



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 04:59 AM EDT

PDB ID : 7SHY
Title : IgE-Fc in complex with omalizumab scFv
Authors : Pennington, L.F.; Jardetzky, T.J.; Kleinboelting, S.
Deposited on : 2021-10-11
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

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:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

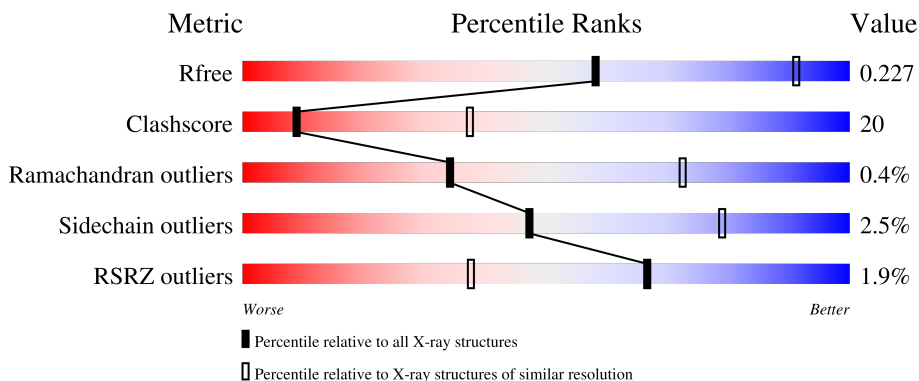
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.






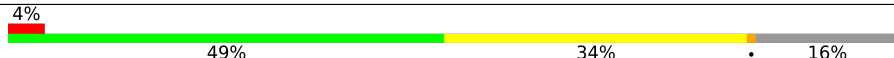


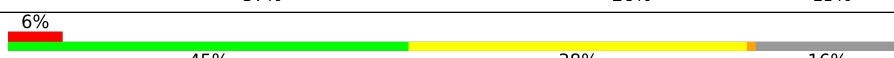




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	122	66% (green), 33% (yellow), . (grey)
1	E	122	75% (green), 25% (yellow), . (grey)
1	I	122	65% (green), 33% (yellow), .. (grey)
1	K	122	2% (red), 63% (green), 34% (yellow), .. (grey)
2	D	134	61% (green), 22% (yellow), . (grey), 15% (grey)

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	134	
2	J	134	
2	L	134	
3	A	247	
3	B	247	
3	G	247	
3	H	247	
4	M	6	
5	N	6	
6	O	4	
7	P	7	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MAN	H	601	-	-	X	-
4	NAG	M	1	X	-	-	-
4	NAG	M	2	-	-	X	-
6	NAG	O	1	X	-	X	-
6	BMA	O	3	-	-	X	-
9	NAG	B	601	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 14133 atoms, of which 8 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Omalizumab VH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	I	120	Total 931	C 589	N 162	O 177	S 3	0	0	0
1	K	120	Total 931	C 589	N 162	O 177	S 3	0	0	0
1	C	121	Total 937	C 592	N 163	O 179	S 3	0	0	0
1	E	121	Total 937	C 592	N 163	O 179	S 3	0	0	0

- Molecule 2 is a protein called Omalizumab VL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	J	115	Total 873	C 545	N 142	O 183	S 3	0	0	0
2	L	113	Total 865	C 540	N 140	O 182	S 3	0	0	0
2	D	114	Total 868	C 542	N 141	O 182	S 3	0	0	0
2	F	112	Total 860	C 538	N 139	O 180	S 3	0	0	0

- Molecule 3 is a protein called IgE Fc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	208	Total 1646	C 1031	N 303	O 306	S 6	0	0	0
3	G	209	Total 1650	C 1032	N 304	O 308	S 6	0	0	0
3	H	208	Total 1631	C 1022	N 297	O 306	S 6	0	0	0
3	B	210	Total 1655	C 1036	N 305	O 308	S 6	0	0	0

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	299	ALA	-	expression tag	UNP P01854
A	300	PRO	-	expression tag	UNP P01854
A	301	MET	-	expression tag	UNP P01854
A	302	ALA	-	expression tag	UNP P01854
A	303	GLU	-	expression tag	UNP P01854
A	304	GLY	-	expression tag	UNP P01854
A	305	GLY	-	expression tag	UNP P01854
A	306	GLY	-	expression tag	UNP P01854
A	307	GLN	-	expression tag	UNP P01854
A	308	ASN	-	expression tag	UNP P01854
A	309	HIS	-	expression tag	UNP P01854
A	310	HIS	-	expression tag	UNP P01854
A	311	HIS	-	expression tag	UNP P01854
A	312	HIS	-	expression tag	UNP P01854
A	313	HIS	-	expression tag	UNP P01854
A	314	HIS	-	expression tag	UNP P01854
A	315	HIS	-	expression tag	UNP P01854
A	316	HIS	-	expression tag	UNP P01854
A	317	GLY	-	expression tag	UNP P01854
A	318	GLY	-	expression tag	UNP P01854
A	319	GLU	-	expression tag	UNP P01854
A	320	ASN	-	expression tag	UNP P01854
A	321	LEU	-	expression tag	UNP P01854
A	322	TYR	-	expression tag	UNP P01854
A	323	PHE	-	expression tag	UNP P01854
A	324	GLN	-	expression tag	UNP P01854
A	325	GLY	-	expression tag	UNP P01854
A	326	GLY	-	expression tag	UNP P01854
A	327	SER	-	expression tag	UNP P01854
G	299	ALA	-	expression tag	UNP P01854
G	300	PRO	-	expression tag	UNP P01854
G	301	MET	-	expression tag	UNP P01854
G	302	ALA	-	expression tag	UNP P01854
G	303	GLU	-	expression tag	UNP P01854
G	304	GLY	-	expression tag	UNP P01854
G	305	GLY	-	expression tag	UNP P01854
G	306	GLY	-	expression tag	UNP P01854
G	307	GLN	-	expression tag	UNP P01854
G	308	ASN	-	expression tag	UNP P01854
G	309	HIS	-	expression tag	UNP P01854
G	310	HIS	-	expression tag	UNP P01854
G	311	HIS	-	expression tag	UNP P01854

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	312	HIS	-	expression tag	UNP P01854
G	313	HIS	-	expression tag	UNP P01854
G	314	HIS	-	expression tag	UNP P01854
G	315	HIS	-	expression tag	UNP P01854
G	316	HIS	-	expression tag	UNP P01854
G	317	GLY	-	expression tag	UNP P01854
G	318	GLY	-	expression tag	UNP P01854
G	319	GLU	-	expression tag	UNP P01854
G	320	ASN	-	expression tag	UNP P01854
G	321	LEU	-	expression tag	UNP P01854
G	322	TYR	-	expression tag	UNP P01854
G	323	PHE	-	expression tag	UNP P01854
G	324	GLN	-	expression tag	UNP P01854
G	325	GLY	-	expression tag	UNP P01854
G	326	GLY	-	expression tag	UNP P01854
G	327	SER	-	expression tag	UNP P01854
H	299	ALA	-	expression tag	UNP P01854
H	300	PRO	-	expression tag	UNP P01854
H	301	MET	-	expression tag	UNP P01854
H	302	ALA	-	expression tag	UNP P01854
H	303	GLU	-	expression tag	UNP P01854
H	304	GLY	-	expression tag	UNP P01854
H	305	GLY	-	expression tag	UNP P01854
H	306	GLY	-	expression tag	UNP P01854
H	307	GLN	-	expression tag	UNP P01854
H	308	ASN	-	expression tag	UNP P01854
H	309	HIS	-	expression tag	UNP P01854
H	310	HIS	-	expression tag	UNP P01854
H	311	HIS	-	expression tag	UNP P01854
H	312	HIS	-	expression tag	UNP P01854
H	313	HIS	-	expression tag	UNP P01854
H	314	HIS	-	expression tag	UNP P01854
H	315	HIS	-	expression tag	UNP P01854
H	316	HIS	-	expression tag	UNP P01854
H	317	GLY	-	expression tag	UNP P01854
H	318	GLY	-	expression tag	UNP P01854
H	319	GLU	-	expression tag	UNP P01854
H	320	ASN	-	expression tag	UNP P01854
H	321	LEU	-	expression tag	UNP P01854
H	322	TYR	-	expression tag	UNP P01854
H	323	PHE	-	expression tag	UNP P01854
H	324	GLN	-	expression tag	UNP P01854

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	325	GLY	-	expression tag	UNP P01854
H	326	GLY	-	expression tag	UNP P01854
H	327	SER	-	expression tag	UNP P01854
B	299	ALA	-	expression tag	UNP P01854
B	300	PRO	-	expression tag	UNP P01854
B	301	MET	-	expression tag	UNP P01854
B	302	ALA	-	expression tag	UNP P01854
B	303	GLU	-	expression tag	UNP P01854
B	304	GLY	-	expression tag	UNP P01854
B	305	GLY	-	expression tag	UNP P01854
B	306	GLY	-	expression tag	UNP P01854
B	307	GLN	-	expression tag	UNP P01854
B	308	ASN	-	expression tag	UNP P01854
B	309	HIS	-	expression tag	UNP P01854
B	310	HIS	-	expression tag	UNP P01854
B	311	HIS	-	expression tag	UNP P01854
B	312	HIS	-	expression tag	UNP P01854
B	313	HIS	-	expression tag	UNP P01854
B	314	HIS	-	expression tag	UNP P01854
B	315	HIS	-	expression tag	UNP P01854
B	316	HIS	-	expression tag	UNP P01854
B	317	GLY	-	expression tag	UNP P01854
B	318	GLY	-	expression tag	UNP P01854
B	319	GLU	-	expression tag	UNP P01854
B	320	ASN	-	expression tag	UNP P01854
B	321	LEU	-	expression tag	UNP P01854
B	322	TYR	-	expression tag	UNP P01854
B	323	PHE	-	expression tag	UNP P01854
B	324	GLN	-	expression tag	UNP P01854
B	325	GLY	-	expression tag	UNP P01854
B	326	GLY	-	expression tag	UNP P01854
B	327	SER	-	expression tag	UNP P01854

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(2-3)-[alpha-L-fucopyranose-(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			ZeroOcc	AltConf	Trace	
			Total	C	N				O
4	M	6	71	40	2	29	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[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.

ta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	N	6	72	40	2	30	0	0	0

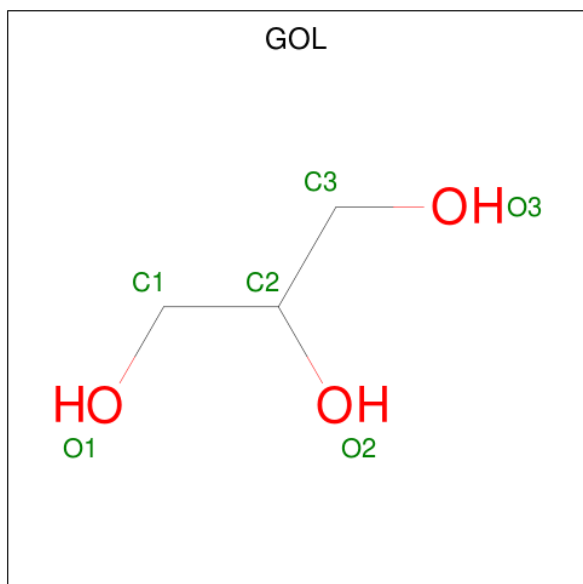
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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.

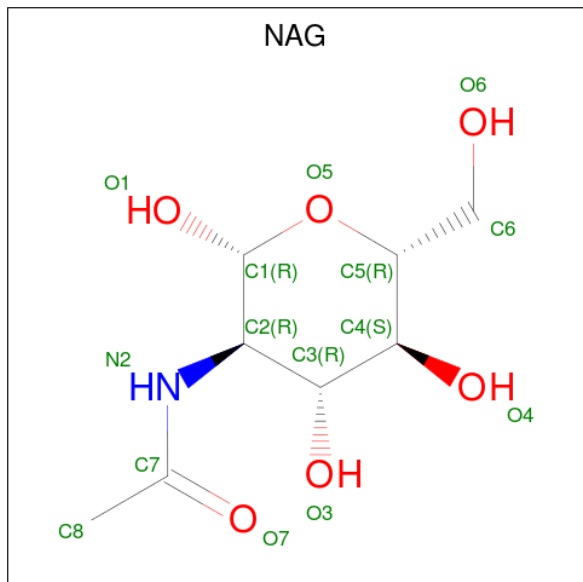
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	P	7	83	46	2	35	0	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



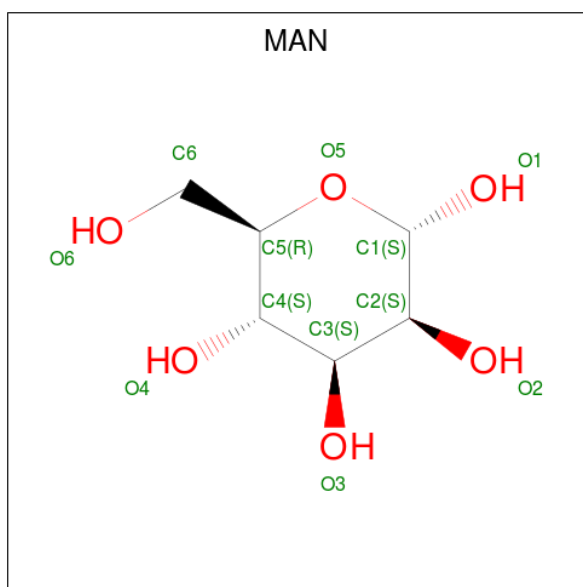
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
8	D	1	14	3	8	3	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 10 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	C	O	0	0
			11	6	5		

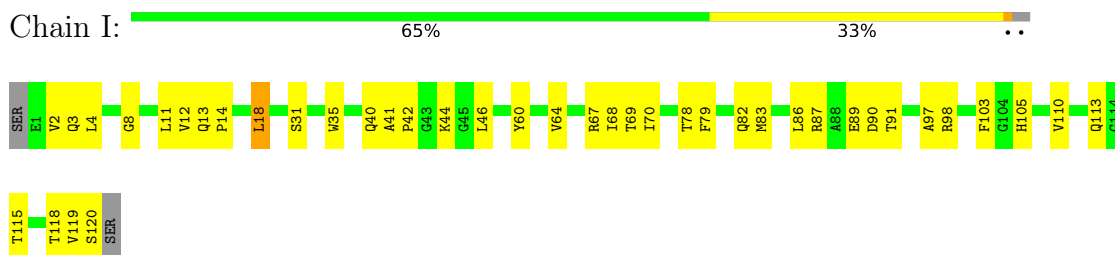
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	K	1	Total	O	0	0
			1	1		
11	L	1	Total	O	0	0
			1	1		
11	D	1	Total	O	0	0
			1	1		
11	G	2	Total	O	0	0
			2	2		
11	B	1	Total	O	0	0
			1	1		

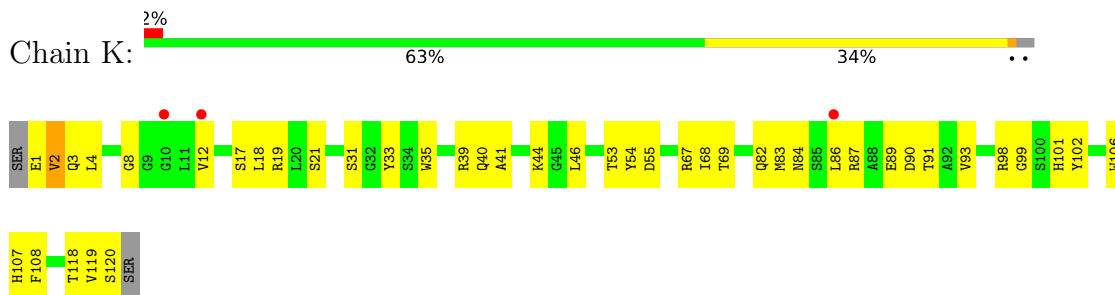
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

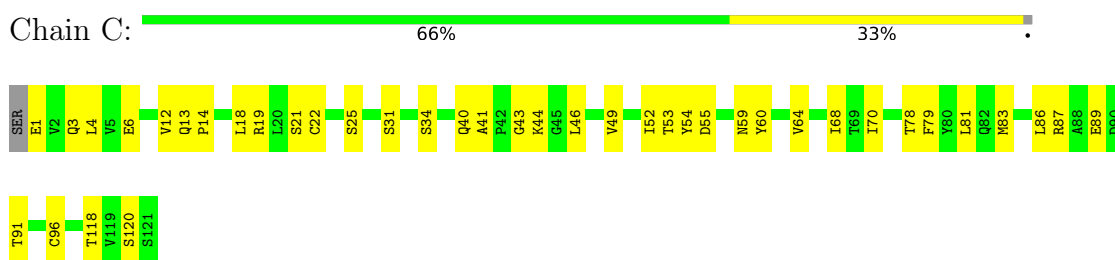
- Molecule 1: Omalizumab VH



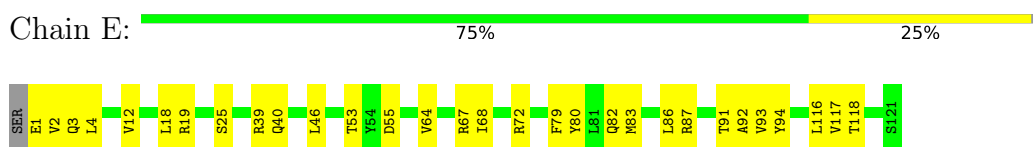
- Molecule 1: Omalizumab VH



- Molecule 1: Omalizumab VH



- Molecule 1: Omalizumab VH



- Molecule 2: Omalizumab VL

Chain M:  33% 67%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

- Molecule 5: beta-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[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

Chain N:  67% 33%

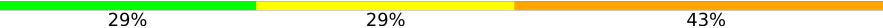
MAG1
MAG2
BMA3
MAN4
BMA5
MAN6

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

Chain O:  25% 75%

MAG1
MAG2
BMA3
MAN4

- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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

Chain P:  29% 29% 43%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.50Å 179.09Å 91.52Å 90.00° 111.66° 90.00°	Depositor
Resolution (Å)	39.93 – 3.00 49.62 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.93-3.00) 97.9 (49.62-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.14	Depositor
R, R_{free}	0.173 , 0.230 0.167 , 0.227	Depositor DCC
R_{free} test set	2308 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	87.8	Xtrriage
Anisotropy	0.450	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14133	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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, FUC, MAN, BMA, GOL

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	C	0.58	0/963	0.75	0/1310
1	E	0.53	0/963	0.71	0/1310
1	I	0.54	0/957	0.74	1/1302 (0.1%)
1	K	0.45	0/957	0.66	0/1302
2	D	0.55	0/888	0.74	0/1205
2	F	0.51	0/880	0.70	0/1195
2	J	0.58	1/893 (0.1%)	0.72	0/1212
2	L	0.47	0/885	0.69	0/1201
3	A	0.42	0/1688	0.66	1/2298 (0.0%)
3	B	0.49	0/1697	0.68	0/2310
3	G	0.53	0/1692	0.75	2/2305 (0.1%)
3	H	0.43	0/1672	0.66	0/2279
All	All	0.50	1/14135 (0.0%)	0.70	4/19229 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	46	LYS	C-N	-5.88	1.20	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	348	LEU	CA-CB-CG	6.55	130.38	115.30
3	A	479	LEU	CB-CG-CD1	-6.17	100.51	111.00
3	G	372	LEU	CA-CB-CG	5.76	128.54	115.30
1	I	18	LEU	CA-CB-CG	5.43	127.79	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	424	HIS	Peptide

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	C	937	0	886	30	0
1	E	937	0	886	35	0
1	I	931	0	881	34	0
1	K	931	0	881	41	0
2	D	868	0	814	27	0
2	F	860	0	808	16	0
2	J	873	0	816	22	0
2	L	865	0	814	20	1
3	A	1646	0	1630	91	0
3	B	1655	0	1636	71	1
3	G	1650	0	1626	67	0
3	H	1631	0	1603	114	0
4	M	71	0	60	9	0
5	N	72	0	61	4	0
6	O	50	0	43	15	0
7	P	83	0	70	4	0
8	D	6	8	8	0	0
9	A	14	0	13	1	0
9	B	14	0	13	1	0
9	H	14	0	13	1	0
10	H	11	0	10	6	0
11	B	1	0	0	0	0
11	D	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	G	2	0	0	0	0
11	K	1	0	0	0	0
11	L	1	0	0	0	0
All	All	14125	8	13572	561	1

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 20.

The worst 5 of 561 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)
3:H:479:LEU:HG	3:H:523:ILE:HB	1.30	1.13
1:K:68:ILE:HD12	1:K:83:MET:HG2	1.37	1.06
1:E:64:VAL:HB	1:E:68:ILE:HD12	1.37	1.04
1:C:68:ILE:HD11	1:C:81:LEU:HD11	1.38	1.04
3:H:396:THR:HG21	6:O:1:NAG:C7	1.91	1.00

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:85:GLU:OE2	3:B:458:ASP:OD2[4_557]	2.06	0.14

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 X-ray entries followed by that with respect to entries of similar resolution.

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	C	119/122 (98%)	115 (97%)	4 (3%)	0	100 100
1	E	119/122 (98%)	113 (95%)	6 (5%)	0	100 100
1	I	118/122 (97%)	112 (95%)	6 (5%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	118/122 (97%)	114 (97%)	3 (2%)	1 (1%)	19	57
2	D	112/134 (84%)	107 (96%)	5 (4%)	0	100	100
2	F	110/134 (82%)	106 (96%)	4 (4%)	0	100	100
2	J	113/134 (84%)	109 (96%)	4 (4%)	0	100	100
2	L	111/134 (83%)	105 (95%)	6 (5%)	0	100	100
3	A	206/247 (83%)	197 (96%)	9 (4%)	0	100	100
3	B	208/247 (84%)	195 (94%)	11 (5%)	2 (1%)	15	53
3	G	207/247 (84%)	198 (96%)	7 (3%)	2 (1%)	15	53
3	H	206/247 (83%)	190 (92%)	14 (7%)	2 (1%)	15	53
All	All	1747/2012 (87%)	1661 (95%)	79 (4%)	7 (0%)	34	72

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	383	ASN
3	G	368	GLY
3	H	436	THR
3	H	481	ASN
3	B	383	ASN

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 X-ray entries followed by that with respect to entries of similar resolution.

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	C	99/100 (99%)	94 (95%)	5 (5%)	24	60
1	E	99/100 (99%)	98 (99%)	1 (1%)	76	91
1	I	98/100 (98%)	96 (98%)	2 (2%)	55	83
1	K	98/100 (98%)	97 (99%)	1 (1%)	76	91
2	D	96/113 (85%)	92 (96%)	4 (4%)	30	66
2	F	96/113 (85%)	91 (95%)	5 (5%)	23	59
2	J	96/113 (85%)	93 (97%)	3 (3%)	40	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	97/113 (86%)	92 (95%)	5 (5%)	23	59
3	A	184/212 (87%)	179 (97%)	5 (3%)	44	77
3	B	184/212 (87%)	183 (100%)	1 (0%)	88	96
3	G	184/212 (87%)	180 (98%)	4 (2%)	52	81
3	H	181/212 (85%)	179 (99%)	2 (1%)	73	90
All	All	1512/1700 (89%)	1474 (98%)	38 (2%)	47	79

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	512	THR
2	F	34	ASP
3	H	339	TYR
2	F	9	SER
3	B	434	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	481	ASN
3	H	484	GLN
3	B	477	GLN
3	B	371	ASN
3	B	424	HIS

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](#)

23 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	M	1	3,4	14,14,15	2.30	1 (7%)	17,19,21	1.35	2 (11%)
4	NAG	M	2	4	14,14,15	0.55	0	17,19,21	1.44	3 (17%)
4	BMA	M	3	4	11,11,12	1.47	1 (9%)	15,15,17	1.87	7 (46%)
4	MAN	M	4	4	11,11,12	1.37	2 (18%)	15,15,17	1.08	0
4	MAN	M	5	4	11,11,12	1.99	4 (36%)	15,15,17	1.51	3 (20%)
4	FUC	M	6	4	10,10,11	1.58	1 (10%)	14,14,16	1.91	6 (42%)
5	NAG	N	1	3,5	14,14,15	0.31	0	17,19,21	0.53	0
5	NAG	N	2	5	14,14,15	0.25	0	17,19,21	0.58	0
5	BMA	N	3	5	11,11,12	1.96	3 (27%)	15,15,17	1.37	1 (6%)
5	MAN	N	4	5	11,11,12	1.57	3 (27%)	15,15,17	1.09	1 (6%)
5	BMA	N	5	5	11,11,12	1.35	1 (9%)	15,15,17	1.24	1 (6%)
5	MAN	N	6	5	11,11,12	1.02	0	15,15,17	1.40	2 (13%)
6	NAG	O	1	3,6	14,14,15	0.60	0	17,19,21	1.62	4 (23%)
6	NAG	O	2	6	14,14,15	0.49	0	17,19,21	0.75	0
6	BMA	O	3	6	11,11,12	1.83	3 (27%)	15,15,17	2.57	7 (46%)
6	MAN	O	4	6	11,11,12	1.29	1 (9%)	15,15,17	1.45	1 (6%)
7	NAG	P	1	3,7	14,14,15	0.27	0	17,19,21	0.41	0
7	NAG	P	2	7	14,14,15	0.24	0	17,19,21	0.57	0
7	BMA	P	3	7	11,11,12	1.13	0	15,15,17	2.02	3 (20%)
7	MAN	P	4	7	11,11,12	1.29	1 (9%)	15,15,17	1.04	1 (6%)
7	MAN	P	5	7	11,11,12	1.14	1 (9%)	15,15,17	1.29	2 (13%)
7	MAN	P	6	7	11,11,12	1.73	2 (18%)	15,15,17	1.72	3 (20%)
7	MAN	P	7	7	11,11,12	1.05	0	15,15,17	0.97	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	M	1	3,4	1/1/5/7	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1	NAG	O5-C1	-8.39	1.30	1.43
4	M	6	FUC	C1-C2	4.51	1.62	1.52
7	P	6	MAN	C1-C2	4.23	1.61	1.52
4	M	5	MAN	C1-C2	4.11	1.61	1.52
4	M	5	MAN	C2-C3	3.68	1.57	1.52

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	3	BMA	C1-O5-C5	-6.36	103.57	112.19
7	P	3	BMA	C1-O5-C5	5.64	119.83	112.19
5	N	6	MAN	C1-O5-C5	4.60	118.42	112.19
7	P	6	MAN	C1-O5-C5	4.48	118.27	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	4	MAN	C1-O5-C5	4.46	118.24	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	1	NAG	C1
6	O	1	NAG	C1

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	2	NAG	C3-C2-N2-C7
7	P	1	NAG	O5-C5-C6-O6
5	N	5	BMA	O5-C5-C6-O6
4	M	5	MAN	O5-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

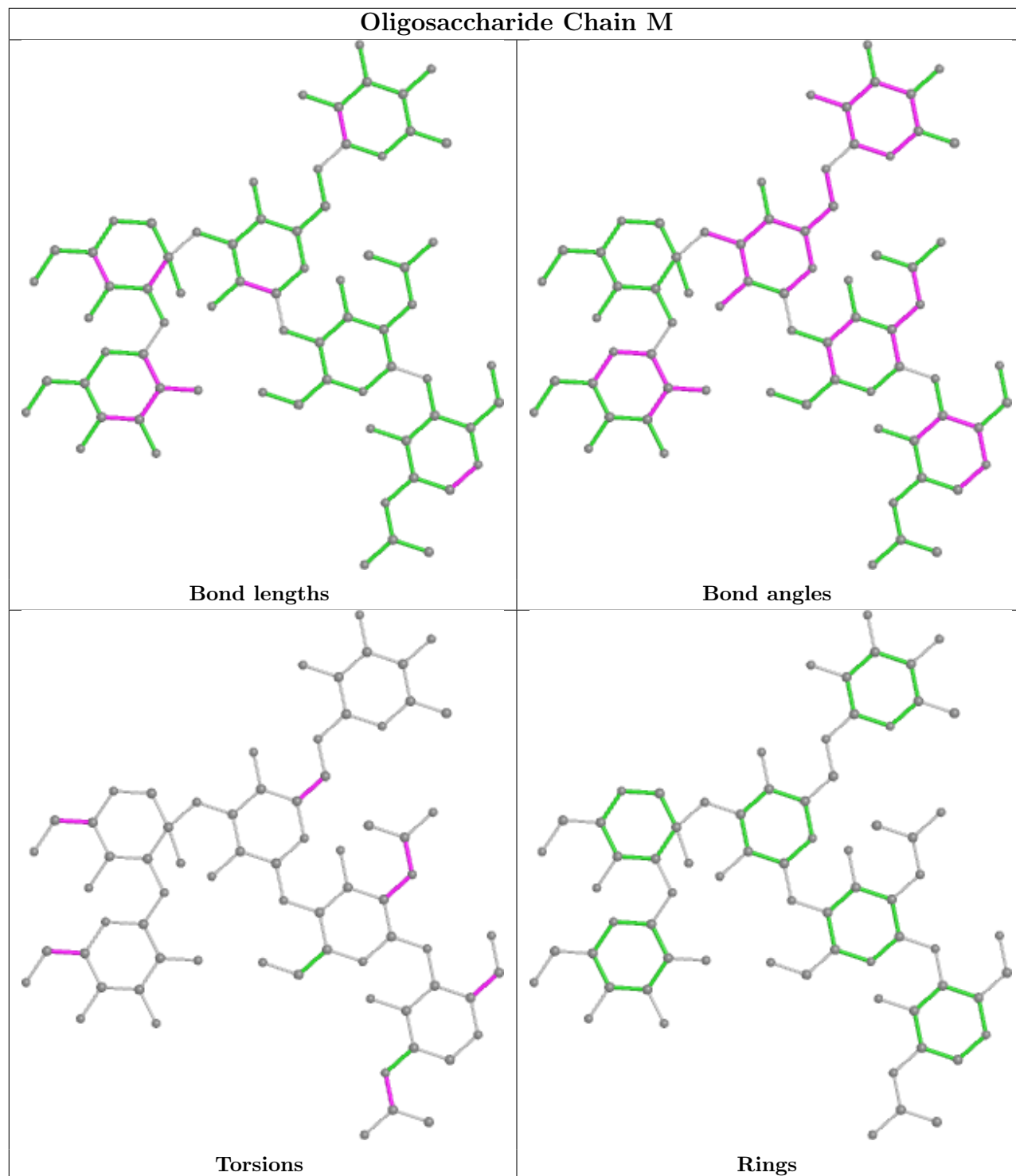
Mol	Chain	Res	Type	Atoms
6	O	4	MAN	C1-C2-C3-C4-C5-O5

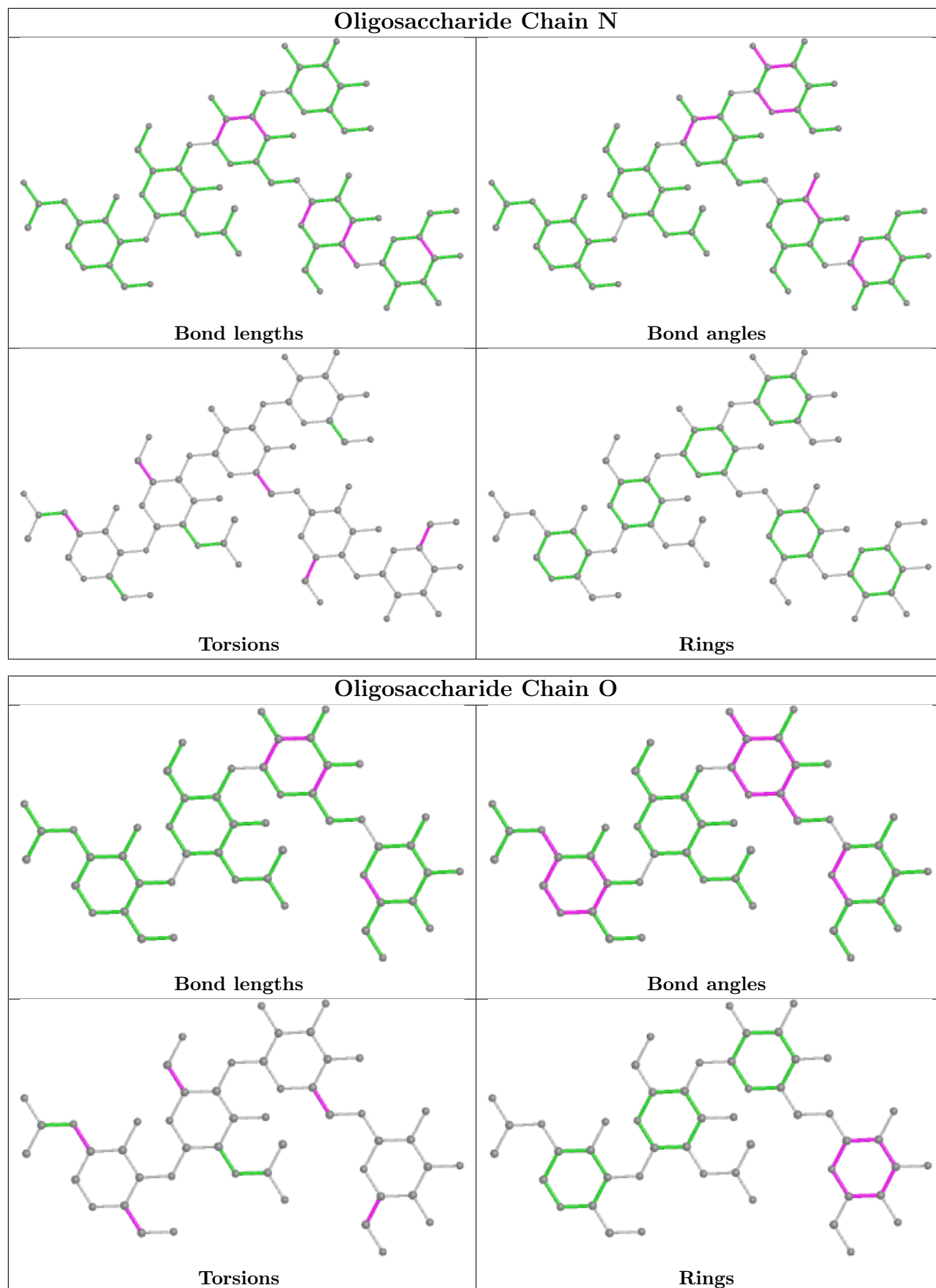
15 monomers are involved in 32 short contacts:

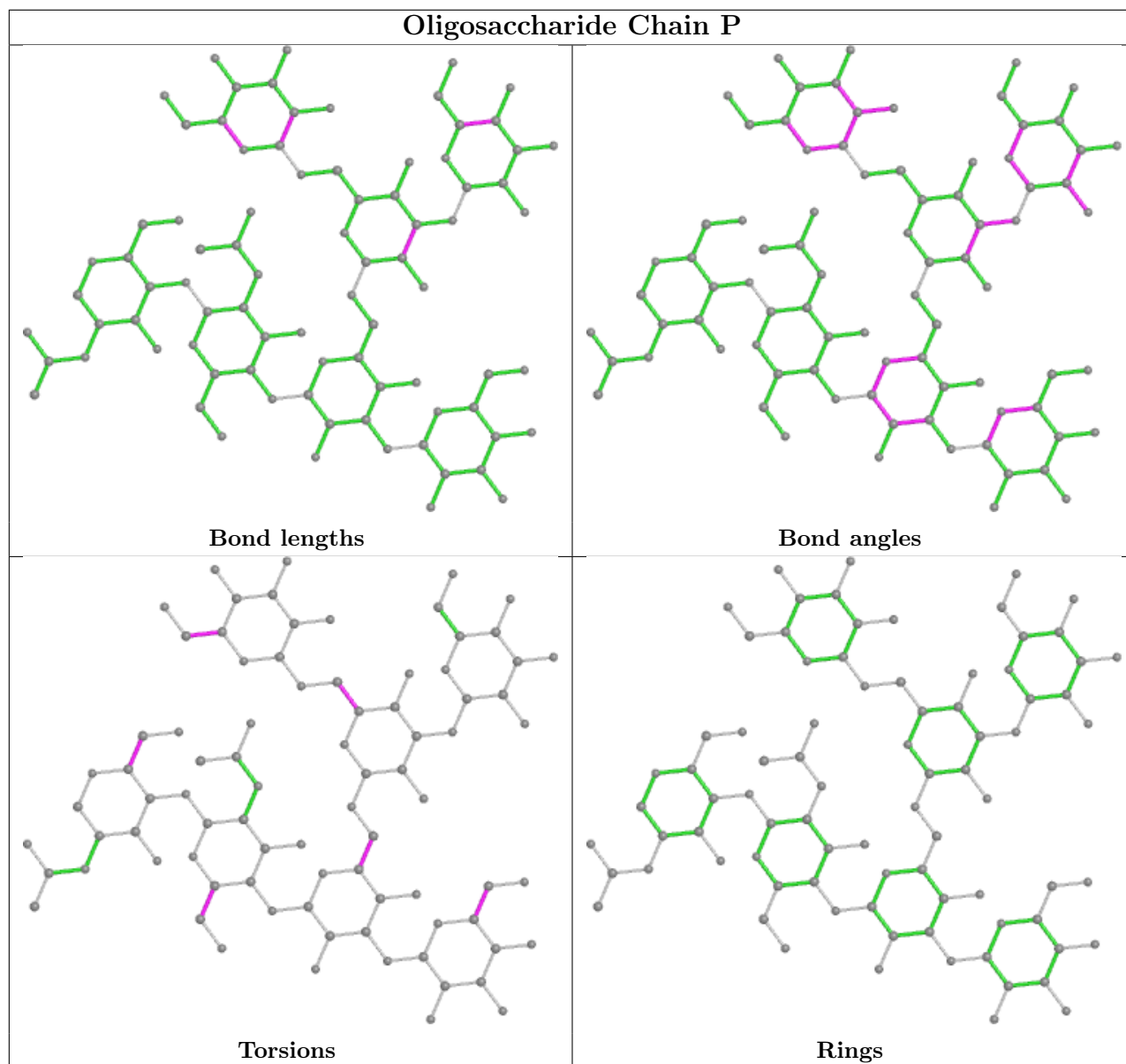
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	2	NAG	1	0
6	O	3	BMA	8	0
4	M	3	BMA	1	0
6	O	4	MAN	1	0
6	O	2	NAG	1	0
5	N	1	NAG	3	0
7	P	6	MAN	3	0
5	N	4	MAN	1	0
7	P	5	MAN	1	0
7	P	4	MAN	3	0
5	N	5	BMA	1	0
6	O	1	NAG	7	0
4	M	2	NAG	7	0
4	M	4	MAN	1	0
4	M	5	MAN	1	0

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](#)

5 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
9	NAG	B	601	-	14,14,15	0.49	0	17,19,21	0.53	0
8	GOL	D	201	-	5,5,5	0.48	0	5,5,5	0.43	0
9	NAG	A	601	3	14,14,15	0.83	1 (7%)	17,19,21	0.65	0
9	NAG	H	602	3	14,14,15	0.74	0	17,19,21	1.21	2 (11%)
10	MAN	H	601	-	11,11,12	1.13	1 (9%)	15,15,17	1.40	3 (20%)

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
9	NAG	B	601	-	-	1/6/23/26	0/1/1/1
8	GOL	D	201	-	-	2/4/4/4	-
9	NAG	A	601	3	-	2/6/23/26	0/1/1/1
9	NAG	H	602	3	-	3/6/23/26	0/1/1/1
10	MAN	H	601	-	-	2/2/19/22	1/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	601	NAG	O5-C1	2.85	1.48	1.43
10	H	601	MAN	C2-C3	2.30	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	602	NAG	C3-C4-C5	2.76	115.17	110.24
10	H	601	MAN	O2-C2-C1	2.52	114.30	109.15
10	H	601	MAN	O3-C3-C2	2.50	114.78	109.99
10	H	601	MAN	C1-O5-C5	2.34	115.36	112.19
9	H	602	NAG	C2-N2-C7	2.05	125.82	122.90

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	201	GOL	C1-C2-C3-O3
9	H	602	NAG	C3-C2-N2-C7
9	A	601	NAG	C4-C5-C6-O6
10	H	601	MAN	C4-C5-C6-O6
9	A	601	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	H	601	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	601	NAG	1	0
9	A	601	NAG	1	0
9	H	602	NAG	1	0
10	H	601	MAN	6	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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	121/122 (99%)	-0.31	0 100 100	51, 68, 98, 135	0
1	E	121/122 (99%)	-0.22	0 100 100	50, 73, 124, 140	0
1	I	120/122 (98%)	-0.25	0 100 100	47, 65, 111, 136	0
1	K	120/122 (98%)	-0.05	3 (2%) 57 29	66, 91, 126, 136	0
2	D	114/134 (85%)	-0.44	0 100 100	57, 77, 110, 145	0
2	F	112/134 (83%)	-0.46	0 100 100	59, 81, 106, 135	0
2	J	115/134 (85%)	-0.34	0 100 100	54, 72, 109, 151	0
2	L	113/134 (84%)	-0.54	0 100 100	64, 88, 121, 140	0
3	A	208/247 (84%)	0.06	11 (5%) 26 10	63, 129, 182, 229	0
3	B	210/247 (85%)	-0.24	3 (1%) 75 49	53, 102, 164, 243	0
3	G	209/247 (84%)	-0.30	2 (0%) 82 59	60, 85, 161, 195	0
3	H	208/247 (84%)	0.26	15 (7%) 15 4	75, 127, 205, 249	0
All	All	1771/2012 (88%)	-0.20	34 (1%) 66 37	47, 89, 167, 249	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	397	LEU	3.7
1	K	12	VAL	3.6
3	A	399	VAL	3.5
3	A	360	VAL	3.5
3	A	390	GLU	3.5

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

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

6.3 Carbohydrates

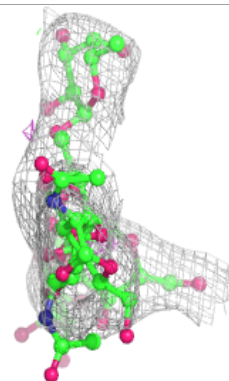
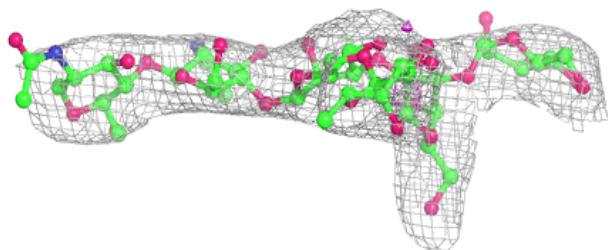
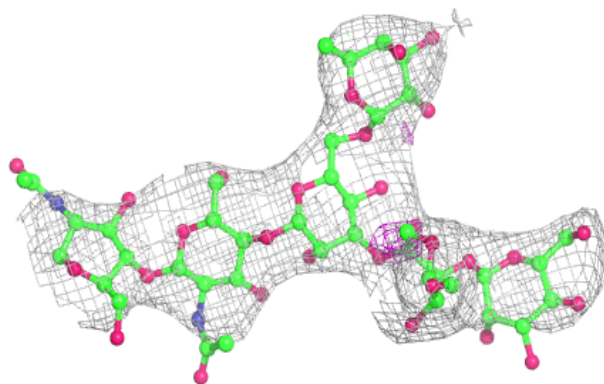
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	N	5	11/12	0.69	0.30	139,153,168,173	0
4	MAN	M	5	11/12	0.72	0.29	121,137,145,145	0
6	NAG	O	1	14/15	0.80	0.36	142,157,186,193	0
4	MAN	M	4	11/12	0.81	0.15	92,125,145,147	0
6	NAG	O	2	14/15	0.82	0.27	129,141,149,149	0
7	MAN	P	6	11/12	0.82	0.43	109,151,168,173	0
6	BMA	O	3	11/12	0.83	0.11	117,143,155,157	0
6	MAN	O	4	11/12	0.84	0.15	127,142,150,150	0
5	MAN	N	4	11/12	0.85	0.15	124,132,144,155	0
5	MAN	N	6	11/12	0.86	0.18	129,140,145,146	0
4	BMA	M	3	11/12	0.86	0.17	119,130,145,150	0
7	MAN	P	5	11/12	0.88	0.17	121,157,160,161	0
4	NAG	M	2	14/15	0.88	0.35	114,137,155,164	0
7	BMA	P	3	11/12	0.89	0.12	119,134,142,143	0
7	NAG	P	1	14/15	0.90	0.12	108,131,138,142	0
7	MAN	P	4	11/12	0.90	0.15	138,141,155,156	0
4	FUC	M	6	10/11	0.91	0.14	103,131,135,135	0
7	MAN	P	7	11/12	0.91	0.15	107,130,142,147	0
7	NAG	P	2	14/15	0.93	0.16	120,132,137,141	0
5	BMA	N	3	11/12	0.93	0.08	107,129,139,144	0
4	NAG	M	1	14/15	0.94	0.26	128,147,166,166	0
5	NAG	N	1	14/15	0.95	0.09	92,111,118,125	0
5	NAG	N	2	14/15	0.97	0.11	104,114,124,126	0

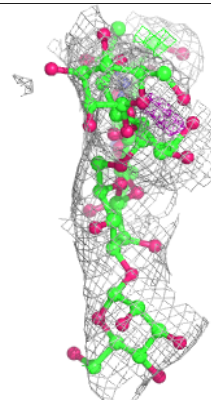
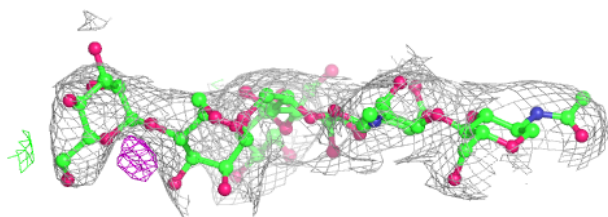
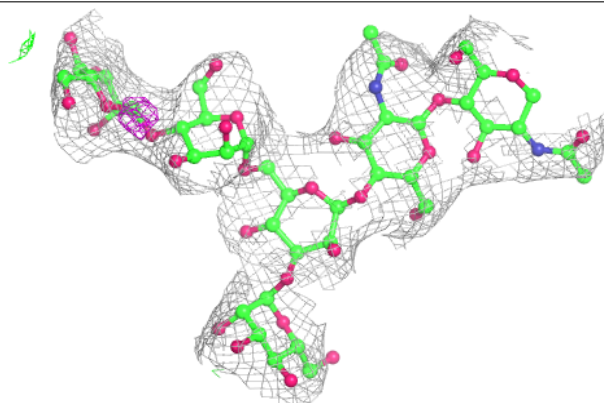
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

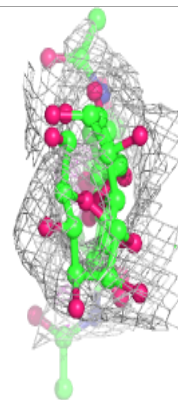
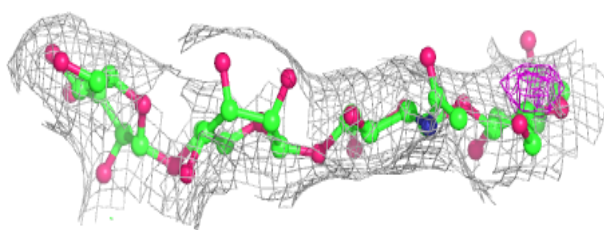
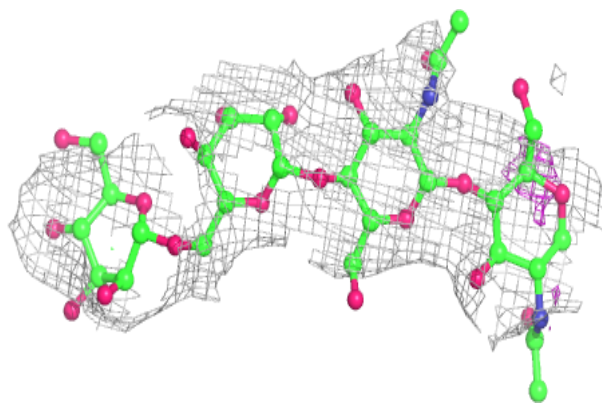
**Electron density around Chain N:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

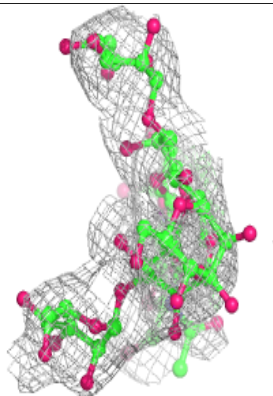
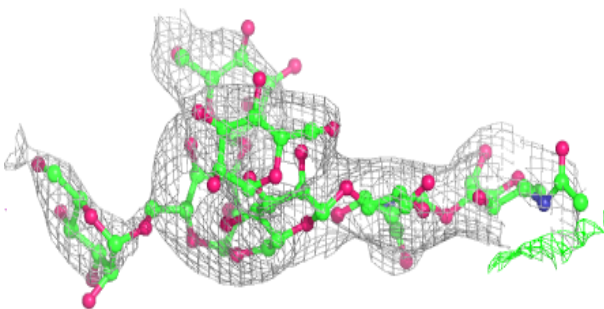
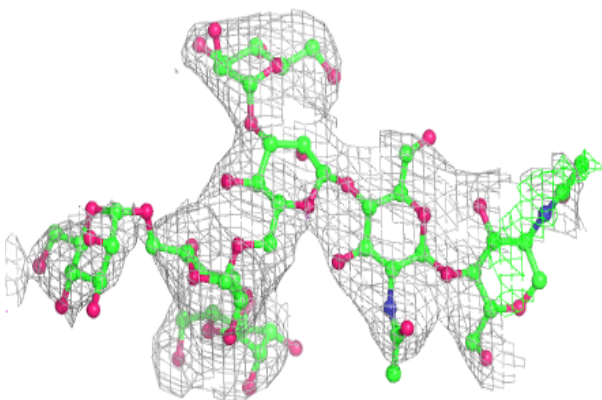


Electron density around Chain O:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain P:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	NAG	B	601	14/15	0.38	0.45	159,167,170,172	0
9	NAG	A	601	14/15	0.67	0.34	126,166,170,171	0
9	NAG	H	602	14/15	0.81	0.17	136,148,150,155	0
10	MAN	H	601	11/12	0.90	0.10	118,127,133,135	0
8	GOL	D	201	6/6	0.91	0.22	67,100,120,134	0

6.5 Other polymers [i](#)

There are no such residues in this entry.