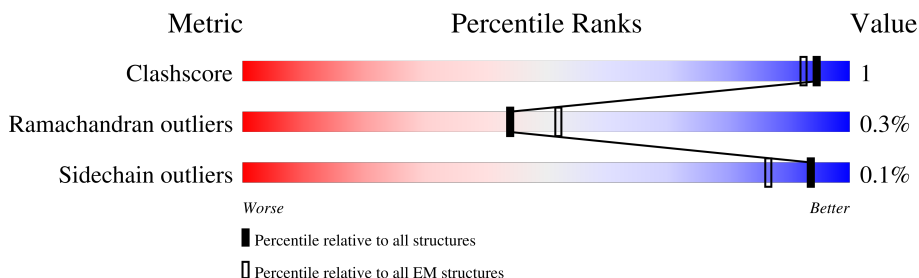
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



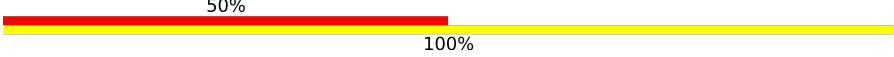
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	516	<div style="display: flex; justify-content: space-between;"> 8% 79% 5% 16% </div>
2	B	153	<div style="display: flex; justify-content: space-between;"> 5% 73% 6% 21% </div>
3	H	125	<div style="display: flex; justify-content: space-between;"> 22% 92% 7% </div>
4	L	128	<div style="display: flex; justify-content: space-between;"> 27% 78% 7% 15% </div>
5	C	2	<div style="display: flex; justify-content: space-between;"> 50% 100% </div>
5	D	2	<div style="display: flex; justify-content: space-between;"> 50% 100% </div>
5	F	2	<div style="display: flex; justify-content: space-between;"> 50% 100% </div>
5	G	2	<div style="display: flex; justify-content: space-between;"> 50% 100% </div>

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Mol	Chain	Length	Quality of chain
6	E	4	 A horizontal bar chart representing the quality of chain. The bar is divided into two segments: a red segment on the left and a yellow segment on the right. The red segment is labeled '50%' and the yellow segment is labeled '100%'. The total length of the bar represents 100% of the chain's quality.

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6530 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 HIV-1 Envelope Glycoprotein BG505 SOSIP.664 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	432	3405	2142	600	635	28	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	expression tag	UNP Q2N0S6
A	-3	ASP	-	expression tag	UNP Q2N0S6
A	-2	ALA	-	expression tag	UNP Q2N0S6
A	-1	MET	-	expression tag	UNP Q2N0S6
A	0	LYS	-	expression tag	UNP Q2N0S6
A	1	ARG	-	expression tag	UNP Q2N0S6
A	2	GLY	-	expression tag	UNP Q2N0S6
A	3	LEU	-	expression tag	UNP Q2N0S6
A	4	CYS	-	expression tag	UNP Q2N0S6
A	5	CYS	-	expression tag	UNP Q2N0S6
A	6	VAL	-	expression tag	UNP Q2N0S6
A	7	LEU	-	expression tag	UNP Q2N0S6
A	8	LEU	-	expression tag	UNP Q2N0S6
A	9	LEU	-	expression tag	UNP Q2N0S6
A	10	CYS	-	expression tag	UNP Q2N0S6
A	11	GLY	-	expression tag	UNP Q2N0S6
A	12	ALA	-	expression tag	UNP Q2N0S6
A	13	VAL	-	expression tag	UNP Q2N0S6
A	14	PHE	-	expression tag	UNP Q2N0S6
A	15	VAL	-	expression tag	UNP Q2N0S6
A	16	SER	-	expression tag	UNP Q2N0S6
A	17	PRO	-	expression tag	UNP Q2N0S6
A	18	SER	-	expression tag	UNP Q2N0S6
A	19	GLN	-	expression tag	UNP Q2N0S6
A	20	GLU	-	expression tag	UNP Q2N0S6
A	21	ILE	-	expression tag	UNP Q2N0S6
A	22	HIS	-	expression tag	UNP Q2N0S6
A	23	ALA	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	24	ARG	-	expression tag	UNP Q2N0S6
A	25	PHE	-	expression tag	UNP Q2N0S6
A	26	ARG	-	expression tag	UNP Q2N0S6
A	27	ARG	-	expression tag	UNP Q2N0S6
A	28	GLY	-	expression tag	UNP Q2N0S6
A	29	ALA	-	expression tag	UNP Q2N0S6
A	30	ARG	-	expression tag	UNP Q2N0S6
A	332	ASN	THR	engineered mutation	UNP Q2N0S6
A	501	CYS	ALA	engineered mutation	UNP Q2N0S6
A	509	ARG	-	expression tag	UNP Q2N0S6
A	510	ARG	-	expression tag	UNP Q2N0S6
A	511	ARG	-	expression tag	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called HIV-1 Envelope Glycoprotein BG505 SOSIP.664 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	121	971	616	167	182	6	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 3 is a protein called RM20A3 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	124	943	595	161	182	5	0	0

- Molecule 4 is a protein called RM20A3 Fab Light Chain.

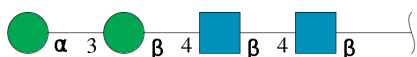
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	109	811	505	136	167	3	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



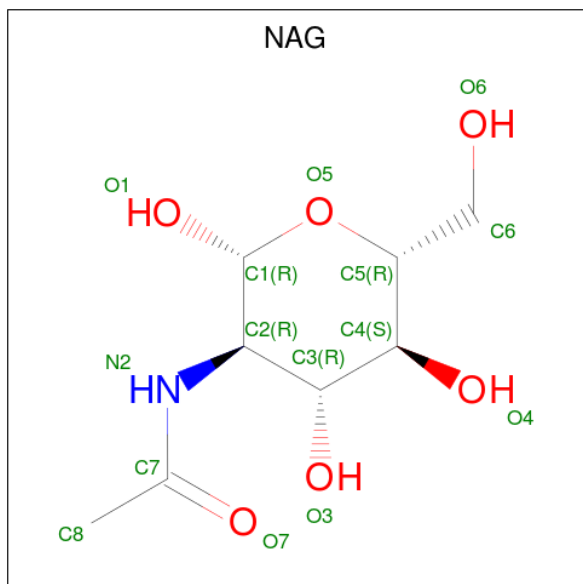
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	C	2	28	16	2	10	0	0
5	D	2	28	16	2	10	0	0
5	F	2	28	16	2	10	0	0
5	G	2	28	16	2	10	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	E	4	50	28	2	20	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

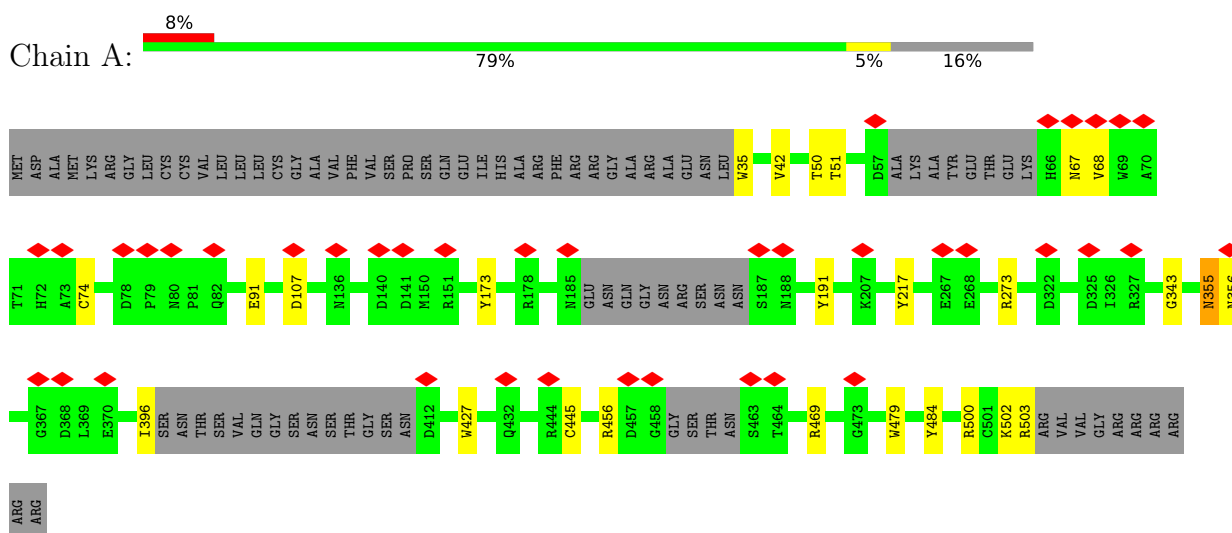


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 182	C 104	N 13	O 65	0
7	A	1	Total 182	C 104	N 13	O 65	0
7	A	1	Total 182	C 104	N 13	O 65	0
7	A	1	Total 182	C 104	N 13	O 65	0
7	A	1	Total 182	C 104	N 13	O 65	0
7	A	1	Total 182	C 104	N 13	O 65	0
7	A	1	Total 182	C 104	N 13	O 65	0
7	A	1	Total 182	C 104	N 13	O 65	0
7	A	1	Total 182	C 104	N 13	O 65	0
7	A	1	Total 182	C 104	N 13	O 65	0
7	A	1	Total 182	C 104	N 13	O 65	0
7	A	1	Total 182	C 104	N 13	O 65	0
7	A	1	Total 182	C 104	N 13	O 65	0
7	A	1	Total 182	C 104	N 13	O 65	0
7	A	1	Total 182	C 104	N 13	O 65	0
7	B	1	Total 56	C 32	N 4	O 20	0
7	B	1	Total 56	C 32	N 4	O 20	0
7	B	1	Total 56	C 32	N 4	O 20	0
7	B	1	Total 56	C 32	N 4	O 20	0

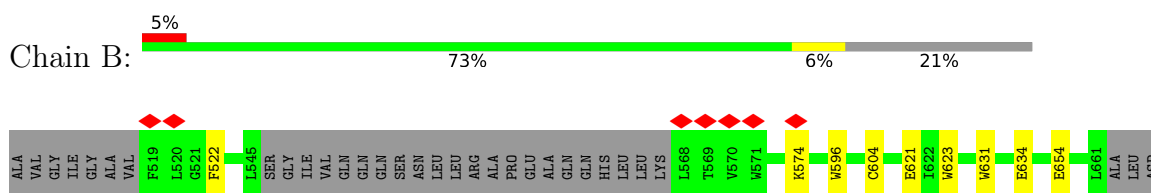
3 Residue-property plots

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.

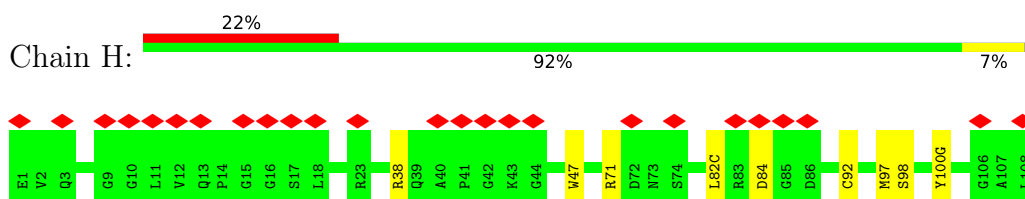
- Molecule 1: HIV-1 Envelope Glycoprotein BG505 SOSIP.664 gp120



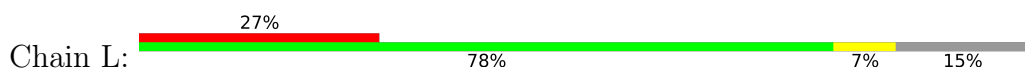
- Molecule 2: HIV-1 Envelope Glycoprotein BG505 SOSIP.664 gp41

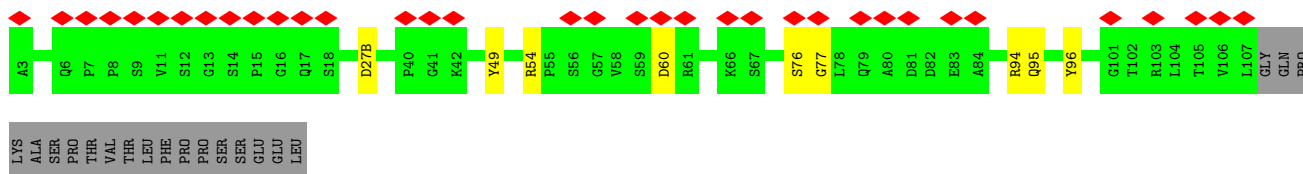


- Molecule 3: RM20A3 Fab Heavy Chain



- Molecule 4: RM20A3 Fab Light Chain





- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	46104	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.103	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	288.4, 288.4, 288.4	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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: NAG, MAN, BMA

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	1.21	11/3476 (0.3%)	0.88	8/4718 (0.2%)
2	B	1.34	10/989 (1.0%)	0.80	0/1341
3	H	1.33	6/963 (0.6%)	0.97	0/1300
4	L	1.15	2/830 (0.2%)	0.95	2/1129 (0.2%)
All	All	1.24	29/6258 (0.5%)	0.89	10/8488 (0.1%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	100(G)	TYR	CG-CD1	-7.23	1.29	1.39
1	A	42	VAL	CB-CG1	-6.50	1.39	1.52
4	L	96	TYR	CB-CG	-6.34	1.42	1.51
2	B	634	GLU	CD-OE1	-6.33	1.18	1.25
3	H	100(G)	TYR	CD1-CE1	-6.17	1.30	1.39
3	H	38	ARG	CB-CG	-6.03	1.36	1.52
1	A	91	GLU	CD-OE1	-5.90	1.19	1.25
1	A	74	CYS	CB-SG	-5.80	1.72	1.81
2	B	522	PHE	CB-CG	-5.75	1.41	1.51
3	H	71	ARG	CD-NE	-5.68	1.36	1.46
1	A	445	CYS	CB-SG	-5.63	1.72	1.81
1	A	217	TYR	CB-CG	-5.58	1.43	1.51
1	A	427	TRP	CE2-CZ2	-5.56	1.30	1.39
1	A	191	TYR	CG-CD1	-5.50	1.32	1.39
3	H	92	CYS	CB-SG	-5.49	1.72	1.81
2	B	623	TRP	CZ3-CH2	-5.41	1.31	1.40
2	B	604	CYS	CB-SG	-5.38	1.73	1.81
3	H	47	TRP	CD2-CE2	-5.38	1.34	1.41
1	A	500	ARG	CZ-NH2	-5.31	1.26	1.33
1	A	479	TRP	CE2-CZ2	-5.29	1.30	1.39
2	B	654	GLU	CD-OE1	-5.27	1.19	1.25
4	L	49	TYR	CB-CG	-5.20	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	596	TRP	CZ3-CH2	-5.20	1.31	1.40
2	B	631	TRP	CD2-CE2	-5.17	1.35	1.41
2	B	596	TRP	CD2-CE2	-5.14	1.35	1.41
1	A	35	TRP	CZ3-CH2	-5.13	1.31	1.40
2	B	623	TRP	CD2-CE2	-5.12	1.35	1.41
2	B	623	TRP	NE1-CE2	-5.10	1.30	1.37
1	A	484	TYR	CB-CG	-5.05	1.44	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	500	ARG	NE-CZ-NH2	-9.98	115.31	120.30
1	A	469	ARG	NE-CZ-NH2	-8.71	115.94	120.30
4	L	54	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	A	500	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	273	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	A	456	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	217	TYR	CB-CG-CD1	-6.12	117.33	121.00
1	A	469	ARG	NE-CZ-NH1	6.10	123.35	120.30
4	L	96	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	A	173	TYR	CB-CG-CD2	-5.02	117.99	121.00

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	3405	0	3343	7	0
2	B	971	0	948	2	0
3	H	943	0	915	2	0
4	L	811	0	767	3	0
5	C	28	0	25	0	0
5	D	28	0	25	0	0
5	F	28	0	25	0	0
5	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	50	0	41	0	0
7	A	182	0	169	0	0
7	B	56	0	52	2	0
All	All	6530	0	6335	14	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.

All (14) 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:621:GLU:OE2	7:B:702:NAG:H62	1.88	0.73
1:A:355:ASN:N	1:A:355:ASN:OD1	2.30	0.64
7:B:702:NAG:O7	7:B:702:NAG:O3	2.17	0.60
3:H:84:ASP:OD1	3:H:84:ASP:N	2.33	0.59
4:L:60:ASP:OD1	4:L:60:ASP:N	2.44	0.48
3:H:97:MET:HG2	3:H:98:SER:H	1.81	0.45
4:L:94:ARG:O	4:L:95:GLN:HB2	2.17	0.45
1:A:67:ASN:OD1	1:A:68:VAL:N	2.52	0.43
1:A:50:THR:OG1	1:A:51:THR:N	2.52	0.42
1:A:502:LYS:O	1:A:503:ARG:C	2.56	0.42
1:A:343:GLY:HA2	1:A:396:ILE:HD12	2.01	0.41
1:A:356:ASN:OD1	1:A:356:ASN:N	2.46	0.41
4:L:76:SER:OG	4:L:77:GLY:N	2.47	0.41
1:A:107:ASP:OD1	2:B:574:LYS:NZ	2.54	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	422/516 (82%)	412 (98%)	10 (2%)	0	100	100
2	B	117/153 (76%)	115 (98%)	2 (2%)	0	100	100
3	H	122/125 (98%)	116 (95%)	5 (4%)	1 (1%)	19	58
4	L	107/128 (84%)	98 (92%)	8 (8%)	1 (1%)	17	56
All	All	768/922 (83%)	741 (96%)	25 (3%)	2 (0%)	44	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	82(C)	LEU
4	L	27(B)	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	387/456 (85%)	386 (100%)	1 (0%)	92	96
2	B	105/129 (81%)	105 (100%)	0	100	100
3	H	101/102 (99%)	101 (100%)	0	100	100
4	L	89/106 (84%)	89 (100%)	0	100	100
All	All	682/793 (86%)	681 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	355	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	1	5,1	14,14,15	2.06	2 (14%)	17,19,21	0.95	1 (5%)
5	NAG	C	2	5	14,14,15	2.21	2 (14%)	17,19,21	0.83	0
5	NAG	D	1	5,1	14,14,15	2.12	3 (21%)	17,19,21	0.83	1 (5%)
5	NAG	D	2	5	14,14,15	2.20	2 (14%)	17,19,21	0.75	0
6	NAG	E	1	6,1	14,14,15	1.98	2 (14%)	17,19,21	1.09	1 (5%)
6	NAG	E	2	6	14,14,15	2.18	2 (14%)	17,19,21	0.90	0
6	BMA	E	3	6	11,11,12	1.90	2 (18%)	15,15,17	1.15	1 (6%)
6	MAN	E	4	6	11,11,12	1.79	2 (18%)	15,15,17	1.31	2 (13%)
5	NAG	F	1	5,1	14,14,15	2.15	3 (21%)	17,19,21	1.03	1 (5%)
5	NAG	F	2	5	14,14,15	2.18	3 (21%)	17,19,21	1.18	3 (17%)
5	NAG	G	1	5,1	14,14,15	2.10	2 (14%)	17,19,21	1.08	3 (17%)
5	NAG	G	2	5	14,14,15	2.24	2 (14%)	17,19,21	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	1/6/23/26	0/1/1/1
5	NAG	D	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	D	2	5	-	1/6/23/26	0/1/1/1
6	NAG	E	1	6,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	E	2	6	-	0/6/23/26	0/1/1/1
6	BMA	E	3	6	-	1/2/19/22	0/1/1/1
6	MAN	E	4	6	-	2/2/19/22	0/1/1/1
5	NAG	F	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	NAG	G	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	2	NAG	O5-C1	7.23	1.55	1.43
5	C	2	NAG	O5-C1	7.00	1.54	1.43
5	D	2	NAG	O5-C1	6.99	1.54	1.43
5	F	2	NAG	O5-C1	6.97	1.54	1.43
6	E	2	NAG	O5-C1	6.86	1.54	1.43
5	F	1	NAG	O5-C1	6.57	1.54	1.43
5	D	1	NAG	O5-C1	6.42	1.54	1.43
5	G	1	NAG	O5-C1	6.37	1.53	1.43
6	E	1	NAG	O5-C1	6.24	1.53	1.43
5	C	1	NAG	O5-C1	6.21	1.53	1.43
6	E	3	BMA	O2-C2	-4.24	1.34	1.43
6	E	4	MAN	O2-C2	-4.08	1.34	1.43
6	E	3	BMA	C2-C3	-2.77	1.48	1.52
6	E	2	NAG	C3-C2	-2.74	1.46	1.52
5	F	1	NAG	C3-C2	-2.64	1.46	1.52
5	G	1	NAG	C3-C2	-2.59	1.47	1.52
5	C	1	NAG	C3-C2	-2.59	1.47	1.52
5	D	1	NAG	C3-C2	-2.58	1.47	1.52
6	E	4	MAN	C2-C3	-2.50	1.48	1.52
5	G	2	NAG	C3-C2	-2.44	1.47	1.52
5	C	2	NAG	C3-C2	-2.40	1.47	1.52
5	D	2	NAG	C3-C2	-2.35	1.47	1.52
6	E	1	NAG	C3-C2	-2.33	1.47	1.52
5	F	1	NAG	C1-C2	-2.24	1.49	1.52
5	F	2	NAG	C3-C2	-2.14	1.48	1.52
5	D	1	NAG	C1-C2	-2.09	1.49	1.52
5	F	2	NAG	C4-C3	2.08	1.57	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1	NAG	C3-C4-C5	-3.42	104.13	110.24
6	E	3	BMA	C2-C3-C4	-3.00	105.71	110.89
5	F	2	NAG	C4-C3-C2	-2.85	106.83	111.02
6	E	4	MAN	C1-C2-C3	2.76	113.06	109.67
6	E	4	MAN	C2-C3-C4	-2.67	106.28	110.89
5	F	1	NAG	C3-C4-C5	-2.55	105.68	110.24
5	C	1	NAG	C3-C4-C5	-2.53	105.72	110.24
5	G	1	NAG	O5-C5-C6	-2.26	103.67	107.20
5	G	1	NAG	C3-C4-C5	-2.12	106.47	110.24
5	F	2	NAG	O5-C5-C4	-2.06	105.81	110.83
5	D	1	NAG	C3-C4-C5	-2.06	106.57	110.24
5	G	1	NAG	O5-C1-C2	-2.05	108.06	111.29
5	F	2	NAG	C1-O5-C5	2.04	114.95	112.19

There are no chirality outliers.

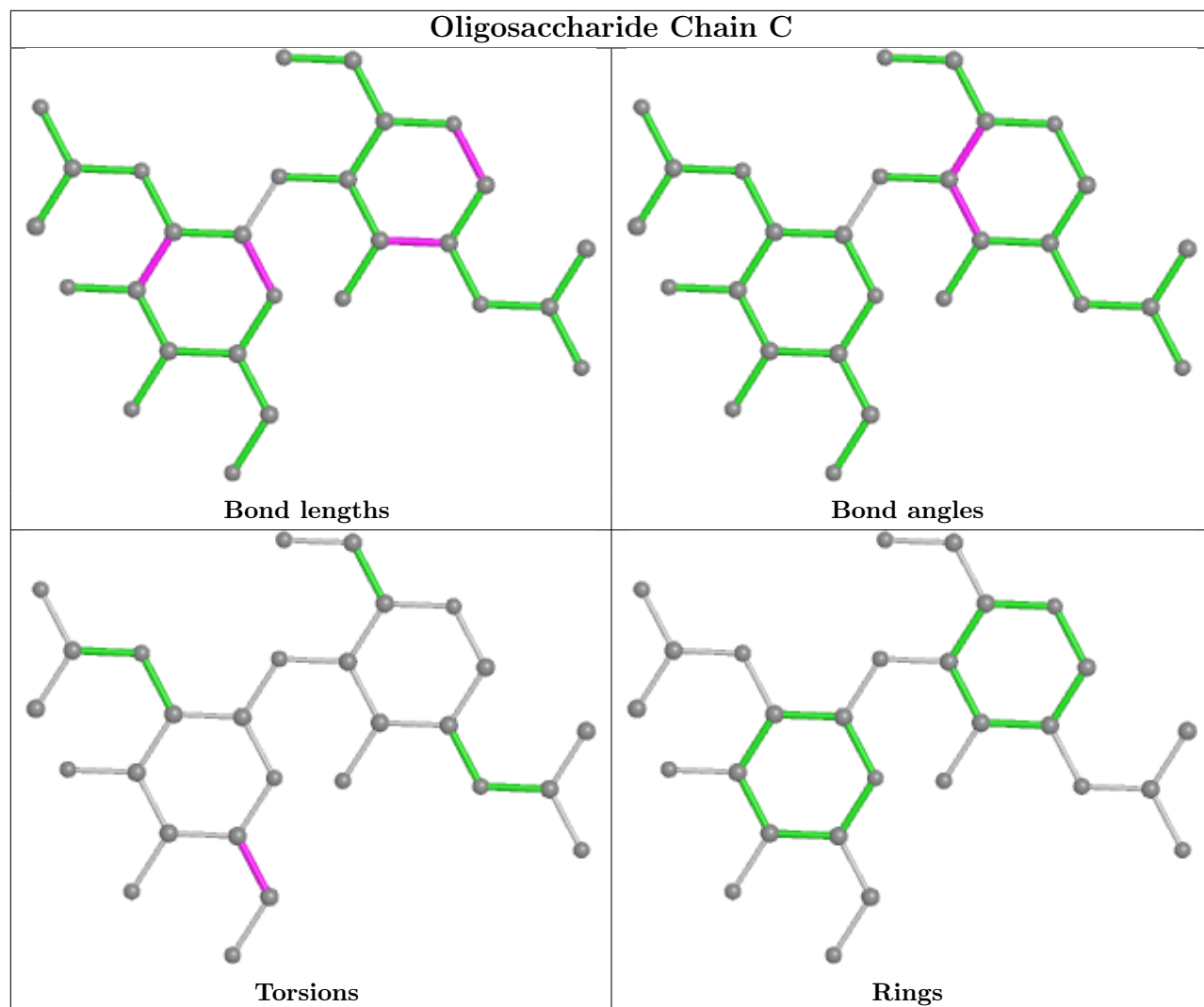
All (10) torsion outliers are listed below:

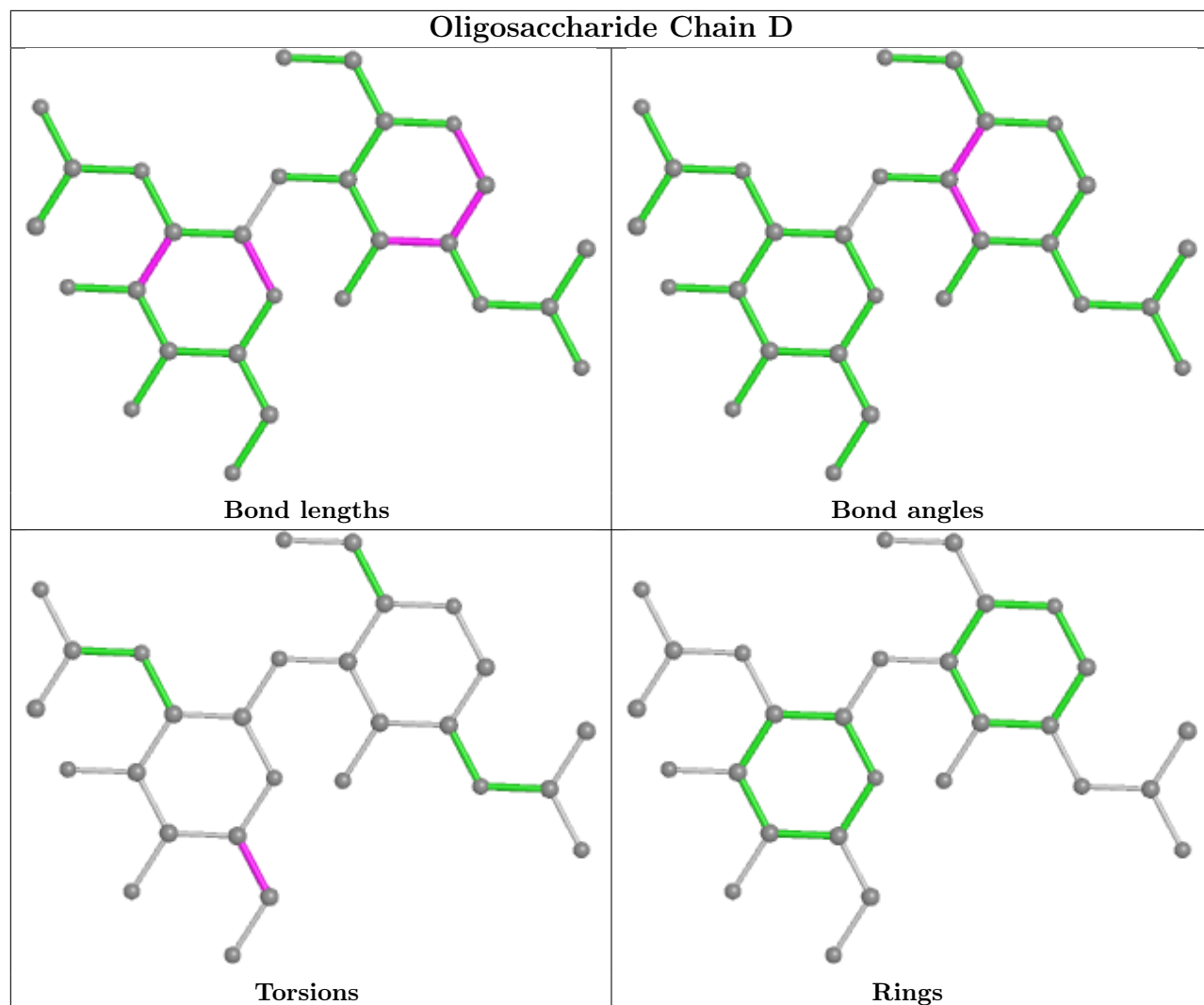
Mol	Chain	Res	Type	Atoms
5	F	1	NAG	O5-C5-C6-O6
6	E	4	MAN	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
6	E	4	MAN	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
6	E	3	BMA	O5-C5-C6-O6
5	C	2	NAG	O5-C5-C6-O6
5	D	2	NAG	O5-C5-C6-O6

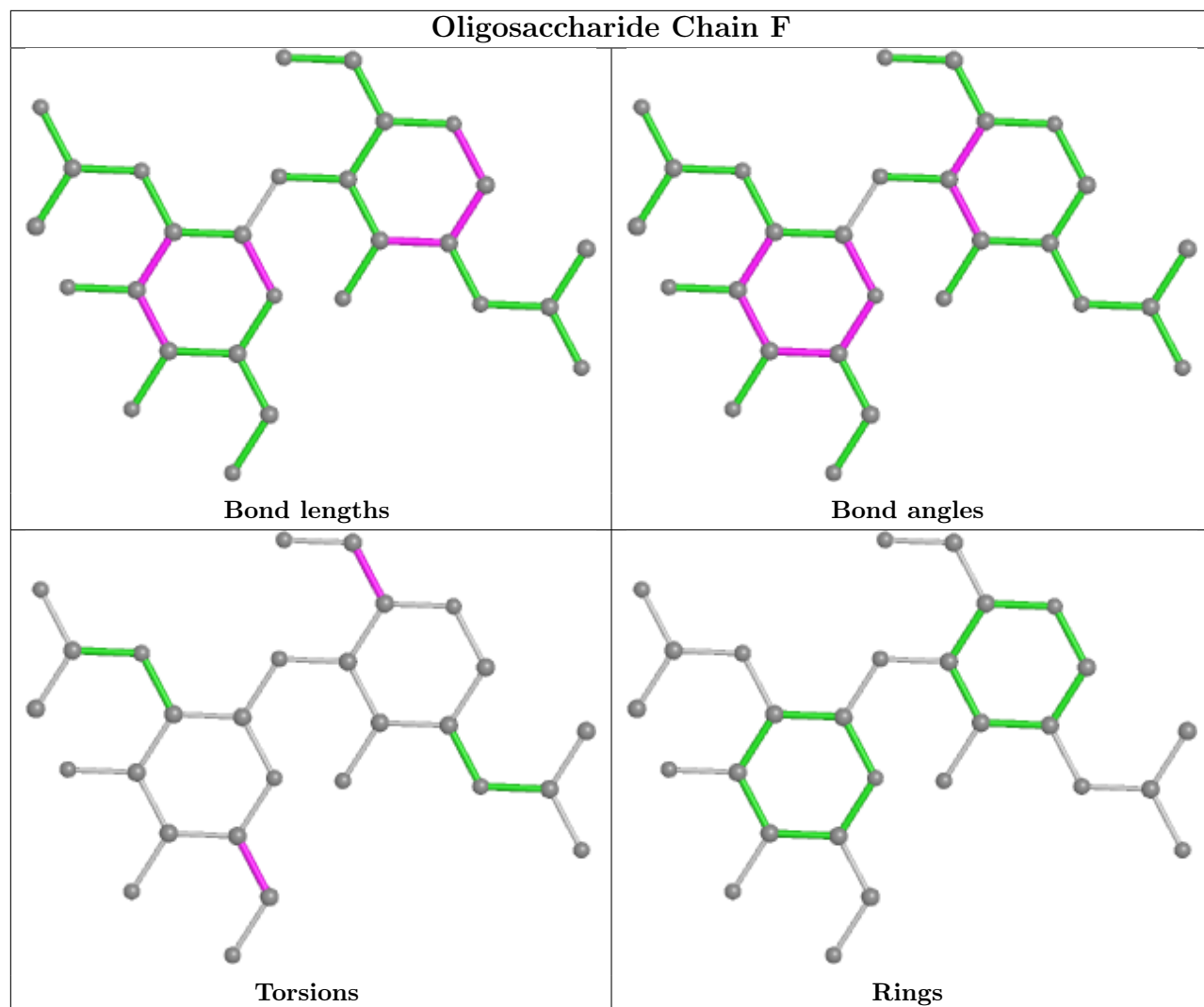
There are no ring outliers.

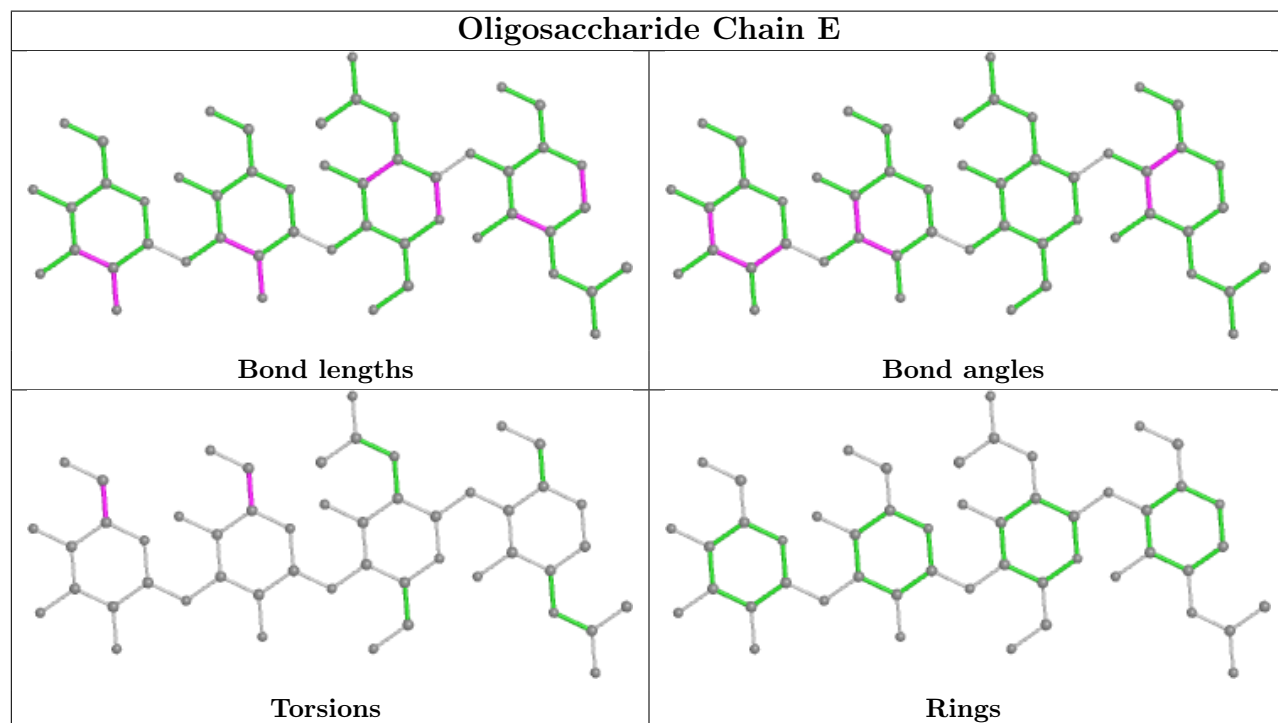
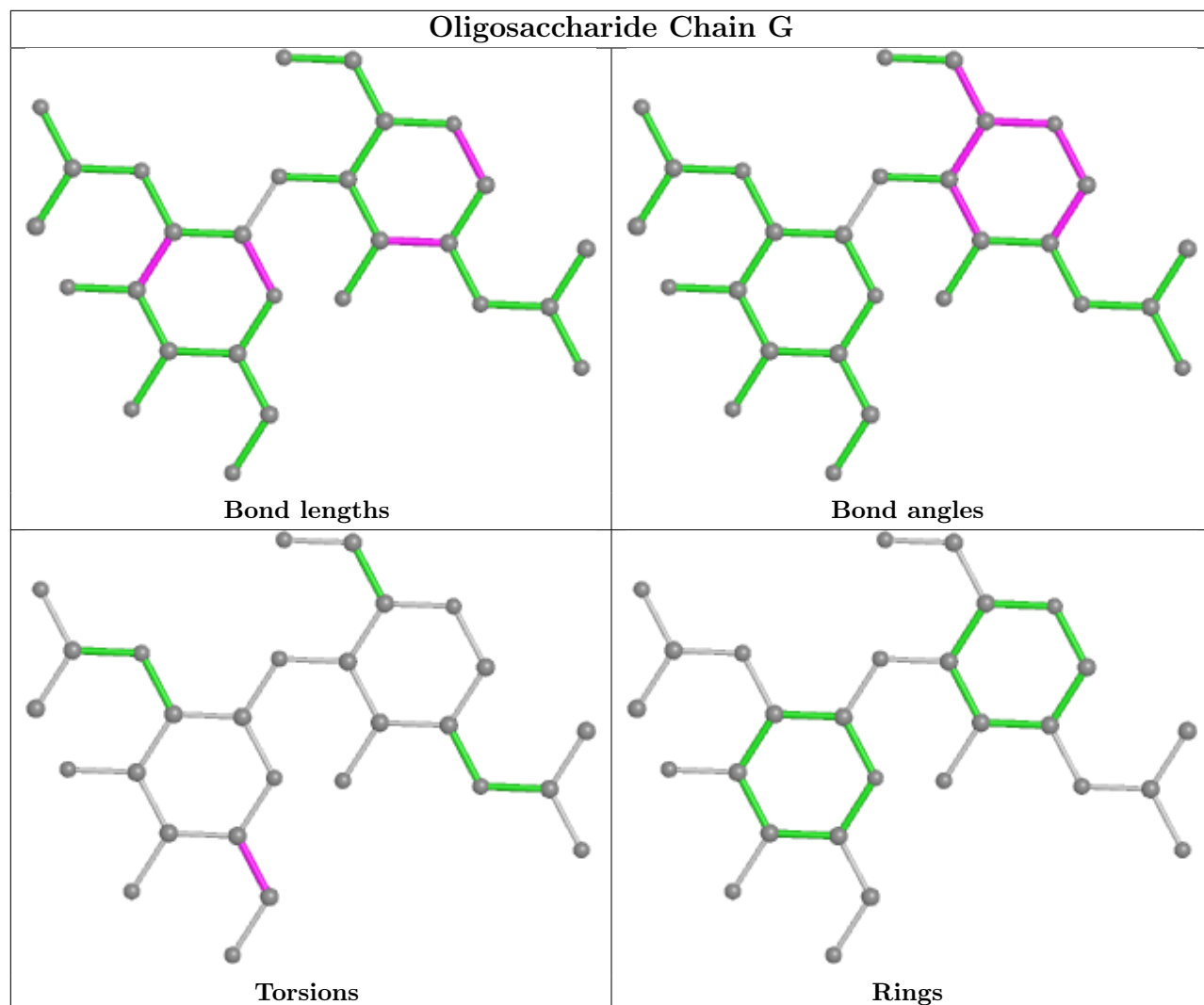
No monomer is involved in short contacts.

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

17 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
7	NAG	A	609	1	14,14,15	2.07	2 (14%)	17,19,21	1.01	1 (5%)
7	NAG	A	615	1	14,14,15	2.17	2 (14%)	17,19,21	0.83	0
7	NAG	B	704	2	14,14,15	0.29	0	17,19,21	0.66	0
7	NAG	A	606	1	14,14,15	2.16	2 (14%)	17,19,21	0.78	0
7	NAG	A	618	1	14,14,15	2.13	2 (14%)	17,19,21	0.98	2 (11%)
7	NAG	B	703	2	14,14,15	0.29	0	17,19,21	0.63	0
7	NAG	B	702	2	14,14,15	0.31	0	17,19,21	0.75	0
7	NAG	A	601	1	14,14,15	2.06	2 (14%)	17,19,21	0.85	1 (5%)
7	NAG	A	614	1	14,14,15	2.04	2 (14%)	17,19,21	0.91	0
7	NAG	A	623	1	14,14,15	2.13	2 (14%)	17,19,21	0.78	1 (5%)
7	NAG	A	603	1	14,14,15	2.10	2 (14%)	17,19,21	0.71	0
7	NAG	A	620	1	14,14,15	2.12	3 (21%)	17,19,21	1.11	2 (11%)
7	NAG	A	616	1	14,14,15	2.10	2 (14%)	17,19,21	0.87	2 (11%)
7	NAG	A	619	1	14,14,15	2.09	2 (14%)	17,19,21	0.70	0
7	NAG	A	617	1	14,14,15	2.05	2 (14%)	17,19,21	0.88	0
7	NAG	B	701	2	14,14,15	0.31	0	17,19,21	0.87	1 (5%)
7	NAG	A	602	1	14,14,15	2.12	2 (14%)	17,19,21	0.81	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
7	NAG	A	609	1	-	1/6/23/26	0/1/1/1
7	NAG	A	615	1	-	2/6/23/26	0/1/1/1
7	NAG	B	704	2	-	3/6/23/26	0/1/1/1
7	NAG	A	606	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	618	1	-	1/6/23/26	0/1/1/1
7	NAG	B	703	2	-	2/6/23/26	0/1/1/1
7	NAG	B	702	2	-	6/6/23/26	0/1/1/1
7	NAG	A	601	1	-	3/6/23/26	0/1/1/1
7	NAG	A	614	1	-	2/6/23/26	0/1/1/1
7	NAG	A	623	1	-	1/6/23/26	0/1/1/1
7	NAG	A	603	1	-	2/6/23/26	0/1/1/1
7	NAG	A	620	1	-	1/6/23/26	0/1/1/1
7	NAG	A	616	1	-	2/6/23/26	0/1/1/1
7	NAG	A	619	1	-	1/6/23/26	0/1/1/1
7	NAG	A	617	1	-	2/6/23/26	0/1/1/1
7	NAG	B	701	2	-	2/6/23/26	0/1/1/1
7	NAG	A	602	1	-	1/6/23/26	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	618	NAG	O5-C1	6.92	1.54	1.43
7	A	602	NAG	O5-C1	6.88	1.54	1.43
7	A	623	NAG	O5-C1	6.87	1.54	1.43
7	A	603	NAG	O5-C1	6.85	1.54	1.43
7	A	619	NAG	O5-C1	6.81	1.54	1.43
7	A	615	NAG	O5-C1	6.79	1.54	1.43
7	A	601	NAG	O5-C1	6.70	1.54	1.43
7	A	606	NAG	O5-C1	6.63	1.54	1.43
7	A	620	NAG	O5-C1	6.59	1.54	1.43
7	A	617	NAG	O5-C1	6.47	1.54	1.43
7	A	616	NAG	O5-C1	6.46	1.54	1.43
7	A	609	NAG	O5-C1	6.45	1.54	1.43
7	A	614	NAG	O5-C1	6.24	1.53	1.43
7	A	606	NAG	C3-C2	-2.83	1.46	1.52
7	A	615	NAG	C3-C2	-2.71	1.46	1.52
7	A	617	NAG	C3-C2	-2.60	1.47	1.52
7	A	616	NAG	C3-C2	-2.57	1.47	1.52
7	A	623	NAG	C3-C2	-2.53	1.47	1.52
7	A	620	NAG	C3-C2	-2.50	1.47	1.52
7	A	602	NAG	C3-C2	-2.44	1.47	1.52
7	A	618	NAG	C3-C2	-2.34	1.47	1.52
7	A	619	NAG	C3-C2	-2.33	1.47	1.52
7	A	614	NAG	C3-C2	-2.31	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	609	NAG	C3-C2	-2.29	1.47	1.52
7	A	620	NAG	C1-C2	-2.12	1.49	1.52
7	A	603	NAG	C3-C2	-2.04	1.48	1.52
7	A	601	NAG	C4-C3	2.03	1.57	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	701	NAG	C1-O5-C5	2.83	116.03	112.19
7	A	609	NAG	C1-O5-C5	-2.82	108.37	112.19
7	A	620	NAG	C2-N2-C7	-2.52	119.31	122.90
7	A	618	NAG	C4-C3-C2	-2.39	107.52	111.02
7	A	618	NAG	C1-O5-C5	-2.32	109.05	112.19
7	A	601	NAG	C4-C3-C2	-2.26	107.70	111.02
7	A	602	NAG	C1-O5-C5	-2.19	109.22	112.19
7	A	616	NAG	C4-C3-C2	-2.08	107.97	111.02
7	A	620	NAG	C4-C3-C2	-2.04	108.03	111.02
7	A	616	NAG	C1-O5-C5	-2.03	109.44	112.19
7	A	623	NAG	C4-C3-C2	-2.00	108.08	111.02

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	702	NAG	C8-C7-N2-C2
7	B	702	NAG	O7-C7-N2-C2
7	A	614	NAG	C4-C5-C6-O6
7	A	603	NAG	O5-C5-C6-O6
7	B	703	NAG	O5-C5-C6-O6
7	A	615	NAG	O5-C5-C6-O6
7	A	617	NAG	O5-C5-C6-O6
7	A	616	NAG	O5-C5-C6-O6
7	A	601	NAG	O5-C5-C6-O6
7	A	601	NAG	C4-C5-C6-O6
7	A	614	NAG	O5-C5-C6-O6
7	B	702	NAG	C1-C2-N2-C7
7	A	603	NAG	C4-C5-C6-O6
7	B	704	NAG	C8-C7-N2-C2
7	B	703	NAG	C4-C5-C6-O6
7	B	704	NAG	O7-C7-N2-C2
7	A	623	NAG	O5-C5-C6-O6
7	A	609	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	A	619	NAG	O5-C5-C6-O6
7	B	704	NAG	O5-C5-C6-O6
7	A	615	NAG	C4-C5-C6-O6
7	B	701	NAG	C4-C5-C6-O6
7	A	606	NAG	O5-C5-C6-O6
7	A	618	NAG	O5-C5-C6-O6
7	A	602	NAG	O5-C5-C6-O6
7	A	620	NAG	O5-C5-C6-O6
7	B	701	NAG	O5-C5-C6-O6
7	A	616	NAG	C4-C5-C6-O6
7	B	702	NAG	C4-C5-C6-O6
7	B	702	NAG	O5-C5-C6-O6
7	A	617	NAG	C4-C5-C6-O6
7	A	601	NAG	C1-C2-N2-C7
7	B	702	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	702	NAG	2	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.

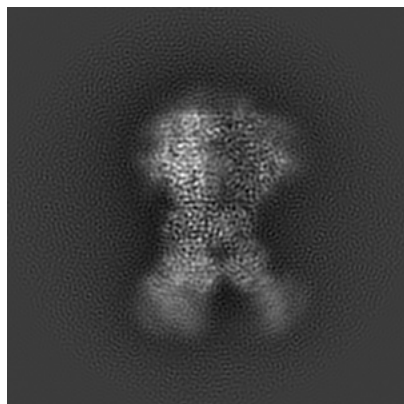
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22111. These allow visual inspection of the internal detail of the map and identification of artifacts.

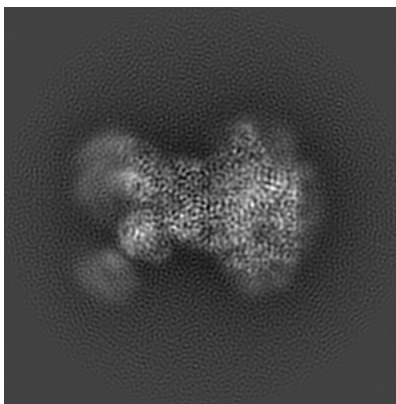
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

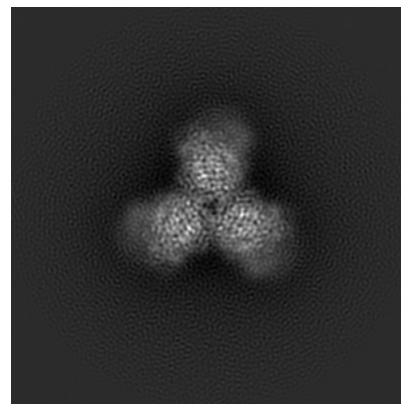
6.1.1 Primary map



X

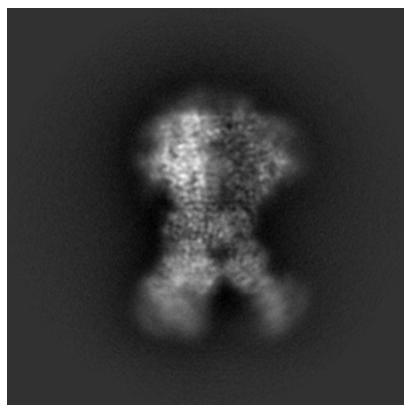


Y

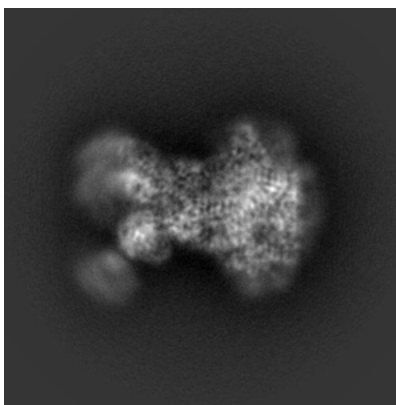


Z

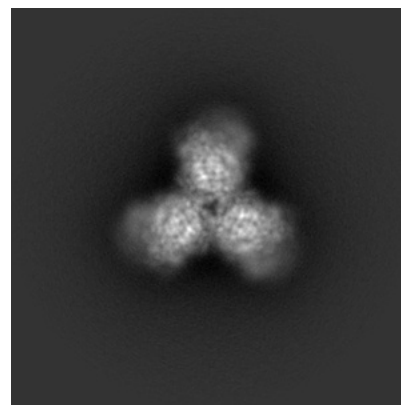
6.1.2 Raw map



X



Y

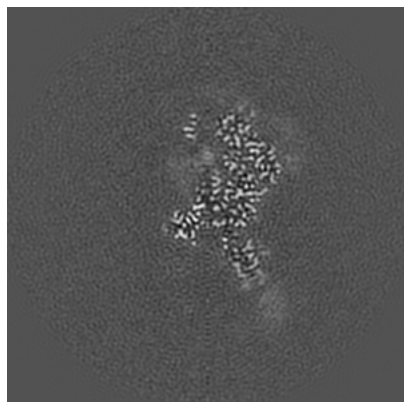


Z

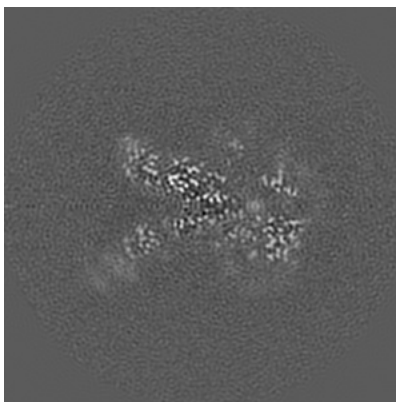
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

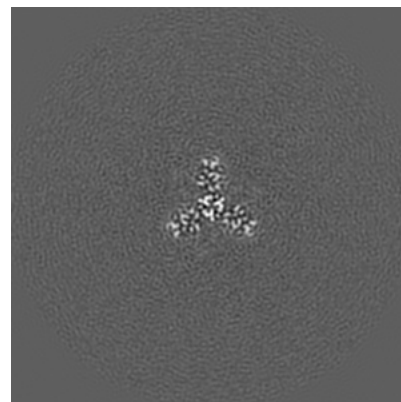
6.2.1 Primary map



X Index: 140

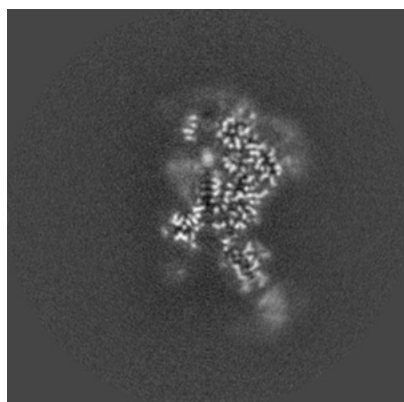


Y Index: 140

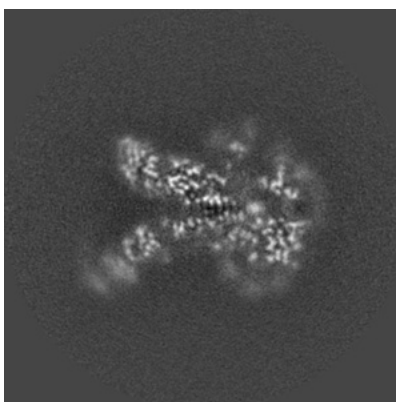


Z Index: 140

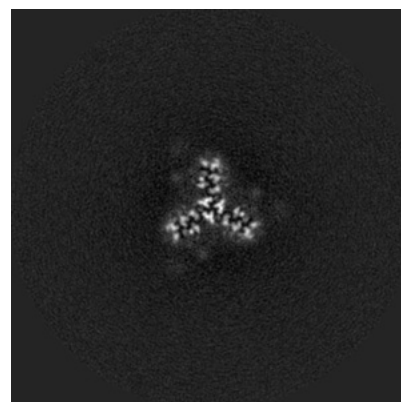
6.2.2 Raw map



X Index: 140



Y Index: 140

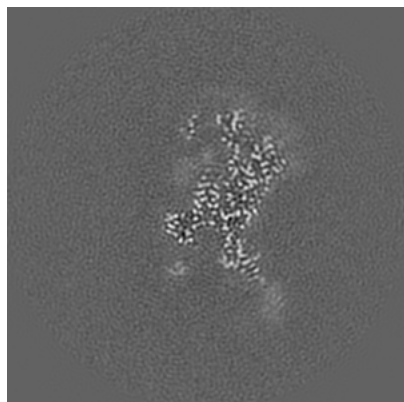


Z Index: 140

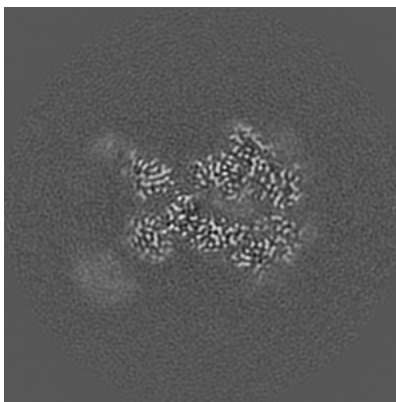
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

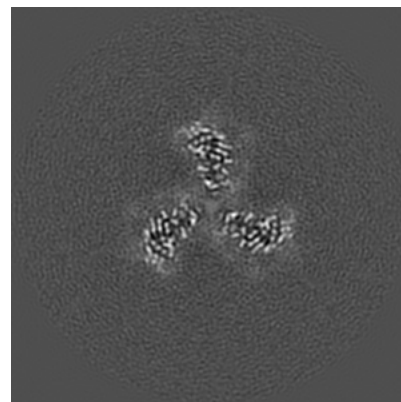
6.3.1 Primary map



X Index: 137

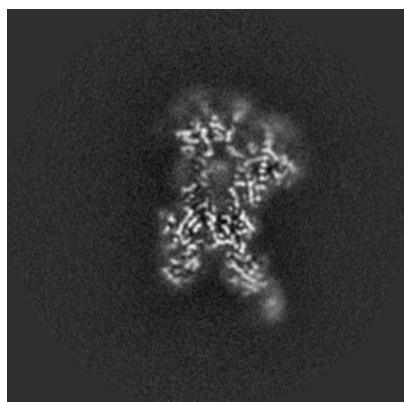


Y Index: 125

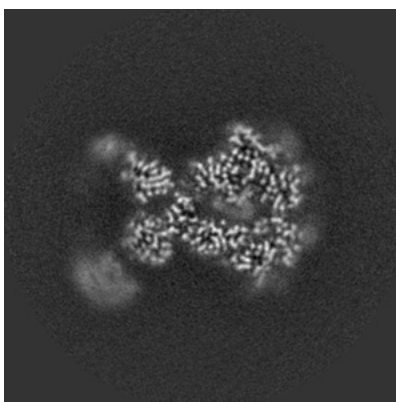


Z Index: 171

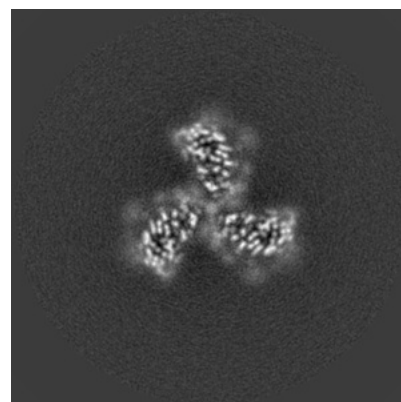
6.3.2 Raw map



X Index: 131



Y Index: 125

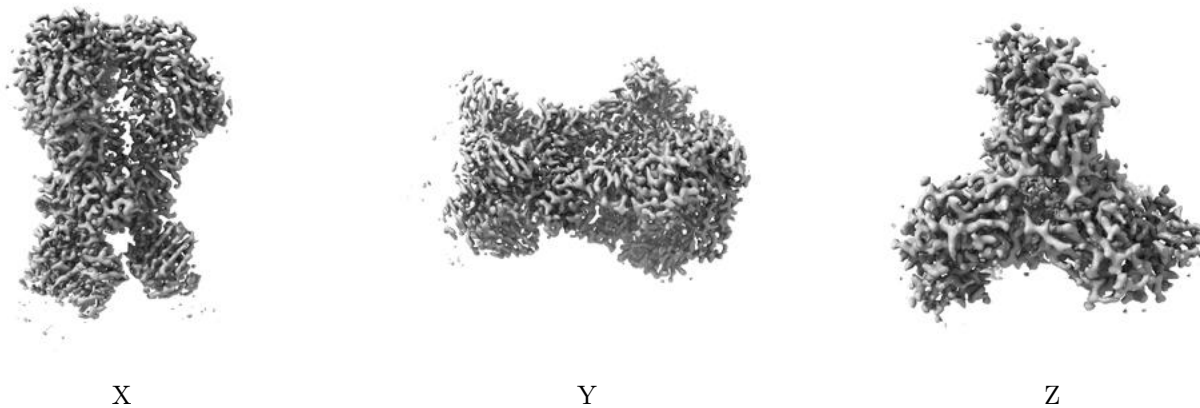


Z Index: 171

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

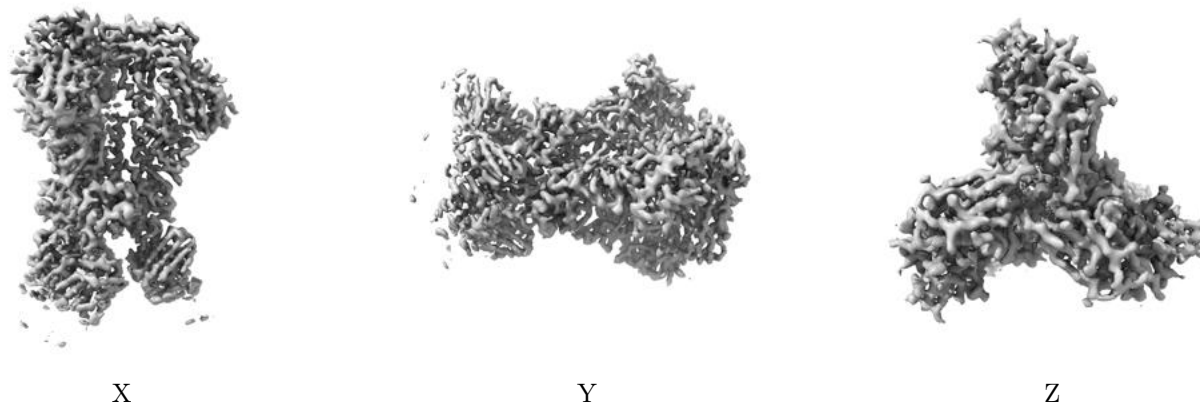
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

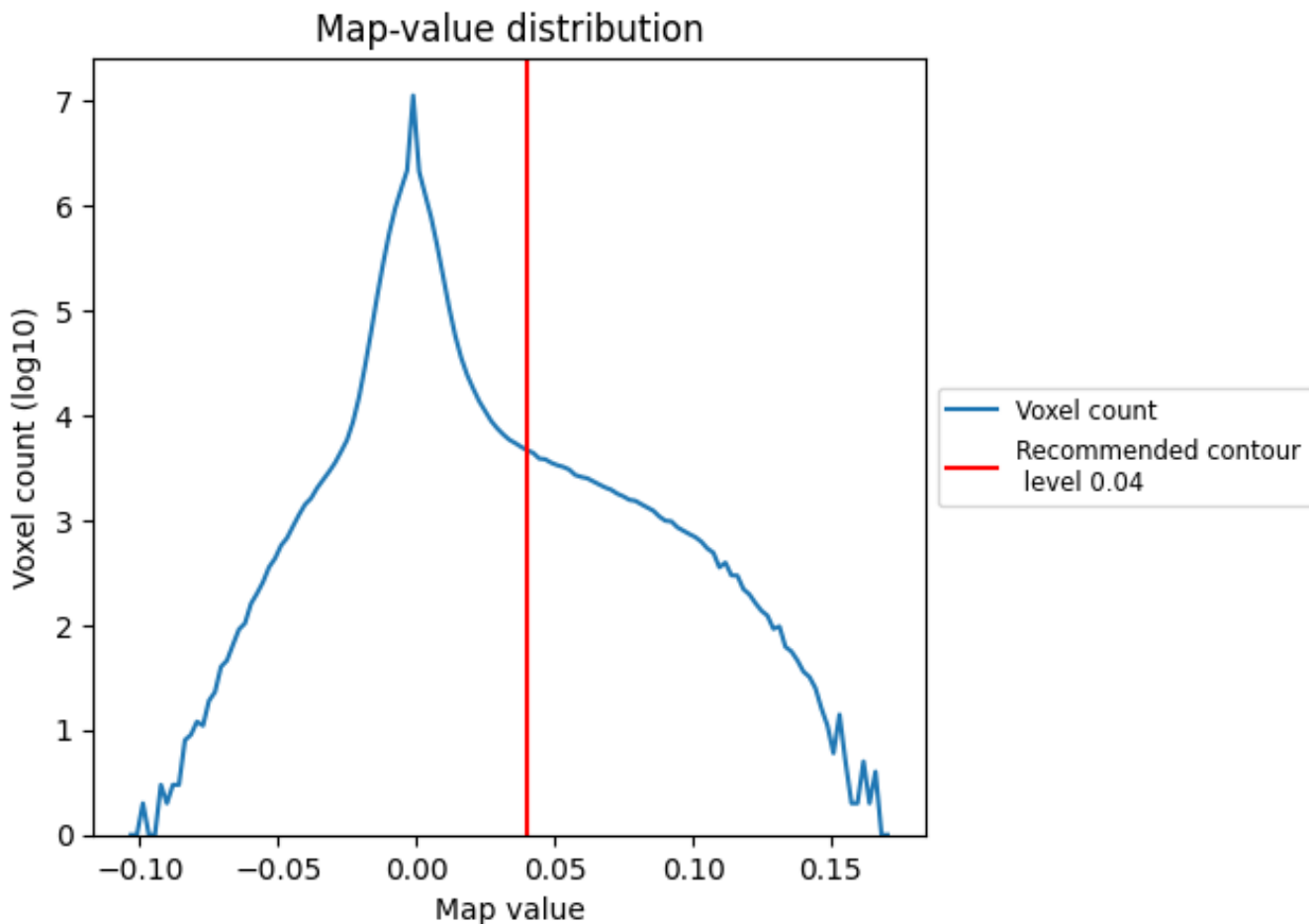
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

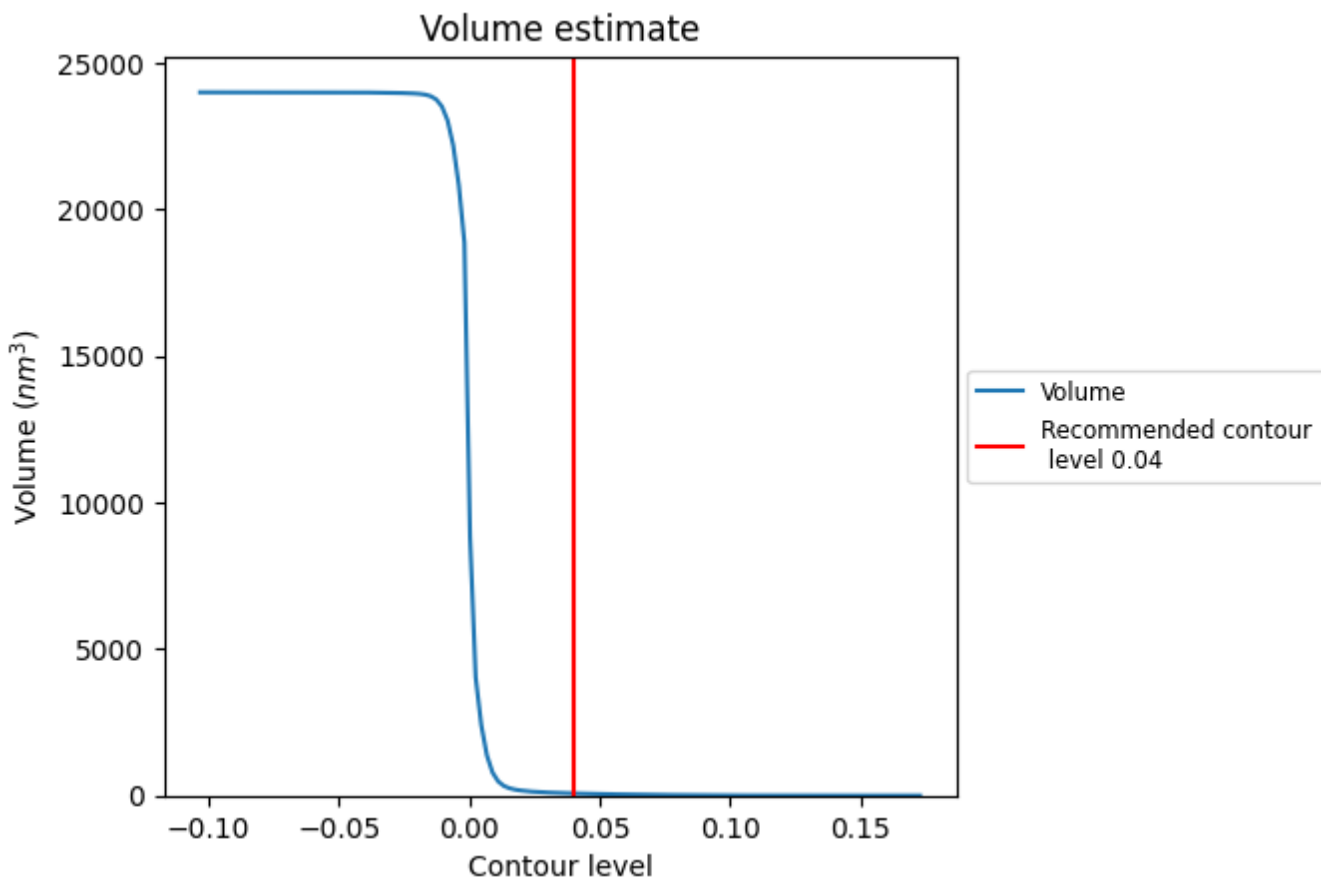
This section contains the results of statistical analysis of the map.

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.

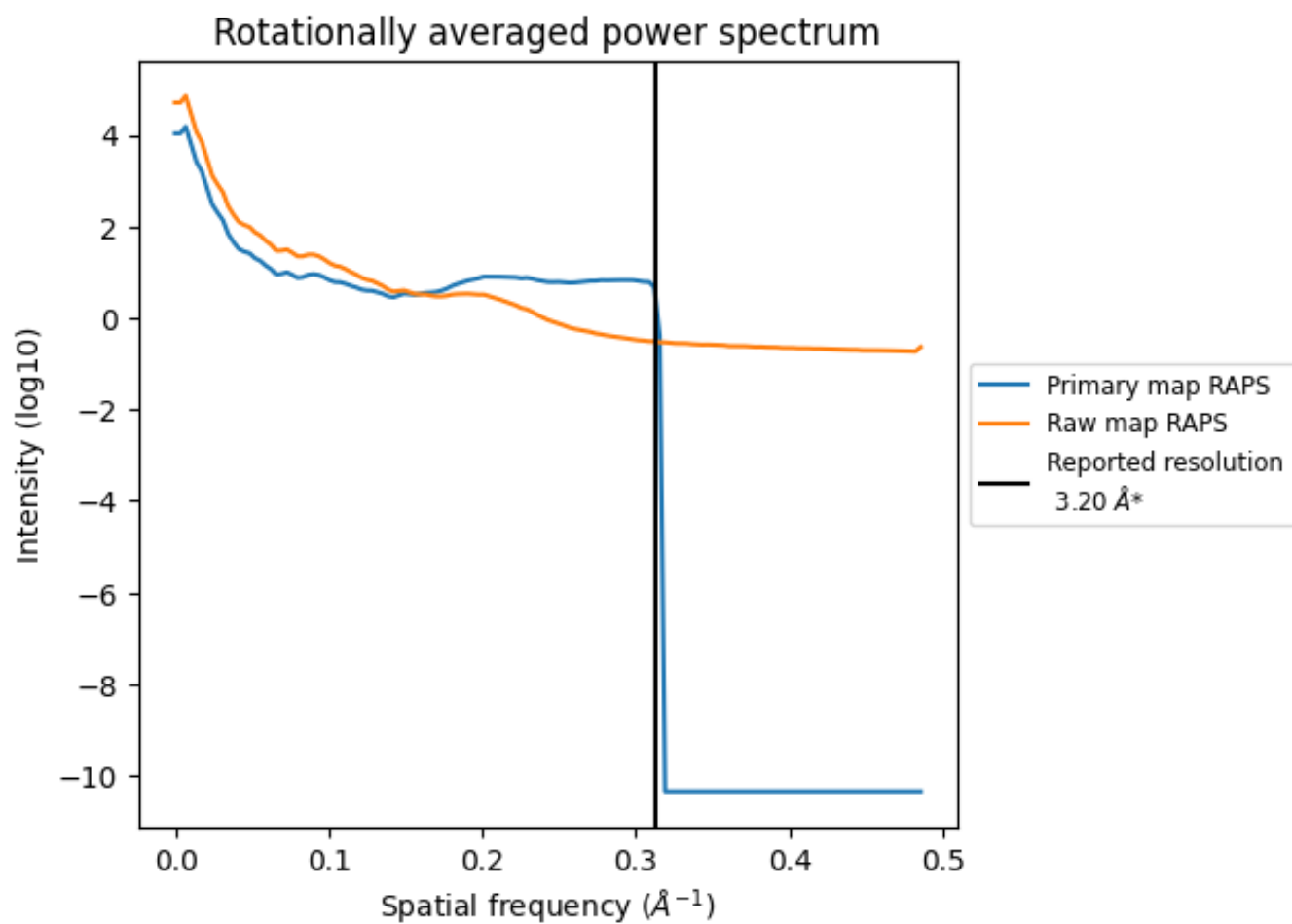
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74 nm³; this corresponds to an approximate mass of 67 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

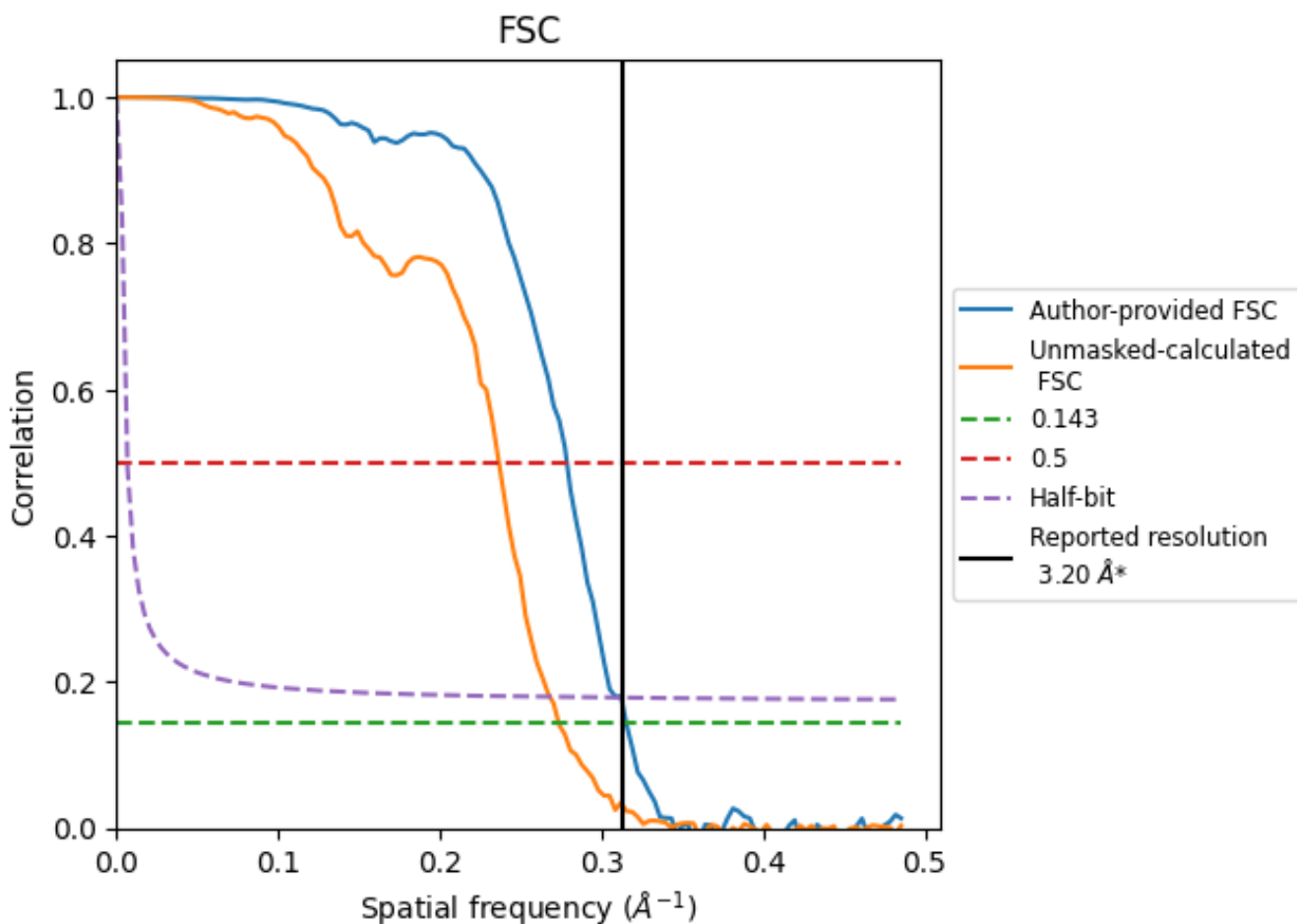


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.17	3.59	3.20
Unmasked-calculated*	3.65	4.23	3.73

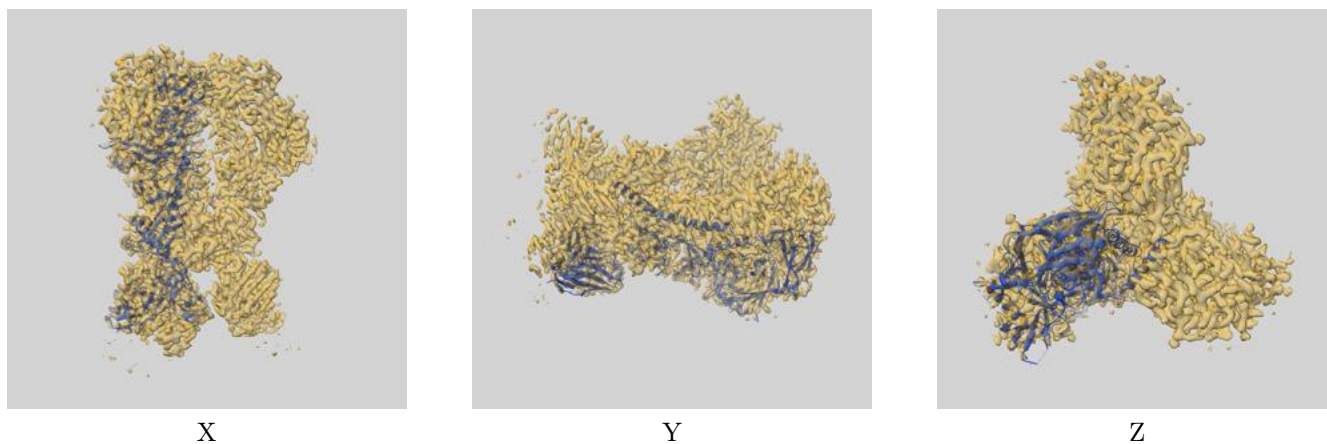
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.65 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

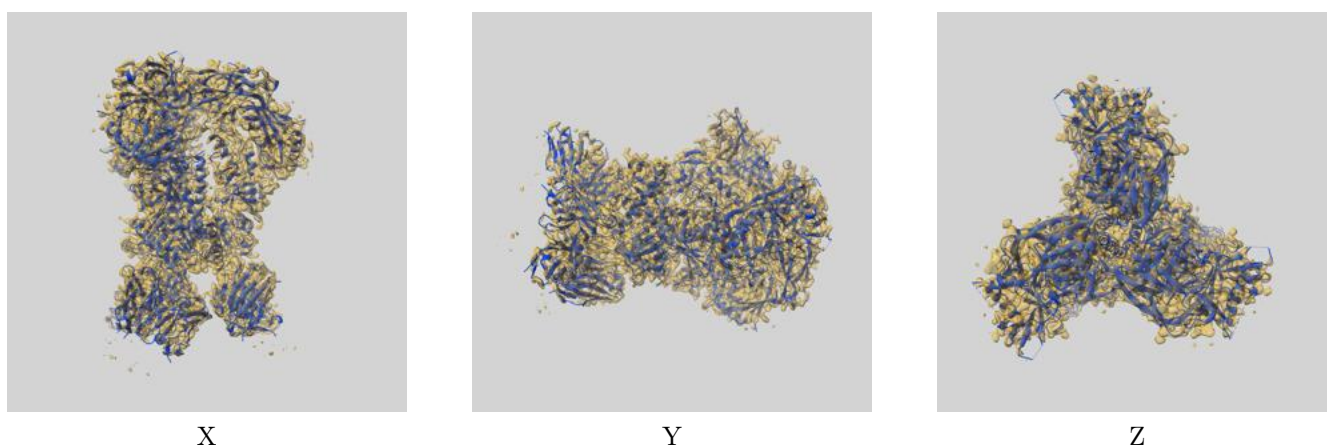
This section contains information regarding the fit between EMDB map EMD-22111 and PDB model 6X9U. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

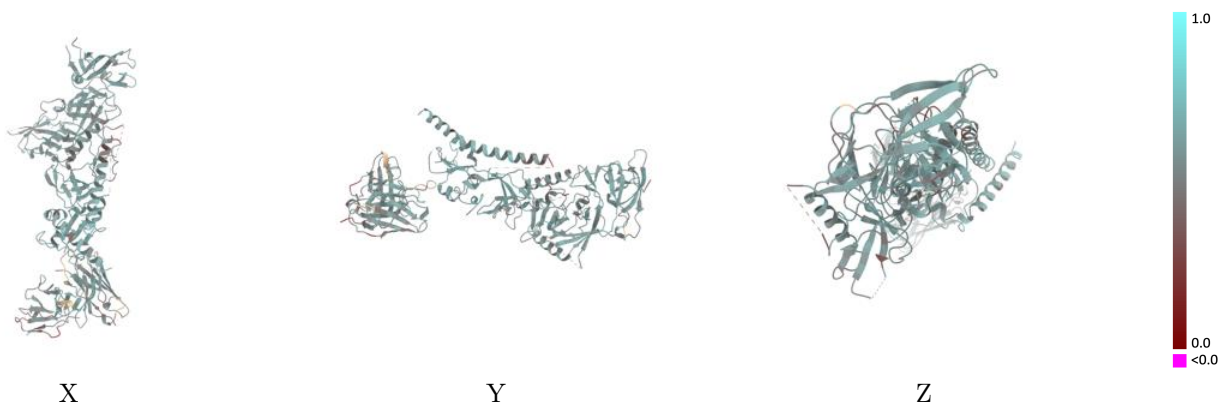


9.1.2 Map-model assembly overlay [i](#)



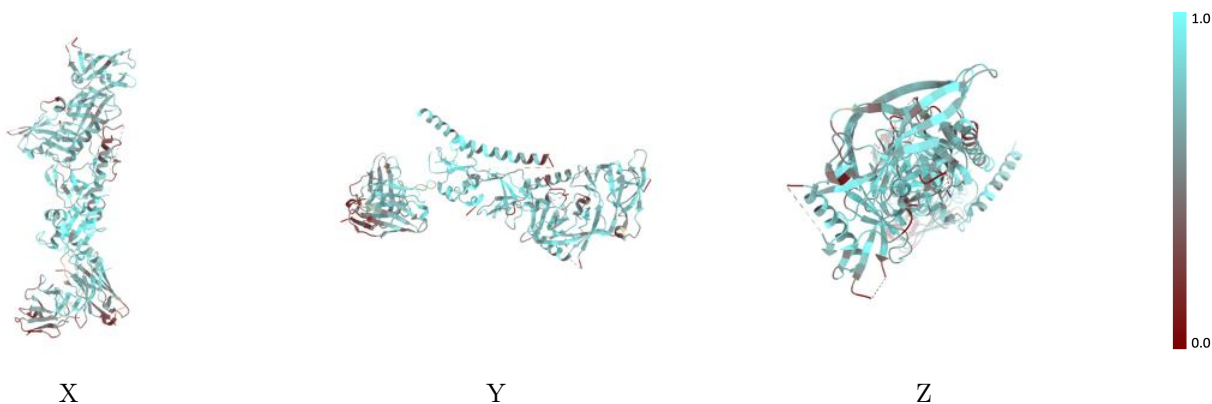
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



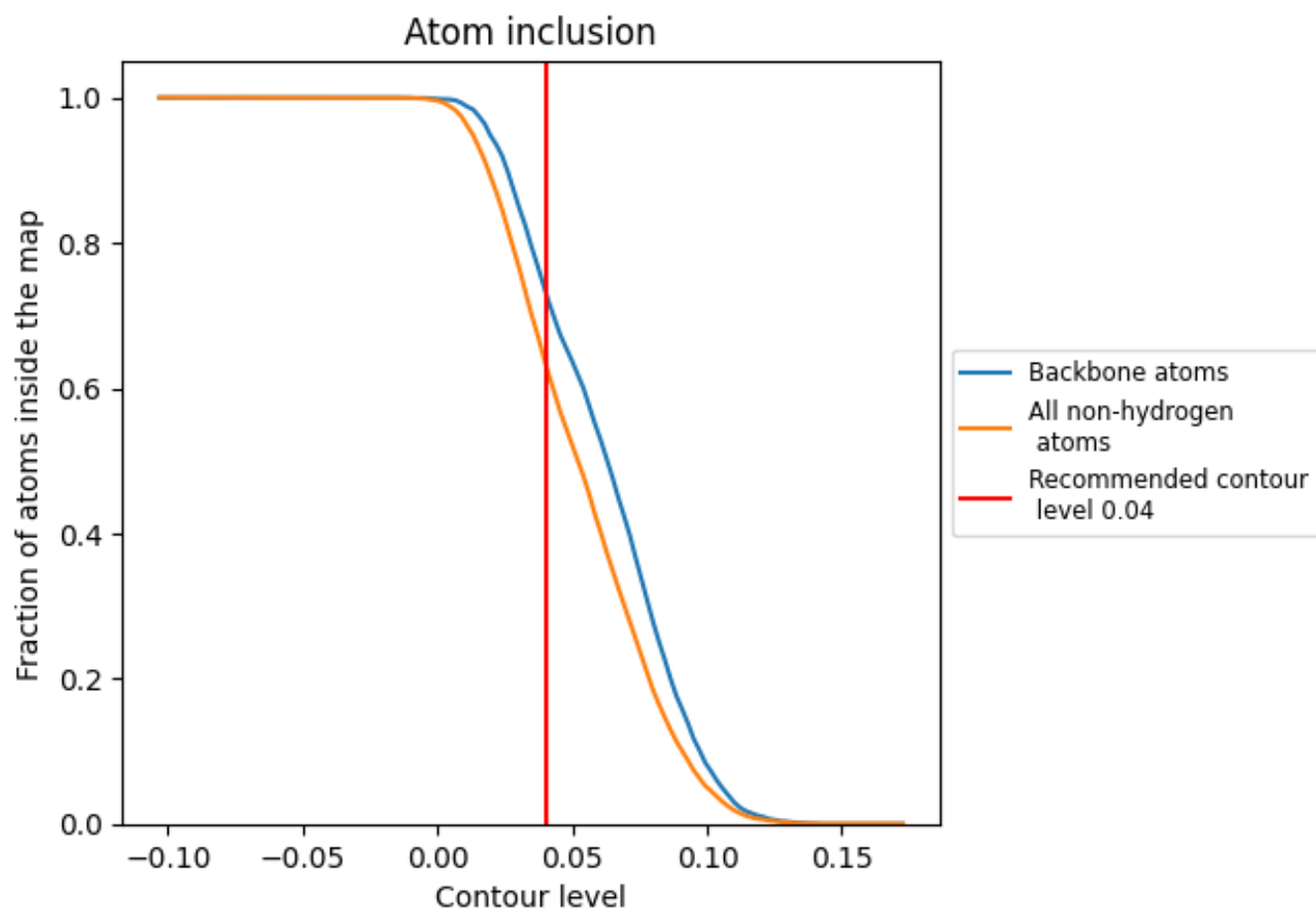
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 63% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6349	 0.5380
A	 0.6601	 0.5460
B	 0.7041	 0.5630
C	 0.2500	 0.4510
D	 0.2500	 0.4740
E	 0.4000	 0.4820
F	 0.3929	 0.4640
G	 0.2500	 0.3680
H	 0.6139	 0.5250
L	 0.5239	 0.5030

