



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:23 PM UTC

PDB ID : 3USU / pdb_00003usu
Title : Crystal structure of Butea monosperma seed lectin
Authors : Abhilash, J.; Geethanandan, K.; Bharath, S.R.; Sadasivan, C.; Haridas, M.
Deposited on : 2011-11-24
Resolution : 2.46 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

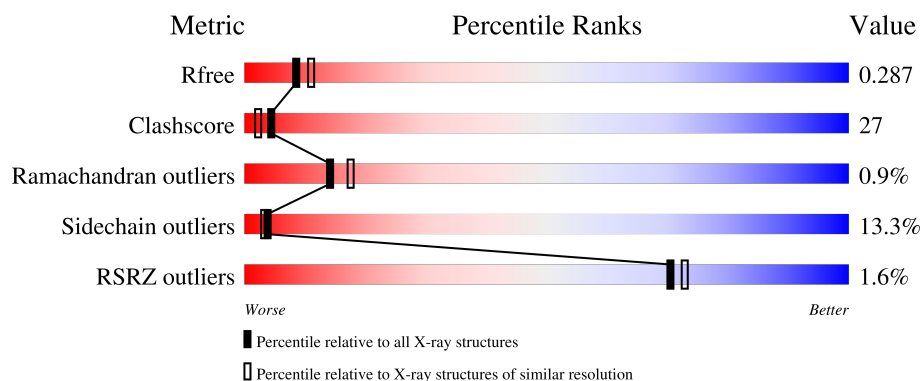
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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.



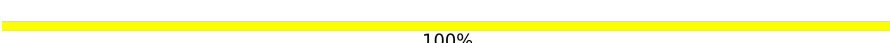
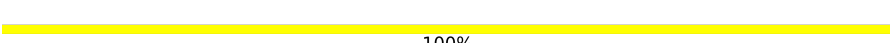
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	A	256	2% 49% 37% 10% . .
1	C	256	3% 55% 36% 6% .
1	E	256	2% 51% 37% 9% . .
1	G	256	2% 51% 36% 10% .
2	B	242	60% 33% 6% .

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Mol	Chain	Length	Quality of chain
2	D	242	 61% 32% 7%
2	F	242	 57% 36% 7%
2	H	242	 57% 35% 7%
3	I	4	 100%
3	K	4	 25% 75%
3	L	4	 50% 50%
4	J	5	 40% 60%
5	M	2	 100%
6	N	2	 100%

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
11	XYP	B	306	-	-	X	-
4	BMA	J	3	-	-	X	-
9	ABU	C	282	-	-	X	-
9	ABU	F	290	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 15748 atoms, of which 0 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.

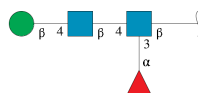
- Molecule 1 is a protein called Lectin Alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	0	0	0
			1892	1227	296	369			
1	C	250	Total	C	N	O	0	0	0
			1892	1227	296	369			
1	E	250	Total	C	N	O	0	0	0
			1892	1227	296	369			
1	G	250	Total	C	N	O	0	0	0
			1892	1227	296	369			

- Molecule 2 is a protein called Lectin Beta Chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	0	0	0
			1828	1184	287	357			
2	D	242	Total	C	N	O	0	0	0
			1828	1184	287	357			
2	F	242	Total	C	N	O	0	0	0
			1828	1184	287	357			
2	H	242	Total	C	N	O	0	0	0
			1828	1184	287	357			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



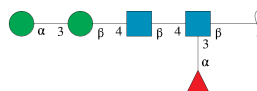
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	4	Total	C	N	O	0	0	0
			49	28	2	19			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	K	4	Total	C	N	O	0	0	0
			49	28	2	19			
3	L	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	5	Total	C	N	O	0	0	0
			60	34	2	24			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	N	2	Total	C	N	O	0	0	0
			24	14	1	9			

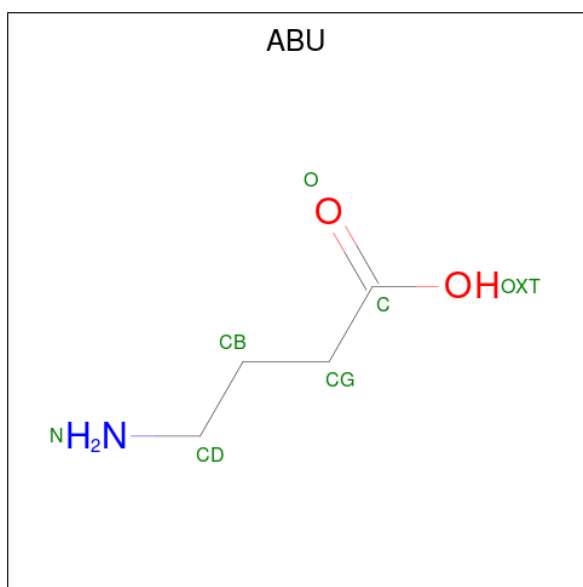
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0
7	D	1	Total Ca 1 1	0	0
7	E	1	Total Ca 1 1	0	0
7	F	1	Total Ca 1 1	0	0
7	G	1	Total Ca 1 1	0	0
7	H	1	Total Ca 1 1	0	0

- Molecule 8 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

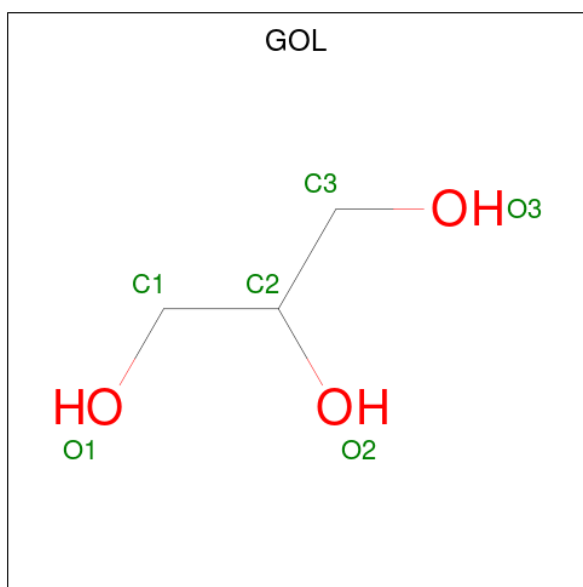
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Mn 1 1	0	0
8	B	1	Total Mn 1 1	0	0
8	C	1	Total Mn 1 1	0	0
8	D	1	Total Mn 1 1	0	0
8	E	1	Total Mn 1 1	0	0
8	F	1	Total Mn 1 1	0	0
8	G	1	Total Mn 1 1	0	0
8	H	1	Total Mn 1 1	0	0

- Molecule 9 is GAMMA-AMINO-BUTANOIC ACID (CCD ID: ABU) (formula: C₄H₉NO₂).



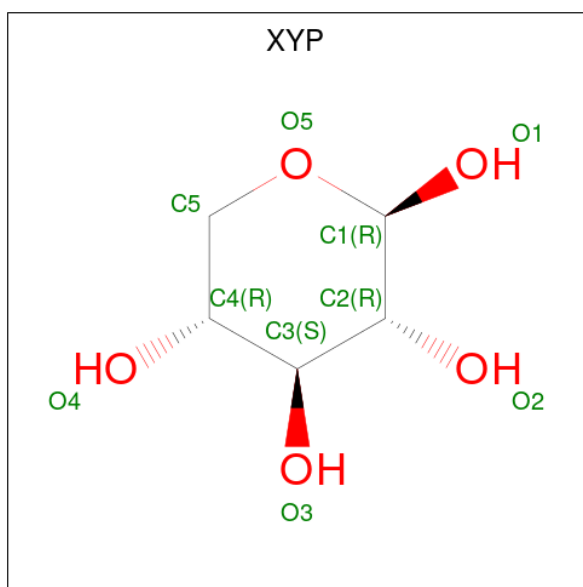
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			7	4	1	2		
9	B	1	Total	C	N	O	0	0
			7	4	1	2		
9	C	1	Total	C	N	O	0	0
			7	4	1	2		
9	D	1	Total	C	N	O	0	0
			7	4	1	2		
9	E	1	Total	C	N	O	0	0
			7	4	1	2		
9	E	1	Total	C	N	O	0	0
			7	4	1	2		
9	F	1	Total	C	N	O	0	0
			7	4	1	2		
9	G	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



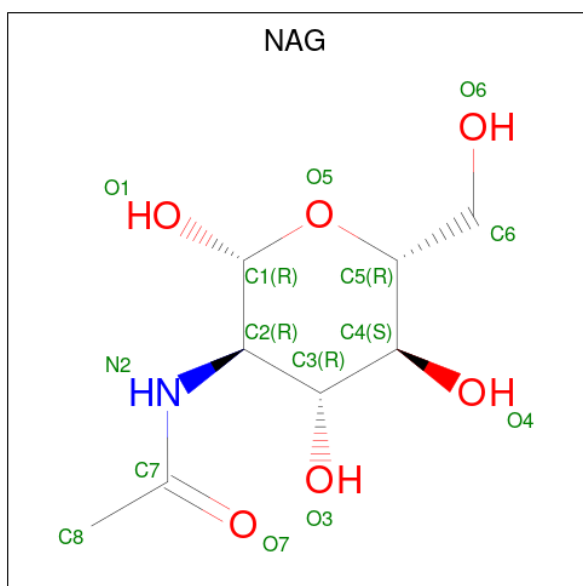
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		
10	B	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		
10	E	1	Total	C	O	0	0
			6	3	3		
10	E	1	Total	C	O	0	0
			6	3	3		
10	G	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is beta-D-xylopyranose (CCD ID: XYP) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			9	5	4		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	D	1	Total	C	N	O	0	0
			14	8	1	5		

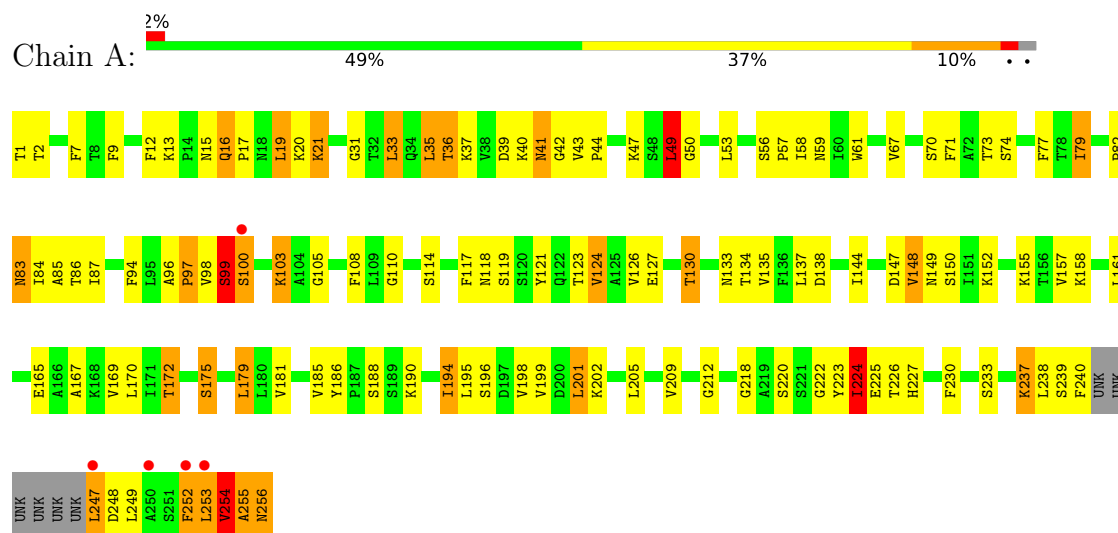
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	65	Total 65	O 65	0	0
13	B	70	Total 70	O 70	0	0
13	C	64	Total 64	O 64	0	0
13	D	47	Total 47	O 47	0	0
13	E	51	Total 51	O 51	0	0
13	F	65	Total 65	O 65	0	0
13	G	60	Total 60	O 60	0	0
13	H	44	Total 44	O 44	0	0

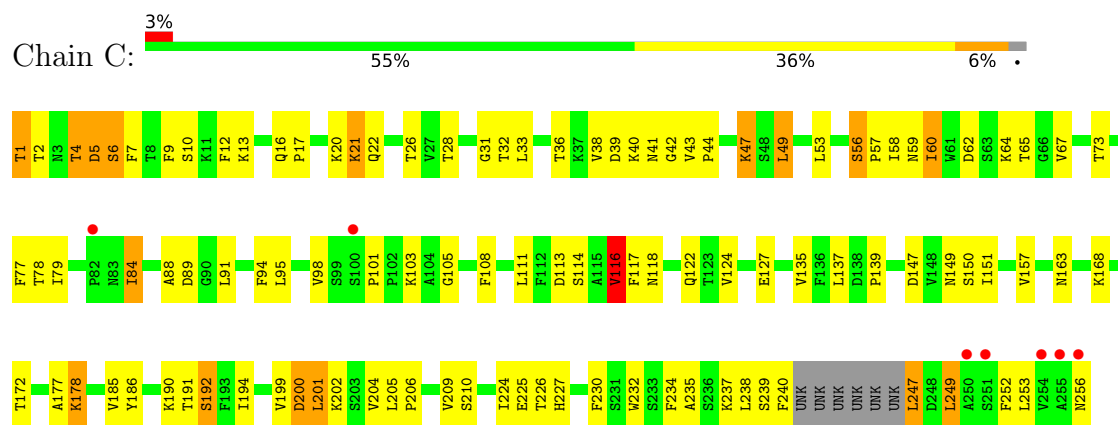
3 Residue-property plots [i](#)

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.

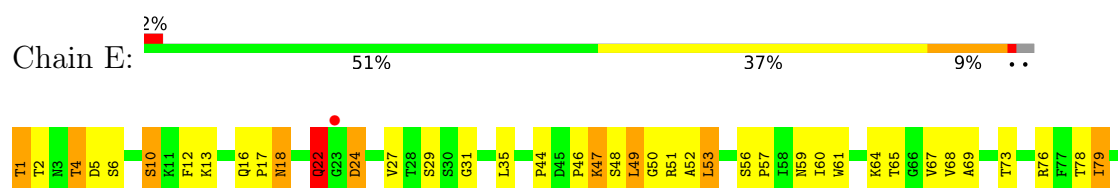
• Molecule 1: Lectin Alpha chain

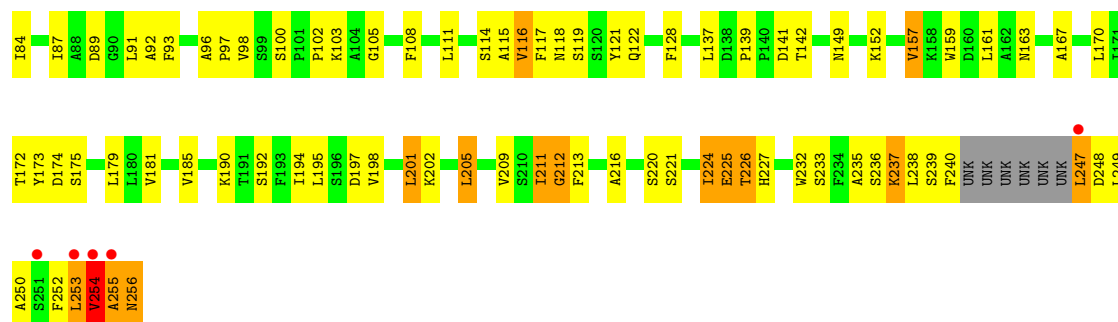


• Molecule 1: Lectin Alpha chain

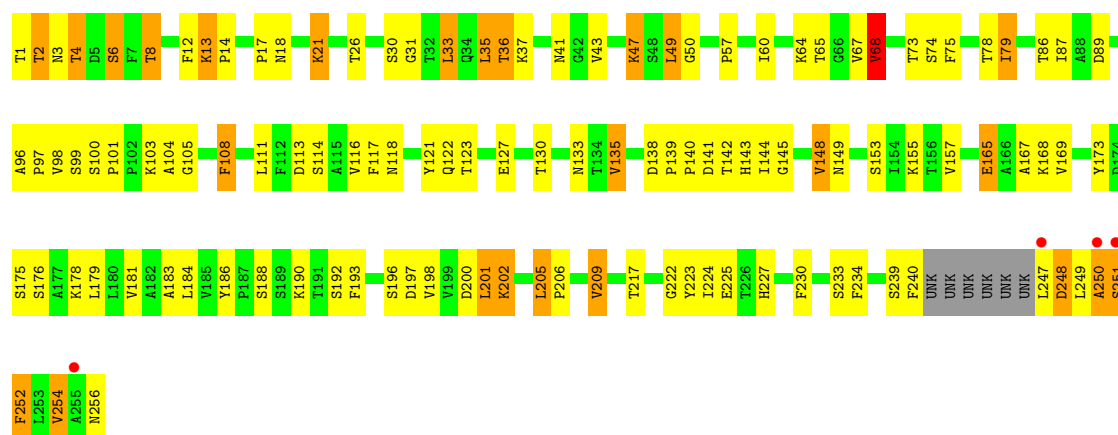


• Molecule 1: Lectin Alpha chain

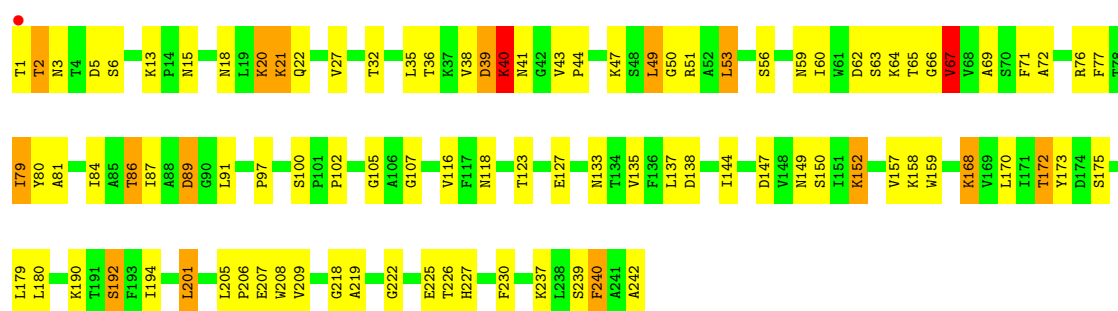




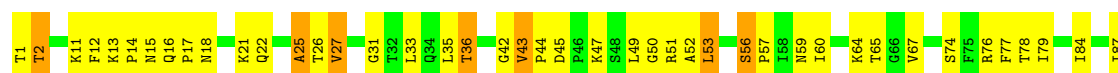
• Molecule 1: Lectin Alpha chain

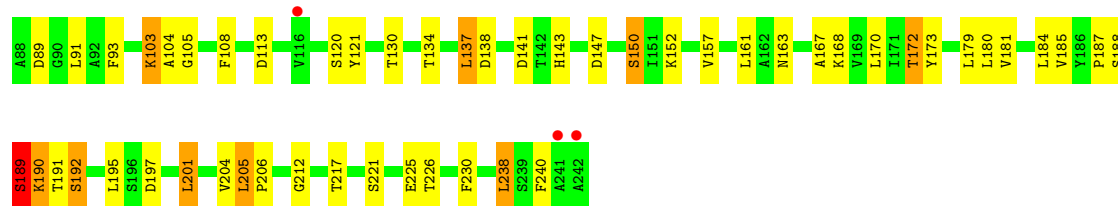


• Molecule 2: Lectin Beta Chain

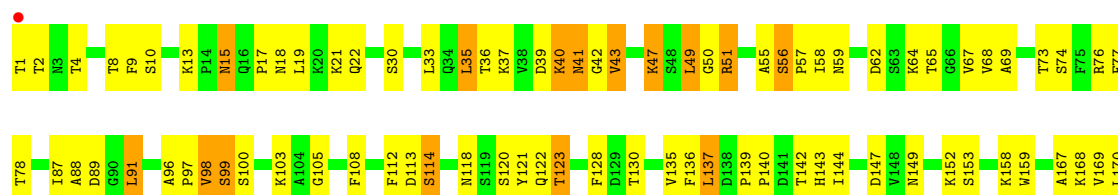


• Molecule 2: Lectin Beta Chain

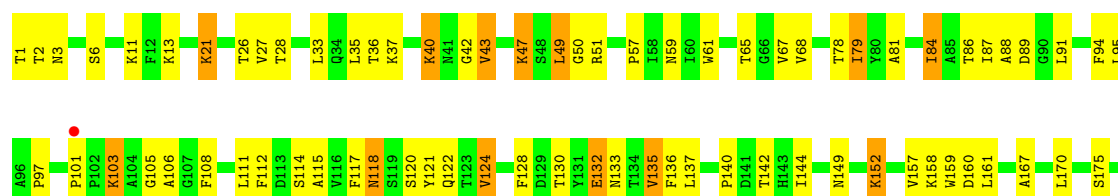




• Molecule 2: Lectin Beta Chain



• Molecule 2: Lectin Beta Chain



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



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



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

Chain L:  50% 50%

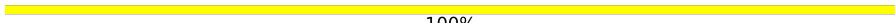
MAG1
MAG2
BMA3
FUC4

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

Chain J:  40% 60%

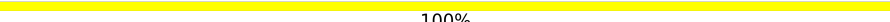
MAG1
MAG2
BMA3
MAI4
FUC5

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

Chain M:  100%

MAG1
MAG2

- Molecule 6: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.45Å 78.91Å 101.85Å 74.30° 76.65° 86.88°	Depositor
Resolution (Å)	69.06 – 2.46 69.06 – 2.46	Depositor EDS
% Data completeness (in resolution range)	94.7 (69.06-2.46) 94.8 (69.06-2.46)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.205 , 0.287 0.206 , 0.287	Depositor DCC
R_{free} test set	3944 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15748	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XYP, GOL, FUC, BMA, MAN, MN, CA, ABU, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.18	5/1939 (0.3%)	1.25	9/2646 (0.3%)
1	C	1.03	4/1939 (0.2%)	1.18	11/2646 (0.4%)
1	E	1.01	3/1939 (0.2%)	1.17	9/2646 (0.3%)
1	G	0.95	0/1939	1.16	10/2646 (0.4%)
2	B	1.11	3/1875 (0.2%)	1.21	5/2560 (0.2%)
2	D	0.96	2/1875 (0.1%)	1.15	9/2560 (0.4%)
2	F	1.07	1/1875 (0.1%)	1.15	2/2560 (0.1%)
2	H	0.92	1/1875 (0.1%)	1.15	9/2560 (0.4%)
All	All	1.03	19/15256 (0.1%)	1.18	64/20824 (0.3%)

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
1	A	0	1
1	C	0	1
1	E	0	1
All	All	0	3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	ILE	N-CA	-6.08	1.38	1.46
2	B	2	THR	C-O	-5.93	1.16	1.24
1	C	232	TRP	NE1-CE2	-5.84	1.31	1.37
2	D	150	SER	C-O	-5.83	1.16	1.24
1	C	101	PRO	CA-C	5.73	1.55	1.51

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	PHE	N-CA-C	11.13	123.50	111.36
2	B	39	ASP	N-CA-C	9.67	122.30	110.41
2	H	2	THR	N-CA-C	9.56	124.11	108.52
1	G	13	LYS	CA-C-N	-8.84	110.65	119.76
1	G	13	LYS	C-N-CA	-8.84	110.65	119.76

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	VAL	Peptide
1	C	247	LEU	Peptide
1	E	22	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1892	0	1874	131	0
1	C	1892	0	1875	99	0
1	E	1892	0	1875	113	0
1	G	1892	0	1875	110	0
2	B	1828	0	1809	108	0
2	D	1828	0	1810	82	0
2	F	1828	0	1810	95	0
2	H	1828	0	1810	108	0
3	I	49	0	43	4	0
3	K	49	0	42	0	0
3	L	49	0	43	1	0
4	J	60	0	47	9	0
5	M	28	0	25	0	0
6	N	24	0	21	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1	0	0	0	0
7	H	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
9	A	7	0	0	3	0
9	B	7	0	0	2	0
9	C	7	0	0	5	0
9	D	7	0	0	0	0
9	E	14	0	0	5	0
9	F	7	0	0	4	0
9	G	7	0	0	0	0
10	A	6	0	8	2	0
10	B	6	0	8	0	0
10	C	6	0	8	1	0
10	D	6	0	8	0	0
10	E	12	0	16	2	0
10	G	6	0	8	0	0
10	H	6	0	8	3	0
11	B	9	0	0	6	0
12	D	14	0	12	0	0
13	A	65	0	0	16	0
13	B	70	0	0	20	0
13	C	64	0	0	13	0
13	D	47	0	0	11	0
13	E	51	0	0	5	0
13	F	65	0	0	12	0
13	G	60	0	0	17	0
13	H	44	0	0	15	0
All	All	15748	0	15035	804	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 27.

The worst 5 of 804 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:238:LEU:HG	13:H:261:HOH:O	1.30	1.28
1:G:101:PRO:HD2	13:G:542:HOH:O	1.34	1.23
11:B:306:XYP:C1	4:J:3:BMA:O2	1.87	1.21
10:H:289:GOL:H2	13:H:411:HOH:O	1.45	1.15
1:A:36:THR:HG21	1:A:227:HIS:HD2	1.04	1.13

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 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	A	246/256 (96%)	229 (93%)	12 (5%)	5 (2%)	6	4
1	C	246/256 (96%)	230 (94%)	13 (5%)	3 (1%)	10	11
1	E	246/256 (96%)	228 (93%)	15 (6%)	3 (1%)	10	11
1	G	246/256 (96%)	231 (94%)	12 (5%)	3 (1%)	10	11
2	B	240/242 (99%)	227 (95%)	11 (5%)	2 (1%)	16	20
2	D	240/242 (99%)	224 (93%)	15 (6%)	1 (0%)	30	37
2	F	240/242 (99%)	230 (96%)	9 (4%)	1 (0%)	30	37
2	H	240/242 (99%)	226 (94%)	14 (6%)	0	100	100
All	All	1944/1992 (98%)	1825 (94%)	101 (5%)	18 (1%)	14	17

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	255	ALA
2	B	40	LYS
1	C	178	LYS
1	E	253	LEU

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	A	210/210 (100%)	174 (83%)	36 (17%)	2	1
1	C	210/210 (100%)	187 (89%)	23 (11%)	6	5
1	E	210/210 (100%)	175 (83%)	35 (17%)	2	1
1	G	210/210 (100%)	175 (83%)	35 (17%)	2	1
2	B	202/202 (100%)	181 (90%)	21 (10%)	7	6
2	D	202/202 (100%)	181 (90%)	21 (10%)	7	6
2	F	202/202 (100%)	178 (88%)	24 (12%)	5	4
2	H	202/202 (100%)	178 (88%)	24 (12%)	5	4
All	All	1648/1648 (100%)	1429 (87%)	219 (13%)	4	3

5 of 219 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	89	ASP
2	F	43	VAL
2	H	40	LYS
1	E	141	ASP
1	E	233	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	149	ASN
2	H	16	GLN
2	H	227	HIS
1	C	149	ASN
1	C	15	ASN

5.3.3 RNA [i](#)

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 ⓘ

21 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
3	NAG	I	1	1,3	14,14,15	0.68	0	17,19,21	1.53	3 (17%)
3	NAG	I	2	3	14,14,15	0.59	0	17,19,21	2.14	4 (23%)
3	BMA	I	3	3	11,11,12	1.28	3 (27%)	15,15,17	2.01	4 (26%)
3	FUC	I	4	3	10,10,11	0.71	0	14,14,16	1.36	2 (14%)
4	NAG	J	1	4,2	14,14,15	0.85	1 (7%)	17,19,21	2.38	3 (17%)
4	NAG	J	2	4	14,14,15	1.04	1 (7%)	17,19,21	2.01	4 (23%)
4	BMA	J	3	4	11,11,12	2.23	3 (27%)	15,15,17	4.11	6 (40%)
4	MAN	J	4	4	11,11,12	6.32	8 (72%)	15,15,17	3.77	8 (53%)
4	FUC	J	5	4	10,10,11	0.72	0	14,14,16	1.24	2 (14%)
3	NAG	K	1	1,3	14,14,15	0.56	0	17,19,21	1.37	2 (11%)
3	NAG	K	2	3	14,14,15	0.57	0	17,19,21	1.60	5 (29%)
3	BMA	K	3	3	11,11,12	0.81	0	15,15,17	1.03	0
3	FUC	K	4	3	10,10,11	4.16	4 (40%)	14,14,16	3.95	5 (35%)
3	NAG	L	1	1,3	14,14,15	1.16	2 (14%)	17,19,21	1.55	4 (23%)
3	NAG	L	2	3	14,14,15	0.70	0	17,19,21	2.40	7 (41%)
3	BMA	L	3	3	11,11,12	0.81	0	15,15,17	1.33	1 (6%)
3	FUC	L	4	3	10,10,11	0.78	0	14,14,16	0.95	1 (7%)
5	NAG	M	1	1,5	14,14,15	0.69	0	17,19,21	1.54	3 (17%)
5	NAG	M	2	5	14,14,15	0.87	1 (7%)	17,19,21	1.94	4 (23%)
6	NAG	N	1	2,6	14,14,15	1.39	3 (21%)	17,19,21	2.68	6 (35%)
6	FUC	N	2	6	10,10,11	3.70	4 (40%)	14,14,16	4.04	8 (57%)

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
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	FUC	I	4	3	-	-	0/1/1/1
4	NAG	J	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	1/2/19/22	0/1/1/1
4	MAN	J	4	4	-	2/2/19/22	0/1/1/1
4	FUC	J	5	4	-	-	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	1/2/19/22	0/1/1/1
3	FUC	K	4	3	-	-	0/1/1/1
3	NAG	L	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	2/2/19/22	0/1/1/1
3	FUC	L	4	3	-	-	0/1/1/1
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
6	NAG	N	1	2,6	-	1/6/23/26	0/1/1/1
6	FUC	N	2	6	-	-	0/1/1/1

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	4	MAN	O5-C5	-12.51	1.19	1.43
3	K	4	FUC	C2-C3	-12.08	1.34	1.52
4	J	4	MAN	O2-C2	9.06	1.62	1.43
4	J	4	MAN	C2-C3	-8.89	1.38	1.52
6	N	2	FUC	C4-C5	-7.12	1.36	1.52

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	3	BMA	O4-C4-C5	11.65	138.01	109.32
3	K	4	FUC	C1-C2-C3	10.75	125.29	109.64
6	N	2	FUC	C6-C5-C4	10.56	132.39	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	3	BMA	O3-C3-C2	9.20	128.82	110.05
4	J	1	NAG	C1-O5-C5	7.66	122.45	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

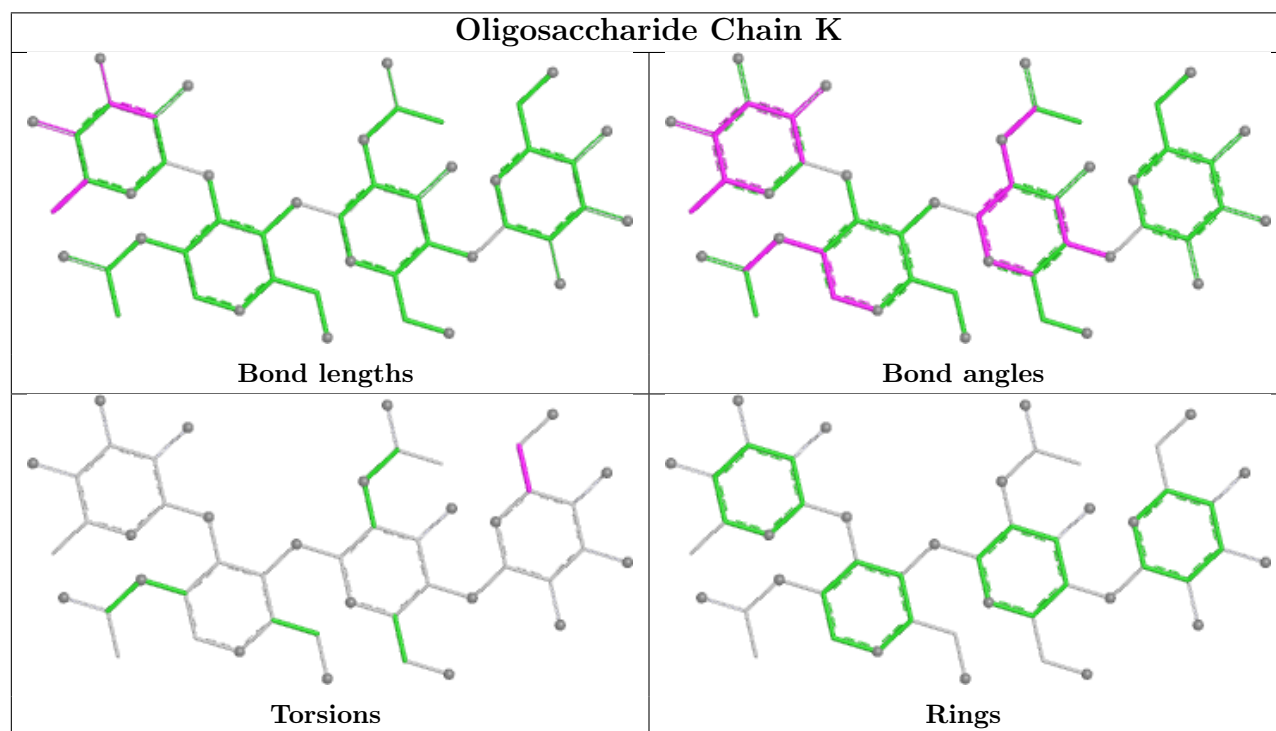
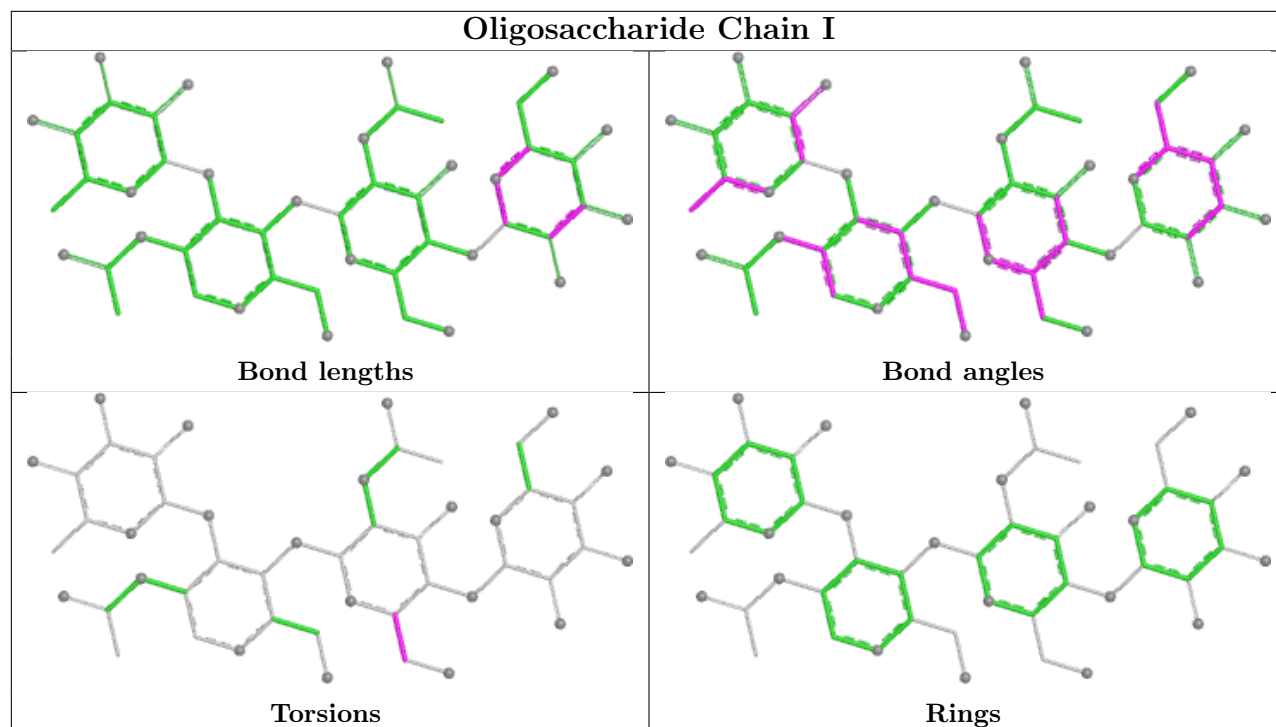
Mol	Chain	Res	Type	Atoms
3	I	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
3	L	3	BMA	C4-C5-C6-O6
4	J	4	MAN	C4-C5-C6-O6

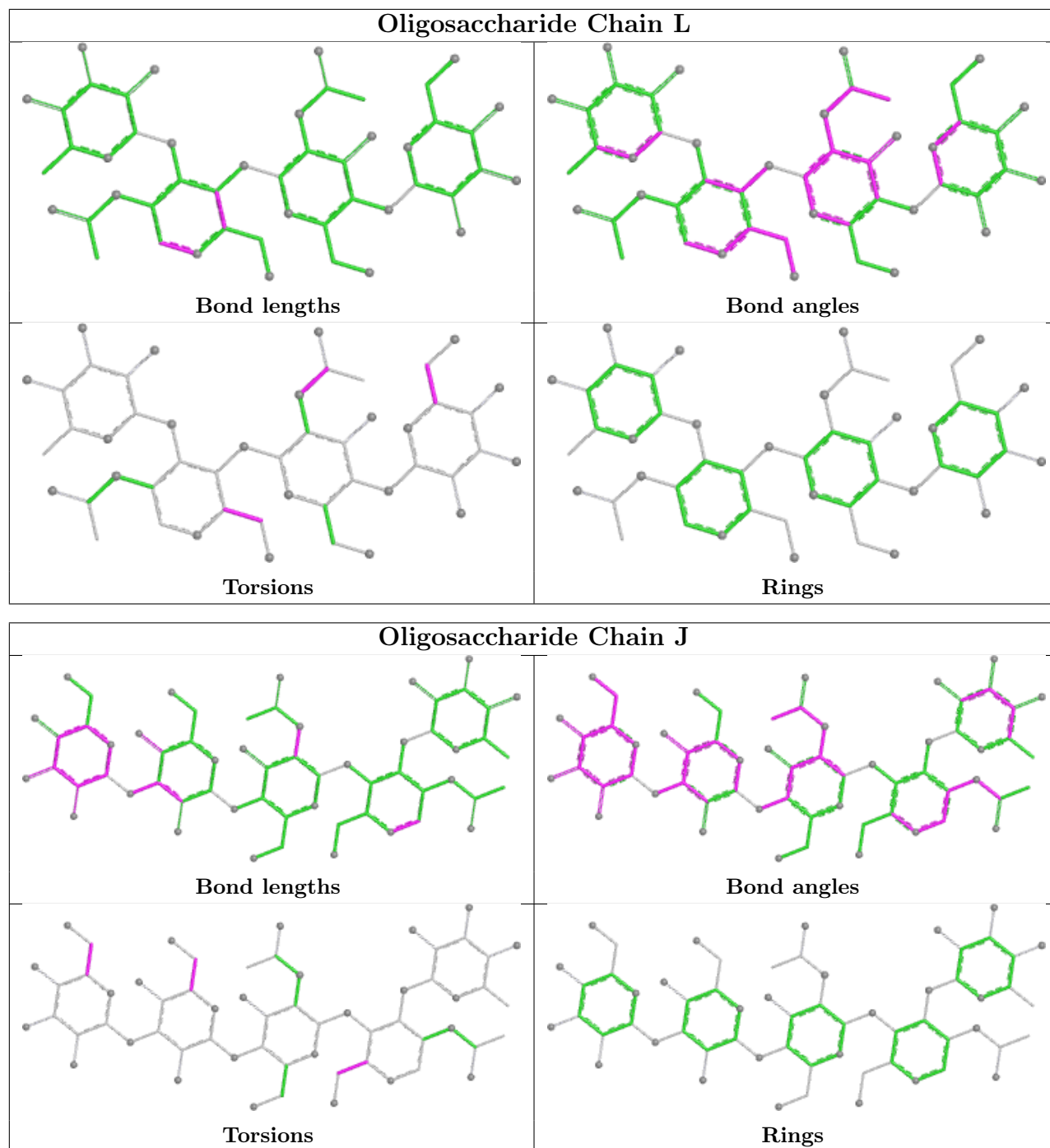
There are no ring outliers.

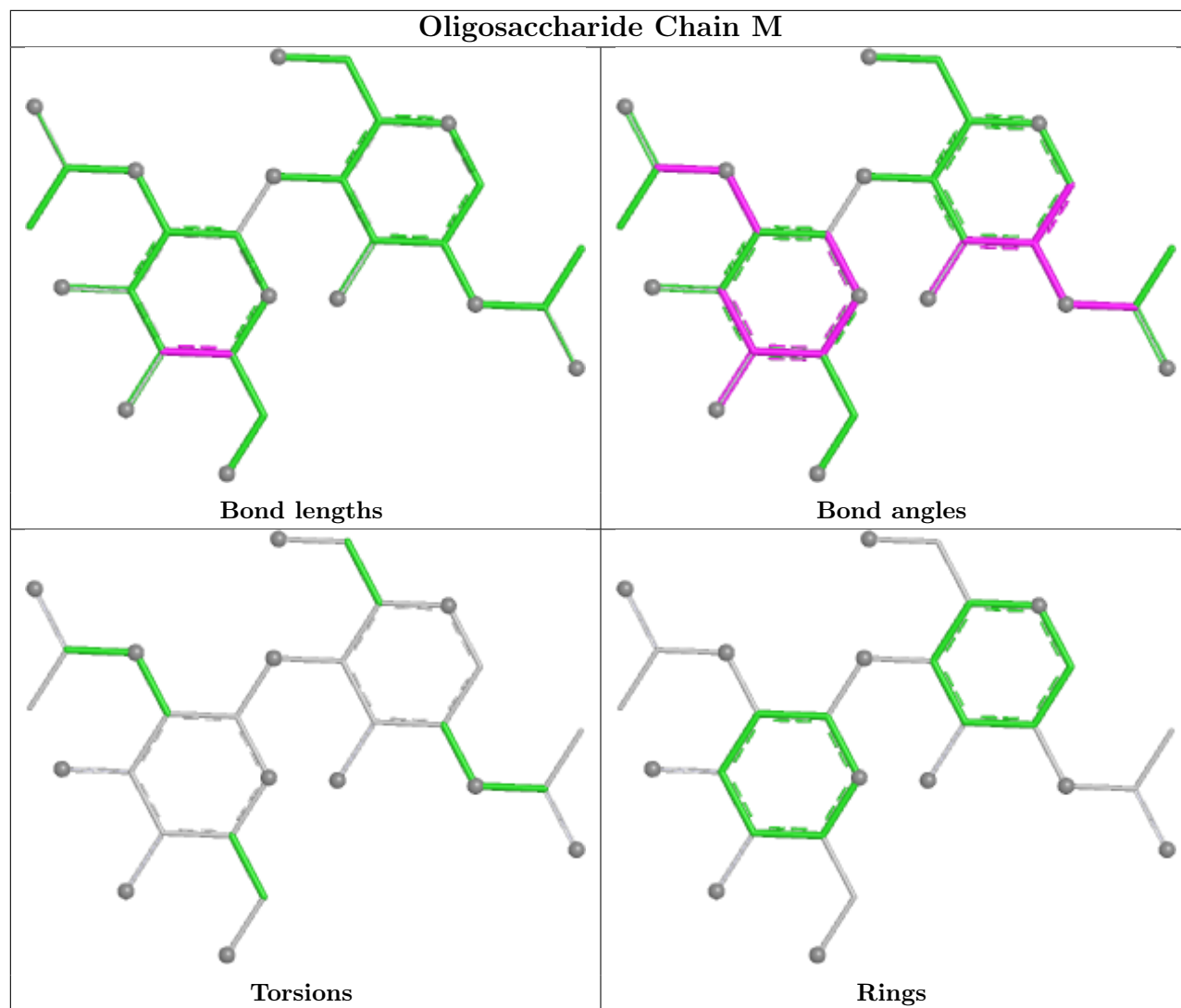
9 monomers are involved in 14 short contacts:

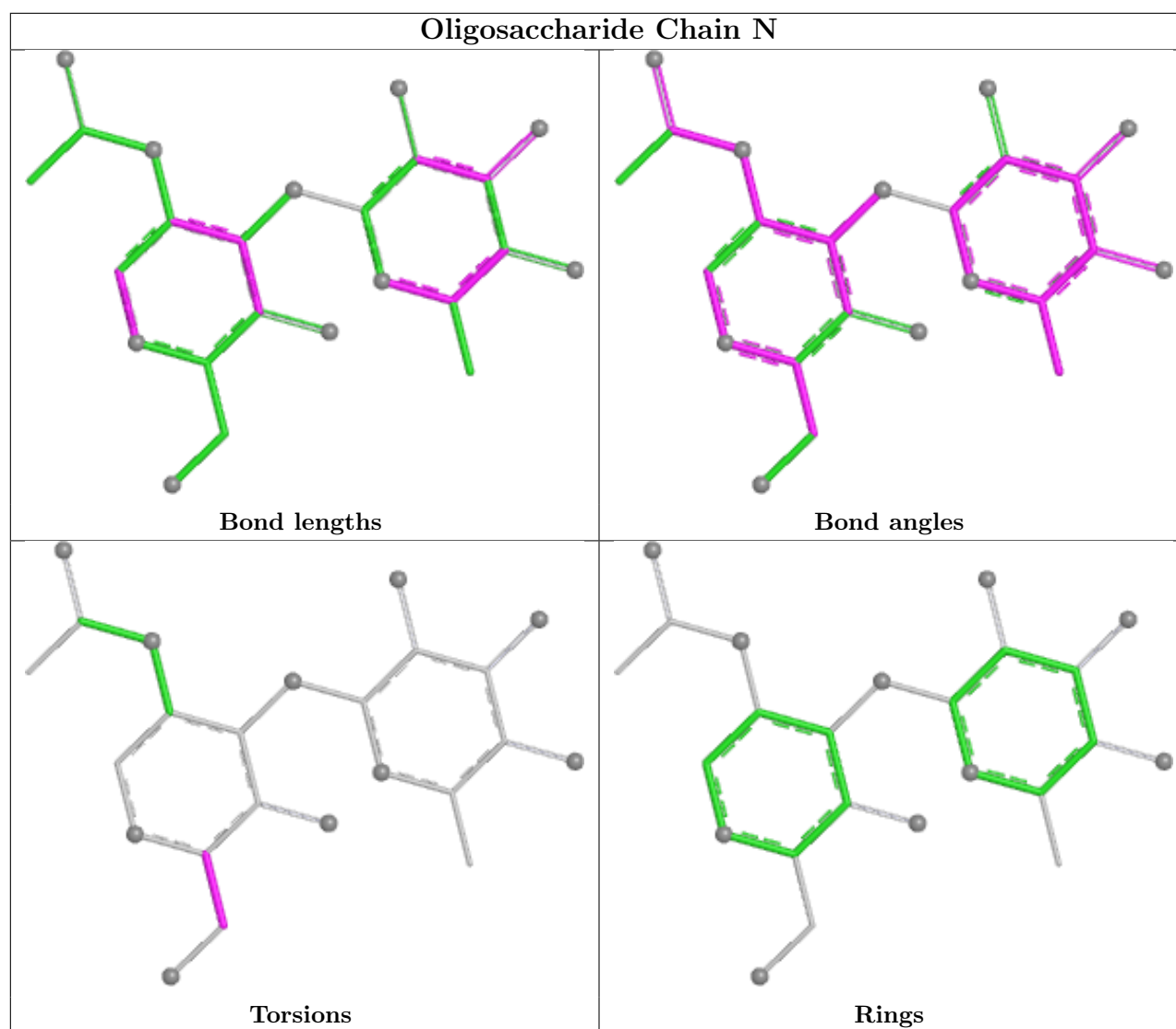
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	4	FUC	1	0
3	L	4	FUC	1	0
3	I	3	BMA	1	0
4	J	4	MAN	2	0
4	J	1	NAG	1	0
3	L	2	NAG	1	0
3	I	1	NAG	2	0
3	I	2	NAG	2	0
4	J	3	BMA	8	0

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](#)

Of 34 ligands modelled in this entry, 16 are monoatomic - leaving 18 for Mogul analysis.

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	$\# Z > 2$
10	GOL	C	283	-	5,5,5	0.35	0	5,5,5	0.76	0
10	GOL	H	289	-	5,5,5	0.31	0	5,5,5	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ABU	E	284	-	6,6,6	1.17	0	6,6,6	1.34	1 (16%)
9	ABU	D	278	-	6,6,6	0.95	0	6,6,6	0.62	0
9	ABU	A	280	-	6,6,6	1.10	1 (16%)	6,6,6	0.67	0
10	GOL	G	287	-	5,5,5	0.32	0	5,5,5	0.36	0
9	ABU	F	290	-	6,6,6	0.86	0	6,6,6	1.22	1 (16%)
11	XYP	B	306	-	9,9,10	2.44	3 (33%)	10,12,14	5.76	5 (50%)
9	ABU	C	282	-	6,6,6	0.79	0	6,6,6	1.17	1 (16%)
9	ABU	B	276	-	6,6,6	1.01	0	6,6,6	0.90	0
10	GOL	B	281	-	5,5,5	0.31	0	5,5,5	1.00	0
9	ABU	E	288	-	6,6,6	0.89	0	6,6,6	0.99	0
10	GOL	A	277	-	5,5,5	0.28	0	5,5,5	0.67	0
9	ABU	G	286	-	6,6,6	0.92	0	6,6,6	0.70	0
10	GOL	D	285	-	5,5,5	0.32	0	5,5,5	0.70	0
12	NAG	D	301	2	14,14,15	1.90	3 (21%)	17,19,21	1.68	4 (23%)
10	GOL	E	279	-	5,5,5	0.28	0	5,5,5	1.23	1 (20%)
10	GOL	E	291	-	5,5,5	0.42	0	5,5,5	0.69	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
10	GOL	C	283	-	-	0/4/4/4	-
10	GOL	H	289	-	-	2/4/4/4	-
9	ABU	E	284	-	-	2/4/4/4	-
9	ABU	D	278	-	-	1/4/4/4	-
9	ABU	A	280	-	-	3/4/4/4	-
10	GOL	G	287	-	-	2/4/4/4	-
9	ABU	F	290	-	-	3/4/4/4	-
11	XYP	B	306	-	-	-	0/1/1/1
9	ABU	C	282	-	-	3/4/4/4	-
9	ABU	B	276	-	-	1/4/4/4	-
10	GOL	B	281	-	-	0/4/4/4	-
9	ABU	E	288	-	-	1/4/4/4	-
10	GOL	A	277	-	-	2/4/4/4	-
9	ABU	G	286	-	-	4/4/4/4	-
10	GOL	D	285	-	-	4/4/4/4	-
12	NAG	D	301	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	E	279	-	-	2/4/4/4	-
10	GOL	E	291	-	-	4/4/4/4	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	306	XYP	O5-C1	5.85	1.54	1.43
12	D	301	NAG	C1-C2	-4.69	1.46	1.52
12	D	301	NAG	C3-C2	-4.09	1.43	1.52
12	D	301	NAG	C2-N2	2.87	1.51	1.46
11	B	306	XYP	C5-C4	2.78	1.58	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	306	XYP	C1-C2-C3	13.75	129.67	109.64
11	B	306	XYP	C5-O5-C1	9.05	126.02	111.42
11	B	306	XYP	O4-C4-C3	-5.84	98.05	110.15
11	B	306	XYP	O4-C4-C5	-4.28	99.42	109.22
12	D	301	NAG	C1-O5-C5	4.19	117.80	112.19

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	277	GOL	C1-C2-C3-O3
10	D	285	GOL	O1-C1-C2-C3
10	D	285	GOL	C1-C2-C3-O3
10	E	279	GOL	O1-C1-C2-C3
10	E	291	GOL	O1-C1-C2-C3

There are no ring outliers.

11 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	283	GOL	1	0
10	H	289	GOL	3	0
9	E	284	ABU	2	0
9	A	280	ABU	3	0
9	F	290	ABU	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	306	XYP	6	0
9	C	282	ABU	5	0
9	B	276	ABU	2	0
9	E	288	ABU	3	0
10	A	277	GOL	2	0
10	E	279	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	A	250/256 (97%)	-0.09	5 (2%) 65 66	12, 20, 30, 48	1 (0%)
1	C	250/256 (97%)	0.00	7 (2%) 55 56	12, 21, 39, 63	0
1	E	250/256 (97%)	0.00	6 (2%) 59 62	14, 24, 40, 59	0
1	G	250/256 (97%)	-0.11	4 (1%) 70 73	14, 22, 35, 52	0
2	B	242/242 (100%)	-0.22	1 (0%) 88 89	11, 18, 26, 35	2 (0%)
2	D	242/242 (100%)	0.05	3 (1%) 76 78	15, 26, 41, 58	0
2	F	242/242 (100%)	-0.15	3 (1%) 76 78	14, 19, 28, 50	1 (0%)
2	H	242/242 (100%)	-0.02	2 (0%) 82 83	17, 26, 39, 55	0
All	All	1968/1992 (98%)	-0.07	31 (1%) 70 73	11, 22, 38, 63	4 (0%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	255	ALA	5.8
2	B	1	THR	5.6
1	E	247	LEU	4.9
2	H	101	PRO	4.2
2	F	242	ALA	4.0

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 [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,

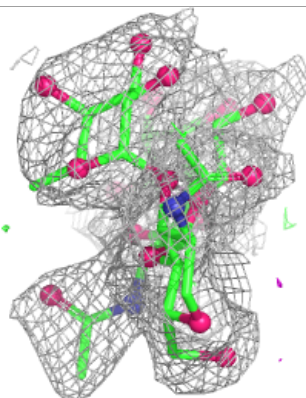
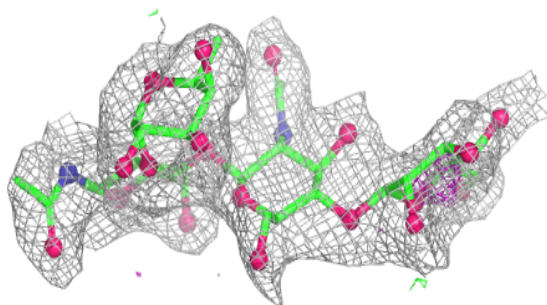
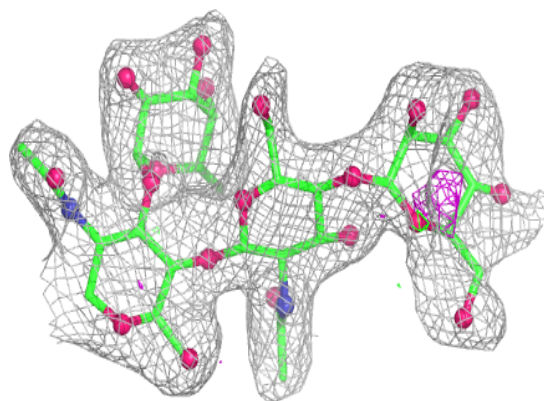
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	FUC	N	2	10/11	0.59	0.20	60,63,68,70	0
5	NAG	M	2	14/15	0.66	0.16	60,70,79,81	0
3	BMA	I	3	11/12	0.69	0.15	39,42,44,46	0
5	NAG	M	1	14/15	0.82	0.13	44,52,59,60	0
3	BMA	K	3	11/12	0.82	0.11	42,46,48,48	0
3	BMA	L	3	11/12	0.82	0.12	42,46,48,49	0
4	MAN	J	4	11/12	0.83	0.14	39,41,44,45	0
4	BMA	J	3	11/12	0.83	0.13	34,38,39,42	0
3	NAG	K	2	14/15	0.88	0.11	36,39,42,42	0
3	NAG	L	1	14/15	0.89	0.11	24,26,28,30	0
6	NAG	N	1	14/15	0.89	0.11	40,46,48,55	0
3	NAG	L	2	14/15	0.89	0.10	32,34,38,40	0
3	NAG	K	1	14/15	0.90	0.10	28,32,33,35	0
3	NAG	I	2	14/15	0.90	0.10	32,33,36,37	0
3	NAG	I	1	14/15	0.93	0.09	26,29,31,32	0
3	FUC	I	4	10/11	0.94	0.09	33,35,37,37	0
3	FUC	L	4	10/11	0.94	0.08	28,30,32,32	0
4	NAG	J	1	14/15	0.94	0.07	20,22,25,25	0
4	NAG	J	2	14/15	0.94	0.09	26,28,31,32	0
3	FUC	K	4	10/11	0.94	0.07	32,34,35,36	0
4	FUC	J	5	10/11	0.95	0.08	25,27,29,30	0

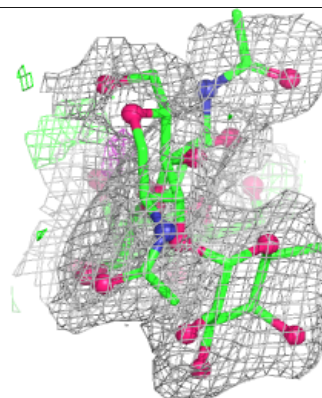
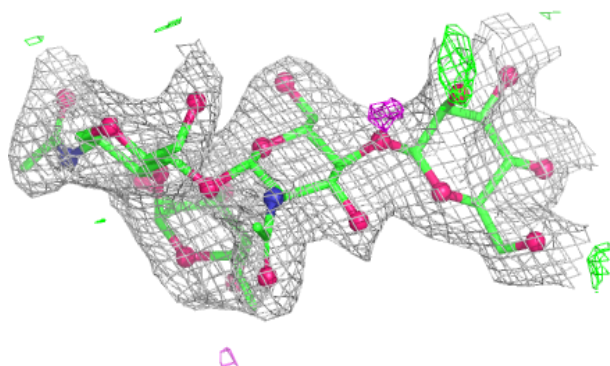
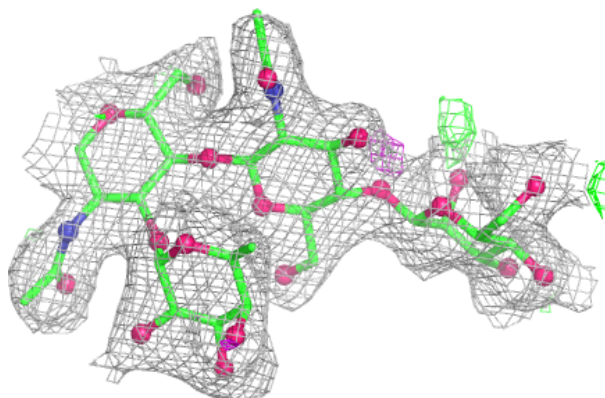
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

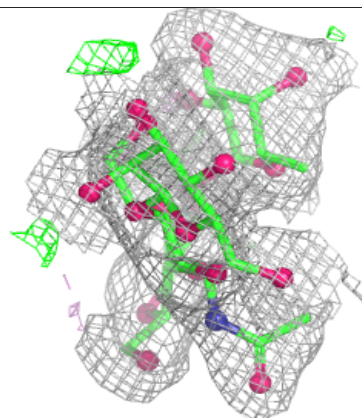
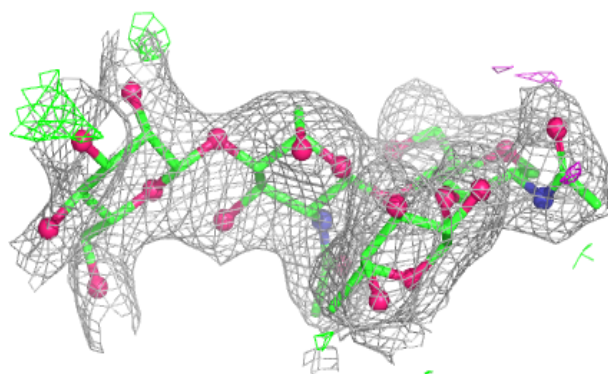
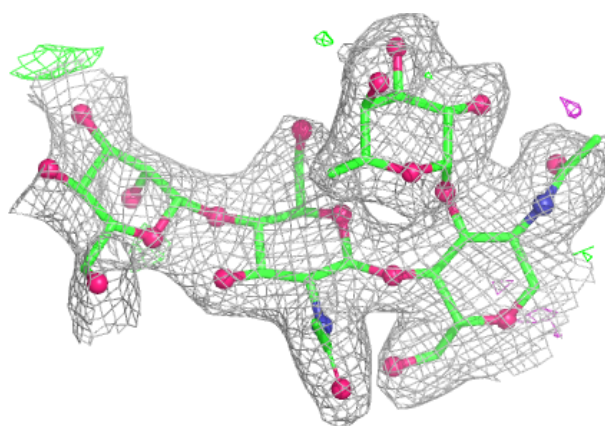
**Electron density around Chain K:**

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

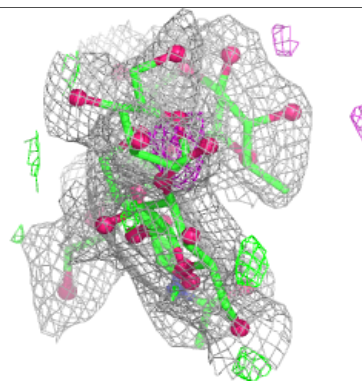
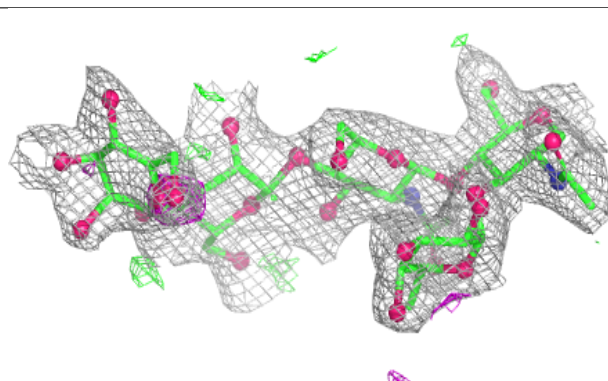
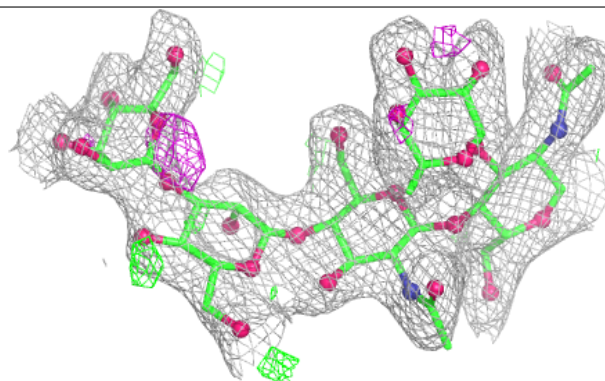


Electron density around Chain L:

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

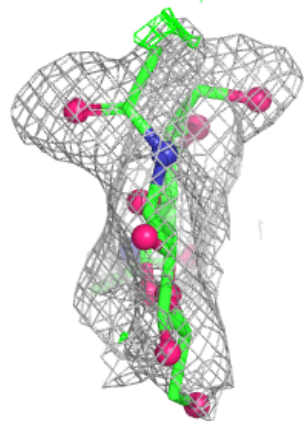
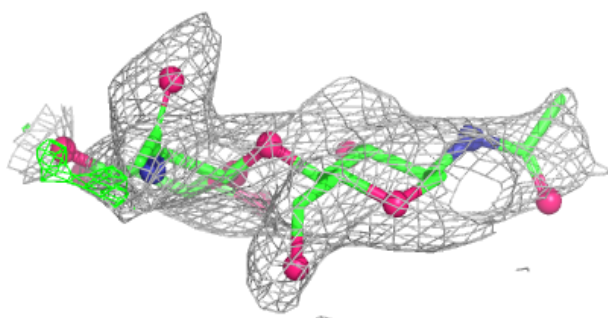
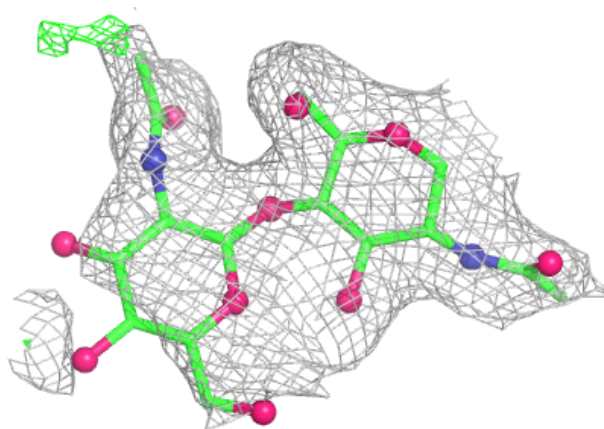
**Electron density around Chain J:**

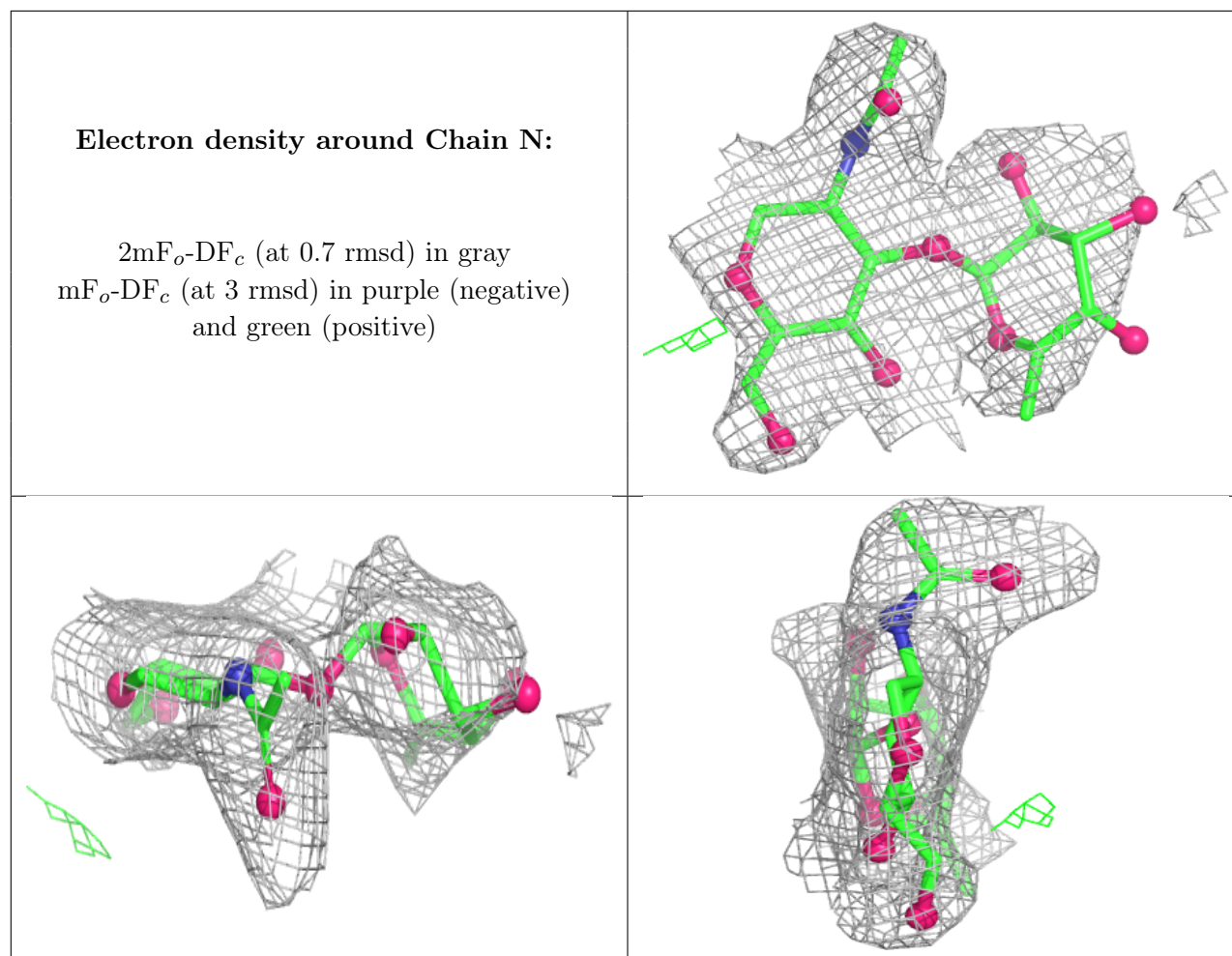
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain M:

$2mF_o - DF_c$ (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	ABU	E	284	7/7	0.79	0.17	25,28,33,33	0
12	NAG	D	301	14/15	0.83	0.12	50,56,59,60	0
11	XYP	B	306	9/10	0.86	0.12	41,41,43,43	0
10	GOL	H	289	6/6	0.88	0.11	29,31,31,34	0
9	ABU	B	276	7/7	0.88	0.15	27,30,34,35	0
10	GOL	A	277	6/6	0.88	0.13	30,33,34,36	0
10	GOL	C	283	6/6	0.89	0.12	25,25,26,26	0
9	ABU	F	290	7/7	0.89	0.17	14,16,20,22	0
9	ABU	D	278	7/7	0.90	0.17	29,30,33,35	0
10	GOL	B	281	6/6	0.91	0.10	20,21,22,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	ABU	E	288	7/7	0.91	0.16	32,36,38,38	0
10	GOL	D	285	6/6	0.91	0.11	32,33,33,34	0
10	GOL	E	291	6/6	0.92	0.10	29,29,31,33	0
9	ABU	A	280	7/7	0.92	0.13	22,24,27,28	0
9	ABU	G	286	7/7	0.92	0.13	31,33,35,37	0
10	GOL	E	279	6/6	0.92	0.11	31,32,33,35	0
9	ABU	C	282	7/7	0.93	0.13	29,30,33,34	0
10	GOL	G	287	6/6	0.95	0.09	29,29,30,31	0
7	CA	D	268	1/1	0.97	0.03	31,31,31,31	0
7	CA	G	270	1/1	0.98	0.02	17,17,17,17	0
8	MN	H	273	1/1	0.98	0.02	23,23,23,23	0
7	CA	B	260	1/1	0.98	0.02	15,15,15,15	0
7	CA	A	264	1/1	0.98	0.02	19,19,19,19	0
7	CA	F	274	1/1	0.98	0.03	23,23,23,23	0
8	MN	E	263	1/1	0.99	0.03	25,25,25,25	0
7	CA	C	266	1/1	0.99	0.02	19,19,19,19	0
7	CA	H	272	1/1	0.99	0.03	30,30,30,30	0
8	MN	B	261	1/1	0.99	0.01	13,13,13,13	0
8	MN	C	267	1/1	0.99	0.01	20,20,20,20	0
8	MN	G	271	1/1	1.00	0.01	19,19,19,19	0
8	MN	A	265	1/1	1.00	0.01	13,13,13,13	0
8	MN	D	269	1/1	1.00	0.02	38,38,38,38	0
7	CA	E	262	1/1	1.00	0.01	20,20,20,20	0
8	MN	F	275	1/1	1.00	0.01	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.