



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:54 PM UTC

PDB ID : 4C2I / pdb_00004c2i
EMDB ID : EMD-2442
Title : Cryo-EM structure of Dengue virus serotype 1 complexed with Fab fragments of human antibody 1F4
Authors : Fibriansah, G.; Tan, J.L.; de Alwis, R.; Smith, S.A.; Ng, T.-S.; Kostyuchenko, V.A.; Ibarra, K.D.; Harris, E.; de Silva, A.; Crowe Junior, J.E.; Lok, S.-M.
Deposited on : 2013-08-18
Resolution : 6.00 Å (reported)
Based on initial model : 4AZX

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

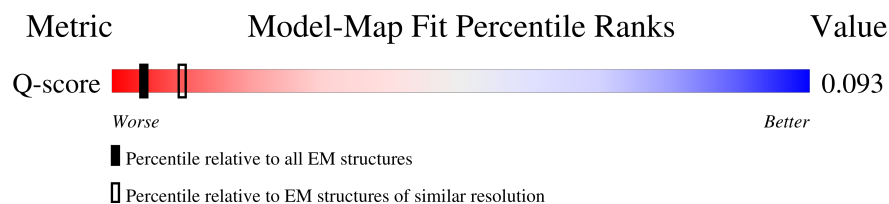
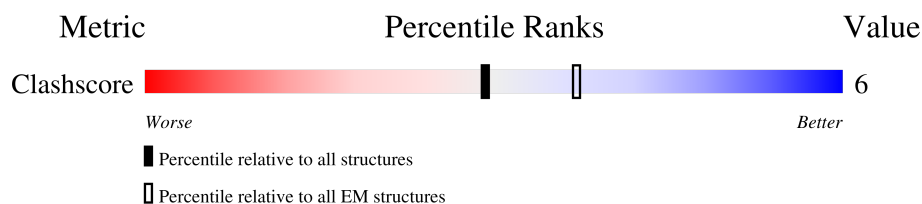
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

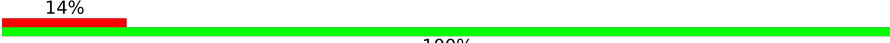
The reported resolution of this entry is 6.00 Å.

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	-
Q-score	-	25397	525 (5.50 - 6.50)

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	495	 14% 100%
1	C	495	 14% 100%
1	E	495	 14% 100%
2	B	75	 23% 96% .
2	D	75	 15% 96% .
2	F	75	 12% 96% .

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Mol	Chain	Length	Quality of chain
3	H	232	41% 97% ..
3	M	232	38% 98% .
4	L	239	30% 88% 12%
4	N	239	32% 88% 12%
5	G	3	100% 33% 67%
5	K	3	67% 33% 67%
6	I	2	50% 100%
6	J	2	100%
6	O	2	100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 2761 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 ENVELOPE PROTEIN.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	A	495	Total C 495 495	0	495
1	C	495	Total C 495 495	0	495
1	E	495	Total C 495 495	0	495

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	SER	GLY	conflict	UNP Q7TGE4
A	8	ASN	SER	conflict	UNP Q7TGE4
A	17	ALA	GLY	conflict	UNP Q7TGE4
A	18	THR	ALA	conflict	UNP Q7TGE4
A	19	GLY	THR	conflict	UNP Q7TGE4
C	7	SER	GLY	conflict	UNP Q7TGE4
C	8	ASN	SER	conflict	UNP Q7TGE4
C	17	ALA	GLY	conflict	UNP Q7TGE4
C	18	THR	ALA	conflict	UNP Q7TGE4
C	19	GLY	THR	conflict	UNP Q7TGE4
E	7	SER	GLY	conflict	UNP Q7TGE4
E	8	ASN	SER	conflict	UNP Q7TGE4
E	17	ALA	GLY	conflict	UNP Q7TGE4
E	18	THR	ALA	conflict	UNP Q7TGE4
E	19	GLY	THR	conflict	UNP Q7TGE4

- Molecule 2 is a protein called POLYPROTEIN.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	B	72	Total C 72 72	0	72
2	D	72	Total C 72 72	0	72

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Mol	Chain	Residues	Atoms		AltConf	Trace
2	F	72	Total	C	0	72
			72	72		

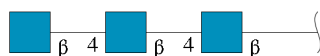
- Molecule 3 is a protein called HEAVY CHAIN FAB FRAGMENT OF ANTIBODY 1F4.

Mol	Chain	Residues	Atoms		AltConf	Trace
3	H	228	Total	C	0	228
			228	228		
3	M	228	Total	C	0	228
			228	228		

- Molecule 4 is a protein called LIGHT CHAIN FAB FRAGMENT OF ANTIBODY 1F4.

Mol	Chain	Residues	Atoms		AltConf	Trace
4	L	211	Total	C	0	211
			211	211		
4	N	211	Total	C	0	211
			211	211		

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



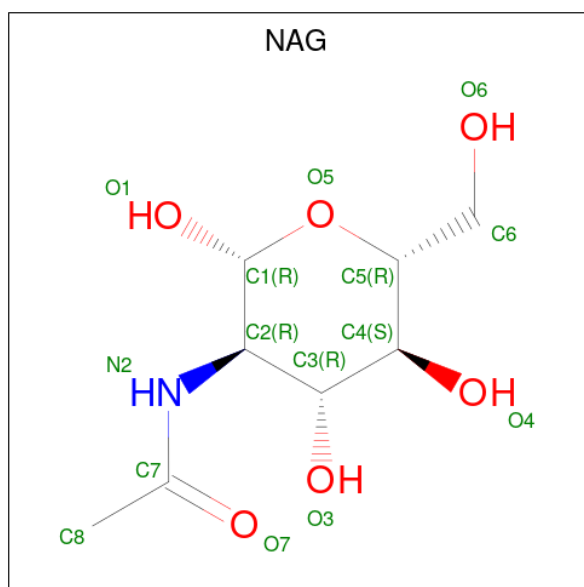
Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	3	Total	C	N	O	0	0
			42	24	3	15		
5	K	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 6 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
6	I	2	Total	C	N	O	0	0
			28	16	2	10		
6	J	2	Total	C	N	O	0	0
			28	16	2	10		
6	O	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

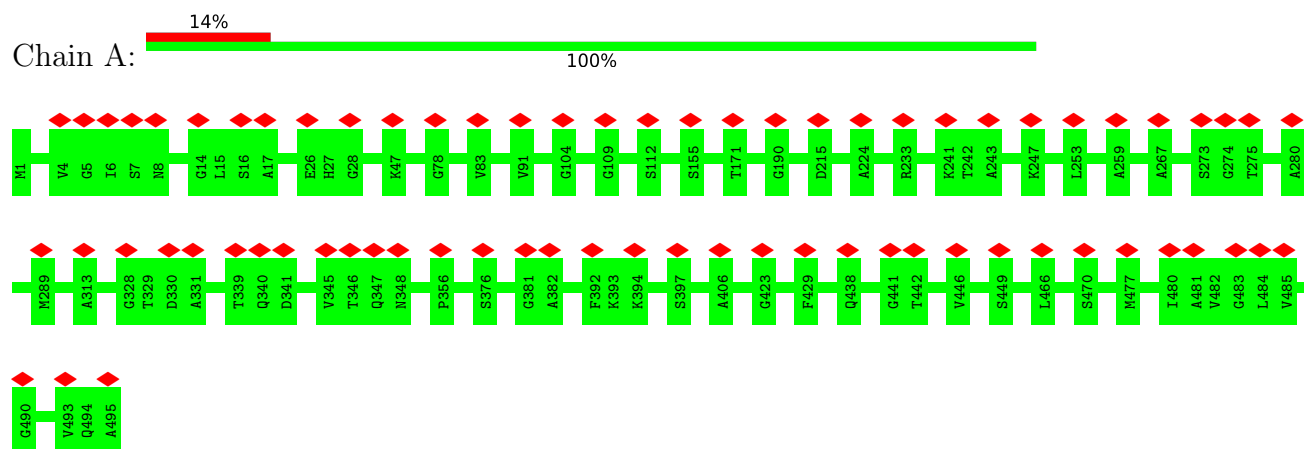


Mol	Chain	Residues	Atoms				AltConf
7	C	1	Total	C	N	O	0
			14	8	1	5	

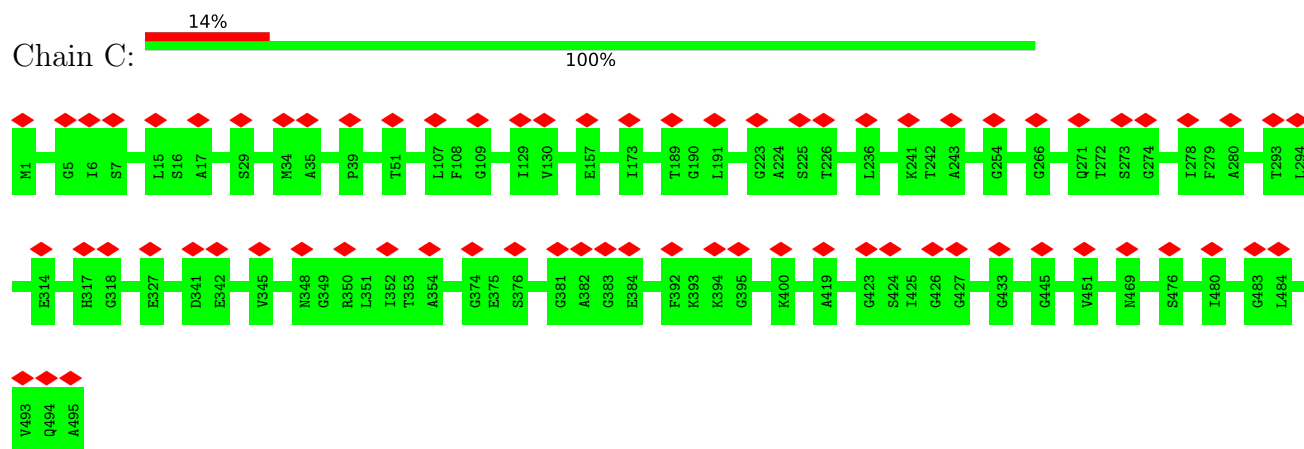
3 Residue-property plots

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.

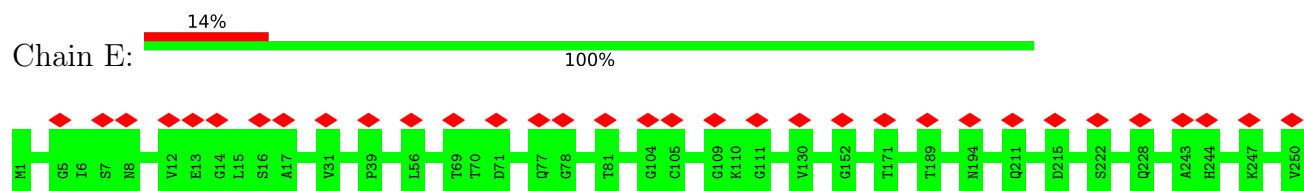
• Molecule 1: ENVELOPE PROTEIN

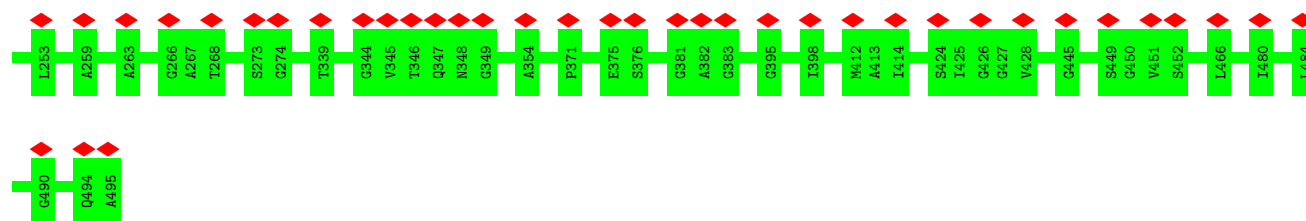


• Molecule 1: ENVELOPE PROTEIN

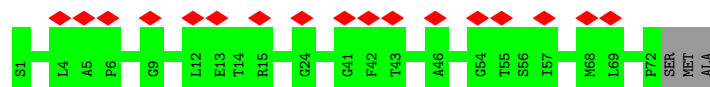


• Molecule 1: ENVELOPE PROTEIN

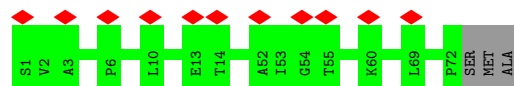




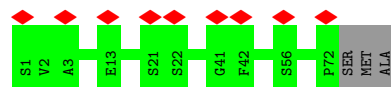
• Molecule 2: POLYPROTEIN



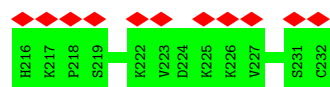
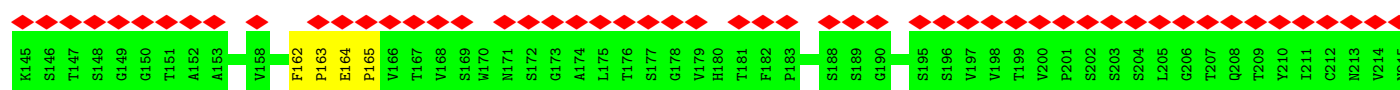
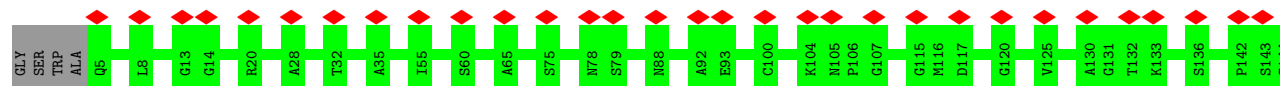
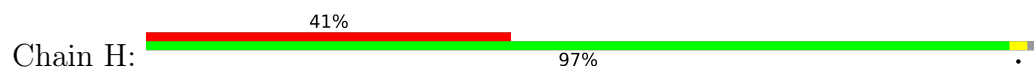
• Molecule 2: POLYPROTEIN



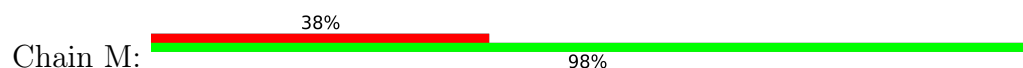
• Molecule 2: POLYPROTEIN

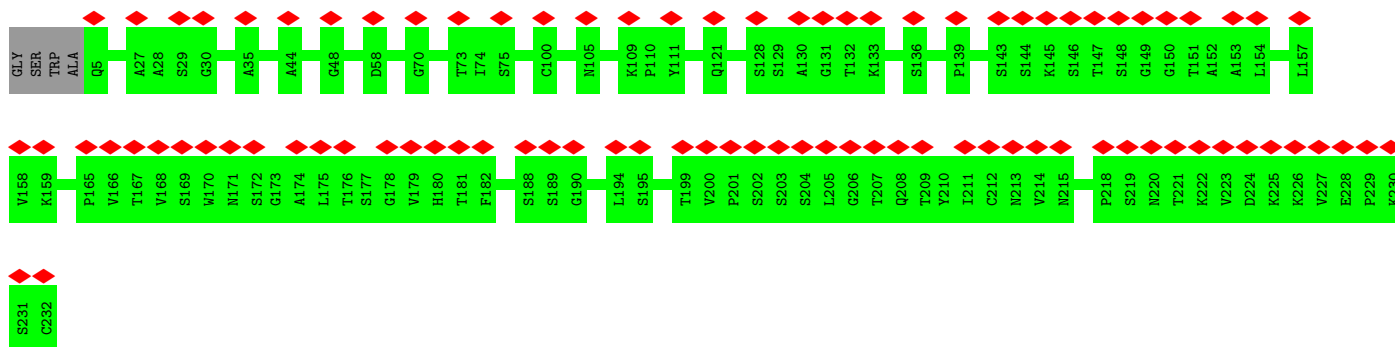


• Molecule 3: HEAVY CHAIN FAB FRAGMENT OF ANTIBODY 1F4

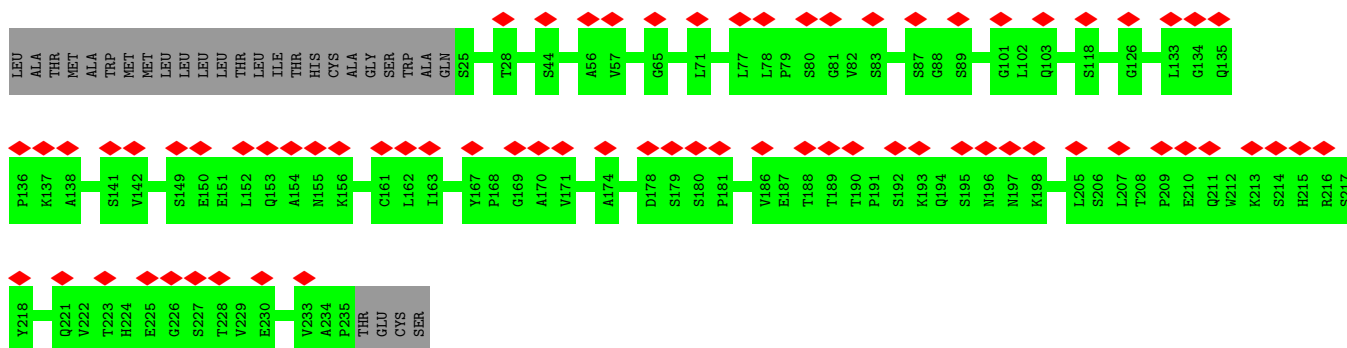
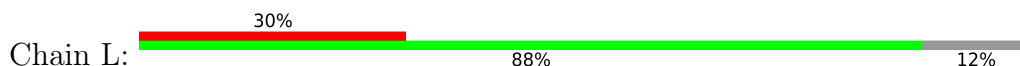


• Molecule 3: HEAVY CHAIN FAB FRAGMENT OF ANTIBODY 1F4

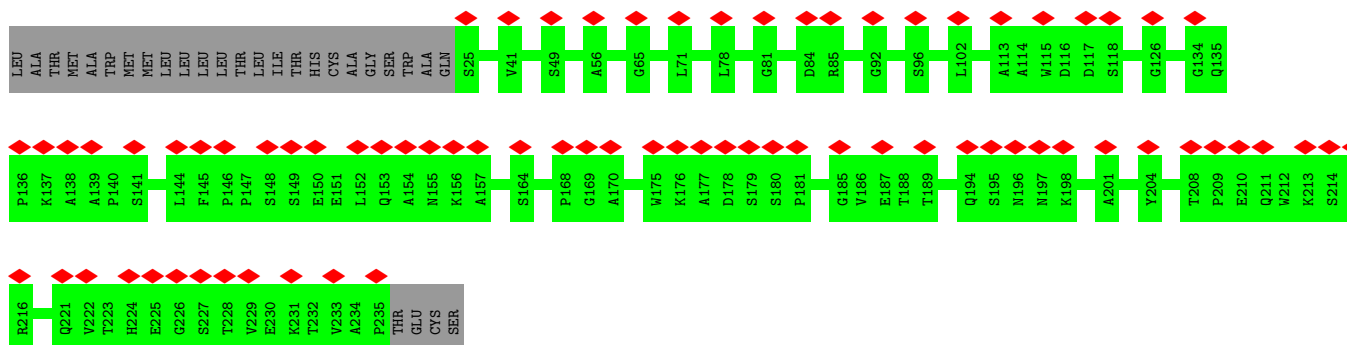
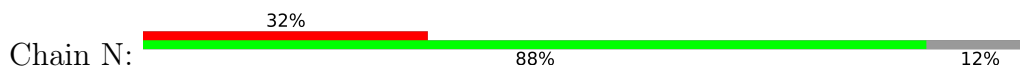




• Molecule 4: LIGHT CHAIN FAB FRAGMENT OF ANTIBODY 1F4



• Molecule 4: LIGHT CHAIN FAB FRAGMENT OF ANTIBODY 1F4



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



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



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



- Molecule 6: 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, I	Depositor
Number of particles used	10270	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	17.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	47000	Depositor
Image detector	FEI FALCON I (4k x 4k)	Depositor
Maximum map value	12.092	Depositor
Minimum map value	-0.769	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2	Depositor
Map size ($\text{\AA}$)	640.0, 640.0, 640.0	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0, 1.0, 1.0	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	495	0	0	0	0
1	C	495	0	0	0	0
1	E	495	0	0	0	0
2	B	72	0	0	0	0
2	D	72	0	0	0	0
2	F	72	0	0	0	0
3	H	228	0	0	2	0
3	M	228	0	0	0	0
4	L	211	0	0	0	0
4	N	211	0	0	0	0
5	G	42	0	37	4	0
5	K	42	0	37	5	0
6	I	28	0	25	4	0
6	J	28	0	24	2	0
6	O	28	0	25	0	0
7	C	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2761	0	161	17	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 6.

All (17) 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)
5:G:1:NAG:H62	5:G:2:NAG:O7	1.41	1.18
5:G:1:NAG:C6	5:G:2:NAG:O7	1.98	1.11
5:G:1:NAG:H61	5:G:2:NAG:O7	1.82	0.78
5:K:1:NAG:O6	5:K:2:NAG:C7	2.33	0.77
5:K:1:NAG:H5	5:K:2:NAG:O7	1.87	0.74
6:I:1:NAG:H62	6:I:2:NAG:O7	1.90	0.72
6:I:1:NAG:H62	6:I:2:NAG:C7	2.20	0.71
5:G:1:NAG:H61	5:G:2:NAG:C7	2.24	0.68
5:K:1:NAG:O6	5:K:2:NAG:C8	2.41	0.68
6:I:1:NAG:C6	6:I:2:NAG:O7	2.45	0.65
5:K:1:NAG:C5	5:K:2:NAG:O7	2.51	0.57
6:I:1:NAG:O6	6:I:2:NAG:O7	2.25	0.48
5:K:1:NAG:O4	5:K:2:NAG:O7	2.33	0.47
6:J:1:NAG:H62	6:J:2:NAG:C7	2.49	0.43
3:H:162:PHE:CA	3:H:163:PRO:CA	2.99	0.40
6:J:1:NAG:H62	6:J:2:NAG:N2	2.35	0.40
3:H:164:GLU:CA	3:H:165:PRO:CA	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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 ⓘ

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	G	1	5	14,14,15	1.83	5 (35%)	17,19,21	1.78	4 (23%)
5	NAG	G	2	5	14,14,15	1.62	3 (21%)	17,19,21	1.53	3 (17%)
5	NAG	G	3	5	14,14,15	1.74	4 (28%)	17,19,21	1.92	4 (23%)
6	NAG	I	1	6	14,14,15	1.36	2 (14%)	17,19,21	2.51	7 (41%)
6	NAG	I	2	6	14,14,15	1.59	3 (21%)	17,19,21	2.24	4 (23%)
6	NAG	J	1	6	14,14,15	1.42	3 (21%)	17,19,21	2.21	7 (41%)
6	NAG	J	2	6	14,14,15	2.01	3 (21%)	17,19,21	2.66	7 (41%)
5	NAG	K	1	5	14,14,15	1.23	2 (14%)	17,19,21	2.34	8 (47%)
5	NAG	K	2	5	14,14,15	1.09	1 (7%)	17,19,21	1.41	1 (5%)
5	NAG	K	3	5	14,14,15	1.70	5 (35%)	17,19,21	1.15	1 (5%)
6	NAG	O	1	6	14,14,15	1.21	2 (14%)	17,19,21	2.25	6 (35%)
6	NAG	O	2	6	14,14,15	2.09	2 (14%)	17,19,21	1.40	3 (17%)

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	G	1	5	-	4/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	NAG	G	3	5	-	2/6/23/26	0/1/1/1
6	NAG	I	1	6	-	2/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1
6	NAG	J	1	6	-	1/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
5	NAG	K	1	5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	1/6/23/26	0/1/1/1
5	NAG	K	3	5	-	0/6/23/26	0/1/1/1
6	NAG	O	1	6	-	4/6/23/26	0/1/1/1
6	NAG	O	2	6	-	1/6/23/26	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	O	2	NAG	C1-C2	-5.95	1.44	1.52
6	J	2	NAG	O5-C1	5.46	1.52	1.43
6	I	2	NAG	C1-C2	-4.35	1.46	1.52
6	O	2	NAG	C2-N2	-4.24	1.39	1.46
5	K	3	NAG	C4-C5	-3.62	1.45	1.53
5	G	1	NAG	O4-C4	3.26	1.51	1.43
5	G	2	NAG	C1-C2	3.12	1.56	1.52
5	G	3	NAG	C1-C2	-3.10	1.48	1.52
6	J	1	NAG	O4-C4	3.03	1.50	1.43
5	G	1	NAG	C8-C7	2.99	1.56	1.50
5	K	3	NAG	O5-C1	-2.93	1.38	1.43
6	J	2	NAG	C4-C5	-2.81	1.47	1.53
5	G	2	NAG	C4-C3	-2.77	1.45	1.52
6	I	1	NAG	C8-C7	-2.77	1.44	1.50
5	K	1	NAG	C2-N2	2.75	1.50	1.46
5	G	2	NAG	C4-C5	-2.68	1.47	1.53
6	I	1	NAG	C1-C2	2.65	1.55	1.52
5	G	3	NAG	C4-C5	2.62	1.58	1.53
5	G	3	NAG	O5-C5	-2.57	1.38	1.43
6	J	2	NAG	O5-C5	2.53	1.48	1.43
5	G	3	NAG	O5-C1	2.51	1.47	1.43
5	G	1	NAG	C4-C5	-2.49	1.47	1.53
5	G	1	NAG	C1-C2	2.41	1.55	1.52
6	I	2	NAG	O7-C7	-2.38	1.17	1.23
6	J	1	NAG	C2-N2	-2.35	1.42	1.46
6	O	1	NAG	C4-C5	2.32	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	3	NAG	O5-C5	2.30	1.47	1.43
6	J	1	NAG	C4-C5	2.25	1.57	1.53
5	K	1	NAG	C7-N2	-2.22	1.27	1.34
5	K	2	NAG	O5-C1	-2.22	1.40	1.43
5	K	3	NAG	C7-N2	-2.14	1.27	1.34
5	G	1	NAG	C2-N2	2.12	1.49	1.46
6	I	2	NAG	C4-C3	2.10	1.57	1.52
6	O	1	NAG	O4-C4	2.08	1.48	1.43
5	K	3	NAG	C4-C3	2.06	1.57	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	2	NAG	O5-C1-C2	-7.80	99.22	111.29
6	I	2	NAG	O5-C1-C2	-6.83	100.72	111.29
5	K	1	NAG	C1-C2-N2	6.10	120.04	110.43
6	I	1	NAG	O5-C1-C2	-5.48	102.81	111.29
6	J	2	NAG	C2-N2-C7	5.27	129.96	122.90
6	J	1	NAG	C2-N2-C7	5.27	129.96	122.90
6	I	1	NAG	C4-C3-C2	4.82	118.09	111.02
5	G	3	NAG	C2-N2-C7	4.25	128.60	122.90
6	O	1	NAG	C4-C3-C2	4.15	117.10	111.02
5	G	3	NAG	C1-C2-N2	3.99	116.73	110.43
5	G	3	NAG	O4-C4-C5	3.86	118.84	109.32
6	O	1	NAG	C3-C4-C5	-3.86	103.23	110.23
6	O	1	NAG	C1-C2-N2	3.72	116.29	110.43
6	I	1	NAG	O5-C5-C4	-3.54	102.22	110.83
5	K	2	NAG	O4-C4-C5	3.46	117.84	109.32
6	I	1	NAG	O4-C4-C5	-3.41	100.92	109.32
6	O	1	NAG	O3-C3-C4	3.38	118.35	110.38
6	J	1	NAG	O5-C1-C2	-3.35	106.11	111.29
5	G	2	NAG	O5-C1-C2	-3.27	106.23	111.29
5	G	1	NAG	O5-C5-C4	-3.26	102.90	110.83
6	J	1	NAG	O4-C4-C3	-3.20	102.84	110.38
5	K	1	NAG	O7-C7-C8	-3.19	116.38	122.05
5	G	1	NAG	O7-C7-C8	-3.14	116.46	122.05
5	G	2	NAG	C1-O5-C5	-3.13	107.99	112.19
6	I	2	NAG	O5-C5-C6	3.11	113.72	107.66
6	O	2	NAG	C4-C3-C2	3.10	115.56	111.02
6	O	1	NAG	O4-C4-C3	-3.04	103.20	110.38
6	J	1	NAG	O7-C7-C8	-2.99	116.73	122.05
6	O	1	NAG	O5-C5-C6	-2.95	101.92	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	1	NAG	O5-C5-C4	-2.90	103.78	110.83
5	G	2	NAG	C4-C3-C2	2.88	115.23	111.02
5	K	1	NAG	O5-C1-C2	-2.85	106.87	111.29
6	I	1	NAG	C8-C7-N2	-2.73	111.59	116.12
5	G	1	NAG	O7-C7-N2	2.64	126.66	121.98
6	I	2	NAG	O4-C4-C5	2.54	115.58	109.32
5	G	3	NAG	C3-C4-C5	-2.53	105.64	110.23
5	K	1	NAG	O5-C5-C6	-2.49	102.81	107.66
6	J	1	NAG	C8-C7-N2	2.42	120.14	116.12
5	K	1	NAG	O3-C3-C2	2.42	114.42	109.40
6	O	2	NAG	C6-C5-C4	2.38	118.86	113.02
6	O	2	NAG	O4-C4-C3	2.38	115.98	110.38
5	K	1	NAG	O4-C4-C3	-2.34	104.86	110.38
6	I	2	NAG	O6-C6-C5	2.31	119.21	111.33
6	I	1	NAG	C6-C5-C4	2.31	118.69	113.02
5	K	1	NAG	C3-C4-C5	-2.26	106.14	110.23
6	J	2	NAG	O4-C4-C5	-2.20	103.90	109.32
5	K	1	NAG	C8-C7-N2	2.18	119.74	116.12
6	J	1	NAG	O3-C3-C2	2.12	113.81	109.40
6	J	2	NAG	C3-C4-C5	-2.10	106.42	110.23
5	K	3	NAG	O7-C7-C8	-2.10	118.32	122.05
6	J	2	NAG	C4-C3-C2	-2.09	107.95	111.02
6	J	2	NAG	C1-C2-N2	-2.05	107.21	110.43
6	I	1	NAG	O4-C4-C3	2.02	115.14	110.38
6	J	2	NAG	O3-C3-C2	2.02	113.59	109.40
5	G	1	NAG	C2-N2-C7	-2.01	120.21	122.90

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	J	1	NAG	C1-C2-N2-C7
6	O	1	NAG	C1-C2-N2-C7
6	I	1	NAG	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
5	G	3	NAG	O5-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
5	G	3	NAG	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
6	O	1	NAG	C4-C5-C6-O6
6	O	1	NAG	C3-C2-N2-C7

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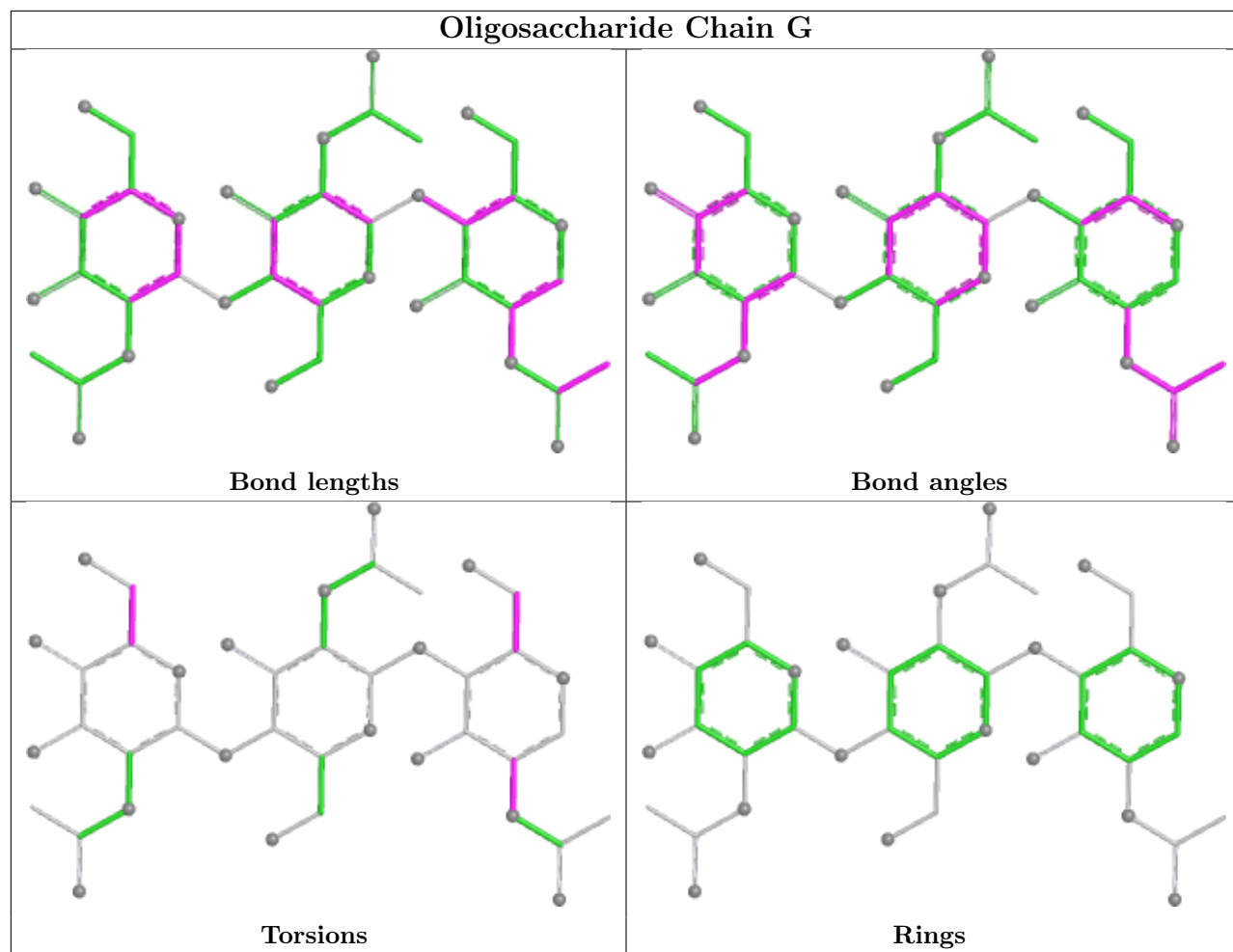
Mol	Chain	Res	Type	Atoms
6	I	2	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
5	G	1	NAG	C1-C2-N2-C7
6	I	2	NAG	O5-C5-C6-O6
6	O	2	NAG	C3-C2-N2-C7
5	K	2	NAG	C1-C2-N2-C7
5	G	1	NAG	C3-C2-N2-C7
5	G	1	NAG	C4-C5-C6-O6

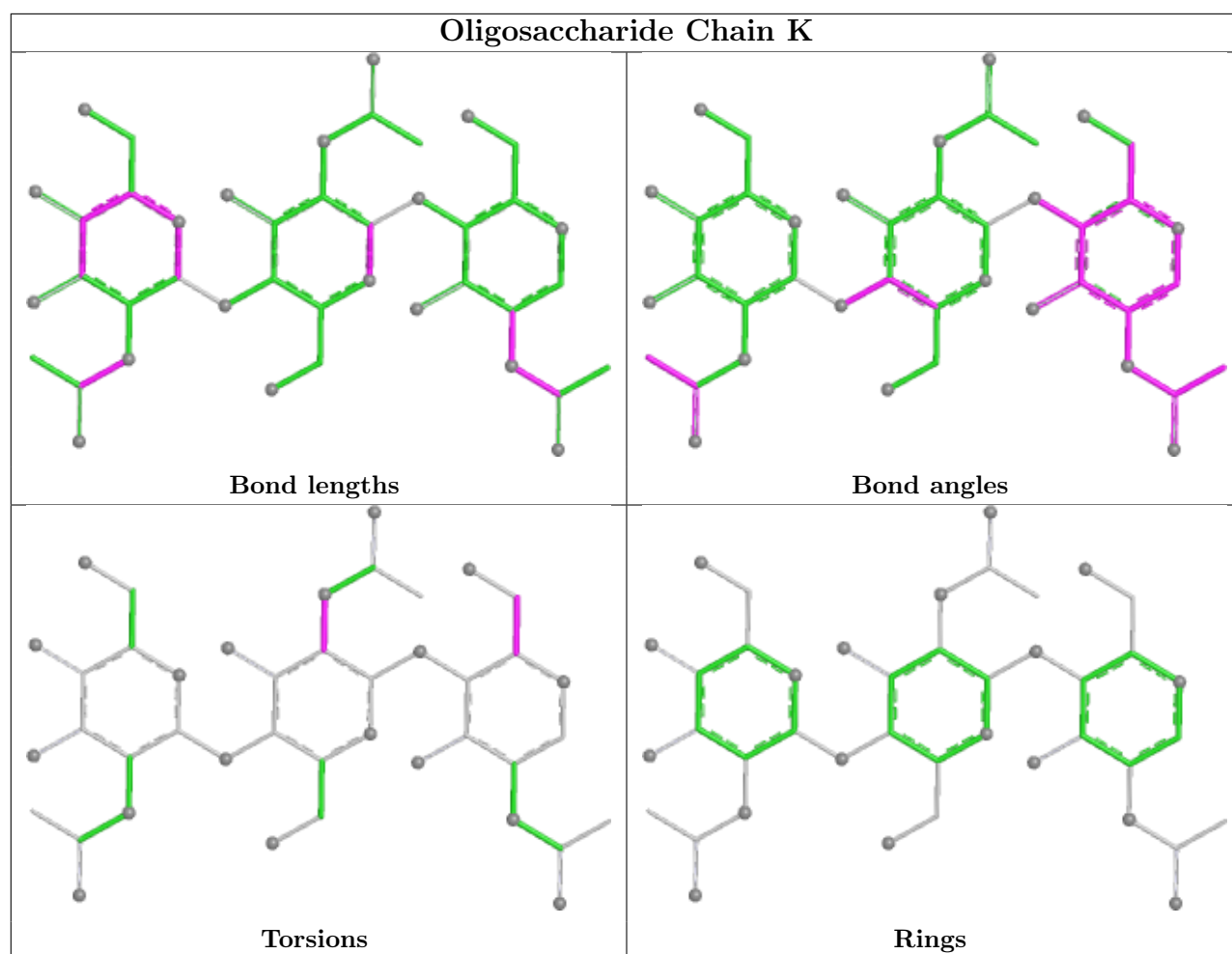
There are no ring outliers.

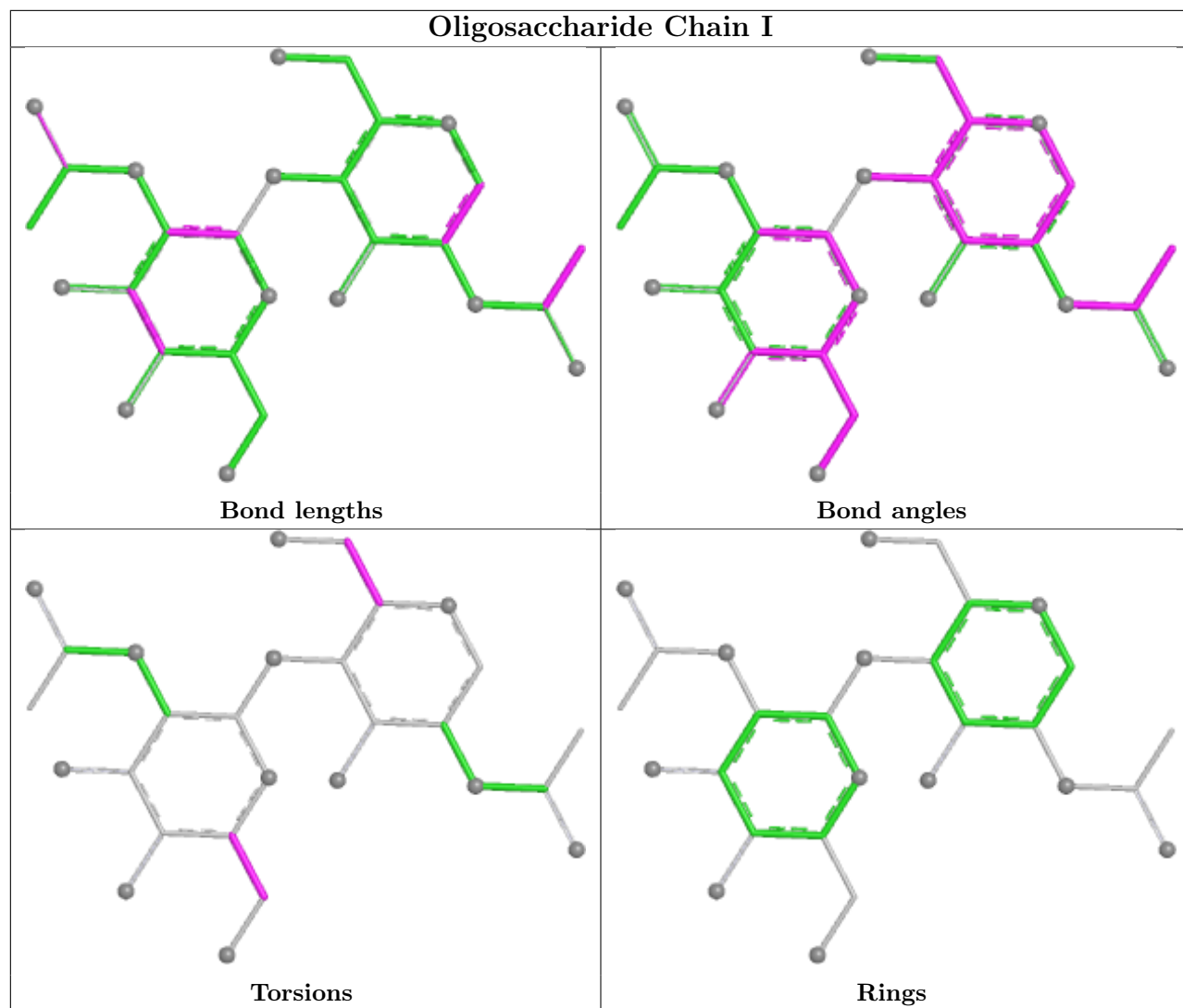
8 monomers are involved in 15 short contacts:

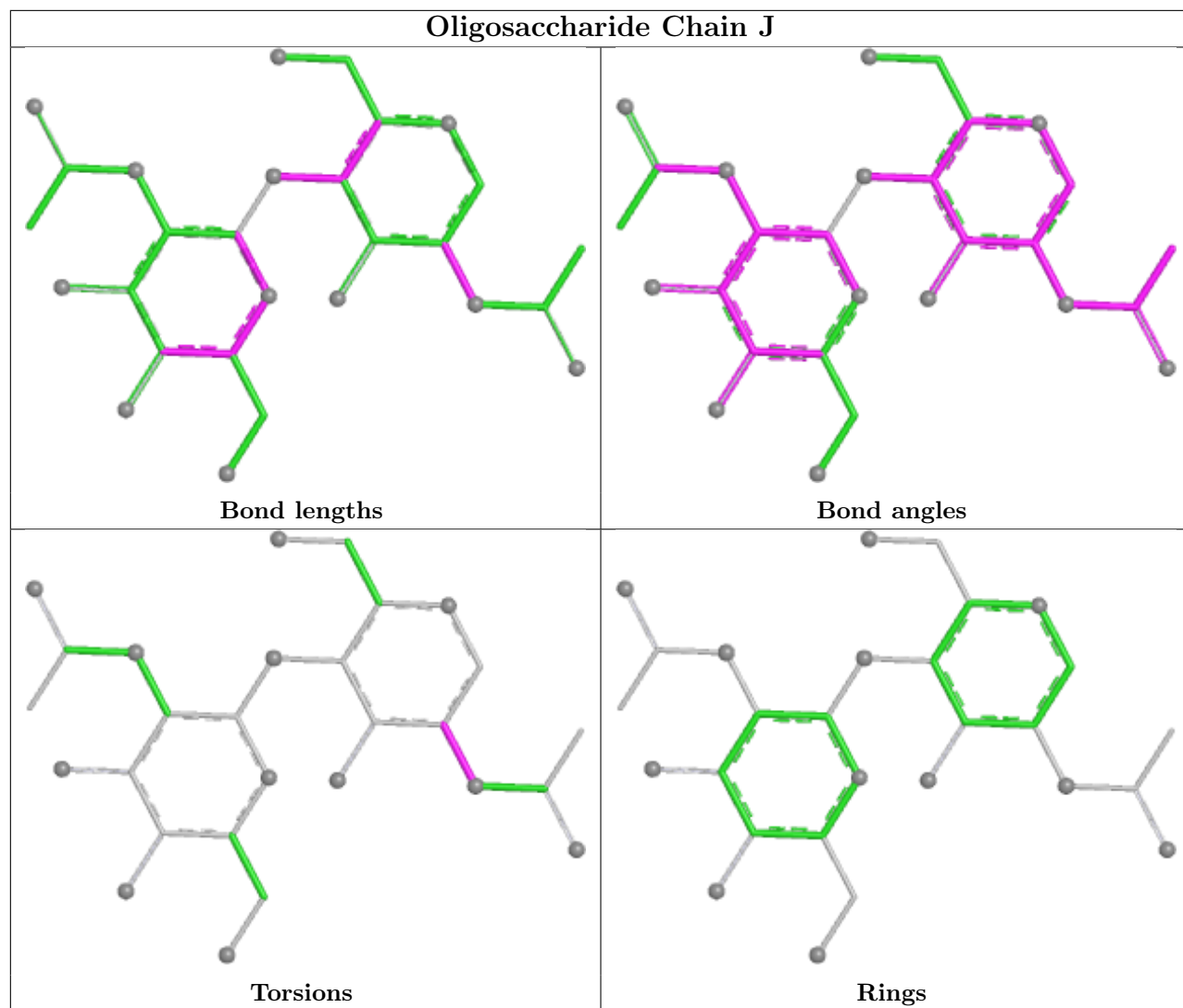
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1	NAG	5	0
6	I	1	NAG	4	0
5	G	1	NAG	4	0
5	G	2	NAG	4	0
6	I	2	NAG	4	0
6	J	2	NAG	2	0
5	K	2	NAG	5	0
6	J	1	NAG	2	0

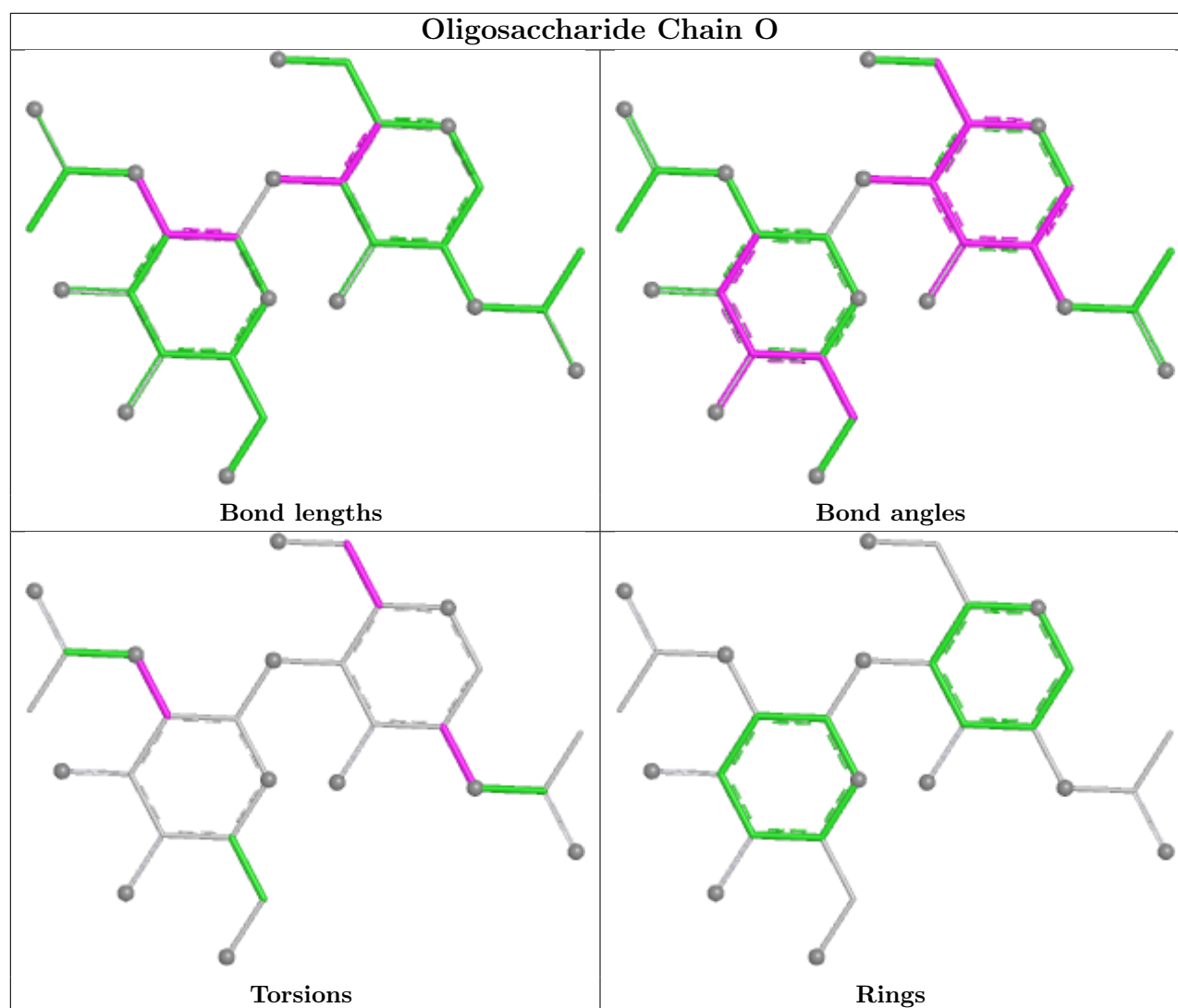
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

1 ligand is 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	C	1501	-	14,14,15	1.75	3 (21%)	17,19,21	1.75	3 (17%)

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	C	1501	-	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1501	NAG	C1-C2	-3.93	1.47	1.52
7	C	1501	NAG	O5-C1	3.49	1.49	1.43
7	C	1501	NAG	O3-C3	2.42	1.49	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1501	NAG	C2-N2-C7	4.59	129.04	122.90
7	C	1501	NAG	C1-C2-N2	2.64	114.59	110.43
7	C	1501	NAG	O5-C1-C2	-2.26	107.79	111.29

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1501	NAG	C3-C2-N2-C7

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.

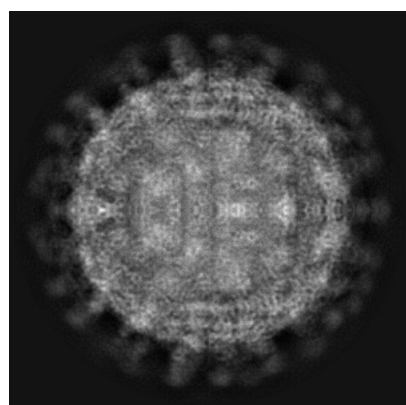
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2442. These allow visual inspection of the internal detail of the map and identification of artifacts.

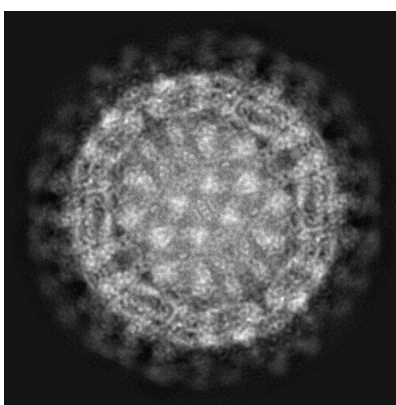
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

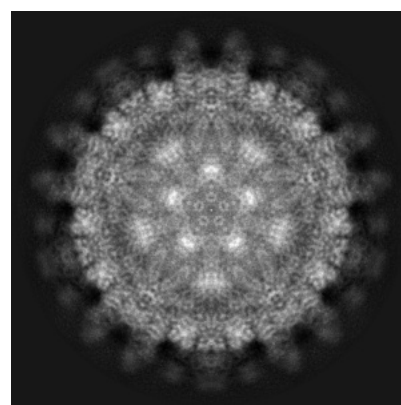
6.1.1 Primary map



X



Y

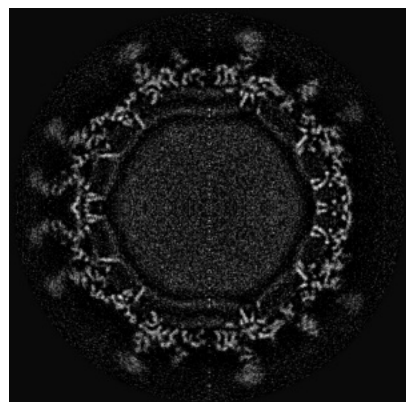


Z

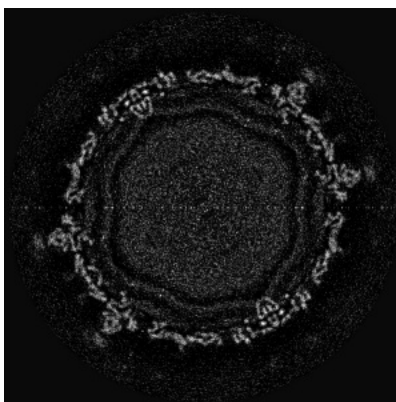
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

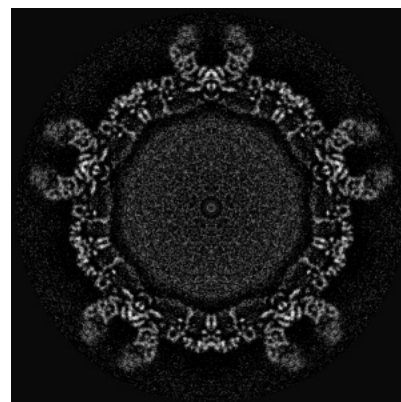
6.2.1 Primary map



X Index: 320



Y Index: 320

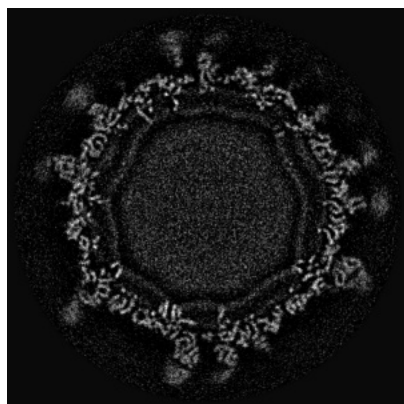


Z Index: 320

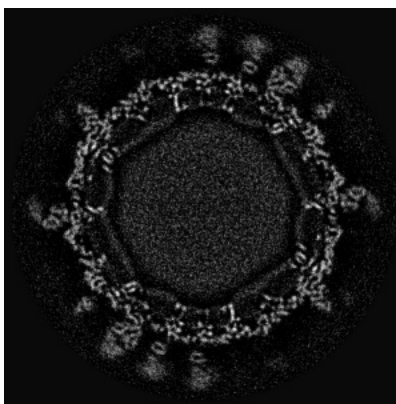
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

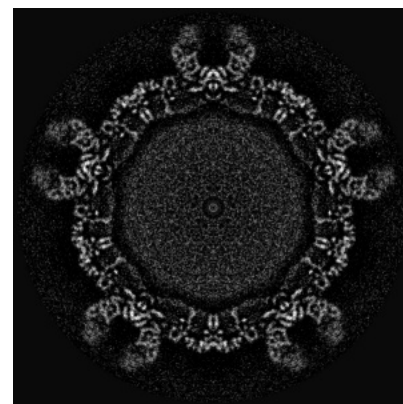
6.3.1 Primary map



X Index: 364



Y Index: 371

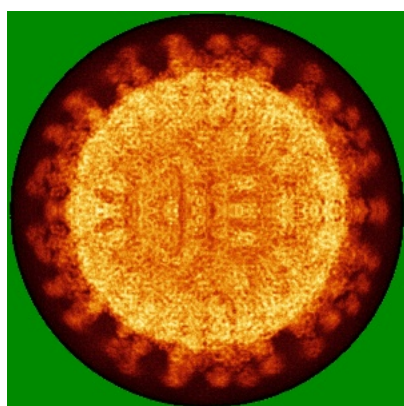


Z Index: 320

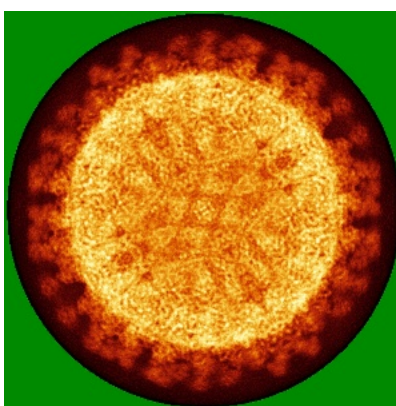
The images above show the largest variance slices of the map in three orthogonal directions.

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

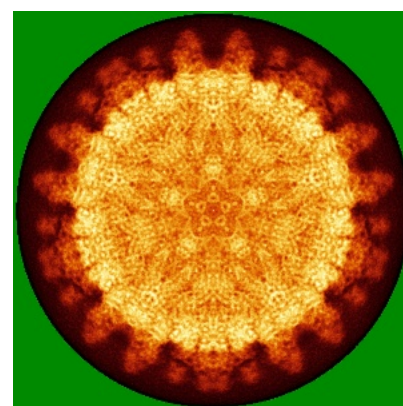
6.4.1 Primary map



X



Y

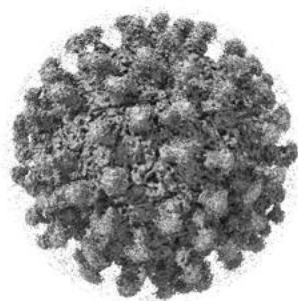


Z

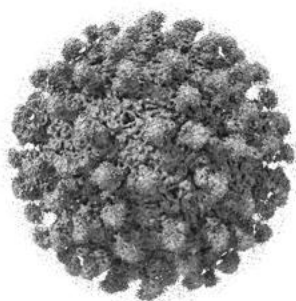
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

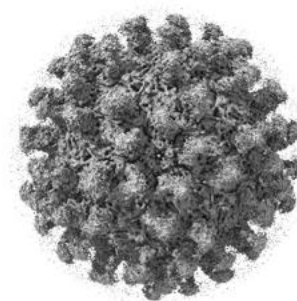
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

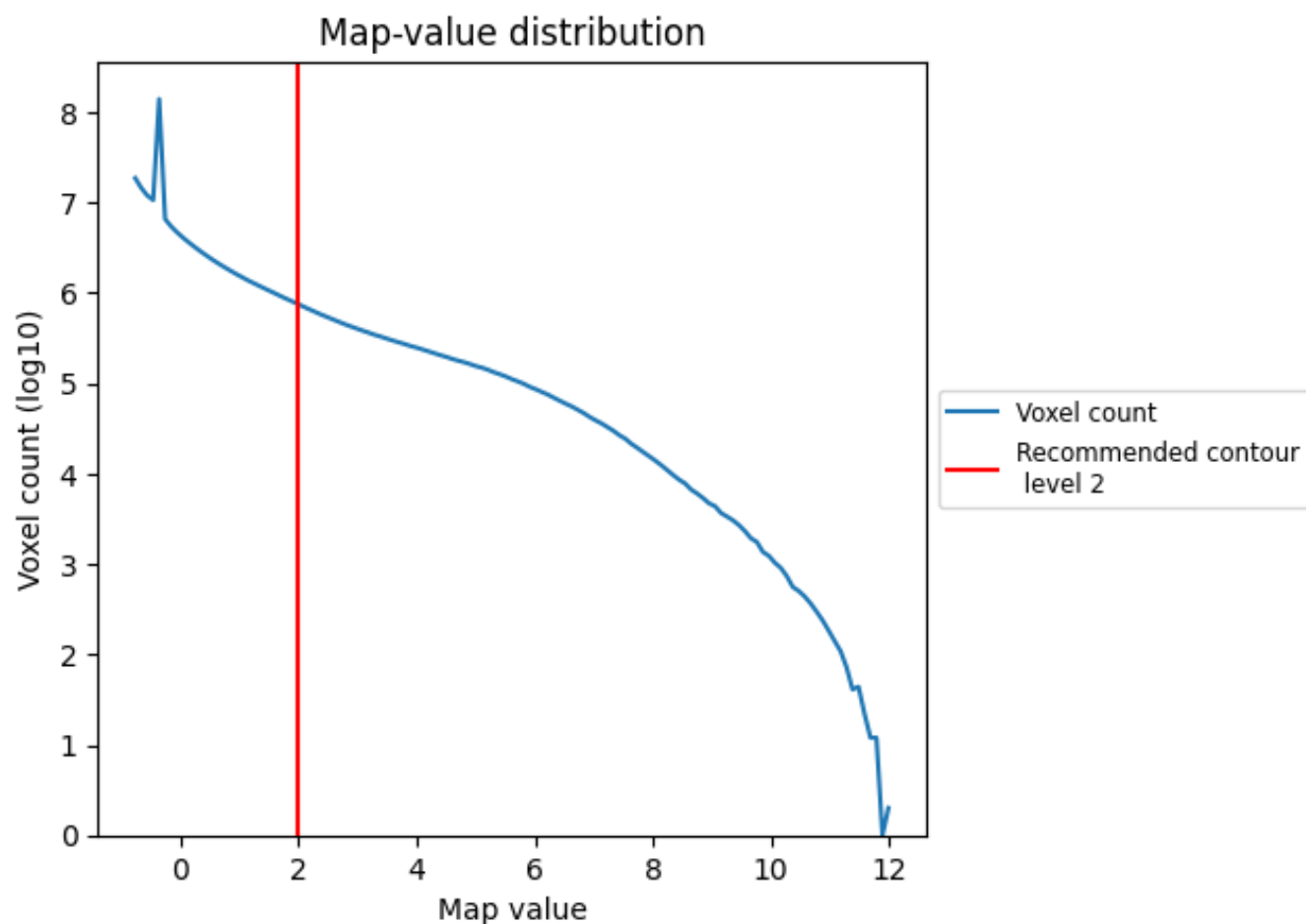
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

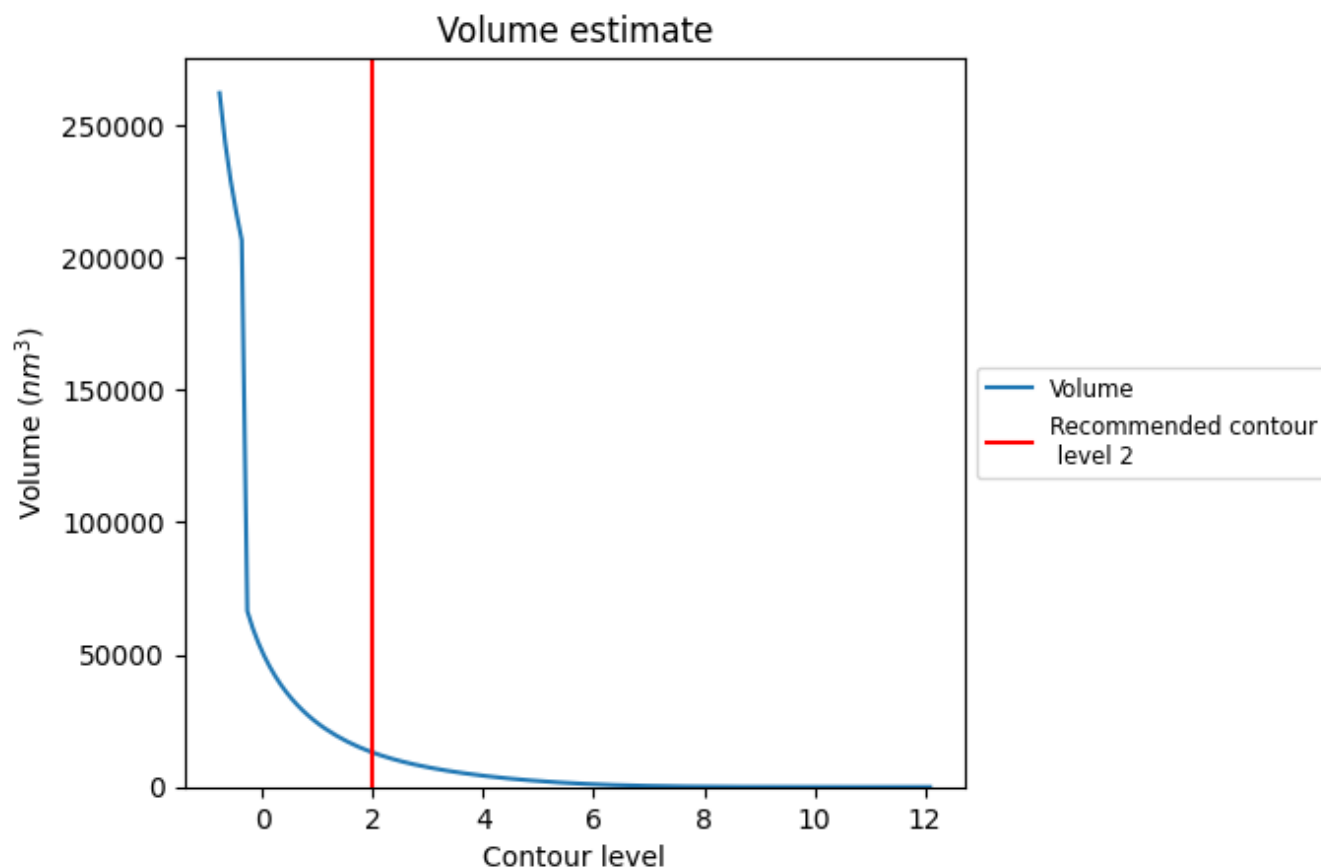
This section contains the results of statistical analysis of the map.

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.

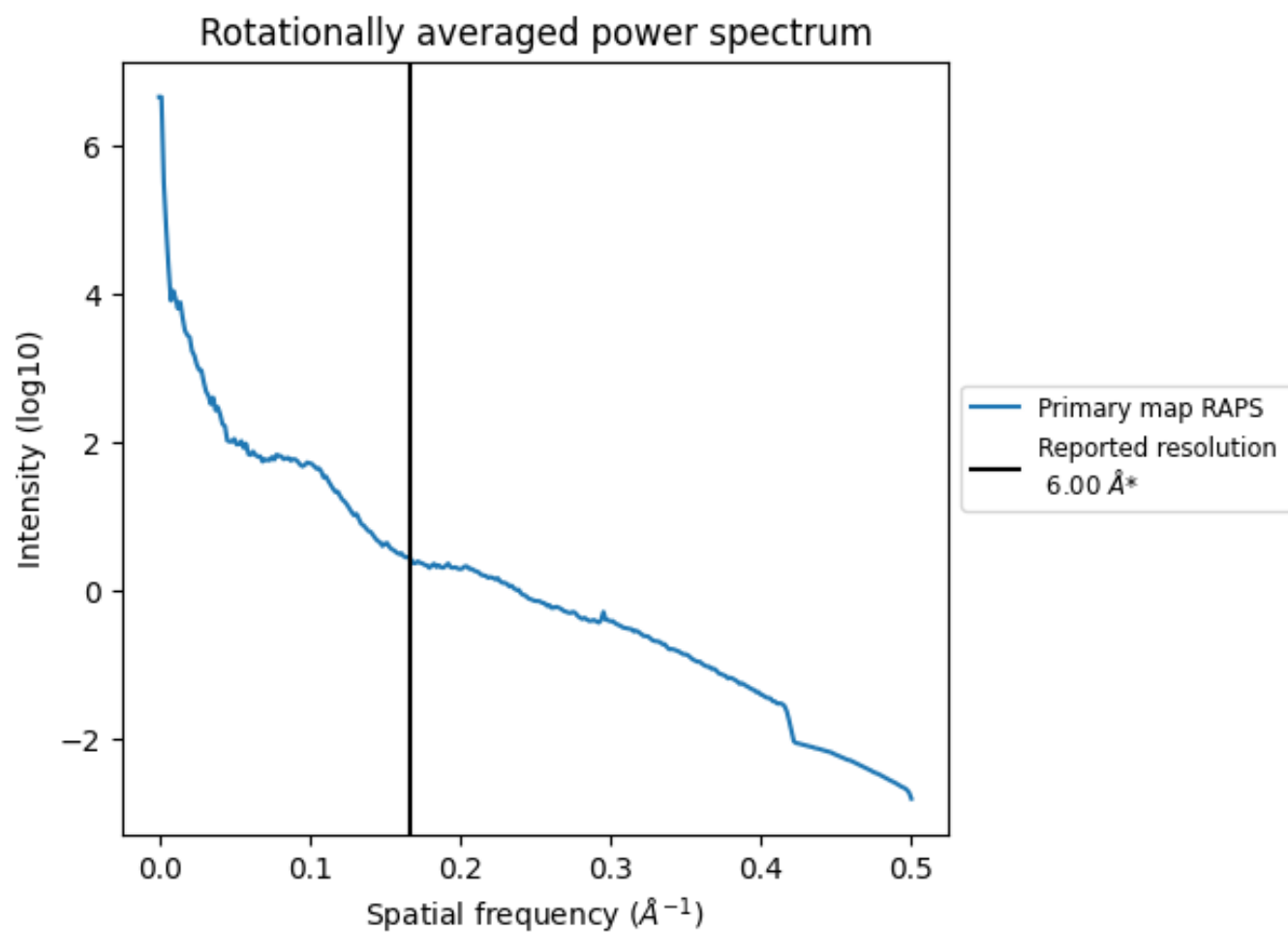
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 13042 nm^3 ; this corresponds to an approximate mass of 11781 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 0.167 Å⁻¹

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

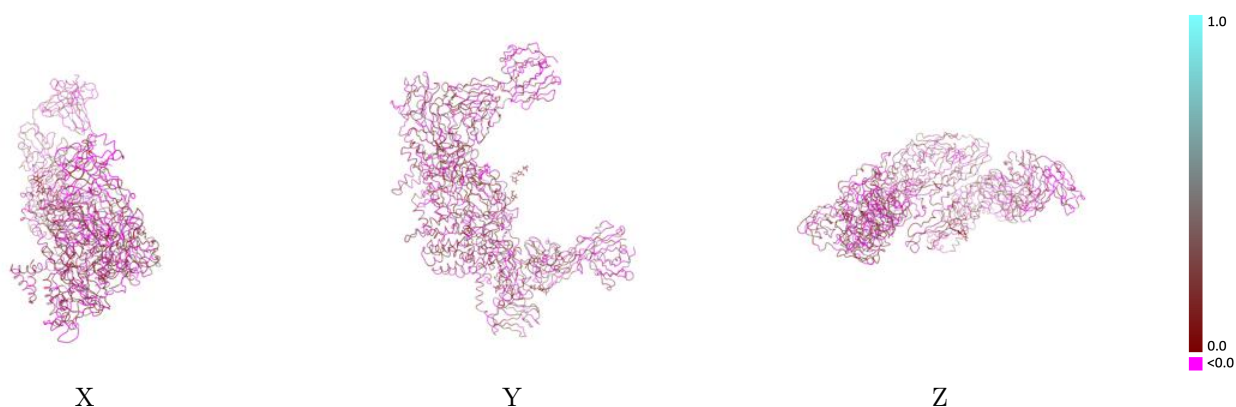
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2442 and PDB model 4C2I. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

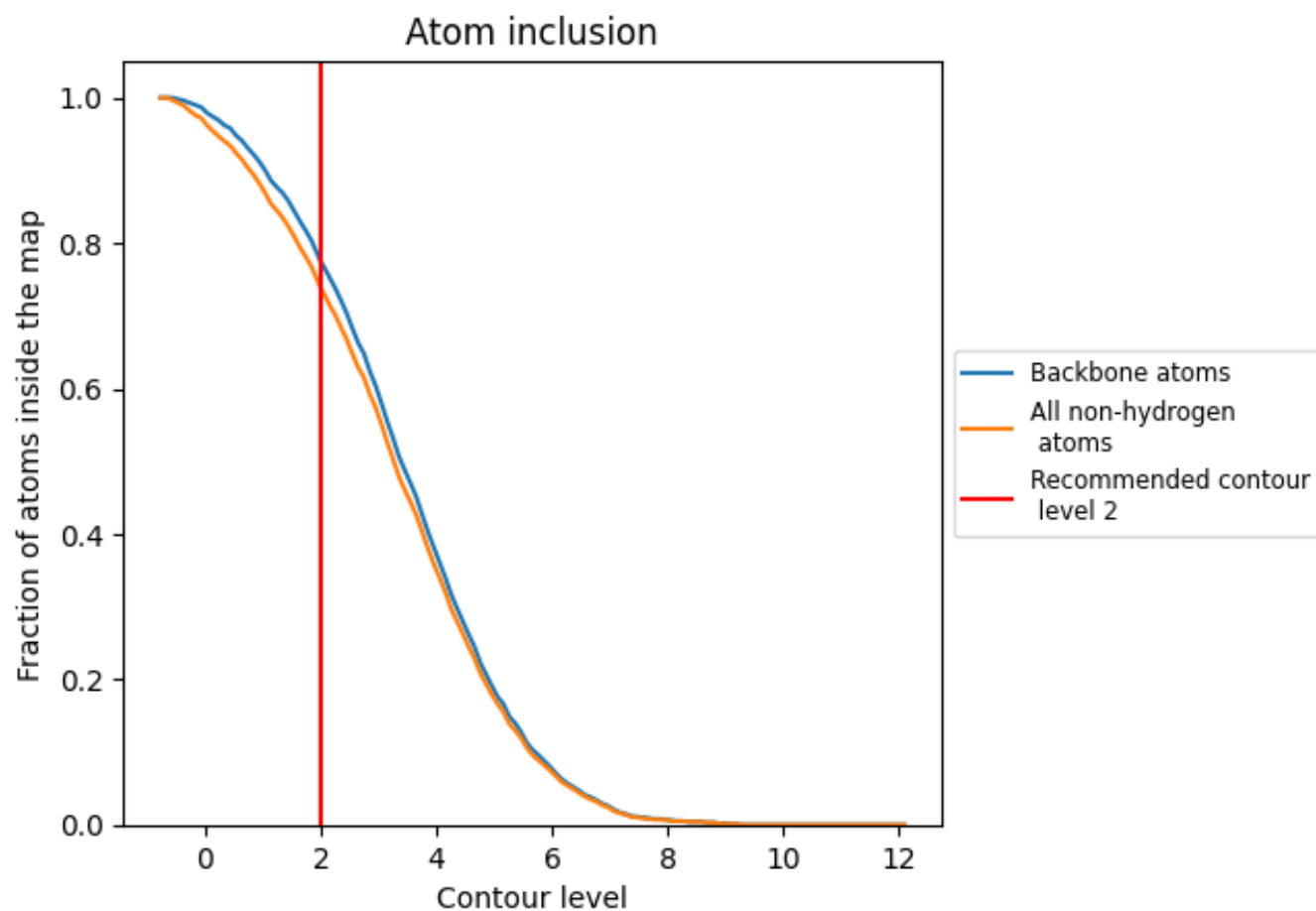


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 74% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7380	 0.0930
A	 0.8570	 0.1100
B	 0.7640	 0.1040
C	 0.8490	 0.1240
D	 0.8470	 0.1000
E	 0.8570	 0.1090
F	 0.8750	 0.1250
G	 0.1430	 0.0550
H	 0.5830	 0.0560
I	 0.3210	 0.1460
J	 0.2140	 0.0980
K	 0.2140	 0.0760
L	 0.6590	 0.1040
M	 0.6100	 0.0460
N	 0.6400	 0.0370
O	 0.0710	 -0.1650

