



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2021 – 04:06 PM EDT

PDB ID : 2ERJ  
Title : Crystal structure of the heterotrimeric interleukin-2 receptor in complex with interleukin-2  
Authors : Debler, E.W.; Stauber, D.J.; Wilson, I.A.  
Deposited on : 2005-10-25  
Resolution : 3.00 Å(reported)

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We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

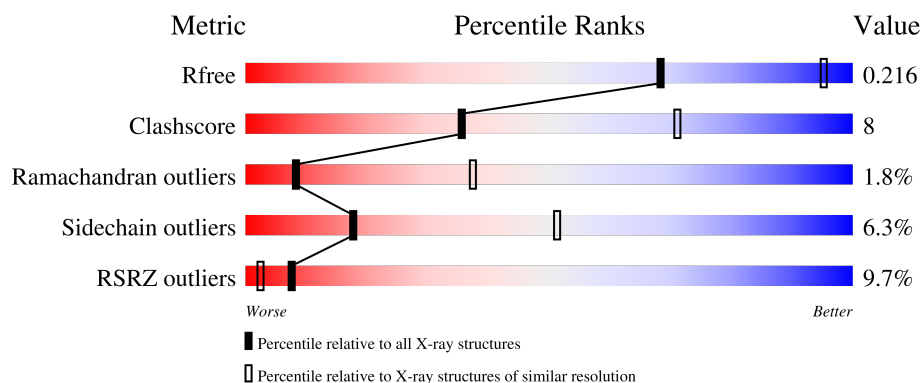
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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  $\geq 3$ , 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	225	<div> <div>8%</div> <div>40%</div> <div>15%</div> <div>•</div> <div>42%</div> </div>
1	E	225	<div> <div>7%</div> <div>43%</div> <div>14%</div> <div>•</div> <div>42%</div> </div>
2	B	219	<div> <div>7%</div> <div>71%</div> <div>20%</div> <div>•</div> <div>7%</div> </div>
2	F	219	<div> <div>5%</div> <div>73%</div> <div>17%</div> <div>•</div> <div>8%</div> </div>
3	C	247	<div> <div>4%</div> <div>60%</div> <div>17%</div> <div>•</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	247	
4	D	133	
4	H	133	
5	I	4	
5	M	4	
6	J	2	
7	K	3	
7	O	3	
8	L	2	
8	P	2	
9	N	3	

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
5	NAG	I	2	-	-	-	X
8	NAG	L	2	-	-	-	X
8	NAG	P	1	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11187 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 Interleukin-2 receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			1028	637	185	191	15			
1	E	131	Total	C	N	O	S	0	0	0
			1033	640	186	192	15			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	cloning artifact	UNP P01589
A	-3	MET	-	cloning artifact	UNP P01589
A	-2	LEU	-	cloning artifact	UNP P01589
A	-1	SER	-	cloning artifact	UNP P01589
A	0	LEU	-	cloning artifact	UNP P01589
A	49	SER	ASN	engineered mutation	UNP P01589
A	68	SER	ASN	engineered mutation	UNP P01589
A	213	THR	-	expression tag	UNP P01589
A	214	GLY	-	expression tag	UNP P01589
A	215	HIS	-	expression tag	UNP P01589
A	216	HIS	-	expression tag	UNP P01589
A	217	HIS	-	expression tag	UNP P01589
A	218	HIS	-	expression tag	UNP P01589
A	219	HIS	-	expression tag	UNP P01589
A	220	HIS	-	expression tag	UNP P01589
E	-4	GLY	-	cloning artifact	UNP P01589
E	-3	MET	-	cloning artifact	UNP P01589
E	-2	LEU	-	cloning artifact	UNP P01589
E	-1	SER	-	cloning artifact	UNP P01589
E	0	LEU	-	cloning artifact	UNP P01589
E	49	SER	ASN	engineered mutation	UNP P01589
E	68	SER	ASN	engineered mutation	UNP P01589
E	213	THR	-	expression tag	UNP P01589
E	214	GLY	-	expression tag	UNP P01589
E	215	HIS	-	expression tag	UNP P01589

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Chain	Residue	Modelled	Actual	Comment	Reference
E	216	HIS	-	expression tag	UNP P01589
E	217	HIS	-	expression tag	UNP P01589
E	218	HIS	-	expression tag	UNP P01589
E	219	HIS	-	expression tag	UNP P01589
E	220	HIS	-	expression tag	UNP P01589

- Molecule 2 is a protein called Interleukin-2 receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	204	Total	C	N	O	S	0	0	0
			1676	1065	298	303	10			
2	F	201	Total	C	N	O	S	0	0	0
			1654	1051	294	299	10			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	cloning artifact	UNP P14784
B	-3	MET	-	cloning artifact	UNP P14784
B	-2	LEU	-	cloning artifact	UNP P14784
B	-1	SER	-	cloning artifact	UNP P14784
B	0	LEU	-	cloning artifact	UNP P14784
B	207	THR	-	expression tag	UNP P14784
B	208	GLY	-	expression tag	UNP P14784
B	209	HIS	-	expression tag	UNP P14784
B	210	HIS	-	expression tag	UNP P14784
B	211	HIS	-	expression tag	UNP P14784
B	212	HIS	-	expression tag	UNP P14784
B	213	HIS	-	expression tag	UNP P14784
B	214	HIS	-	expression tag	UNP P14784
F	-4	GLY	-	cloning artifact	UNP P14784
F	-3	MET	-	cloning artifact	UNP P14784
F	-2	LEU	-	cloning artifact	UNP P14784
F	-1	SER	-	cloning artifact	UNP P14784
F	0	LEU	-	cloning artifact	UNP P14784
F	207	THR	-	expression tag	UNP P14784
F	208	GLY	-	expression tag	UNP P14784
F	209	HIS	-	expression tag	UNP P14784
F	210	HIS	-	expression tag	UNP P14784
F	211	HIS	-	expression tag	UNP P14784
F	212	HIS	-	expression tag	UNP P14784
F	213	HIS	-	expression tag	UNP P14784

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Chain	Residue	Modelled	Actual	Comment	Reference
F	214	HIS	-	expression tag	UNP P14784

- Molecule 3 is a protein called Cytokine receptor common gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	195	Total	C	N	O	S	0	0	0
			1655	1052	294	301	8			
3	G	195	Total	C	N	O	S	0	0	0
			1655	1052	294	301	8			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	cloning artifact	UNP P31785
C	-3	MET	-	cloning artifact	UNP P31785
C	-2	LEU	-	cloning artifact	UNP P31785
C	-1	SER	-	cloning artifact	UNP P31785
C	0	LEU	-	cloning artifact	UNP P31785
C	53	GLN	ASN	engineered mutation	UNP P31785
C	234	ARG	-	expression tag	UNP P31785
C	235	THR	-	expression tag	UNP P31785
C	236	GLY	-	expression tag	UNP P31785
C	237	HIS	-	expression tag	UNP P31785
C	238	HIS	-	expression tag	UNP P31785
C	239	HIS	-	expression tag	UNP P31785
C	240	HIS	-	expression tag	UNP P31785
C	241	HIS	-	expression tag	UNP P31785
C	242	HIS	-	expression tag	UNP P31785
G	-4	GLY	-	cloning artifact	UNP P31785
G	-3	MET	-	cloning artifact	UNP P31785
G	-2	LEU	-	cloning artifact	UNP P31785
G	-1	SER	-	cloning artifact	UNP P31785
G	0	LEU	-	cloning artifact	UNP P31785
G	53	GLN	ASN	engineered mutation	UNP P31785
G	234	ARG	-	expression tag	UNP P31785
G	235	THR	-	expression tag	UNP P31785
G	236	GLY	-	expression tag	UNP P31785
G	237	HIS	-	expression tag	UNP P31785
G	238	HIS	-	expression tag	UNP P31785
G	239	HIS	-	expression tag	UNP P31785
G	240	HIS	-	expression tag	UNP P31785
G	241	HIS	-	expression tag	UNP P31785

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Chain	Residue	Modelled	Actual	Comment	Reference
G	242	HIS	-	expression tag	UNP P31785

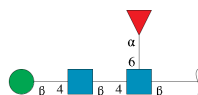
- Molecule 4 is a protein called Interleukin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	131	Total 1068	C 685	N 176	O 201	S 6	0	0	0
4	H	131	Total 1068	C 685	N 176	O 201	S 6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	125	ALA	CYS	engineered mutation	UNP P60568
H	125	ALA	CYS	engineered mutation	UNP P60568

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



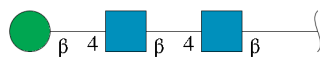
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	4	Total	C	N	O	0	0	0
			49	28	2	19			
5	M	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



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

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



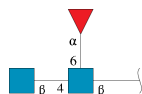
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	O	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 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
8	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

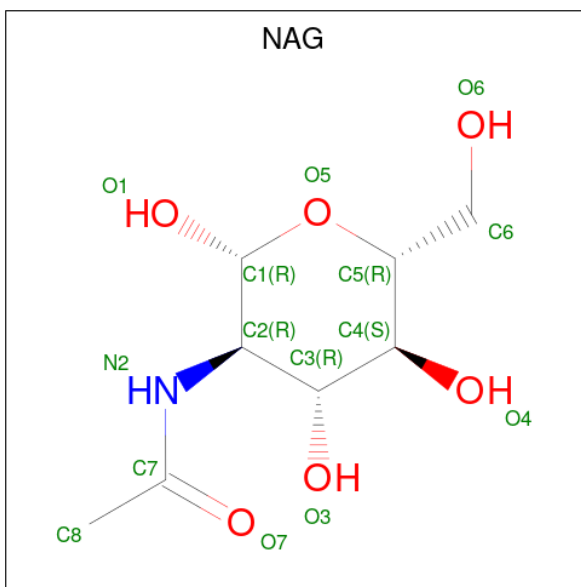
- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	N	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

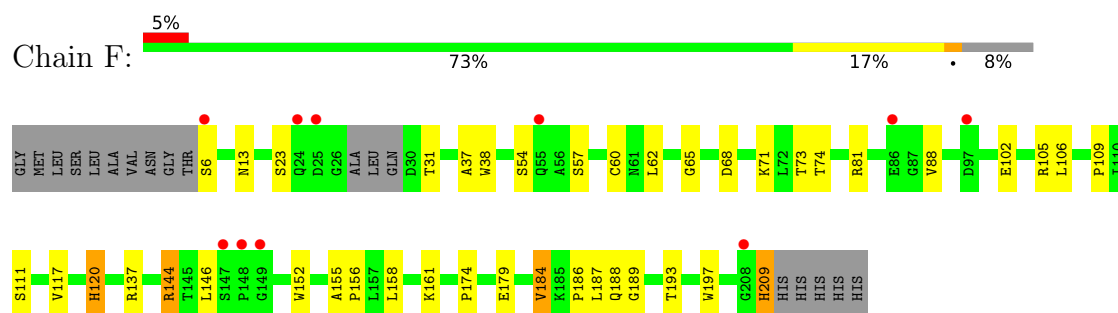




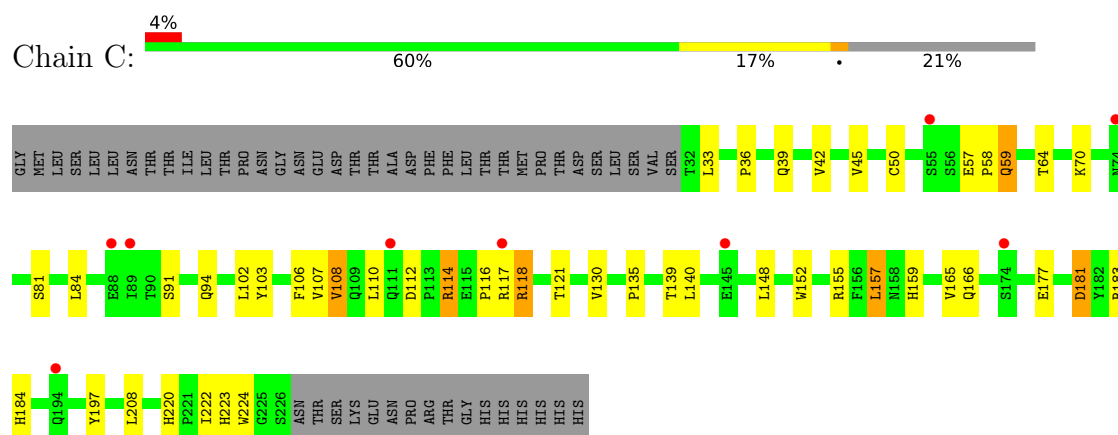
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	G	1	Total	C	N	O	0	0
			14	8	1	5		
10	G	1	Total	C	N	O	0	0
			14	8	1	5		



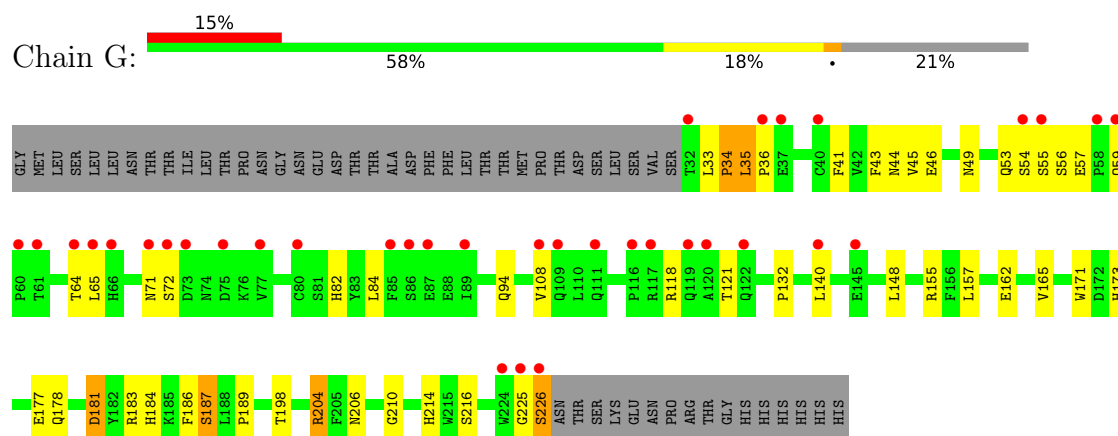
- Molecule 2: Interleukin-2 receptor beta chain



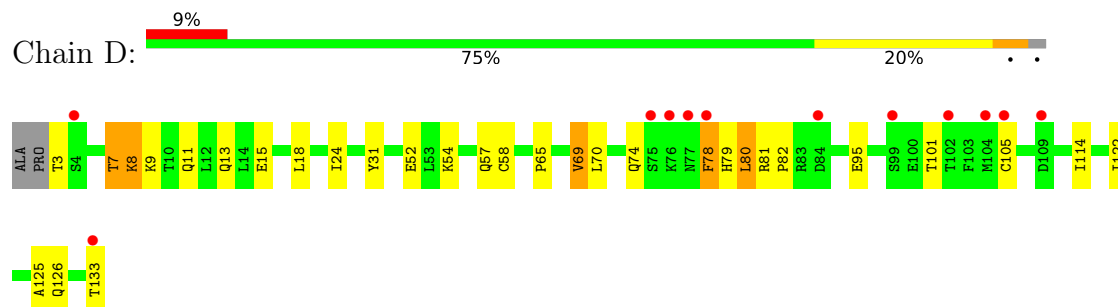
- Molecule 3: Cytokine receptor common gamma chain



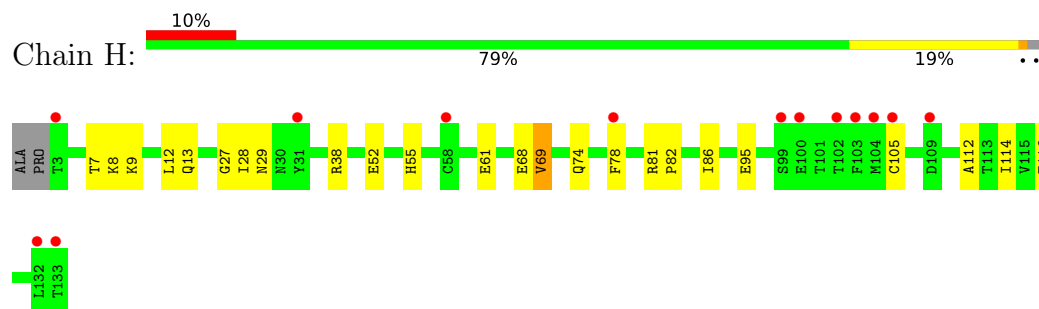
- Molecule 3: Cytokine receptor common gamma chain



- Molecule 4: Interleukin-2



- Molecule 4: Interleukin-2



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



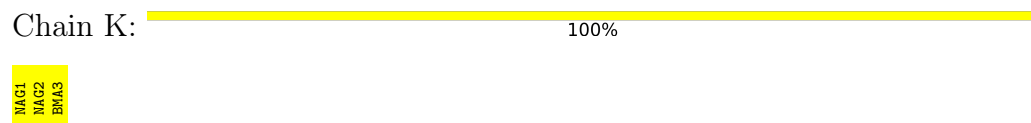
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



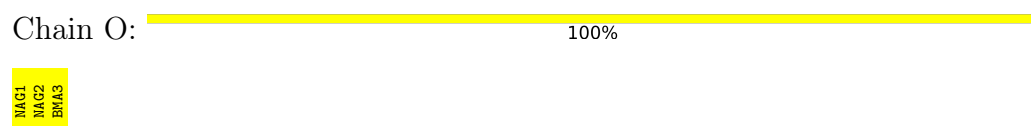
- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose




- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

MAG1  
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  100%

MAG1  
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  33% 67%

MAG1  
MAG2  
FUC3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.27Å 70.55Å 129.24Å 83.85° 82.45° 89.72°	Depositor
Resolution (Å)	129.10 – 3.00 45.45 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.4 (129.10-3.00) 93.4 (45.45-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.220 , 0.263 0.220 , 0.216	Depositor DCC
$R_{free}$ test set	1861 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.4	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 103.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11187	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BMA, NAG, FUC

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	0.43	0/1056	0.55	0/1427
1	E	0.39	0/1061	0.53	0/1434
2	B	0.52	0/1725	0.62	0/2353
2	F	0.54	0/1702	0.62	0/2320
3	C	0.48	0/1710	0.65	0/2329
3	G	0.43	0/1710	0.61	0/2329
4	D	0.48	0/1085	0.61	1/1464 (0.1%)
4	H	0.45	0/1085	0.58	0/1464
All	All	0.47	0/11134	0.60	1/15120 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	80	LEU	CA-CB-CG	5.13	127.11	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	1028	0	967	20	0
1	E	1033	0	972	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1676	0	1615	32	0
2	F	1654	0	1590	31	0
3	C	1655	0	1555	26	0
3	G	1655	0	1555	26	0
4	D	1068	0	1103	16	0
4	H	1068	0	1103	15	0
5	I	49	0	43	0	0
5	M	49	0	43	2	0
6	J	24	0	22	1	0
7	K	39	0	34	0	0
7	O	39	0	34	0	0
8	L	28	0	25	0	0
8	P	28	0	25	0	0
9	N	38	0	34	3	0
10	C	28	0	26	0	0
10	G	28	0	26	0	0
All	All	11187	0	10772	177	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 8.

The worst 5 of 177 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:A:20:TYR:HB3	1:A:24:THR:HG21	1.50	0.93
3:G:33:LEU:N	3:G:34:PRO:HD2	1.89	0.86
1:E:20:TYR:HB3	1:E:24:THR:HG21	1.58	0.85
2:F:81:ARG:NH2	9:N:3:FUC:H61	1.95	0.81
4:H:69:VAL:HG11	4:H:114:ILE:HD12	1.63	0.81

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	126/225 (56%)	108 (86%)	15 (12%)	3 (2%)	6	29
1	E	127/225 (56%)	110 (87%)	14 (11%)	3 (2%)	6	29
2	B	202/219 (92%)	185 (92%)	14 (7%)	3 (2%)	10	42
2	F	197/219 (90%)	181 (92%)	16 (8%)	0	100	100
3	C	193/247 (78%)	171 (89%)	16 (8%)	6 (3%)	4	23
3	G	193/247 (78%)	168 (87%)	19 (10%)	6 (3%)	4	23
4	D	129/133 (97%)	120 (93%)	8 (6%)	1 (1%)	19	57
4	H	129/133 (97%)	121 (94%)	7 (5%)	1 (1%)	19	57
All	All	1296/1648 (79%)	1164 (90%)	109 (8%)	23 (2%)	8	37

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	GLU
1	A	133	GLN
3	C	117	ARG
2	B	148	PRO
3	C	181	ASP

### 5.3.2 Protein sidechains ⓘ

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	114/200 (57%)	106 (93%)	8 (7%)	15	47
1	E	114/200 (57%)	109 (96%)	5 (4%)	28	65
2	B	186/198 (94%)	174 (94%)	12 (6%)	17	50
2	F	184/198 (93%)	173 (94%)	11 (6%)	19	53
3	C	188/236 (80%)	177 (94%)	11 (6%)	19	54
3	G	188/236 (80%)	173 (92%)	15 (8%)	12	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	124/125 (99%)	114 (92%)	10 (8%)	11	40
4	H	124/125 (99%)	119 (96%)	5 (4%)	31	68
All	All	1222/1518 (80%)	1145 (94%)	77 (6%)	18	51

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	35	LEU
3	G	226	SER
3	G	54	SER
3	G	157	LEU
4	H	95	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	139	HIS
2	F	36	HIS
4	H	119	ASN
3	G	82	HIS
4	D	126	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

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	$\# Z  > 2$
5	NAG	I	1	2,5	14,14,15	0.57	0	17,19,21	1.16	1 (5%)
5	NAG	I	2	5	14,14,15	0.59	0	17,19,21	0.87	1 (5%)
5	BMA	I	3	5	11,11,12	0.71	0	15,15,17	1.46	2 (13%)
5	FUC	I	4	5	10,10,11	0.78	0	14,14,16	0.81	0
6	NAG	J	1	2,6	14,14,15	0.50	0	17,19,21	1.38	3 (17%)
6	FUC	J	2	6	10,10,11	0.66	0	14,14,16	0.58	0
7	NAG	K	1	2,7	14,14,15	0.61	0	17,19,21	0.98	1 (5%)
7	NAG	K	2	7	14,14,15	0.53	0	17,19,21	1.04	2 (11%)
7	BMA	K	3	7	11,11,12	0.50	0	15,15,17	1.30	1 (6%)
8	NAG	L	1	8,3	14,14,15	0.67	0	17,19,21	1.29	2 (11%)
8	NAG	L	2	8	14,14,15	0.69	0	17,19,21	1.48	3 (17%)
5	NAG	M	1	2,5	14,14,15	0.66	0	17,19,21	1.05	1 (5%)
5	NAG	M	2	5	14,14,15	0.56	0	17,19,21	0.91	0
5	BMA	M	3	5	11,11,12	0.65	0	15,15,17	1.92	3 (20%)
5	FUC	M	4	5	10,10,11	0.74	0	14,14,16	0.88	1 (7%)
9	NAG	N	1	2,9	14,14,15	0.47	0	17,19,21	1.55	3 (17%)
9	NAG	N	2	9	14,14,15	0.44	0	17,19,21	1.29	1 (5%)
9	FUC	N	3	9	10,10,11	0.59	0	14,14,16	0.94	1 (7%)
7	NAG	O	1	2,7	14,14,15	0.63	0	17,19,21	1.11	1 (5%)
7	NAG	O	2	7	14,14,15	0.54	0	17,19,21	1.38	2 (11%)
7	BMA	O	3	7	11,11,12	0.64	0	15,15,17	1.04	1 (6%)
8	NAG	P	1	8,3	14,14,15	0.66	0	17,19,21	0.96	2 (11%)
8	NAG	P	2	8	14,14,15	0.65	0	17,19,21	1.28	2 (11%)

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	I	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	4/6/23/26	0/1/1/1
5	BMA	I	3	5	-	2/2/19/22	0/1/1/1
5	FUC	I	4	5	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	J	1	2,6	-	2/6/23/26	0/1/1/1
6	FUC	J	2	6	-	-	0/1/1/1
7	NAG	K	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1
7	BMA	K	3	7	-	2/2/19/22	0/1/1/1
8	NAG	L	1	8,3	-	3/6/23/26	0/1/1/1
8	NAG	L	2	8	-	2/6/23/26	0/1/1/1
5	NAG	M	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	FUC	M	4	5	-	-	0/1/1/1
9	NAG	N	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	N	2	9	-	4/6/23/26	0/1/1/1
9	FUC	N	3	9	-	-	0/1/1/1
7	NAG	O	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	O	2	7	-	2/6/23/26	0/1/1/1
7	BMA	O	3	7	-	2/2/19/22	0/1/1/1
8	NAG	P	1	8,3	-	3/6/23/26	0/1/1/1
8	NAG	P	2	8	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	3	BMA	C1-O5-C5	5.34	119.43	112.19
9	N	2	NAG	C1-O5-C5	4.40	118.15	112.19
7	K	3	BMA	C1-O5-C5	3.90	117.47	112.19
5	M	3	BMA	C1-C2-C3	3.76	114.29	109.67
7	O	2	NAG	C1-O5-C5	3.73	117.25	112.19

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

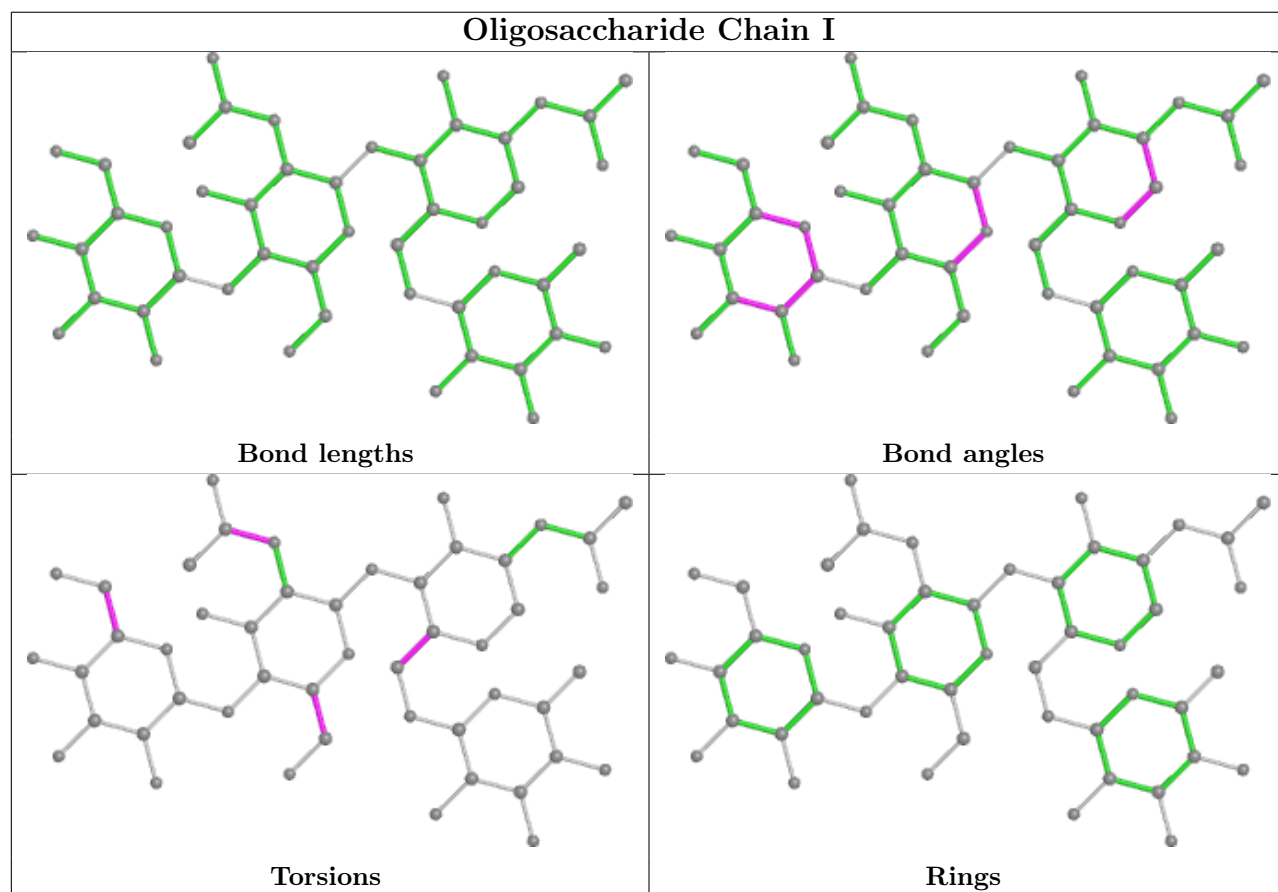
Mol	Chain	Res	Type	Atoms
8	L	2	NAG	C8-C7-N2-C2
8	L	2	NAG	O7-C7-N2-C2
8	P	1	NAG	C3-C2-N2-C7
8	P	1	NAG	C8-C7-N2-C2
8	P	1	NAG	O7-C7-N2-C2

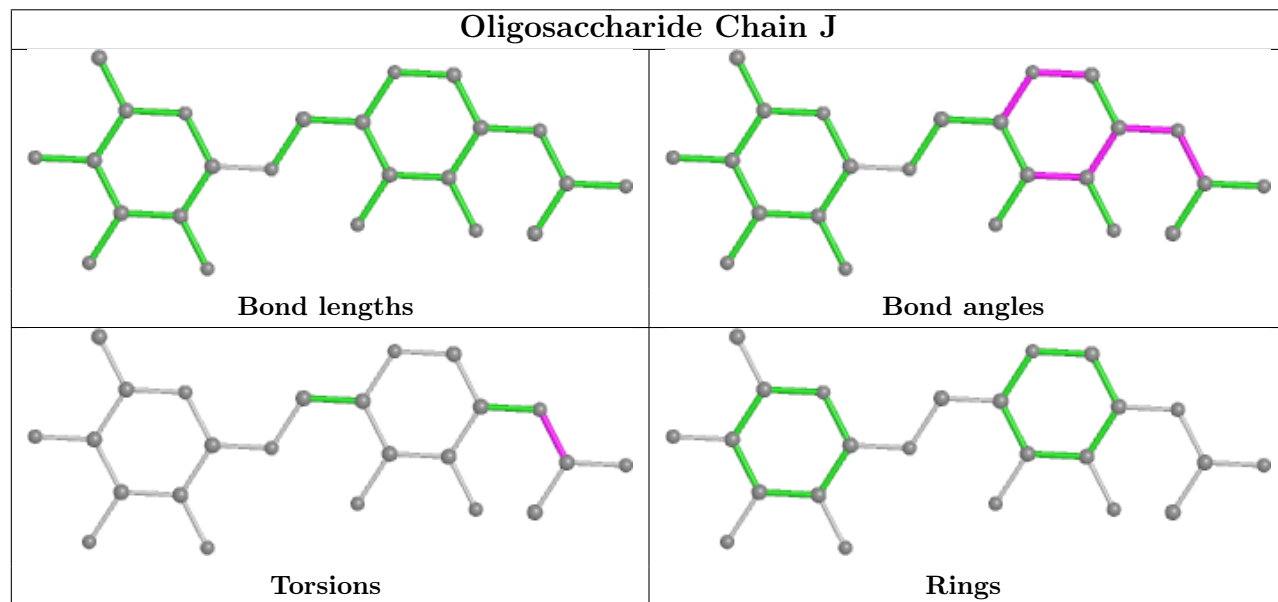
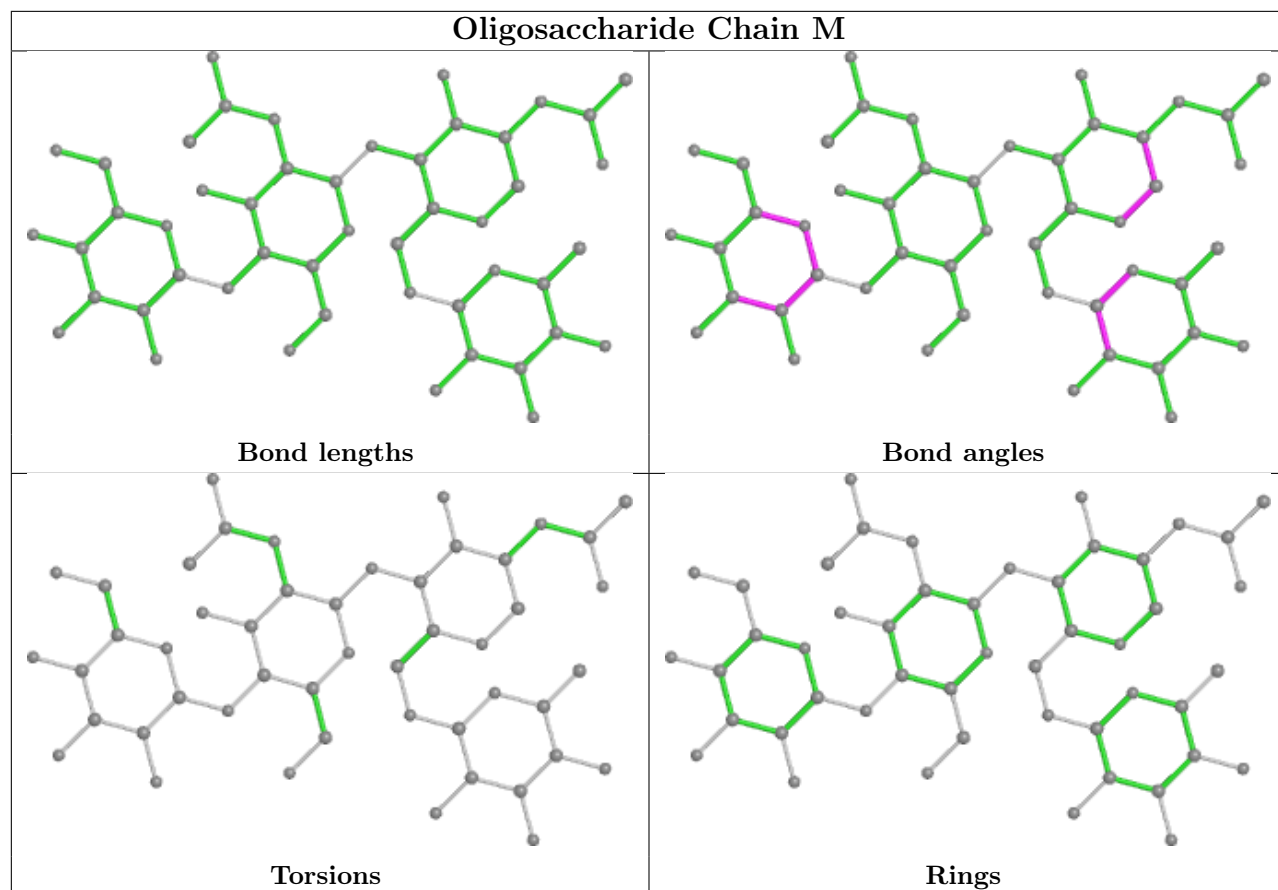
There are no ring outliers.

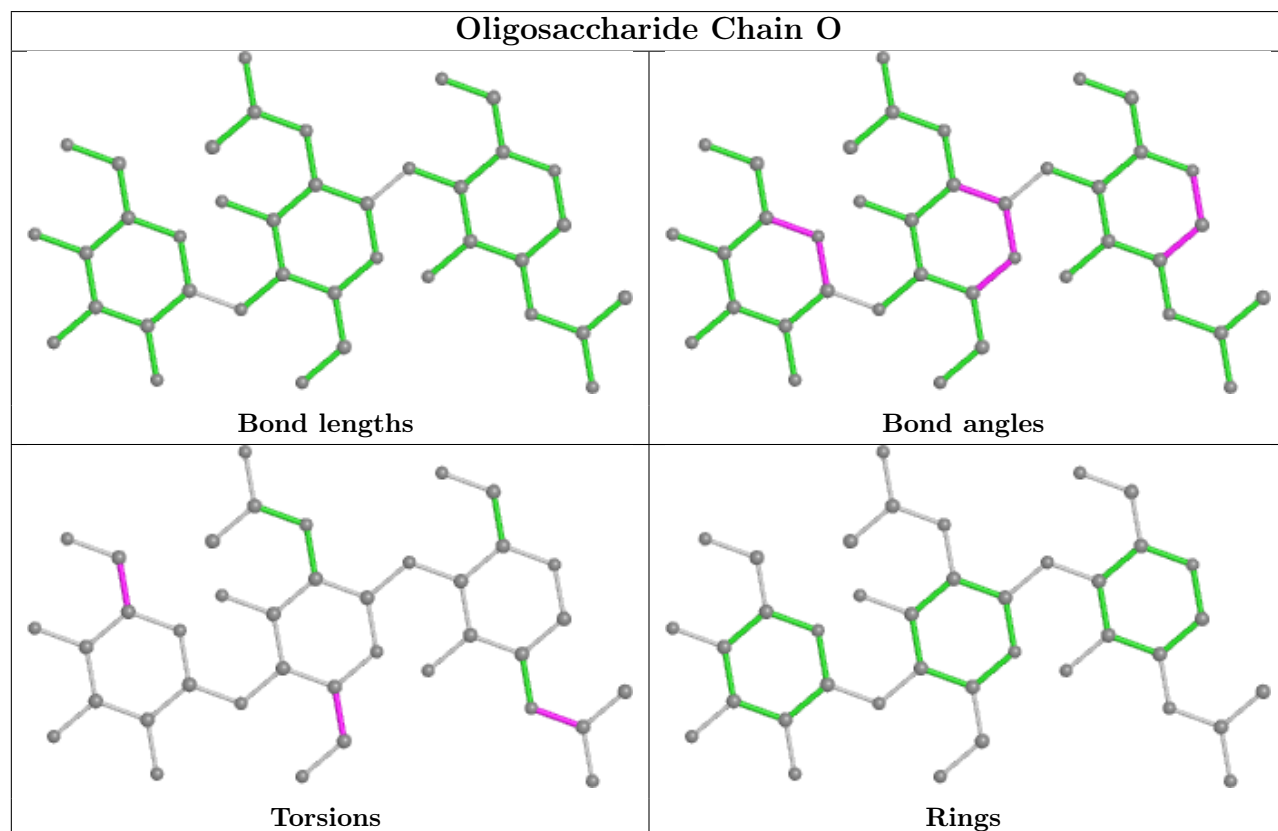
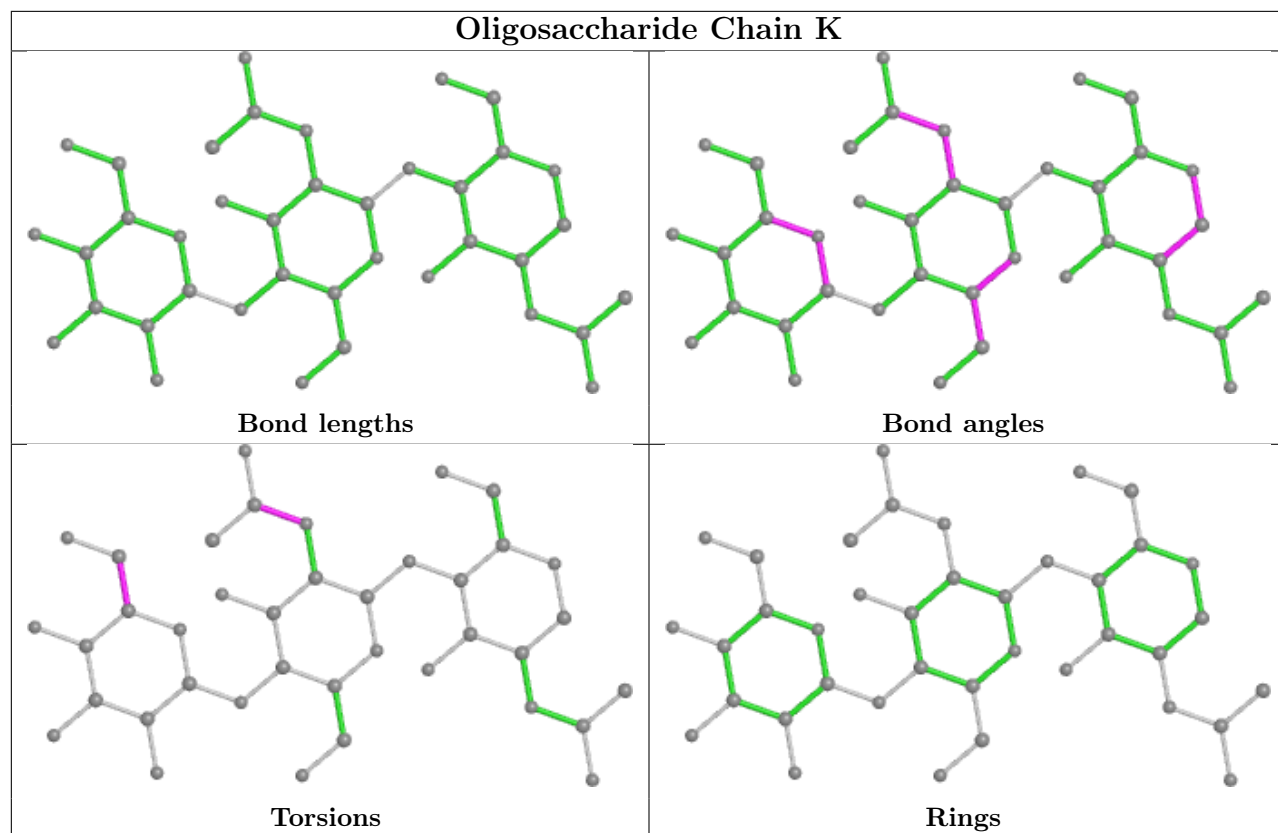
4 monomers are involved in 6 short contacts:

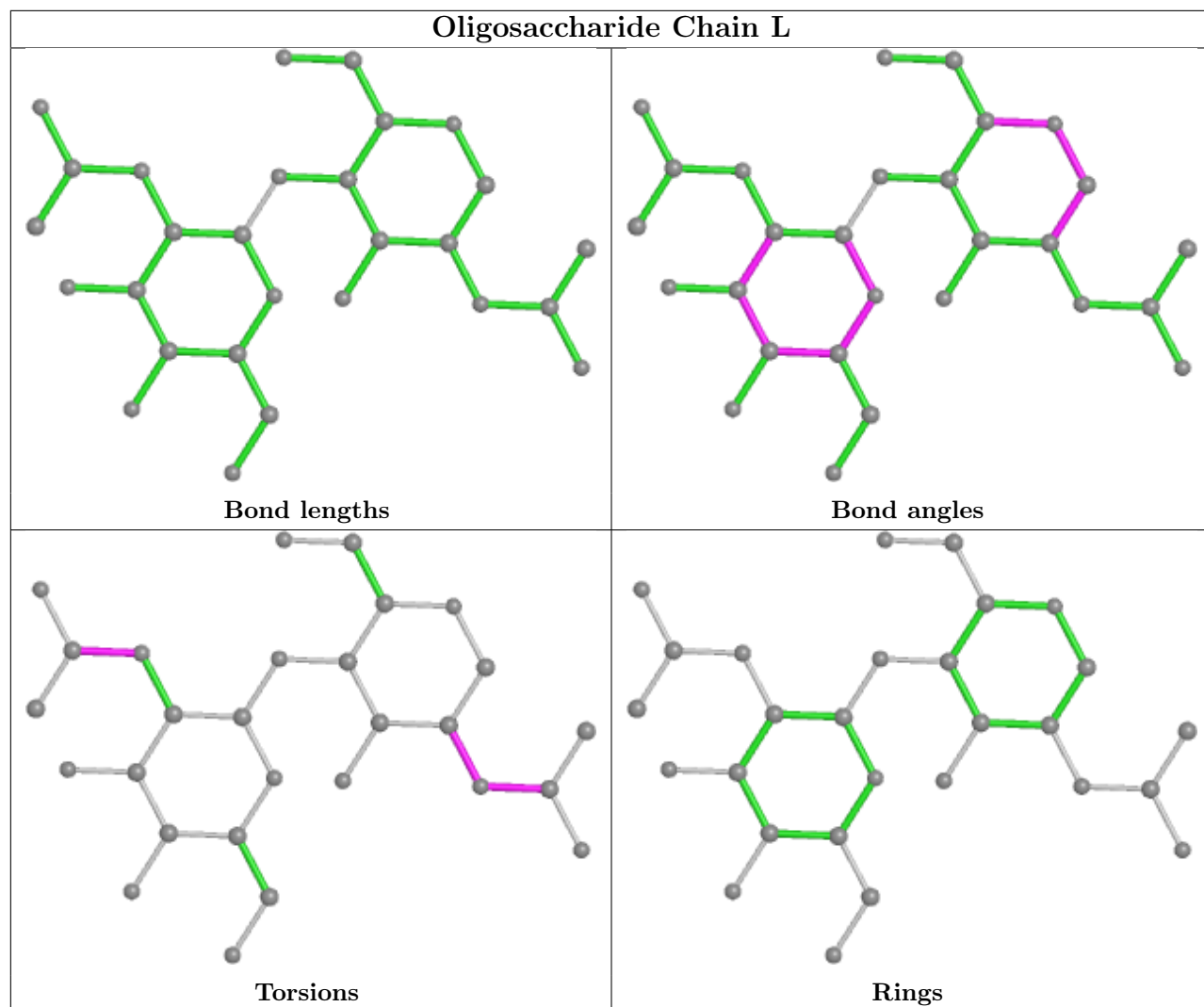
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	N	3	FUC	2	0
6	J	2	FUC	1	0
9	N	1	NAG	1	0
5	M	4	FUC	2	0

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

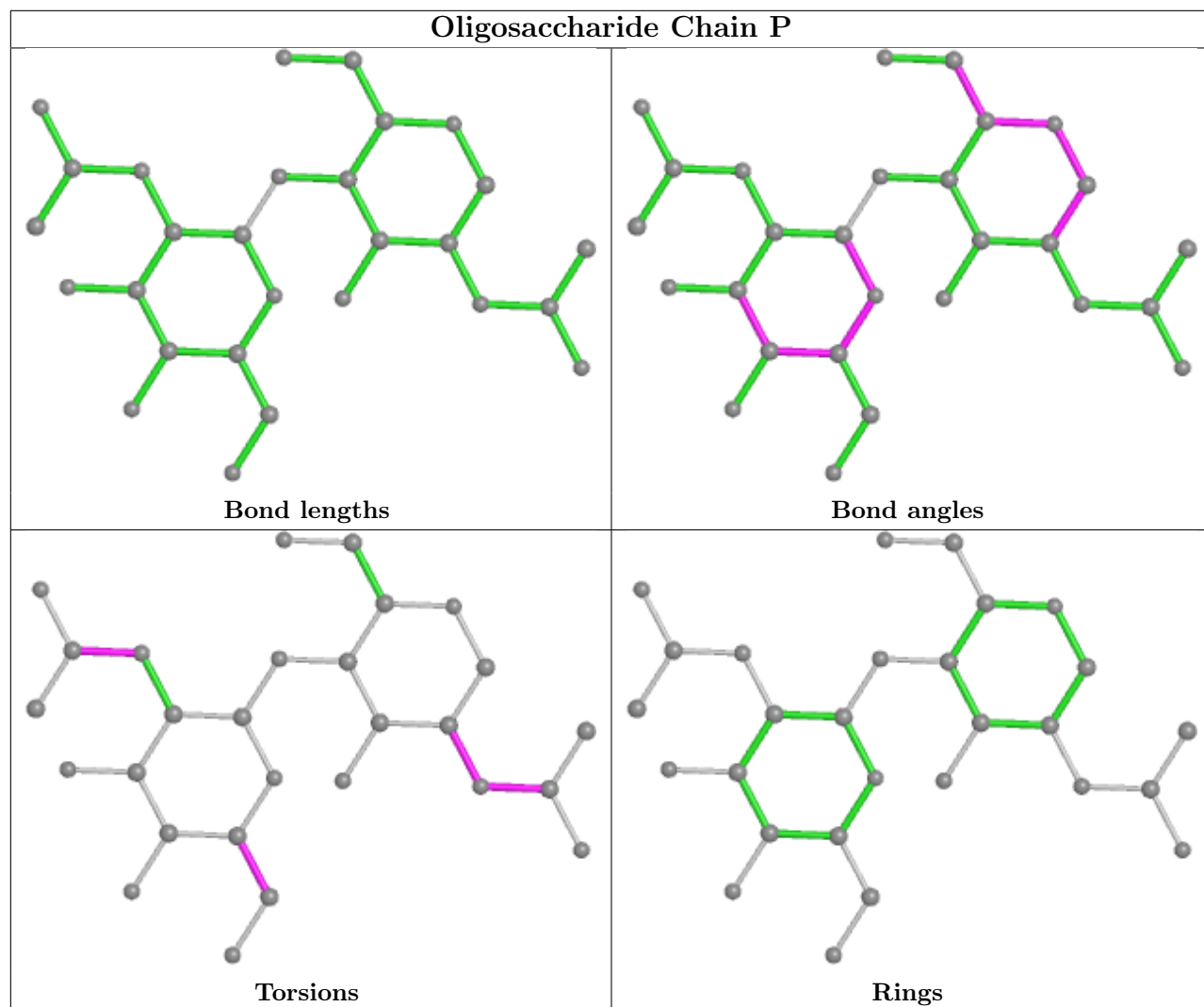


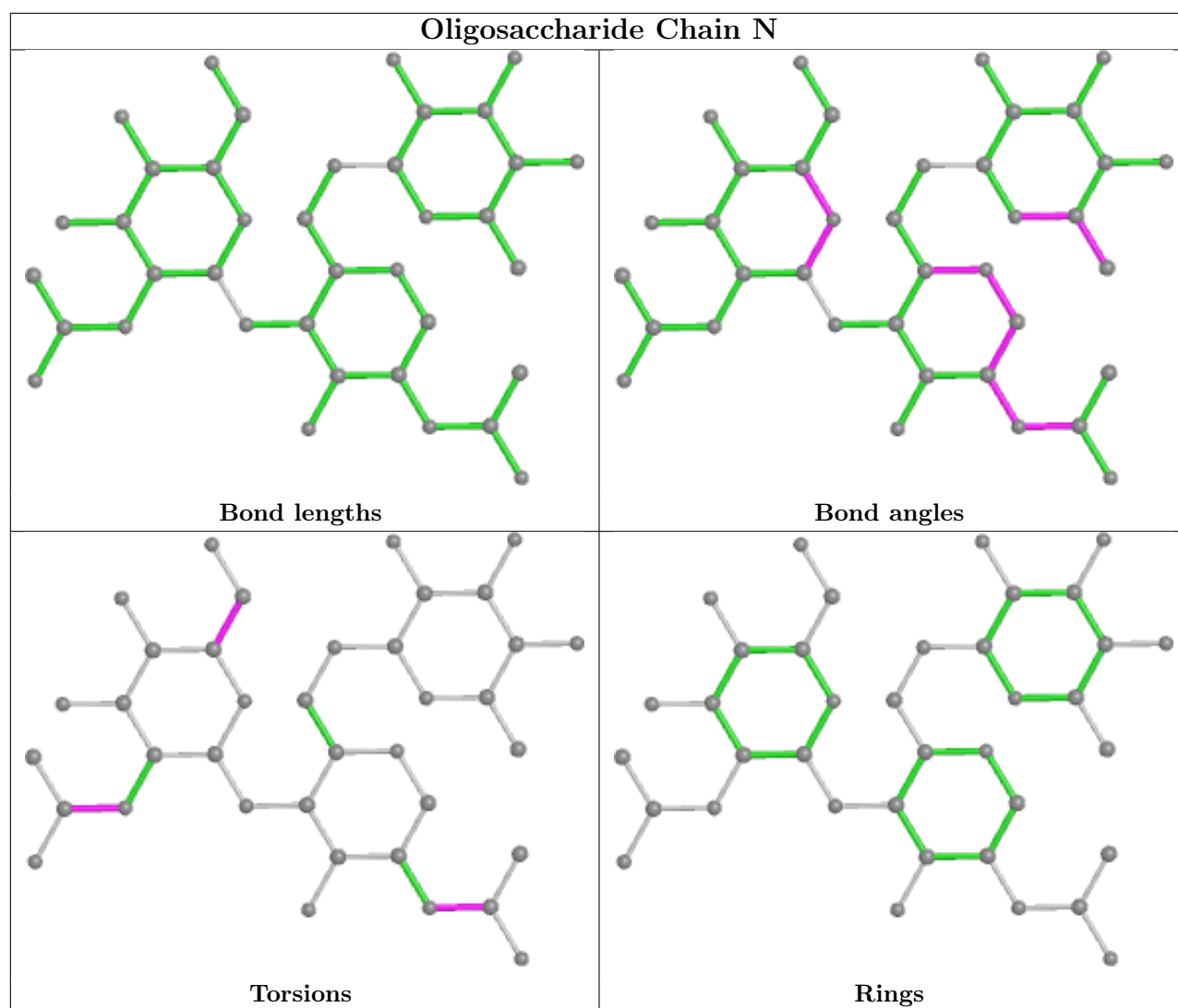












## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
10	NAG	G	400	3	14,14,15	0.54	0	17,19,21	1.61	4 (23%)
10	NAG	C	400	3	14,14,15	0.40	0	17,19,21	1.85	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	NAG	C	500	3	14,14,15	0.53	0	17,19,21	1.38	3 (17%)
10	NAG	G	500	3	14,14,15	0.53	0	17,19,21	1.03	2 (11%)

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	NAG	G	400	3	-	4/6/23/26	0/1/1/1
10	NAG	C	400	3	-	4/6/23/26	0/1/1/1
10	NAG	C	500	3	-	2/6/23/26	0/1/1/1
10	NAG	G	500	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	400	NAG	C1-O5-C5	4.61	118.44	112.19
10	G	400	NAG	O5-C5-C6	3.79	113.15	107.20
10	G	400	NAG	C1-O5-C5	3.35	116.73	112.19
10	C	500	NAG	C1-O5-C5	3.23	116.57	112.19
10	C	400	NAG	O5-C5-C6	3.20	112.22	107.20

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	G	400	NAG	C8-C7-N2-C2
10	G	400	NAG	O7-C7-N2-C2
10	C	400	NAG	O5-C5-C6-O6
10	G	400	NAG	O5-C5-C6-O6
10	G	400	NAG	C4-C5-C6-O6

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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	130/225 (57%)	0.95	17 (13%) 3 1	85, 91, 96, 97	0
1	E	131/225 (58%)	0.81	16 (12%) 4 1	86, 92, 96, 98	0
2	B	204/219 (93%)	0.60	15 (7%) 14 4	82, 91, 96, 100	0
2	F	201/219 (91%)	0.43	10 (4%) 28 10	82, 92, 96, 100	0
3	C	195/247 (78%)	0.54	9 (4%) 32 12	88, 92, 97, 102	0
3	G	195/247 (78%)	1.07	36 (18%) 1 0	87, 93, 97, 102	0
4	D	131/133 (98%)	0.75	12 (9%) 9 3	83, 92, 100, 103	0
4	H	131/133 (98%)	0.72	13 (9%) 7 2	84, 92, 100, 105	0
All	All	1318/1648 (79%)	0.72	128 (9%) 7 2	82, 92, 97, 105	0

The worst 5 of 128 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	54	SER	12.3
4	H	102	THR	9.1
2	F	25	ASP	7.9
1	A	49	SER	7.8
4	H	133	THR	7.8

### 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,

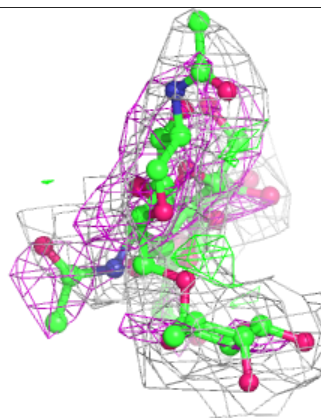
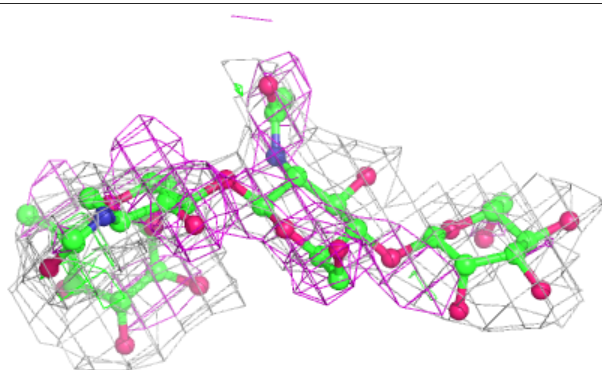
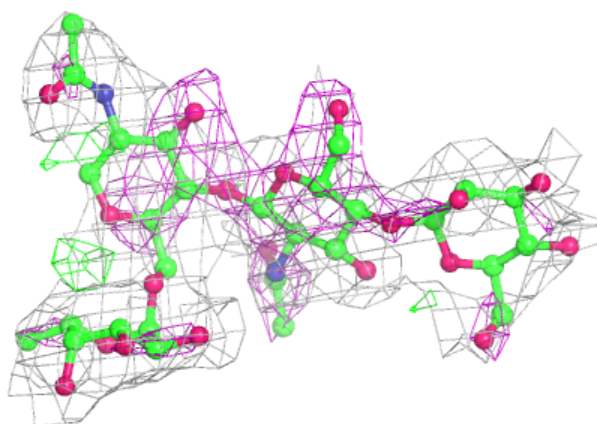
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	BMA	K	3	11/12	0.63	0.32	106,108,109,109	0
5	BMA	M	3	11/12	0.67	0.31	108,110,112,113	0
8	NAG	P	2	14/15	0.70	0.40	114,116,117,117	0
9	NAG	N	2	14/15	0.72	0.33	108,111,112,113	0
9	NAG	N	1	14/15	0.73	0.32	97,98,101,105	0
7	BMA	O	3	11/12	0.76	0.28	97,99,100,101	0
8	NAG	P	1	14/15	0.77	0.48	105,107,110,112	0
5	BMA	I	3	11/12	0.79	0.29	114,116,117,117	0
5	NAG	I	2	14/15	0.79	0.48	101,105,108,111	0
7	NAG	K	2	14/15	0.79	0.28	94,96,99,103	0
8	NAG	L	2	14/15	0.80	0.52	97,99,101,102	0
9	FUC	N	3	10/11	0.82	0.30	102,102,102,102	0
7	NAG	O	2	14/15	0.85	0.22	80,86,88,93	0
5	NAG	I	1	14/15	0.85	0.27	77,85,88,94	0
5	NAG	M	2	14/15	0.87	0.23	91,94,99,104	0
6	NAG	J	1	14/15	0.88	0.16	94,95,96,97	0
6	FUC	J	2	10/11	0.90	0.35	96,97,97,97	0
7	NAG	K	1	14/15	0.90	0.20	85,86,87,90	0
8	NAG	L	1	14/15	0.91	0.22	88,89,91,95	0
5	NAG	M	1	14/15	0.92	0.16	73,79,81,86	0
5	FUC	I	4	10/11	0.92	0.13	72,74,75,76	0
7	NAG	O	1	14/15	0.92	0.19	74,75,78,79	0
5	FUC	M	4	10/11	0.94	0.14	70,70,72,72	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.

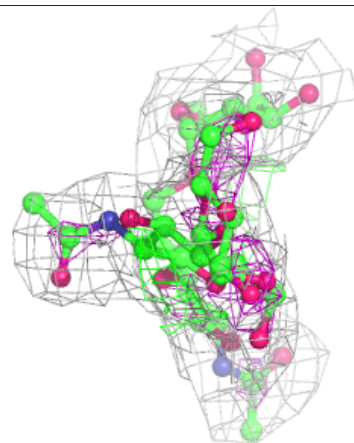
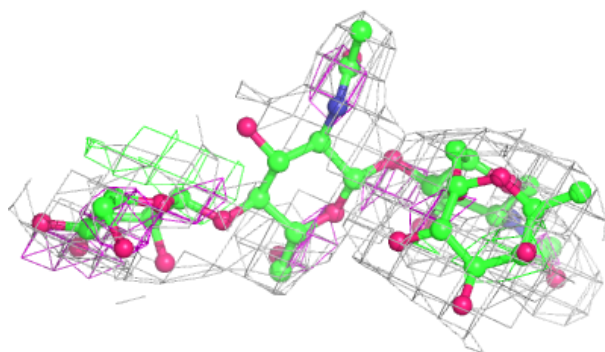
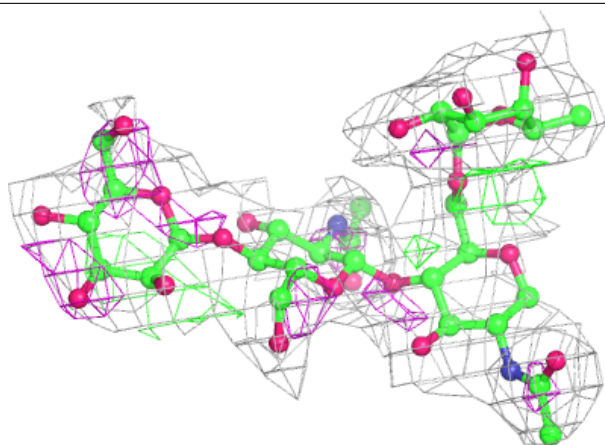
**Electron density around Chain I:**

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

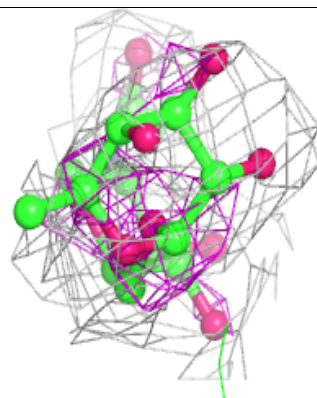
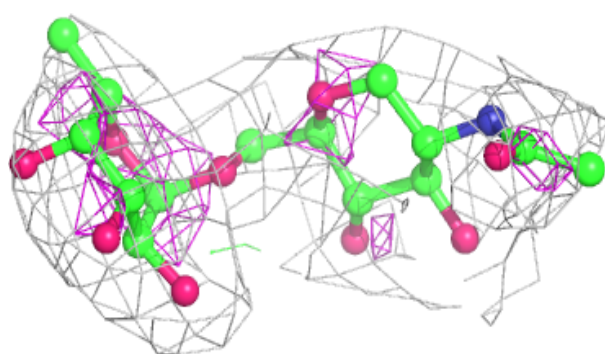
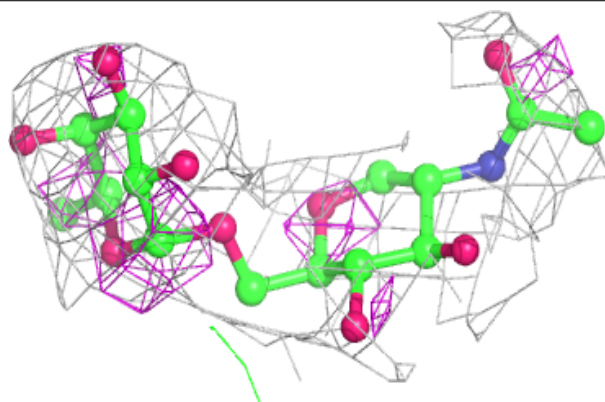


**Electron density around Chain M:**

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

**Electron density around Chain J:**

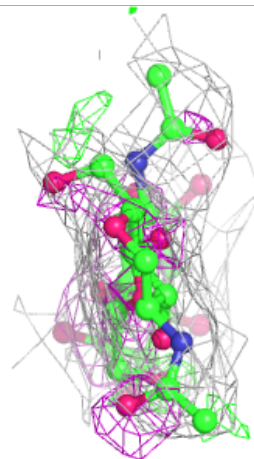
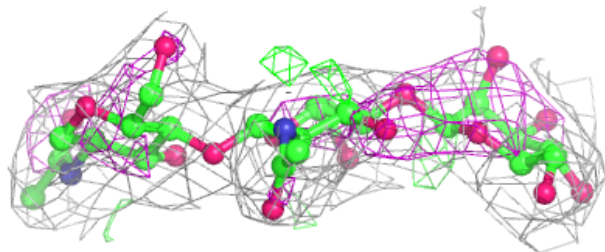
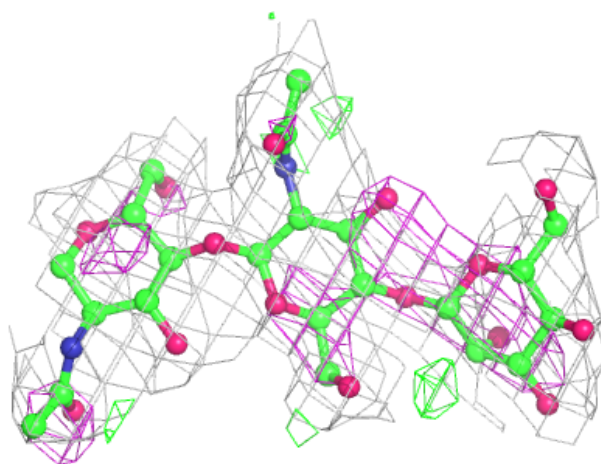
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





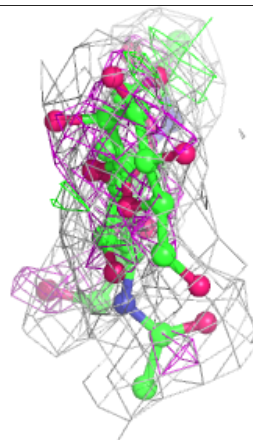
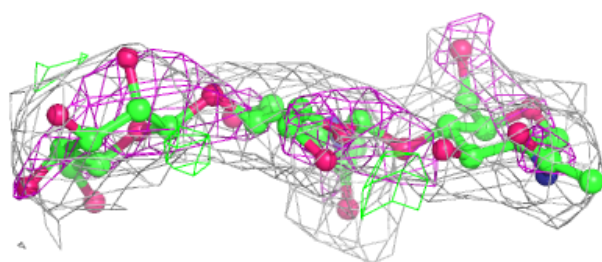
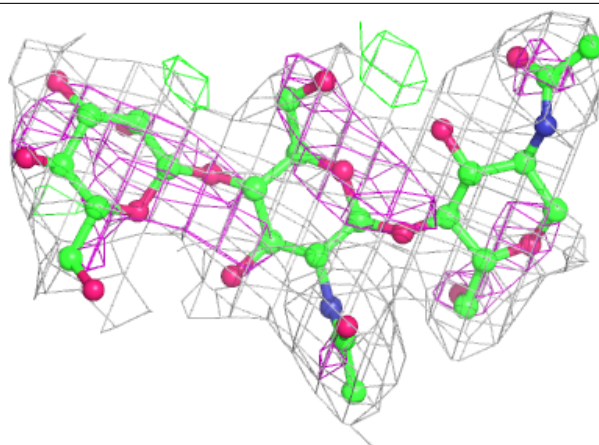
**Electron density around Chain K:**

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



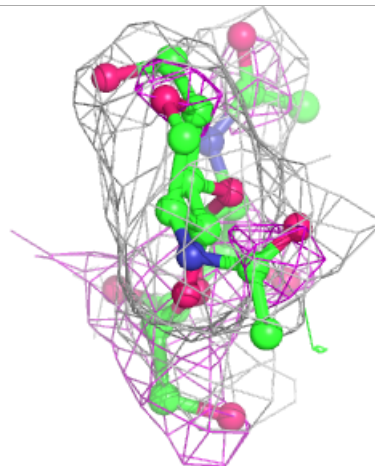
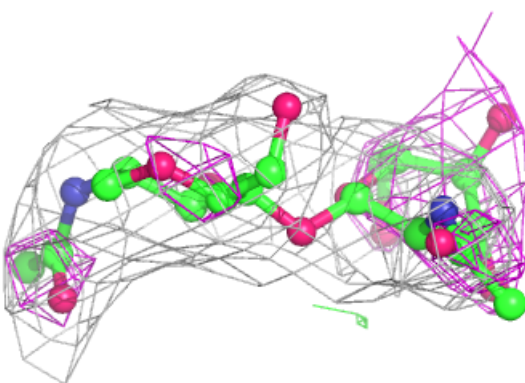
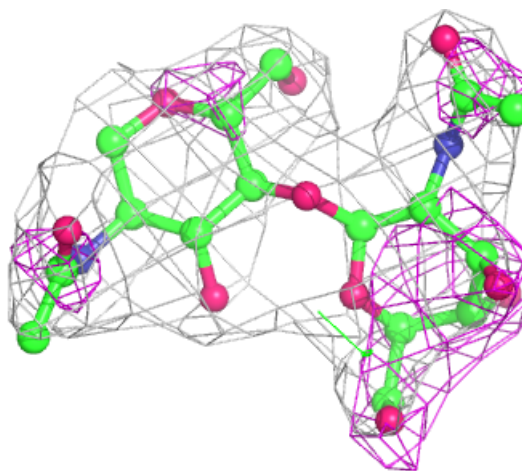
**Electron density around Chain O:**

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



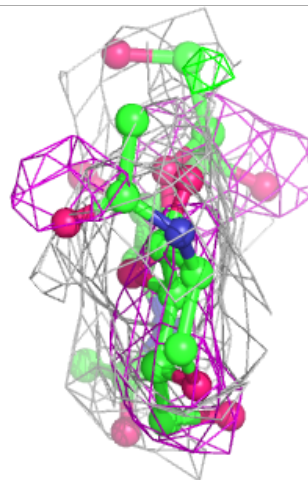
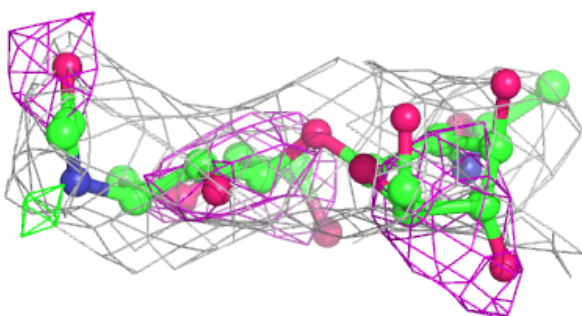
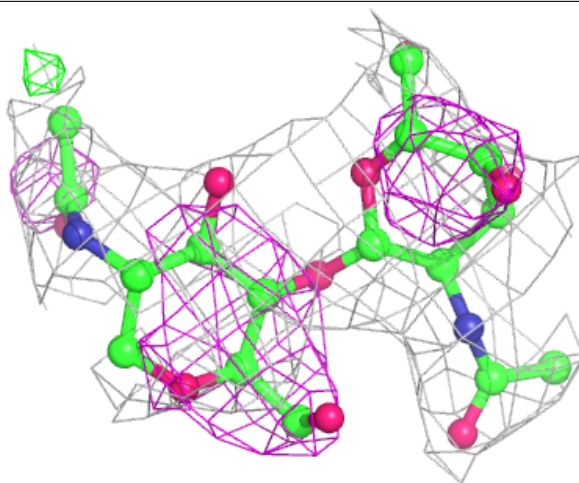
**Electron density around Chain L:**

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



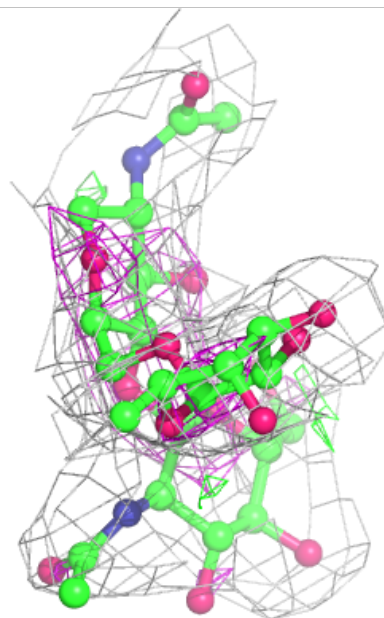
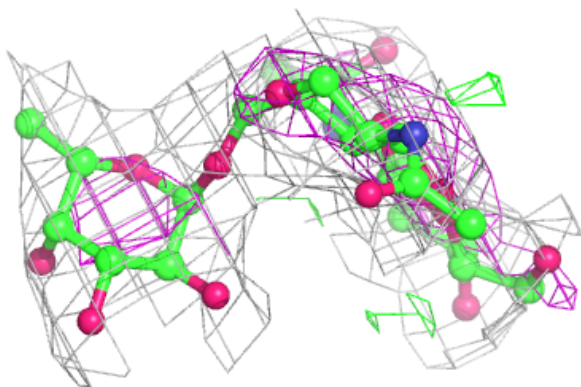
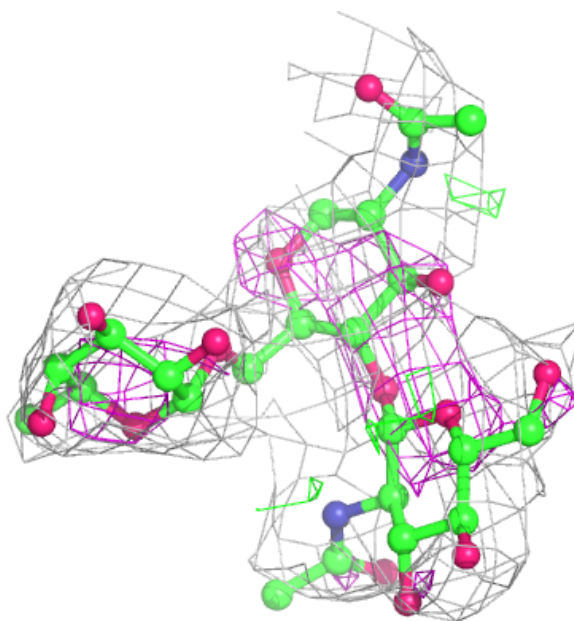
**Electron density around Chain P:**

$2mF_o-DF_c$  (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<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
 mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
 and green (positive)

**6.4 Ligands** ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
10	NAG	G	500	14/15	0.65	0.23	99,101,104,104	0
10	NAG	C	500	14/15	0.66	0.24	94,95,96,96	0
10	NAG	G	400	14/15	0.75	0.18	101,103,104,105	0

*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	NAG	C	400	14/15	0.86	0.13	85,88,88,89	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.