



Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 09:37 PM EST

PDB ID : 7KFE
EMDB ID : EMD-22851
Title : Bundibugyo virus GP (mucin deleted) bound to antibody Fab BDBV-329
Authors : Murin, C.D.; Ward, A.B.
Deposited on : 2020-10-13
Resolution : 6.60 Å (reported)

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

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

A user guide is available at

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

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:

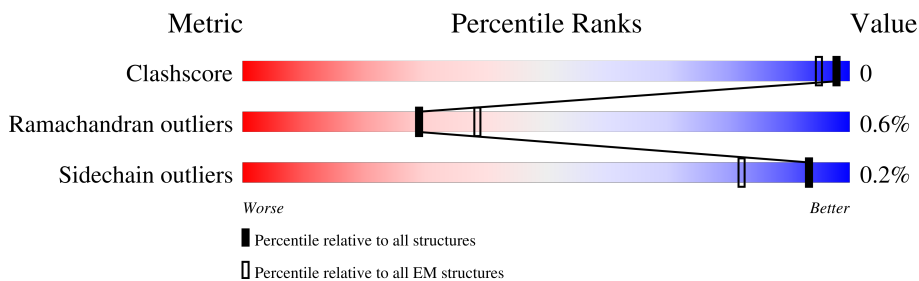
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 6.60 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	G	244	22% (red), 54% (green), 43% (grey)
1	H	244	12% (red), 56% (green), 43% (grey)
2	I	215	26% (red), 47% (green), 50% (grey)
2	J	215	21% (red), 47% (green), 50% (grey)
3	A	343	46% (green), 50% (grey)
3	B	343	58% (green), 6% (yellow), 36% (grey)
3	C	343	60% (green), 36% (grey)
4	D	177	8% (red), 62% (green), 35% (grey)

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Mol	Chain	Length	Quality of chain
4	E	177	 7% 63% 35%
4	F	177	 8% 62% 35%
5	K	5	 20% 100%
5	M	5	 100%
5	O	5	 20% 100%
6	L	2	 100%
6	N	2	 100%

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 11538 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 Antibody BDBV-329 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H	140	1073	683	186	199	5	0	0
1	G	140	1073	683	186	199	5	0	0

- Molecule 2 is a protein called Antibody BDBV-329 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	J	108	810	507	138	162	3	0	0
2	I	108	810	507	138	162	3	0	0

- Molecule 3 is a protein called Spike glycoprotein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	170	1313	836	223	249	5	0	0
3	B	219	1728	1108	292	322	6	0	0
3	C	219	1728	1108	292	322	6	0	0

There are 93 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	313	ILE	-	expression tag	UNP A0A510C2V9
A	314	ASP	-	expression tag	UNP A0A510C2V9
A	315	ILE	-	expression tag	UNP A0A510C2V9
A	316	SER	-	expression tag	UNP A0A510C2V9
A	317	GLU	-	expression tag	UNP A0A510C2V9
A	318	SER	-	expression tag	UNP A0A510C2V9
A	319	THR	-	expression tag	UNP A0A510C2V9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	320	GLU	-	expression tag	UNP A0A510C2V9
A	321	PRO	-	expression tag	UNP A0A510C2V9
A	322	GLY	-	expression tag	UNP A0A510C2V9
A	323	PRO	-	expression tag	UNP A0A510C2V9
A	324	LEU	-	expression tag	UNP A0A510C2V9
A	325	THR	-	expression tag	UNP A0A510C2V9
A	326	ASN	-	expression tag	UNP A0A510C2V9
A	327	THR	-	expression tag	UNP A0A510C2V9
A	328	THR	-	expression tag	UNP A0A510C2V9
A	329	ARG	-	expression tag	UNP A0A510C2V9
A	330	GLY	-	expression tag	UNP A0A510C2V9
A	331	ALA	-	expression tag	UNP A0A510C2V9
A	332	ALA	-	expression tag	UNP A0A510C2V9
A	333	ASN	-	expression tag	UNP A0A510C2V9
A	334	LEU	-	expression tag	UNP A0A510C2V9
A	335	LEU	-	expression tag	UNP A0A510C2V9
A	336	THR	-	expression tag	UNP A0A510C2V9
A	337	GLY	-	expression tag	UNP A0A510C2V9
A	338	SER	-	expression tag	UNP A0A510C2V9
A	339	ARG	-	expression tag	UNP A0A510C2V9
A	340	ARG	-	expression tag	UNP A0A510C2V9
A	341	THR	-	expression tag	UNP A0A510C2V9
A	342	ARG	-	expression tag	UNP A0A510C2V9
A	343	ARG	-	expression tag	UNP A0A510C2V9
B	313	ILE	-	expression tag	UNP A0A510C2V9
B	314	ASP	-	expression tag	UNP A0A510C2V9
B	315	ILE	-	expression tag	UNP A0A510C2V9
B	316	SER	-	expression tag	UNP A0A510C2V9
B	317	GLU	-	expression tag	UNP A0A510C2V9
B	318	SER	-	expression tag	UNP A0A510C2V9
B	319	THR	-	expression tag	UNP A0A510C2V9
B	320	GLU	-	expression tag	UNP A0A510C2V9
B	321	PRO	-	expression tag	UNP A0A510C2V9
B	322	GLY	-	expression tag	UNP A0A510C2V9
B	323	PRO	-	expression tag	UNP A0A510C2V9
B	324	LEU	-	expression tag	UNP A0A510C2V9
B	325	THR	-	expression tag	UNP A0A510C2V9
B	326	ASN	-	expression tag	UNP A0A510C2V9
B	327	THR	-	expression tag	UNP A0A510C2V9
B	328	THR	-	expression tag	UNP A0A510C2V9
B	329	ARG	-	expression tag	UNP A0A510C2V9
B	330	GLY	-	expression tag	UNP A0A510C2V9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	331	ALA	-	expression tag	UNP A0A510C2V9
B	332	ALA	-	expression tag	UNP A0A510C2V9
B	333	ASN	-	expression tag	UNP A0A510C2V9
B	334	LEU	-	expression tag	UNP A0A510C2V9
B	335	LEU	-	expression tag	UNP A0A510C2V9
B	336	THR	-	expression tag	UNP A0A510C2V9
B	337	GLY	-	expression tag	UNP A0A510C2V9
B	338	SER	-	expression tag	UNP A0A510C2V9
B	339	ARG	-	expression tag	UNP A0A510C2V9
B	340	ARG	-	expression tag	UNP A0A510C2V9
B	341	THR	-	expression tag	UNP A0A510C2V9
B	342	ARG	-	expression tag	UNP A0A510C2V9
B	343	ARG	-	expression tag	UNP A0A510C2V9
C	313	ILE	-	expression tag	UNP A0A510C2V9
C	314	ASP	-	expression tag	UNP A0A510C2V9
C	315	ILE	-	expression tag	UNP A0A510C2V9
C	316	SER	-	expression tag	UNP A0A510C2V9
C	317	GLU	-	expression tag	UNP A0A510C2V9
C	318	SER	-	expression tag	UNP A0A510C2V9
C	319	THR	-	expression tag	UNP A0A510C2V9
C	320	GLU	-	expression tag	UNP A0A510C2V9
C	321	PRO	-	expression tag	UNP A0A510C2V9
C	322	GLY	-	expression tag	UNP A0A510C2V9
C	323	PRO	-	expression tag	UNP A0A510C2V9
C	324	LEU	-	expression tag	UNP A0A510C2V9
C	325	THR	-	expression tag	UNP A0A510C2V9
C	326	ASN	-	expression tag	UNP A0A510C2V9
C	327	THR	-	expression tag	UNP A0A510C2V9
C	328	THR	-	expression tag	UNP A0A510C2V9
C	329	ARG	-	expression tag	UNP A0A510C2V9
C	330	GLY	-	expression tag	UNP A0A510C2V9
C	331	ALA	-	expression tag	UNP A0A510C2V9
C	332	ALA	-	expression tag	UNP A0A510C2V9
C	333	ASN	-	expression tag	UNP A0A510C2V9
C	334	LEU	-	expression tag	UNP A0A510C2V9
C	335	LEU	-	expression tag	UNP A0A510C2V9
C	336	THR	-	expression tag	UNP A0A510C2V9
C	337	GLY	-	expression tag	UNP A0A510C2V9
C	338	SER	-	expression tag	UNP A0A510C2V9
C	339	ARG	-	expression tag	UNP A0A510C2V9
C	340	ARG	-	expression tag	UNP A0A510C2V9
C	341	THR	-	expression tag	UNP A0A510C2V9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	342	ARG	-	expression tag	UNP A0A510C2V9
C	343	ARG	-	expression tag	UNP A0A510C2V9

- Molecule 4 is a protein called Envelope glycoprotein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	115	Total	C	N	O	S	0	0
			912	579	159	168	6		
4	E	115	Total	C	N	O	S	0	0
			912	579	159	168	6		
4	F	115	Total	C	N	O	S	0	0
			912	579	159	168	6		

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	641	VAL	-	expression tag	UNP B8XCN0
D	642	GLU	-	expression tag	UNP B8XCN0
D	643	VAL	-	expression tag	UNP B8XCN0
D	644	ASP	-	expression tag	UNP B8XCN0
D	645	ASP	-	expression tag	UNP B8XCN0
D	646	ASP	-	expression tag	UNP B8XCN0
D	647	ASP	-	expression tag	UNP B8XCN0
D	648	LYS	-	expression tag	UNP B8XCN0
D	649	ALA	-	expression tag	UNP B8XCN0
D	650	GLY	-	expression tag	UNP B8XCN0
D	651	TRP	-	expression tag	UNP B8XCN0
D	652	SER	-	expression tag	UNP B8XCN0
D	653	HIS	-	expression tag	UNP B8XCN0
D	654	PRO	-	expression tag	UNP B8XCN0
D	655	GLN	-	expression tag	UNP B8XCN0
D	656	PHE	-	expression tag	UNP B8XCN0
D	657	GLU	-	expression tag	UNP B8XCN0
D	658	LYS	-	expression tag	UNP B8XCN0
D	659	GLY	-	expression tag	UNP B8XCN0
D	660	GLY	-	expression tag	UNP B8XCN0
D	661	GLY	-	expression tag	UNP B8XCN0
D	662	SER	-	expression tag	UNP B8XCN0
D	663	GLY	-	expression tag	UNP B8XCN0
D	664	GLY	-	expression tag	UNP B8XCN0
D	665	GLY	-	expression tag	UNP B8XCN0
D	666	SER	-	expression tag	UNP B8XCN0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	667	GLY	-	expression tag	UNP B8XCNO
D	668	GLY	-	expression tag	UNP B8XCNO
D	669	GLY	-	expression tag	UNP B8XCNO
D	670	SER	-	expression tag	UNP B8XCNO
D	671	TRP	-	expression tag	UNP B8XCNO
D	672	SER	-	expression tag	UNP B8XCNO
D	673	HIS	-	expression tag	UNP B8XCNO
D	674	PRO	-	expression tag	UNP B8XCNO
D	675	GLN	-	expression tag	UNP B8XCNO
D	676	PHE	-	expression tag	UNP B8XCNO
D	677	GLU	-	expression tag	UNP B8XCNO
D	678	LYS	-	expression tag	UNP B8XCNO
E	641	VAL	-	expression tag	UNP B8XCNO
E	642	GLU	-	expression tag	UNP B8XCNO
E	643	VAL	-	expression tag	UNP B8XCNO
E	644	ASP	-	expression tag	UNP B8XCNO
E	645	ASP	-	expression tag	UNP B8XCNO
E	646	ASP	-	expression tag	UNP B8XCNO
E	647	ASP	-	expression tag	UNP B8XCNO
E	648	LYS	-	expression tag	UNP B8XCNO
E	649	ALA	-	expression tag	UNP B8XCNO
E	650	GLY	-	expression tag	UNP B8XCNO
E	651	TRP	-	expression tag	UNP B8XCNO
E	652	SER	-	expression tag	UNP B8XCNO
E	653	HIS	-	expression tag	UNP B8XCNO
E	654	PRO	-	expression tag	UNP B8XCNO
E	655	GLN	-	expression tag	UNP B8XCNO
E	656	PHE	-	expression tag	UNP B8XCNO
E	657	GLU	-	expression tag	UNP B8XCNO
E	658	LYS	-	expression tag	UNP B8XCNO
E	659	GLY	-	expression tag	UNP B8XCNO
E	660	GLY	-	expression tag	UNP B8XCNO
E	661	GLY	-	expression tag	UNP B8XCNO
E	662	SER	-	expression tag	UNP B8XCNO
E	663	GLY	-	expression tag	UNP B8XCNO
E	664	GLY	-	expression tag	UNP B8XCNO
E	665	GLY	-	expression tag	UNP B8XCNO
E	666	SER	-	expression tag	UNP B8XCNO
E	667	GLY	-	expression tag	UNP B8XCNO
E	668	GLY	-	expression tag	UNP B8XCNO
E	669	GLY	-	expression tag	UNP B8XCNO
E	670	SER	-	expression tag	UNP B8XCNO

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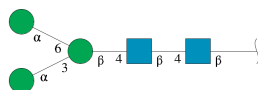
Chain	Residue	Modelled	Actual	Comment	Reference
E	671	TRP	-	expression tag	UNP B8XCN0
E	672	SER	-	expression tag	UNP B8XCN0
E	673	HIS	-	expression tag	UNP B8XCN0
E	674	PRO	-	expression tag	UNP B8XCN0
E	675	GLN	-	expression tag	UNP B8XCN0
E	676	PHE	-	expression tag	UNP B8XCN0
E	677	GLU	-	expression tag	UNP B8XCN0
E	678	LYS	-	expression tag	UNP B8XCN0
F	641	VAL	-	expression tag	UNP B8XCN0
F	642	GLU	-	expression tag	UNP B8XCN0
F	643	VAL	-	expression tag	UNP B8XCN0
F	644	ASP	-	expression tag	UNP B8XCN0
F	645	ASP	-	expression tag	UNP B8XCN0
F	646	ASP	-	expression tag	UNP B8XCN0
F	647	ASP	-	expression tag	UNP B8XCN0
F	648	LYS	-	expression tag	UNP B8XCN0
F	649	ALA	-	expression tag	UNP B8XCN0
F	650	GLY	-	expression tag	UNP B8XCN0
F	651	TRP	-	expression tag	UNP B8XCN0
F	652	SER	-	expression tag	UNP B8XCN0
F	653	HIS	-	expression tag	UNP B8XCN0
F	654	PRO	-	expression tag	UNP B8XCN0
F	655	GLN	-	expression tag	UNP B8XCN0
F	656	PHE	-	expression tag	UNP B8XCN0
F	657	GLU	-	expression tag	UNP B8XCN0
F	658	LYS	-	expression tag	UNP B8XCN0
F	659	GLY	-	expression tag	UNP B8XCN0
F	660	GLY	-	expression tag	UNP B8XCN0
F	661	GLY	-	expression tag	UNP B8XCN0
F	662	SER	-	expression tag	UNP B8XCN0
F	663	GLY	-	expression tag	UNP B8XCN0
F	664	GLY	-	expression tag	UNP B8XCN0
F	665	GLY	-	expression tag	UNP B8XCN0
F	666	SER	-	expression tag	UNP B8XCN0
F	667	GLY	-	expression tag	UNP B8XCN0
F	668	GLY	-	expression tag	UNP B8XCN0
F	669	GLY	-	expression tag	UNP B8XCN0
F	670	SER	-	expression tag	UNP B8XCN0
F	671	TRP	-	expression tag	UNP B8XCN0
F	672	SER	-	expression tag	UNP B8XCN0
F	673	HIS	-	expression tag	UNP B8XCN0
F	674	PRO	-	expression tag	UNP B8XCN0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	675	GLN	-	expression tag	UNP B8XCN0
F	676	PHE	-	expression tag	UNP B8XCN0
F	677	GLU	-	expression tag	UNP B8XCN0
F	678	LYS	-	expression tag	UNP B8XCN0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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
5	K	5	Total	C	N	O	0	0
			61	34	2	25		
5	M	5	Total	C	N	O	0	0
			61	34	2	25		
5	O	5	Total	C	N	O	0	0
			61	34	2	25		

- 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	L	2	Total	C	N	O	0	0
			28	16	2	10		
6	N	2	Total	C	N	O	0	0
			28	16	2	10		

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



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

TRP
ALA
PHE
TRP
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ASN
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• Molecule 3: Spike glycoprotein 1



MET
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I93
L43
S46
L51
R54
K64
E71
Y99
E103
E124
R130
G131
F132
P133
R134
E178

K190
F193
PHE
GLN
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F234
Y241
N257
R265
ARG
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THR
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L273
P279
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• Molecule 4: Envelope glycoprotein 2



GLU
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G599
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H613
T616
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• Molecule 4: Envelope glycoprotein 2



GLU
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LYS
C511
R521
D522
A525
A526
A536
A539
Y543
R587
T616
K617
N618
D621
K622
I623
D624
Q625
ILE
HIS
GLY
ASP
PHE
ILE
ASP
LYS
PRO
LEU
PRO
GLN
THR
ASP
VAL
GLU
VAL
VAL
ASP
ASP
ASP
ASP
LYS
PRO
LEU
PRO
GLN
THR
ASP
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VAL
SER

HIS
PRO
GLN
PHE
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TRP
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PHE
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LYS

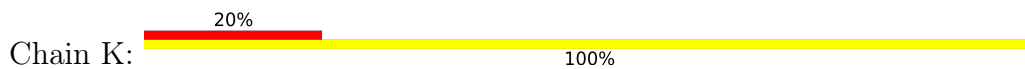
• Molecule 4: Envelope glycoprotein 2



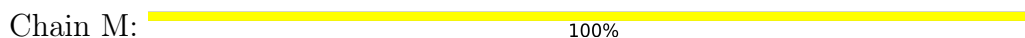
GLU
ILE
THR
LEU
ARG
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ALA
LYS
C511
A525
A538
A539
Y543
T544
E545
R559
R596
W597
I603
D607
H613
D614
K617
M618
I619
T620
D621
K622
I623
D624
Q625
ILE
HIS
ASP
PHE
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ASP
LYS
PRO
LEU
PRO
GLN
THR
ASP
VAL
VAL
ASP

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LYS
ALA
GLY
TRP
SER
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GLY
GLY
SER
GLY
GLY
GLY
GLY
GLY
SER
TRP
HIS
PRO
GLN
PHE
GLU
LYS

• Molecule 5: alpha-D-mannopyranose-(1-3)-[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



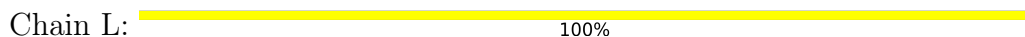
● Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



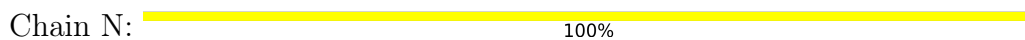
● Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



● Molecule 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, Not provided	
Number of particles used	45640	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	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	0.116	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0289	Depositor
Map size (Å)	331.19998, 331.19998, 331.19998	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	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, BMA, 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	G	1.02	0/1100	1.03	2/1494 (0.1%)
1	H	1.02	0/1100	1.06	3/1494 (0.2%)
2	I	1.11	5/829 (0.6%)	0.99	2/1124 (0.2%)
2	J	1.10	4/829 (0.5%)	0.99	1/1124 (0.1%)
3	A	1.22	10/1343 (0.7%)	1.07	9/1824 (0.5%)
3	B	1.24	11/1770 (0.6%)	1.10	12/2407 (0.5%)
3	C	1.23	16/1770 (0.9%)	0.99	3/2407 (0.1%)
4	D	1.06	0/935	0.99	5/1274 (0.4%)
4	E	1.08	2/935 (0.2%)	0.96	2/1274 (0.2%)
4	F	1.13	5/935 (0.5%)	0.98	3/1274 (0.2%)
All	All	1.14	53/11546 (0.5%)	1.03	42/15696 (0.3%)

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	178	GLU	CG-CD	-8.28	1.39	1.51
3	A	193	PHE	CG-CD1	7.59	1.50	1.38
3	B	193	PHE	CG-CD2	7.18	1.49	1.38
3	C	193	PHE	CG-CD1	7.14	1.49	1.38
3	B	193	PHE	CG-CD1	6.96	1.49	1.38
3	C	193	PHE	CG-CD2	6.95	1.49	1.38
3	B	151	TYR	CB-CG	-6.77	1.41	1.51
4	F	543	TYR	CB-CG	-6.75	1.41	1.51
3	B	241	TYR	CB-CG	-6.51	1.41	1.51
2	J	37	TYR	CB-CG	-6.45	1.42	1.51
3	A	193	PHE	CG-CD2	6.44	1.48	1.38
2	I	37	TYR	CB-CG	-6.39	1.42	1.51
3	B	151	TYR	CD1-CE1	-6.39	1.29	1.39
4	F	543	TYR	CD1-CE1	-6.39	1.29	1.39
2	I	1	GLU	CB-CG	6.34	1.64	1.52
2	J	1	GLU	CB-CG	6.19	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	151	TYR	CB-CG	-6.18	1.42	1.51
3	A	151	TYR	CD1-CE1	-5.95	1.30	1.39
3	B	178	GLU	CD-OE2	-5.93	1.19	1.25
3	B	265	ARG	NE-CZ	5.90	1.40	1.33
3	C	124	GLU	CD-OE2	-5.85	1.19	1.25
4	F	597	TRP	CB-CG	-5.78	1.39	1.50
3	C	265	ARG	NE-CZ	5.77	1.40	1.33
3	B	134	ARG	CG-CD	-5.77	1.37	1.51
3	B	193	PHE	CE1-CZ	5.67	1.48	1.37
2	I	90	GLN	CG-CD	-5.61	1.38	1.51
3	C	178	GLU	CD-OE2	-5.58	1.19	1.25
3	C	241	TYR	CB-CG	-5.57	1.43	1.51
4	E	543	TYR	CB-CG	-5.52	1.43	1.51
3	C	178	GLU	CD-OE1	-5.44	1.19	1.25
3	C	99	TYR	CB-CG	-5.42	1.43	1.51
3	A	156	GLU	CD-OE2	-5.42	1.19	1.25
3	A	100	GLU	CD-OE1	-5.35	1.19	1.25
3	A	71	GLU	CD-OE2	-5.34	1.19	1.25
3	B	99	TYR	CG-CD1	-5.32	1.32	1.39
3	C	134	ARG	CG-CD	-5.29	1.38	1.51
2	I	92	TYR	CE2-CZ	-5.25	1.31	1.38
4	F	597	TRP	CZ3-CH2	-5.23	1.31	1.40
3	C	193	PHE	CE1-CZ	5.20	1.47	1.37
3	C	132	PHE	CB-CG	-5.19	1.42	1.51
3	A	193	PHE	CE2-CZ	5.17	1.47	1.37
3	A	193	PHE	CE1-CZ	5.16	1.47	1.37
3	C	103	GLU	CD-OE1	-5.14	1.20	1.25
2	J	90	GLN	CG-CD	-5.13	1.39	1.51
4	E	543	TYR	CD1-CE1	-5.11	1.31	1.39
3	A	220	TYR	CB-CG	-5.11	1.44	1.51
2	J	50	TYR	CB-CG	-5.11	1.44	1.51
3	C	193	PHE	CE2-CZ	5.09	1.47	1.37
3	C	71	GLU	CD-OE1	-5.08	1.20	1.25
4	F	597	TRP	NE1-CE2	-5.07	1.30	1.37
3	B	245	GLU	CD-OE1	-5.02	1.20	1.25
3	C	273	LEU	CB-CG	5.02	1.67	1.52
2	I	50	TYR	CB-CG	-5.01	1.44	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	67	ARG	NE-CZ-NH2	-11.50	114.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	151	TYR	CB-CG-CD1	-10.27	114.84	121.00
3	A	151	TYR	CB-CG-CD1	-9.97	115.02	121.00
4	F	543	TYR	CB-CG-CD1	-9.71	115.17	121.00
3	B	99	TYR	CB-CG-CD1	-8.76	115.75	121.00
4	E	543	TYR	CB-CG-CD1	-8.70	115.78	121.00
4	D	587	ARG	NE-CZ-NH2	-7.33	116.64	120.30
3	B	172	ARG	NE-CZ-NH2	-7.27	116.67	120.30
4	D	596	ARG	NE-CZ-NH2	-7.13	116.73	120.30
3	A	172	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	H	56	GLY	N-CA-C	-7.03	95.52	113.10
4	E	587	ARG	NE-CZ-NH2	-7.02	116.79	120.30
4	D	543	TYR	CB-CG-CD1	-6.81	116.91	121.00
3	A	130	ARG	NE-CZ-NH2	-6.56	117.02	120.30
2	J	33	TYR	CB-CG-CD2	-6.53	117.08	121.00
1	G	56	GLY	N-CA-C	-6.50	96.86	113.10
4	F	559	ARG	NE-CZ-NH2	-6.49	117.06	120.30
3	C	265	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	I	33	TYR	CB-CG-CD2	-6.21	117.27	121.00
3	B	136	ARG	NE-CZ-NH2	-6.21	117.20	120.30
4	D	580	ARG	NE-CZ-NH1	6.19	123.39	120.30
2	I	92	TYR	CB-CG-CD2	-6.18	117.29	121.00
3	A	99	TYR	CB-CG-CD1	-6.12	117.33	121.00
3	C	130	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	G	127	MET	CG-SD-CE	5.86	109.57	100.20
3	B	223	ASP	CB-CG-OD2	-5.81	113.07	118.30
3	B	130	ARG	NE-CZ-NH2	-5.77	117.42	120.30
4	D	534	TYR	CB-CG-CD1	-5.73	117.56	121.00
3	B	261	TYR	CB-CG-CD2	-5.73	117.56	121.00
3	B	85	ARG	NE-CZ-NH2	-5.54	117.53	120.30
3	B	89	ARG	NE-CZ-NH1	5.52	123.06	120.30
3	C	54	ARG	NE-CZ-NH2	-5.41	117.60	120.30
3	B	265	ARG	NE-CZ-NH1	5.37	122.98	120.30
4	F	596	ARG	NE-CZ-NH2	-5.37	117.62	120.30
3	A	132	PHE	CB-CG-CD1	-5.36	117.05	120.80
3	A	109	TYR	CB-CG-CD1	-5.35	117.79	121.00
3	B	241	TYR	CB-CG-CD1	-5.31	117.81	121.00
3	A	132	PHE	CB-CG-CD2	5.30	124.51	120.80
1	H	67	ARG	NE-CZ-NH1	5.25	122.92	120.30
3	A	172	ARG	NE-CZ-NH1	5.24	122.92	120.30
3	A	89	ARG	NE-CZ-NH1	5.21	122.90	120.30
3	B	172	ARG	NE-CZ-NH1	5.07	122.83	120.30

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	G	1073	0	1059	3	0
1	H	1073	0	1059	0	0
2	I	810	0	785	2	0
2	J	810	0	785	1	0
3	A	1313	0	1289	0	0
3	B	1728	0	1691	3	0
3	C	1728	0	1691	0	0
4	D	912	0	876	0	0
4	E	912	0	876	1	0
4	F	912	0	876	0	0
5	K	61	0	52	0	0
5	M	61	0	52	0	0
5	O	61	0	52	0	0
6	L	28	0	24	0	0
6	N	28	0	25	0	0
7	B	14	0	13	0	0
7	C	14	0	13	0	0
All	All	11538	0	11218	9	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 0.

All (9) 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:G:99:GLY:O	1:G:100:LEU:HB3	2.13	0.49
2:J:37:TYR:CZ	2:J:88:TYR:HB2	2.48	0.48
3:B:113:ILE:HG23	3:B:225:PHE:CZ	2.48	0.48
2:I:37:TYR:CZ	2:I:88:TYR:HB2	2.50	0.47
2:I:61:ASP:OD1	2:I:61:ASP:N	2.48	0.46
3:B:241:TYR:HB2	3:B:274:ILE:HG12	1.97	0.45
1:G:99:GLY:O	1:G:100:LEU:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:ARG:O	1:G:121:GLN:NE2	2.50	0.45
3:B:64:LYS:NZ	4:E:522:ASP:OD2	2.52	0.42

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	G	138/244 (57%)	130 (94%)	5 (4%)	3 (2%)	6	35
1	H	138/244 (57%)	129 (94%)	7 (5%)	2 (1%)	11	46
2	I	106/215 (49%)	105 (99%)	1 (1%)	0	100	100
2	J	106/215 (49%)	105 (99%)	1 (1%)	0	100	100
3	A	166/343 (48%)	160 (96%)	6 (4%)	0	100	100
3	B	213/343 (62%)	208 (98%)	5 (2%)	0	100	100
3	C	213/343 (62%)	207 (97%)	6 (3%)	0	100	100
4	D	113/177 (64%)	106 (94%)	6 (5%)	1 (1%)	17	57
4	E	113/177 (64%)	108 (96%)	4 (4%)	1 (1%)	17	57
4	F	113/177 (64%)	107 (95%)	5 (4%)	1 (1%)	17	57
All	All	1419/2478 (57%)	1365 (96%)	46 (3%)	8 (1%)	29	66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	102	SER
1	G	102	SER
1	H	30	ASP
1	G	30	ASP
1	G	100	LEU

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Mol	Chain	Res	Type
4	D	582	PHE
4	F	539	ALA
4	E	539	ALA

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	G	111/201 (55%)	111 (100%)	0	100	100
1	H	111/201 (55%)	111 (100%)	0	100	100
2	I	88/184 (48%)	88 (100%)	0	100	100
2	J	88/184 (48%)	88 (100%)	0	100	100
3	A	143/303 (47%)	143 (100%)	0	100	100
3	B	190/303 (63%)	189 (100%)	1 (0%)	88	93
3	C	190/303 (63%)	189 (100%)	1 (0%)	88	93
4	D	96/146 (66%)	96 (100%)	0	100	100
4	E	96/146 (66%)	96 (100%)	0	100	100
4	F	96/146 (66%)	95 (99%)	1 (1%)	76	86
All	All	1209/2117 (57%)	1206 (100%)	3 (0%)	93	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	229	MET
3	C	257	ASN
4	F	618	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	6	GLN

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](#)

19 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	K	1	4,5	14,14,15	2.18	5 (35%)	17,19,21	1.39	3 (17%)
5	NAG	K	2	5	14,14,15	2.05	6 (42%)	17,19,21	0.99	2 (11%)
5	BMA	K	3	5	11,11,12	1.40	2 (18%)	15,15,17	0.62	0
5	MAN	K	4	5	11,11,12	2.04	6 (54%)	15,15,17	0.72	0
5	MAN	K	5	5	11,11,12	1.91	5 (45%)	15,15,17	0.74	0
6	NAG	L	1	6,3	14,14,15	2.15	6 (42%)	17,19,21	6.83	2 (11%)
6	NAG	L	2	6	14,14,15	2.01	7 (50%)	17,19,21	1.90	3 (17%)
5	NAG	M	1	4,5	14,14,15	2.30	5 (35%)	17,19,21	1.30	3 (17%)
5	NAG	M	2	5	14,14,15	2.10	7 (50%)	17,19,21	1.03	1 (5%)
5	BMA	M	3	5	11,11,12	1.48	3 (27%)	15,15,17	0.64	0
5	MAN	M	4	5	11,11,12	2.00	6 (54%)	15,15,17	0.70	0
5	MAN	M	5	5	11,11,12	1.93	5 (45%)	15,15,17	0.68	0
6	NAG	N	1	6,3	14,14,15	2.24	6 (42%)	17,19,21	1.98	3 (17%)
6	NAG	N	2	6	14,14,15	1.97	5 (35%)	17,19,21	0.99	2 (11%)
5	NAG	O	1	4,5	14,14,15	2.27	6 (42%)	17,19,21	1.18	2 (11%)
5	NAG	O	2	5	14,14,15	2.03	7 (50%)	17,19,21	0.99	0
5	BMA	O	3	5	11,11,12	1.42	2 (18%)	15,15,17	0.63	0
5	MAN	O	4	5	11,11,12	1.99	6 (54%)	15,15,17	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	O	5	5	11,11,12	1.94	5 (45%)	15,15,17	0.70	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	K	1	4,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	MAN	K	4	5	-	0/2/19/22	0/1/1/1
5	MAN	K	5	5	-	0/2/19/22	0/1/1/1
6	NAG	L	1	6,3	-	1/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
5	NAG	M	1	4,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	1/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	0/2/19/22	0/1/1/1
5	MAN	M	5	5	-	0/2/19/22	0/1/1/1
6	NAG	N	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
5	NAG	O	1	4,5	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	1/6/23/26	0/1/1/1
5	BMA	O	3	5	-	0/2/19/22	0/1/1/1
5	MAN	O	4	5	-	0/2/19/22	0/1/1/1
5	MAN	O	5	5	-	0/2/19/22	0/1/1/1

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1	NAG	C1-C2	6.21	1.61	1.52
5	O	1	NAG	C1-C2	6.01	1.61	1.52
5	K	1	NAG	C1-C2	5.65	1.60	1.52
6	N	1	NAG	C1-C2	5.57	1.60	1.52
5	K	2	NAG	C1-C2	4.97	1.59	1.52
6	L	1	NAG	C1-C2	4.87	1.59	1.52
5	M	2	NAG	C1-C2	4.56	1.59	1.52
6	L	2	NAG	C1-C2	4.47	1.59	1.52
6	N	2	NAG	C1-C2	4.40	1.58	1.52
5	O	2	NAG	C1-C2	4.16	1.58	1.52
5	K	4	MAN	C2-C3	3.37	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	4	MAN	O5-C5	3.32	1.50	1.43
5	M	4	MAN	C2-C3	3.30	1.57	1.52
5	O	2	NAG	O5-C5	3.24	1.50	1.43
5	O	5	MAN	C2-C3	3.24	1.57	1.52
5	O	4	MAN	C2-C3	3.23	1.57	1.52
5	K	5	MAN	C2-C3	3.22	1.57	1.52
5	M	2	NAG	O5-C5	3.22	1.50	1.43
5	M	5	MAN	C2-C3	3.22	1.57	1.52
6	N	2	NAG	O5-C5	3.19	1.49	1.43
5	O	4	MAN	O5-C5	3.18	1.49	1.43
5	M	4	MAN	O5-C5	3.17	1.49	1.43
5	O	5	MAN	O5-C5	3.14	1.49	1.43
6	L	2	NAG	O5-C5	3.14	1.49	1.43
6	N	1	NAG	O5-C5	3.12	1.49	1.43
5	M	5	MAN	O5-C5	3.11	1.49	1.43
6	L	1	NAG	O5-C5	3.06	1.49	1.43
5	K	5	MAN	O5-C5	3.03	1.49	1.43
6	L	1	NAG	C3-C2	2.81	1.58	1.52
5	K	1	NAG	O5-C5	2.81	1.49	1.43
5	M	1	NAG	O5-C5	2.75	1.49	1.43
5	M	1	NAG	C3-C2	2.75	1.58	1.52
6	N	1	NAG	O5-C1	2.70	1.48	1.43
6	L	1	NAG	O5-C1	2.69	1.48	1.43
5	K	2	NAG	O5-C5	2.68	1.48	1.43
5	O	1	NAG	O5-C1	2.68	1.48	1.43
5	O	1	NAG	O5-C5	2.67	1.48	1.43
5	O	4	MAN	C1-C2	2.64	1.58	1.52
5	M	4	MAN	C1-C2	2.64	1.58	1.52
5	M	2	NAG	C4-C5	2.63	1.58	1.53
5	K	1	NAG	O5-C1	2.58	1.47	1.43
5	K	4	MAN	C1-C2	2.57	1.58	1.52
5	O	2	NAG	C4-C5	2.57	1.58	1.53
5	M	5	MAN	C1-C2	2.55	1.58	1.52
5	K	5	MAN	C1-C2	2.53	1.58	1.52
5	O	5	MAN	C1-C2	2.52	1.57	1.52
5	M	1	NAG	O5-C1	2.50	1.47	1.43
5	K	2	NAG	C3-C2	2.48	1.57	1.52
5	M	2	NAG	C2-N2	2.46	1.50	1.46
5	K	4	MAN	O5-C1	2.46	1.47	1.43
6	L	2	NAG	C3-C2	2.45	1.57	1.52
5	O	2	NAG	C2-N2	2.44	1.50	1.46
5	O	1	NAG	C2-N2	2.42	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	2	NAG	C2-N2	2.41	1.50	1.46
5	O	5	MAN	C4-C5	2.40	1.58	1.53
5	M	5	MAN	C4-C5	2.39	1.58	1.53
5	K	5	MAN	C4-C5	2.38	1.58	1.53
6	N	2	NAG	C4-C5	2.38	1.58	1.53
5	M	4	MAN	O5-C1	2.38	1.47	1.43
6	N	1	NAG	C4-C5	2.37	1.58	1.53
6	N	2	NAG	C3-C2	2.36	1.57	1.52
6	N	1	NAG	C3-C2	2.36	1.57	1.52
5	O	1	NAG	C3-C2	2.36	1.57	1.52
5	K	2	NAG	C2-N2	2.35	1.50	1.46
5	K	4	MAN	C4-C5	2.34	1.58	1.53
5	O	2	NAG	C4-C3	2.34	1.58	1.52
5	M	4	MAN	C4-C5	2.34	1.58	1.53
6	L	1	NAG	C4-C5	2.33	1.57	1.53
5	O	4	MAN	C4-C5	2.32	1.57	1.53
5	K	1	NAG	C4-C5	2.29	1.57	1.53
6	L	2	NAG	C4-C5	2.29	1.57	1.53
5	O	4	MAN	O5-C1	2.28	1.47	1.43
5	M	2	NAG	C4-C3	2.27	1.58	1.52
5	K	2	NAG	C4-C5	2.26	1.57	1.53
5	M	3	BMA	O5-C5	2.25	1.48	1.43
5	K	3	BMA	O5-C5	2.24	1.48	1.43
5	M	2	NAG	C3-C2	2.24	1.57	1.52
6	L	1	NAG	C4-C3	2.23	1.58	1.52
5	O	2	NAG	C3-C2	2.22	1.57	1.52
5	M	3	BMA	C2-C3	2.20	1.55	1.52
5	K	1	NAG	C2-N2	2.17	1.50	1.46
6	N	2	NAG	O5-C1	2.15	1.47	1.43
6	N	1	NAG	C2-N2	2.14	1.50	1.46
5	O	4	MAN	C4-C3	2.14	1.57	1.52
5	K	3	BMA	C1-C2	2.14	1.57	1.52
5	O	3	BMA	C2-C3	2.14	1.55	1.52
5	M	3	BMA	C1-C2	2.13	1.57	1.52
5	O	3	BMA	O5-C5	2.13	1.47	1.43
5	M	2	NAG	O5-C1	2.11	1.47	1.43
5	M	1	NAG	C2-N2	2.11	1.49	1.46
5	K	2	NAG	C4-C3	2.10	1.57	1.52
5	O	5	MAN	C4-C3	2.08	1.57	1.52
5	M	5	MAN	C4-C3	2.08	1.57	1.52
5	M	4	MAN	C4-C3	2.06	1.57	1.52
5	K	4	MAN	C4-C3	2.06	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	1	NAG	C4-C5	2.06	1.57	1.53
6	L	2	NAG	O5-C1	2.05	1.47	1.43
5	K	5	MAN	C4-C3	2.03	1.57	1.52
6	L	2	NAG	C4-C3	2.02	1.57	1.52
5	O	2	NAG	O5-C1	2.02	1.46	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1	NAG	C2-N2-C7	27.82	162.52	122.90
6	L	2	NAG	C8-C7-N2	6.15	126.51	116.10
6	N	1	NAG	C8-C7-N2	6.06	126.36	116.10
6	N	1	NAG	O7-C7-N2	-3.41	115.67	121.95
6	L	2	NAG	O7-C7-N2	-3.24	116.00	121.95
5	K	1	NAG	O4-C4-C3	-3.24	102.87	110.35
5	M	1	NAG	C8-C7-N2	3.13	121.41	116.10
5	K	1	NAG	O4-C4-C5	-3.00	101.85	109.30
6	L	1	NAG	C8-C7-N2	2.82	120.87	116.10
5	O	1	NAG	O4-C4-C3	-2.62	104.29	110.35
5	K	2	NAG	C8-C7-N2	2.50	120.34	116.10
6	L	2	NAG	O7-C7-C8	-2.46	117.49	122.06
6	N	2	NAG	C8-C7-N2	2.43	120.21	116.10
5	O	1	NAG	C8-C7-N2	2.35	120.08	116.10
5	M	1	NAG	O4-C4-C3	-2.33	104.96	110.35
6	N	1	NAG	O7-C7-C8	-2.20	117.97	122.06
5	K	2	NAG	O7-C7-C8	-2.18	118.01	122.06
5	K	1	NAG	C8-C7-N2	2.11	119.68	116.10
5	M	1	NAG	O7-C7-C8	-2.08	118.19	122.06
6	N	2	NAG	O7-C7-C8	-2.07	118.20	122.06
5	M	2	NAG	C8-C7-N2	2.04	119.55	116.10

There are no chirality outliers.

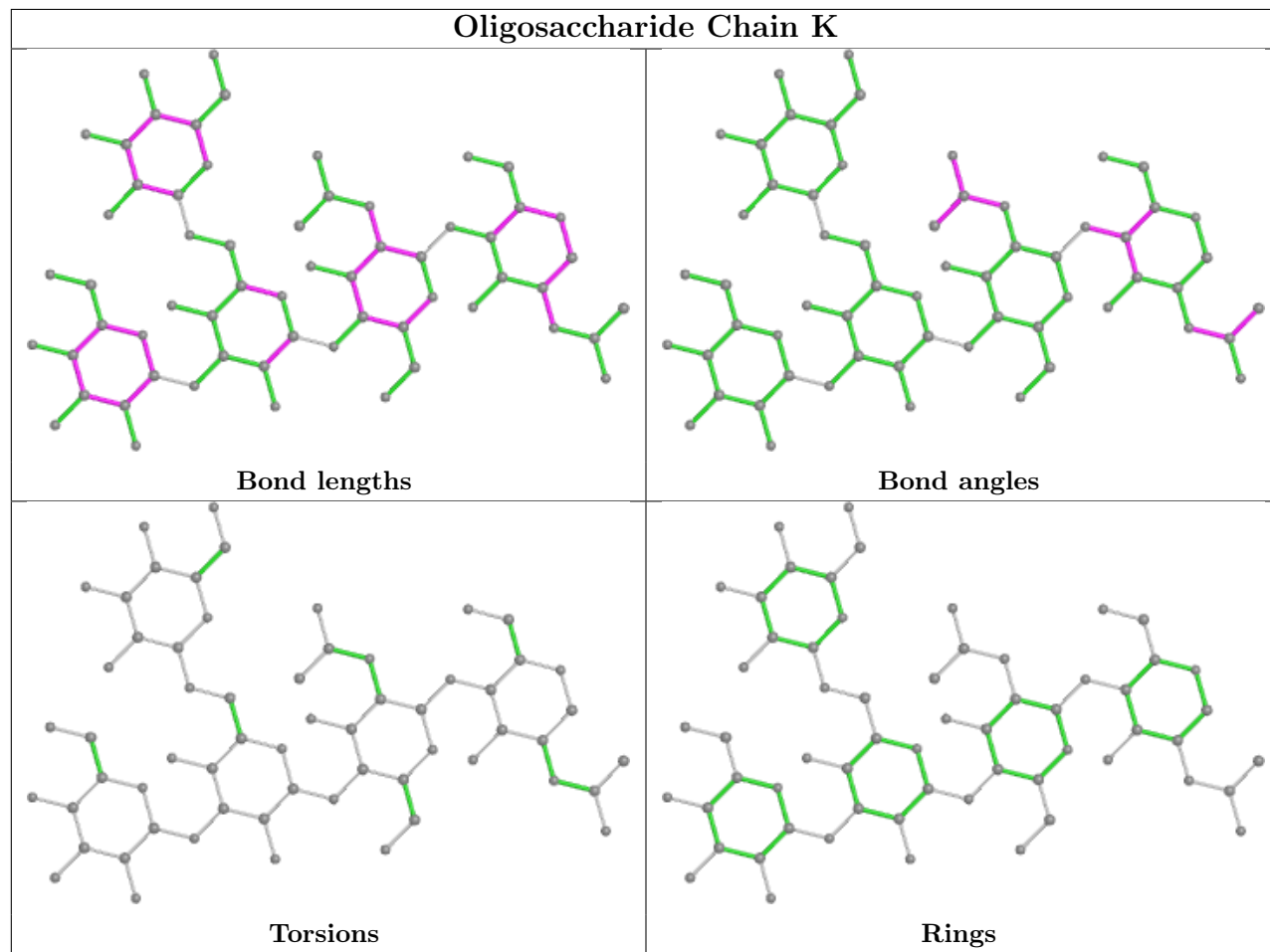
All (7) torsion outliers are listed below:

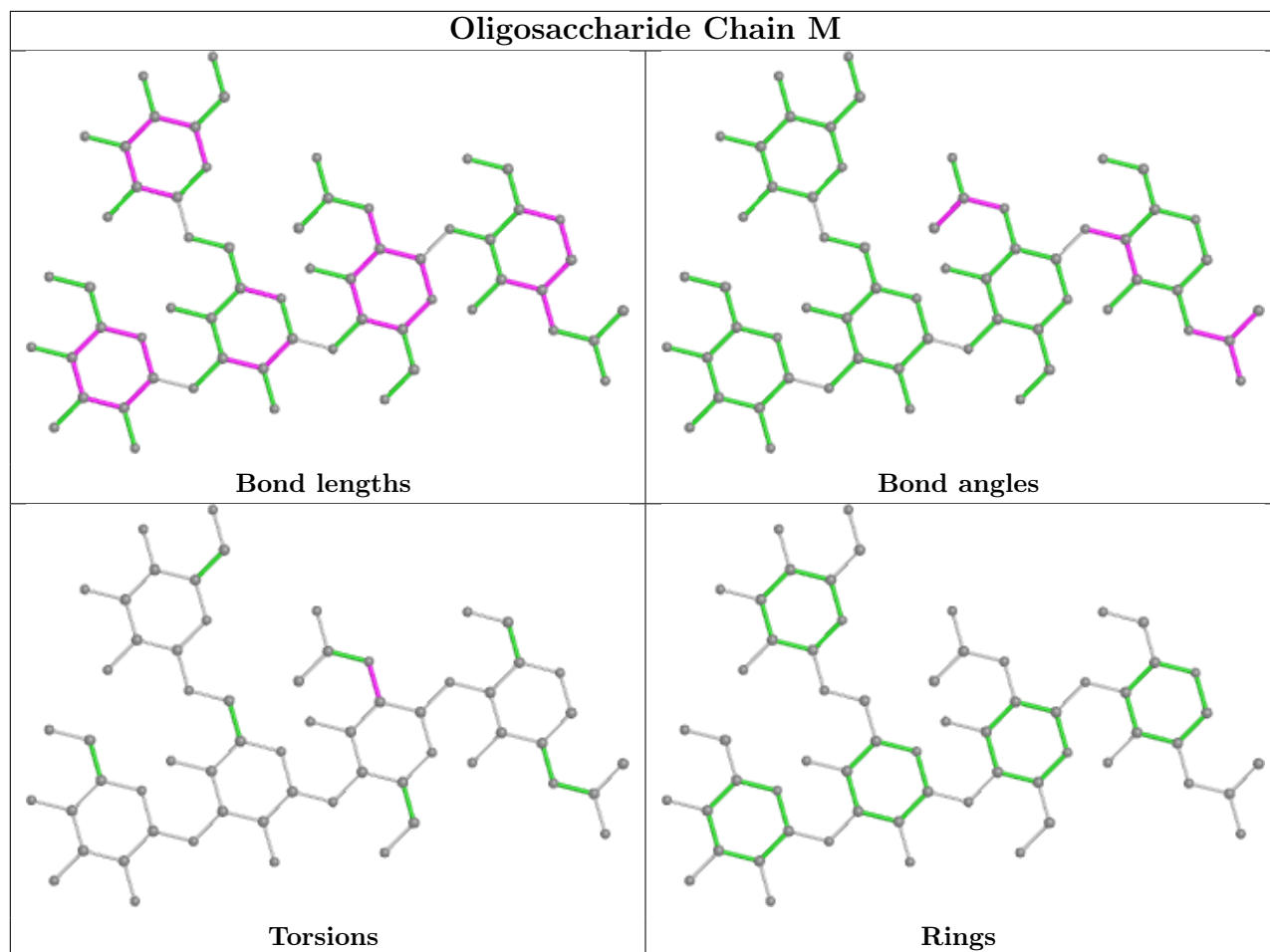
Mol	Chain	Res	Type	Atoms
6	L	1	NAG	C3-C2-N2-C7
6	L	2	NAG	C8-C7-N2-C2
6	L	2	NAG	O7-C7-N2-C2
6	N	1	NAG	C8-C7-N2-C2
6	N	1	NAG	O7-C7-N2-C2
5	M	2	NAG	C3-C2-N2-C7
5	O	2	NAG	C3-C2-N2-C7

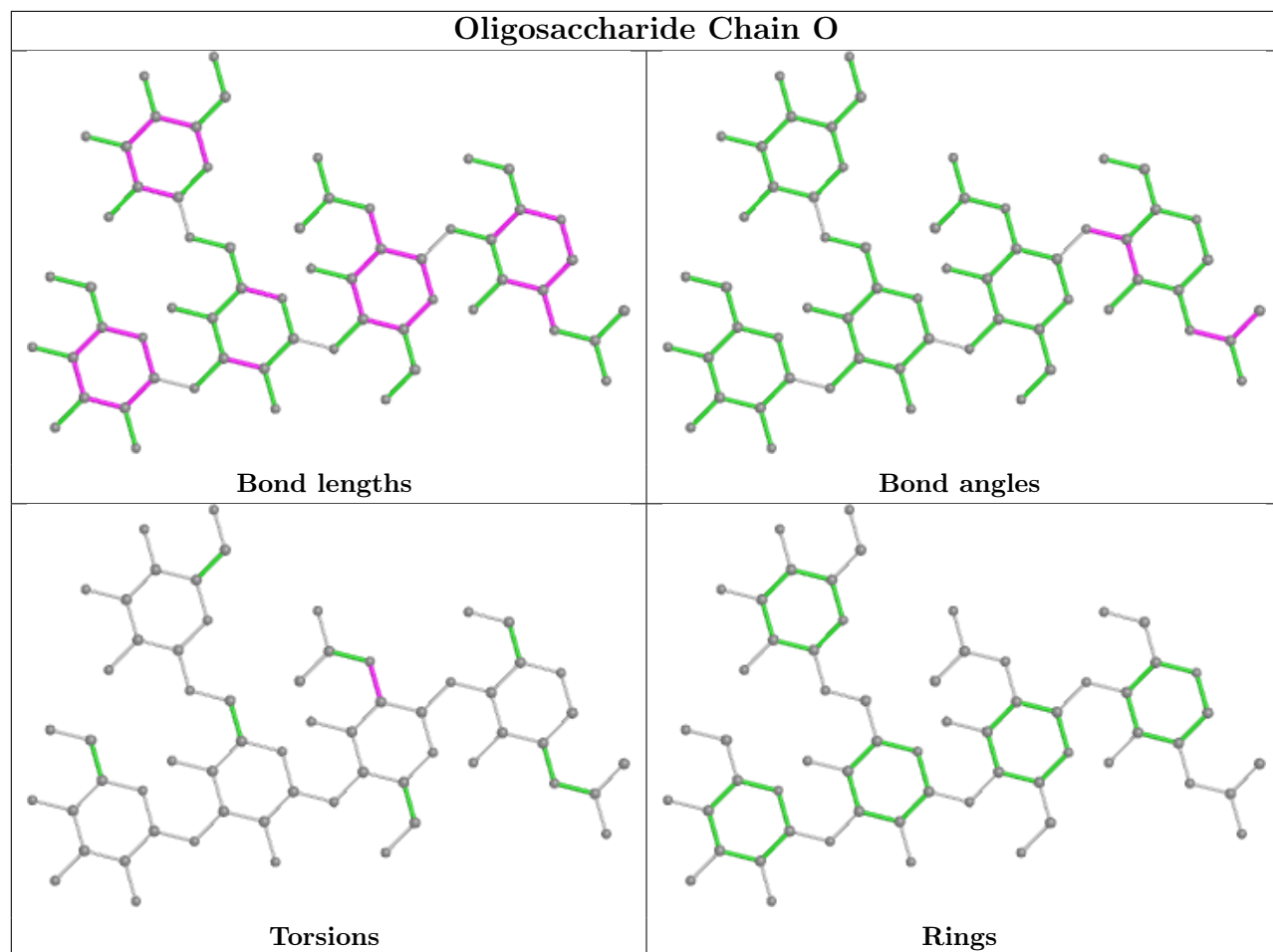
There are no ring outliers.

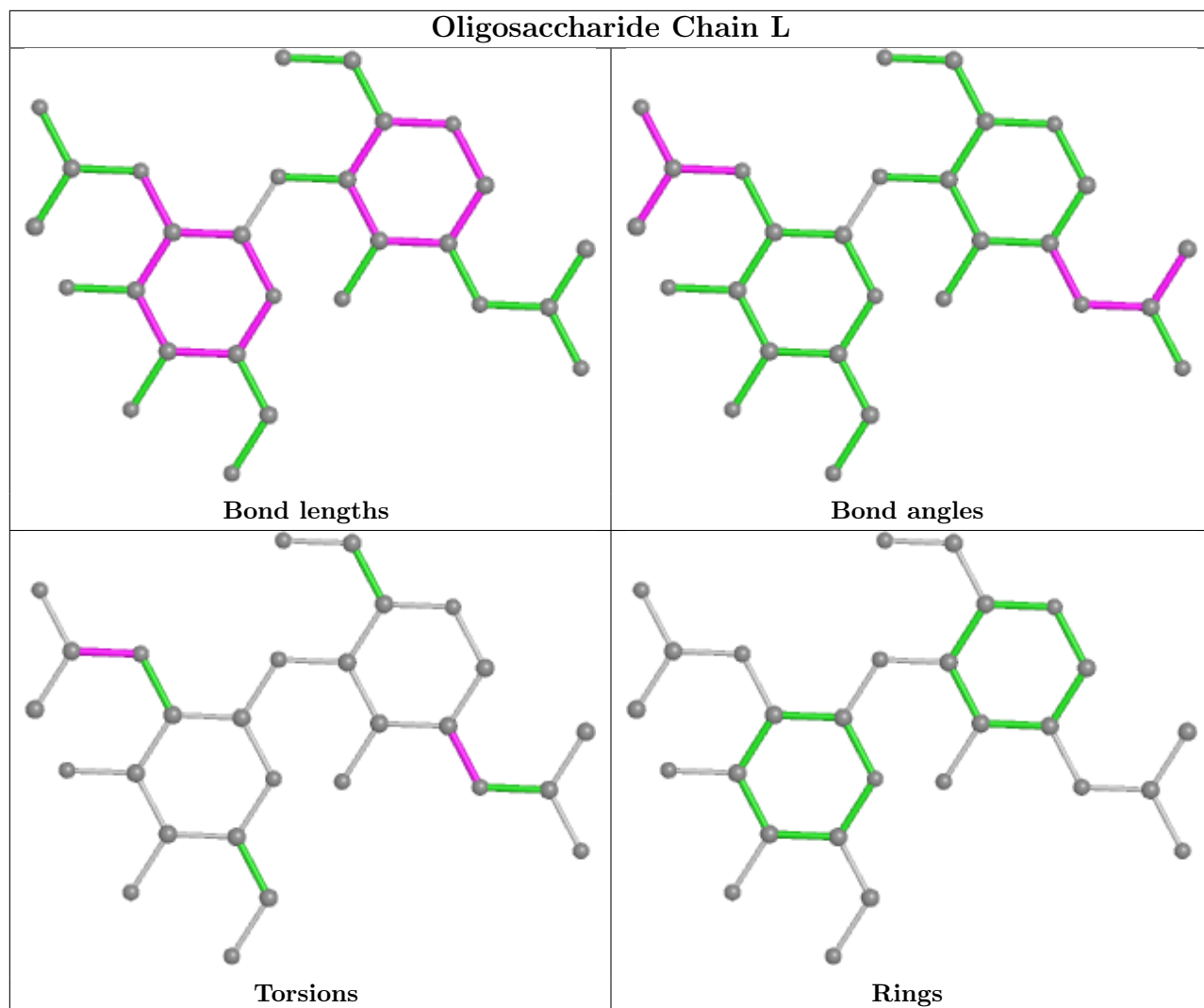
No monomer is involved in short contacts.

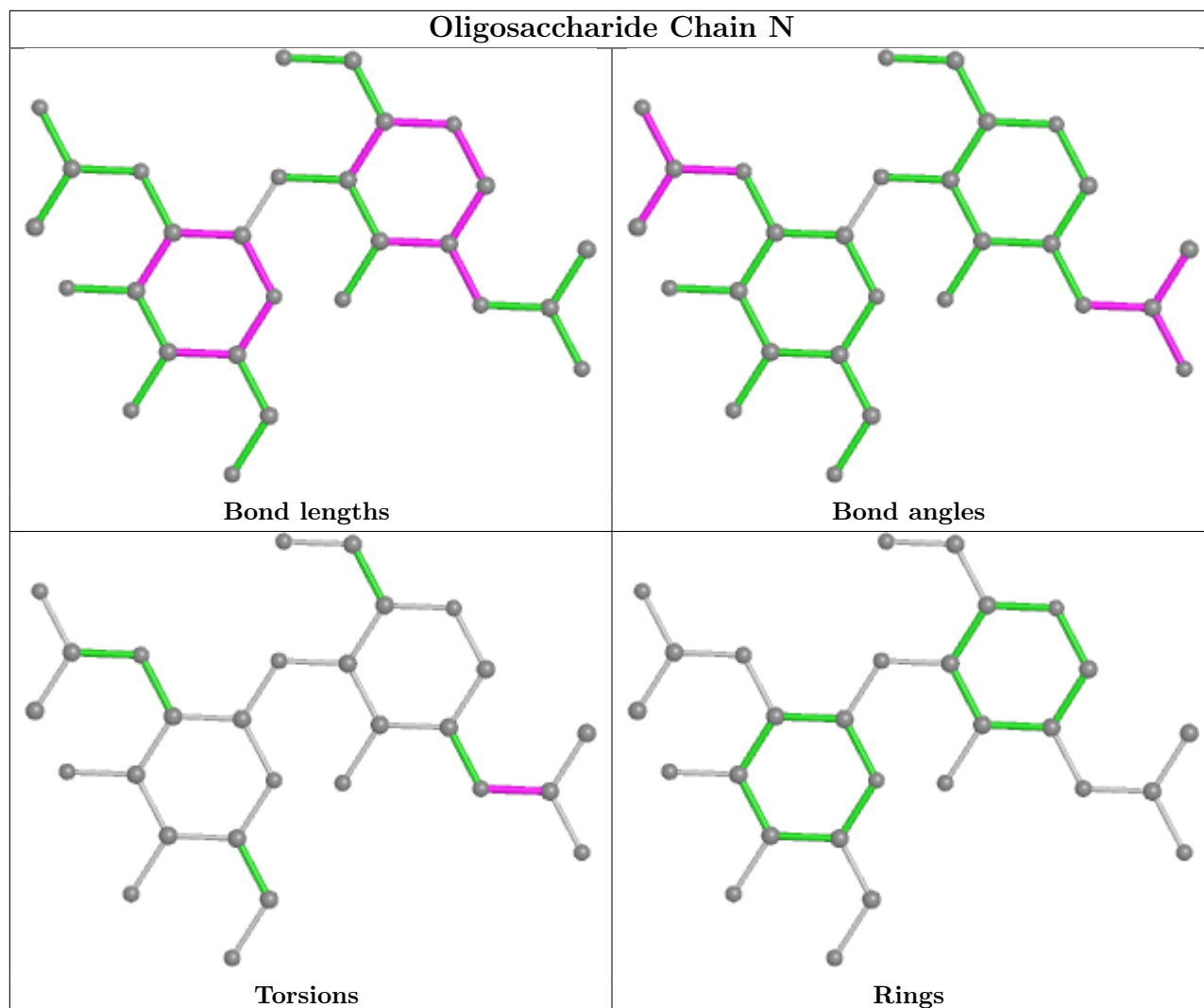
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

2 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	C	401	3	14,14,15	2.18	5 (35%)	17,19,21	0.93	1 (5%)
7	NAG	B	401	3	14,14,15	2.16	5 (35%)	17,19,21	0.94	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	C	401	3	-	0/6/23/26	0/1/1/1
7	NAG	B	401	3	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	401	NAG	C1-C2	5.48	1.60	1.52
7	B	401	NAG	C1-C2	5.30	1.60	1.52
7	B	401	NAG	O5-C5	3.21	1.50	1.43
7	C	401	NAG	O5-C5	3.06	1.49	1.43
7	B	401	NAG	O5-C1	2.78	1.48	1.43
7	C	401	NAG	O5-C1	2.72	1.48	1.43
7	B	401	NAG	C3-C2	2.34	1.57	1.52
7	C	401	NAG	C3-C2	2.31	1.57	1.52
7	C	401	NAG	C4-C5	2.24	1.57	1.53
7	B	401	NAG	C4-C5	2.21	1.57	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	401	NAG	C8-C7-N2	2.03	119.54	116.10
7	C	401	NAG	C8-C7-N2	2.01	119.50	116.10

There are no chirality outliers.

There are no torsion outliers.

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.

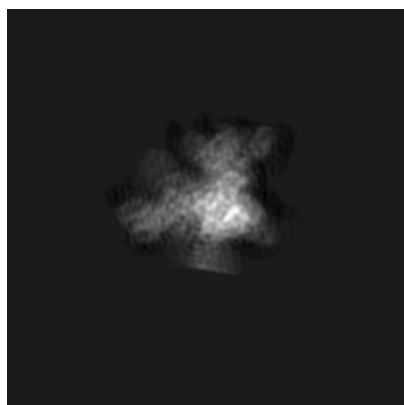
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22851. These allow visual inspection of the internal detail of the map and identification of artifacts.

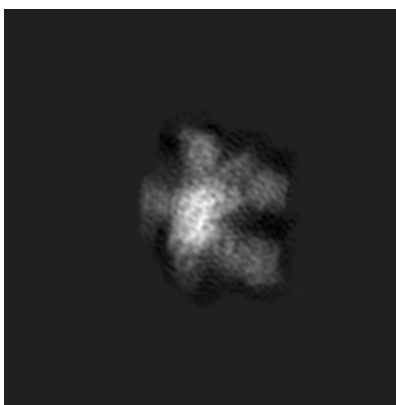
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

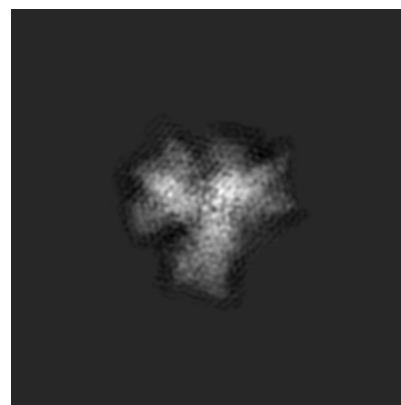
6.1.1 Primary map



X



Y

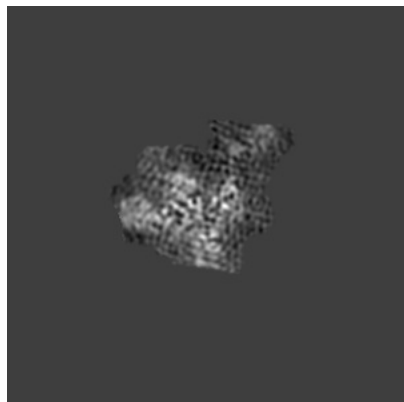


Z

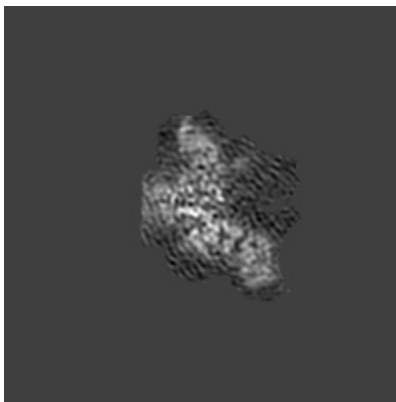
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

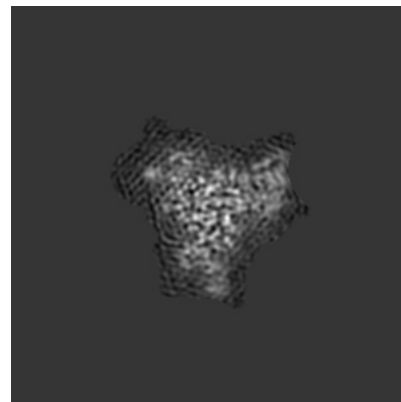
6.2.1 Primary map



X Index: 144



Y Index: 144

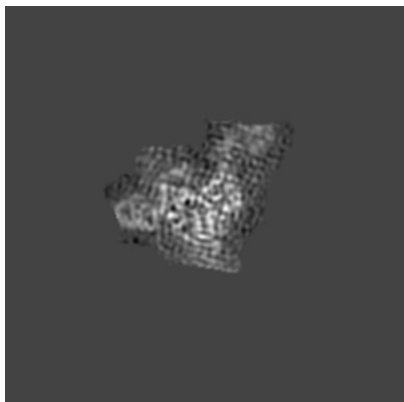


Z Index: 144

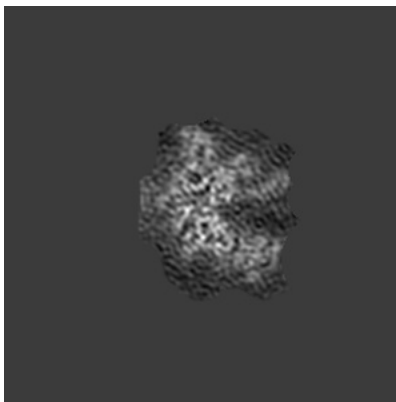
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

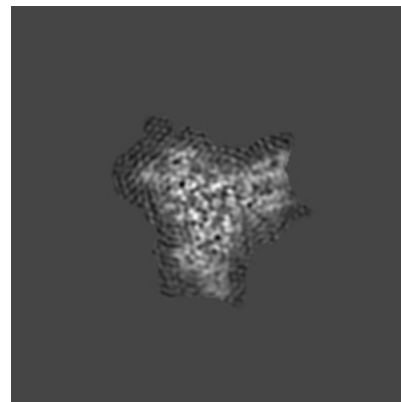
6.3.1 Primary map



X Index: 149



Y Index: 153



Z Index: 142

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0289. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

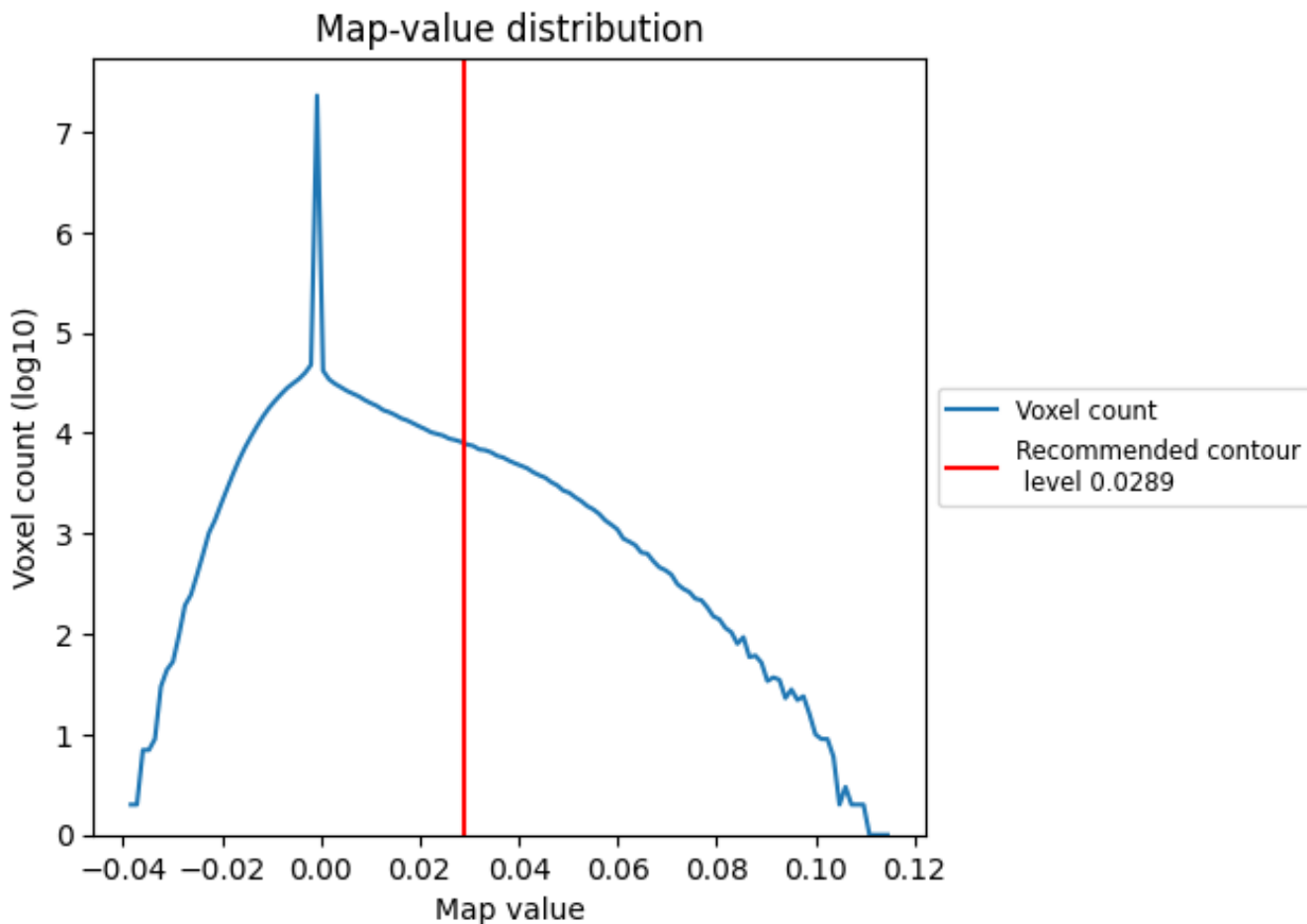
6.5 Mask visualisation

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

7 Map analysis [i](#)

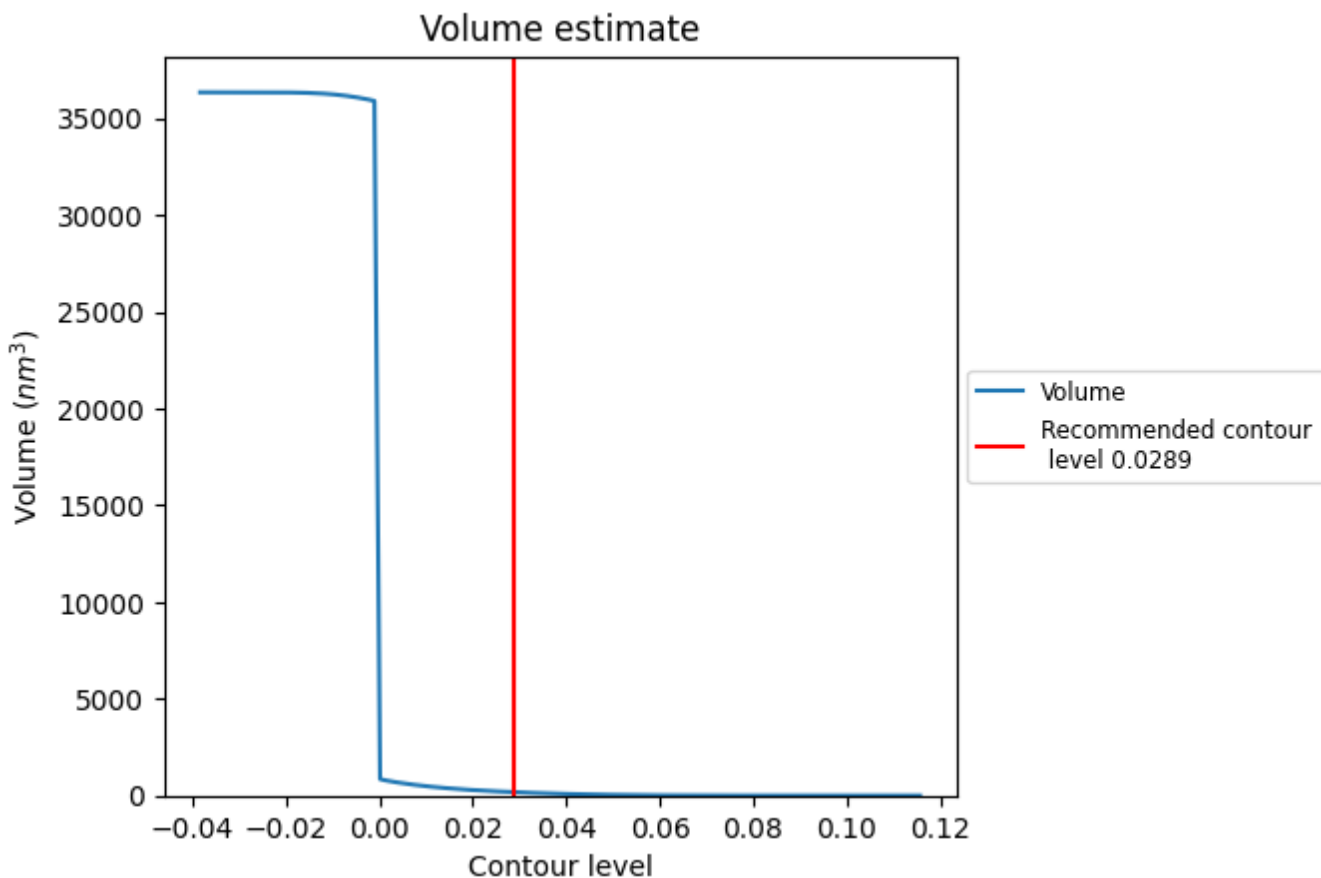
This section contains the results of statistical analysis of the map.

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.

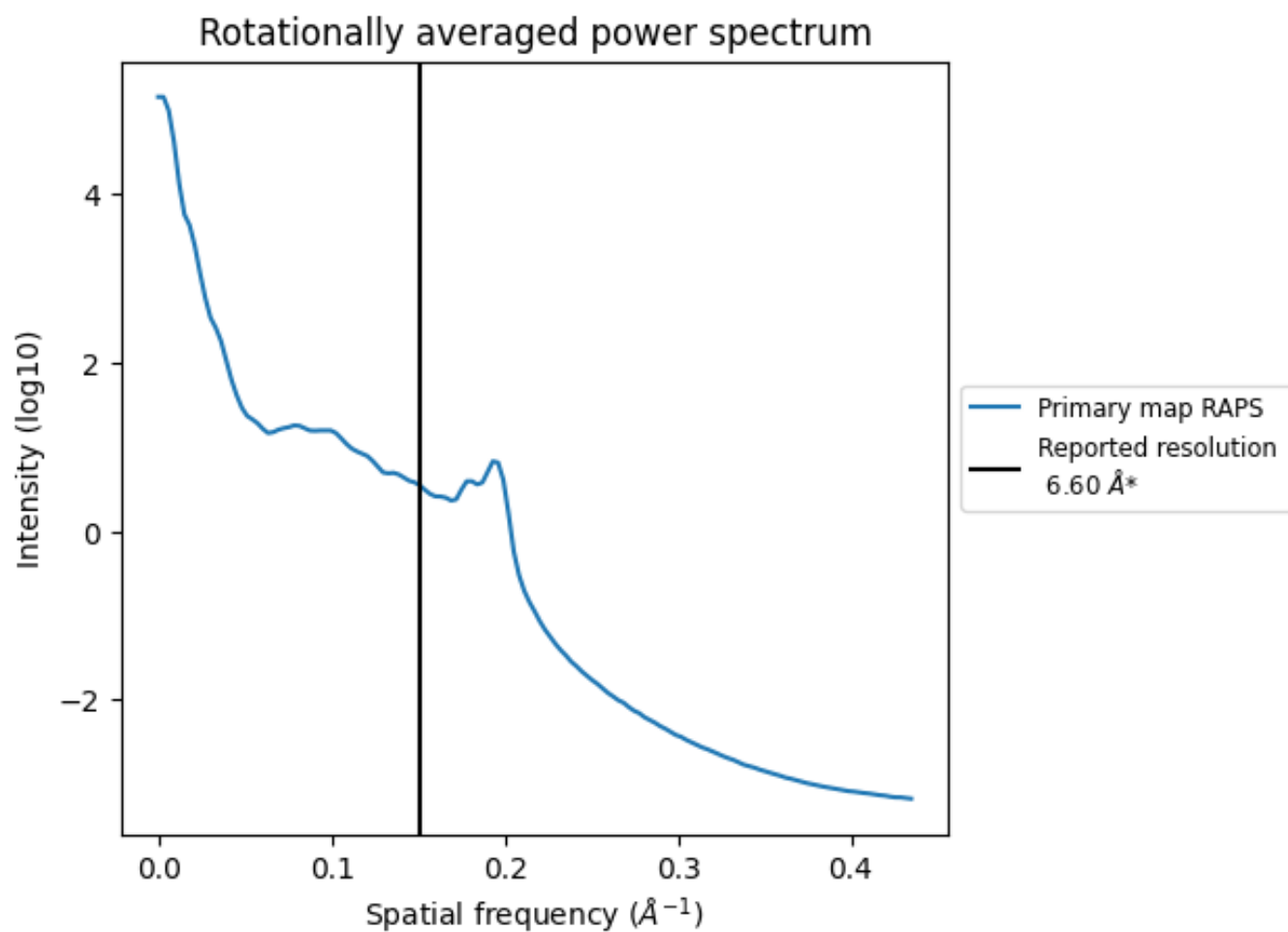
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 176 nm³; this corresponds to an approximate mass of 159 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](#)

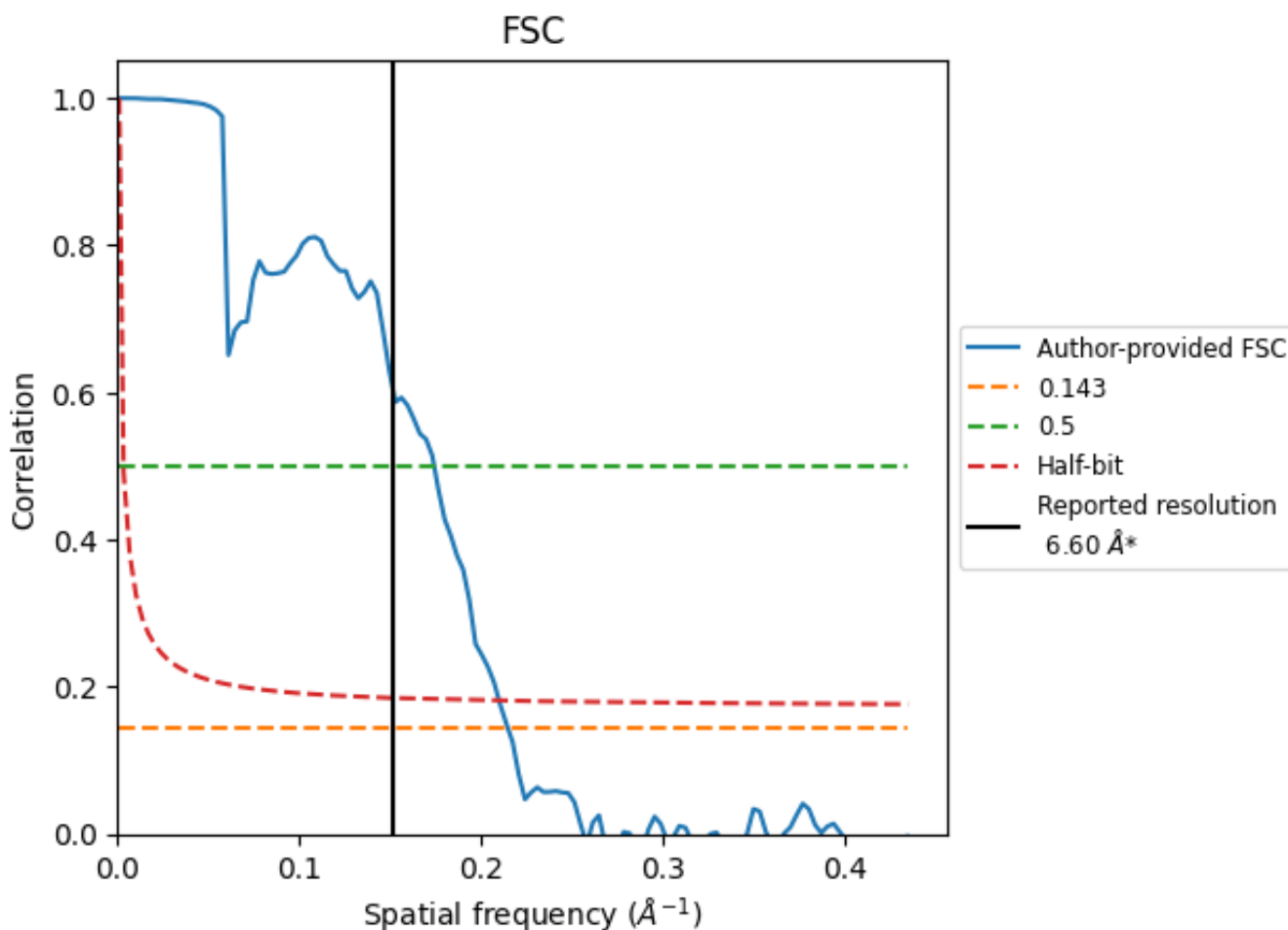


*Reported resolution corresponds to spatial frequency of 0.152\AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.152 Å⁻¹

8.2 Resolution estimates [i](#)

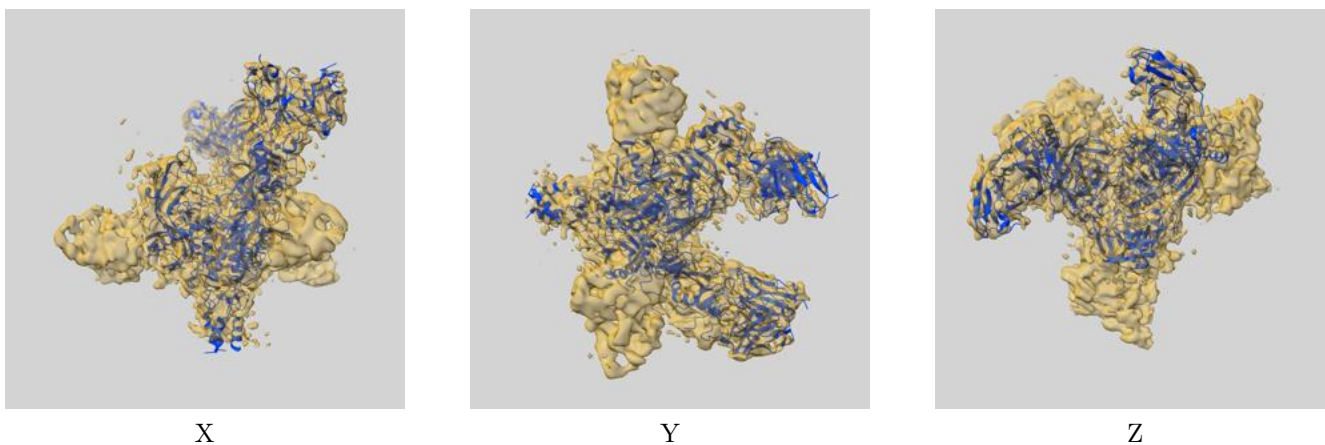
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.60	-	-
Author-provided FSC curve	4.66	5.74	4.76
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.66 differs from the reported value 6.6 by more than 10 %

9 Map-model fit [i](#)

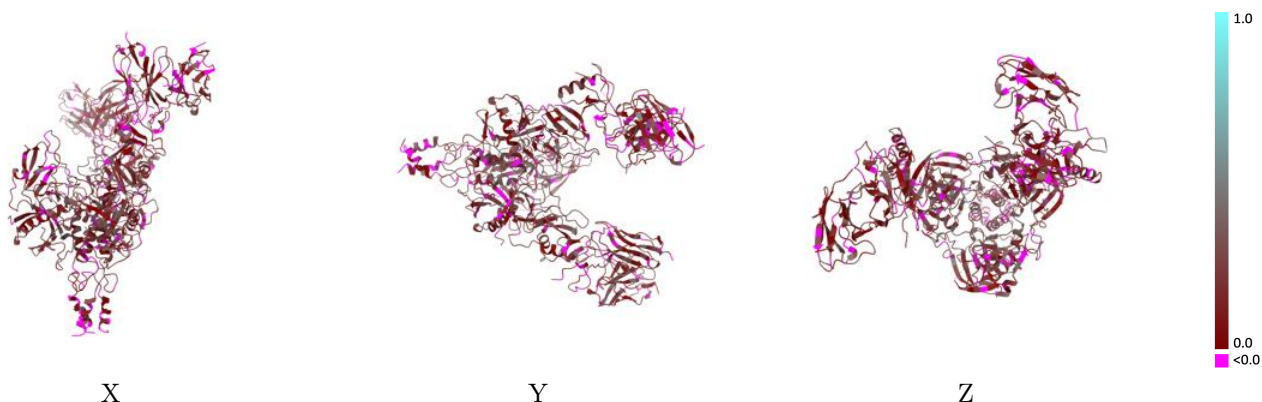
This section contains information regarding the fit between EMDB map EMD-22851 and PDB model 7KFE. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



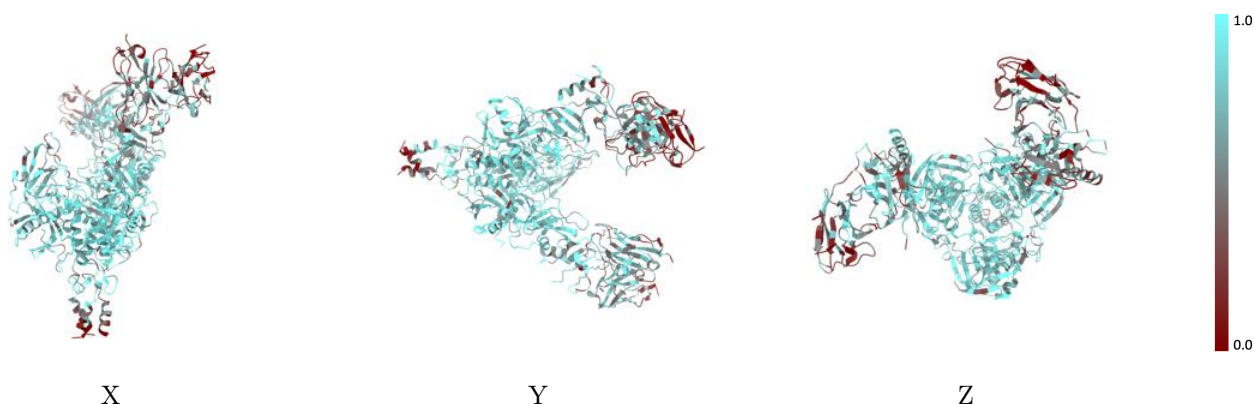
The images above show the 3D surface view of the map at the recommended contour level 0.0289 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



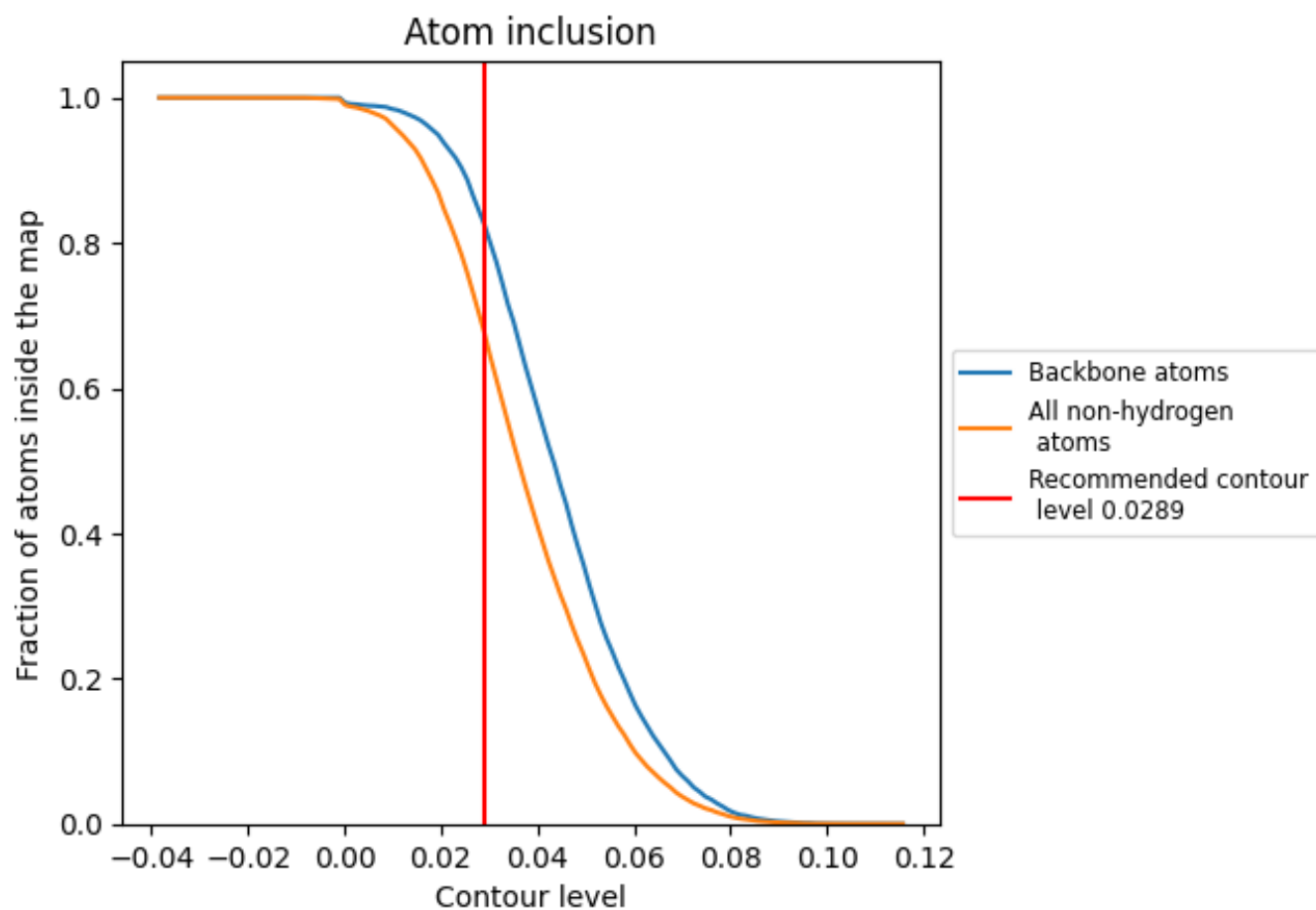
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0289).

































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 68% 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 (0.0289) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6785	 0.1710
A	 0.7725	 0.1910
B	 0.7661	 0.1950
C	 0.7883	 0.2050
D	 0.7330	 0.1720
E	 0.7754	 0.1760
F	 0.7385	 0.1580
G	 0.4875	 0.1170
H	 0.6149	 0.1460
I	 0.3704	 0.1240
J	 0.5082	 0.1490
K	 0.6885	 0.2710
L	 0.5357	 0.2050
M	 0.6557	 0.2920
N	 0.6786	 0.2070
O	 0.6885	 0.2870

