



wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2026 – 11:17 AM EDT

PDB ID : 6CH9 / pdb_00006ch9
Title : Crystal structure of a natively-glycosylated B41 SOSIP.664 HIV-1 Envelope Trimer in complex with the broadly-neutralizing antibodies BG18 and 35O22
Authors : Barnes, C.O.; Bjorkman, P.J.
Deposited on : 2018-02-22
Resolution : 4.85 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

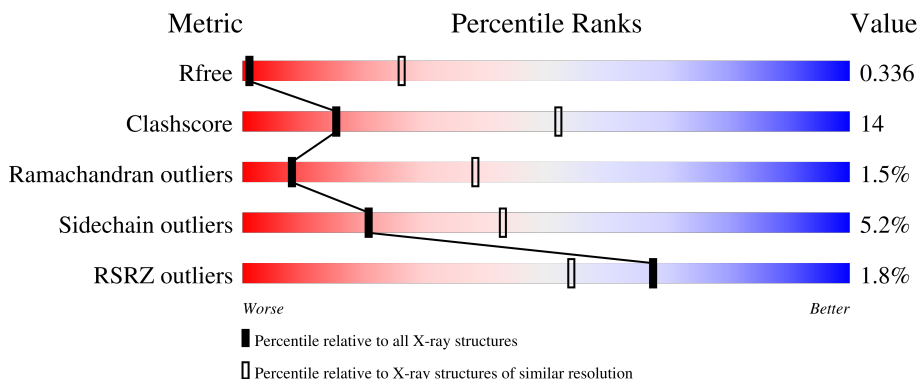
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.85 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	1024 (5.74-3.94)
Clashscore	190562	1007 (5.70-3.98)
Ramachandran outliers	187476	1110 (5.78-3.90)
Sidechain outliers	187428	1091 (5.78-3.90)
RSRZ outliers	180081	1019 (5.74-3.94)

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	B	153	
2	D	243	
3	E	216	
4	G	518	
5	Q	240	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	R	215	
7	A	3	
7	C	3	
7	H	3	
7	J	3	
7	O	3	
7	P	3	
7	T	3	
8	F	4	
9	I	2	
9	K	2	
9	N	2	
10	L	6	
11	M	4	
12	S	5	
13	U	6	

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	NAG	L	1	-	-	X	-
13	NAG	U	1	-	-	X	-
8	MAN	F	4	-	-	X	-
9	NAG	K	1	-	-	X	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 11974 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 Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	136	Total	C	N	O	S	0	0	0
			1094	692	188	206	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP B3UEZ6
B	605	CYS	THR	engineered mutation	UNP B3UEZ6

- Molecule 2 is a protein called 35O22 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	236	Total	C	N	O	S	0	0	0
			1777	1129	296	344	8			

- Molecule 3 is a protein called 35O22 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 4 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	448	Total	C	N	O	S	0	0	0
			3499	2198	617	658	26			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	MET	-	initiating methionine	UNP B3UES2
G	-3	ASP	-	expression tag	UNP B3UES2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	ALA	-	expression tag	UNP B3UES2
G	-1	MET	-	expression tag	UNP B3UES2
G	0	LYS	-	expression tag	UNP B3UES2
G	1	ARG	-	expression tag	UNP B3UES2
G	2	GLY	-	expression tag	UNP B3UES2
G	3	LEU	-	expression tag	UNP B3UES2
G	4	CYS	-	expression tag	UNP B3UES2
G	5	CYS	-	expression tag	UNP B3UES2
G	6	VAL	-	expression tag	UNP B3UES2
G	7	LEU	-	expression tag	UNP B3UES2
G	8	LEU	-	expression tag	UNP B3UES2
G	9	LEU	-	expression tag	UNP B3UES2
G	10	CYS	-	expression tag	UNP B3UES2
G	11	GLY	-	expression tag	UNP B3UES2
G	12	ALA	-	expression tag	UNP B3UES2
G	13	VAL	-	expression tag	UNP B3UES2
G	14	PHE	-	expression tag	UNP B3UES2
G	15	VAL	-	expression tag	UNP B3UES2
G	16	SER	-	expression tag	UNP B3UES2
G	17	PRO	-	expression tag	UNP B3UES2
G	18	SER	-	expression tag	UNP B3UES2
G	19	GLN	-	expression tag	UNP B3UES2
G	20	GLU	-	expression tag	UNP B3UES2
G	21	ILE	-	expression tag	UNP B3UES2
G	22	HIS	-	expression tag	UNP B3UES2
G	23	ALA	-	expression tag	UNP B3UES2
G	24	ARG	-	expression tag	UNP B3UES2
G	25	PHE	-	expression tag	UNP B3UES2
G	26	ARG	-	expression tag	UNP B3UES2
G	27	ARG	-	expression tag	UNP B3UES2
G	28	GLY	-	expression tag	UNP B3UES2
G	29	ALA	-	expression tag	UNP B3UES2
G	30	ARG	-	expression tag	UNP B3UES2
G	501	CYS	ALA	engineered mutation	UNP B3UES2

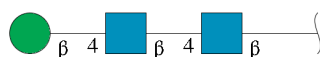
- Molecule 5 is a protein called BG18 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Q	231	Total	C	N	O	S	0	0	0
			1731	1089	298	336	8			

- Molecule 6 is a protein called BG18 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	R	205	Total	C	N	O	S	0	0	0
			1540	963	257	314	6			

- 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.



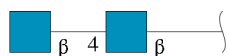
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	A	3	Total	C	N	O		0	0	0
			39	22	2	15				
7	C	3	Total	C	N	O		0	0	0
			39	22	2	15				
7	H	3	Total	C	N	O		0	0	0
			39	22	2	15				
7	J	3	Total	C	N	O		0	0	0
			39	22	2	15				
7	O	3	Total	C	N	O		0	0	0
			39	22	2	15				
7	P	3	Total	C	N	O		0	0	0
			39	22	2	15				
7	T	3	Total	C	N	O		0	0	0
			39	22	2	15				

- Molecule 8 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.



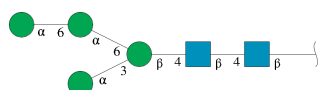
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	4	Total	C	N	O		0	0	0
			50	28	2	20				

- Molecule 9 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
9	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 10 is an oligosaccharide called 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.



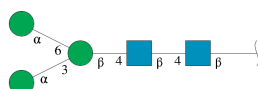
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	L	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 11 is an oligosaccharide called 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.



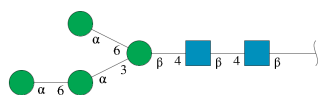
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	M	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



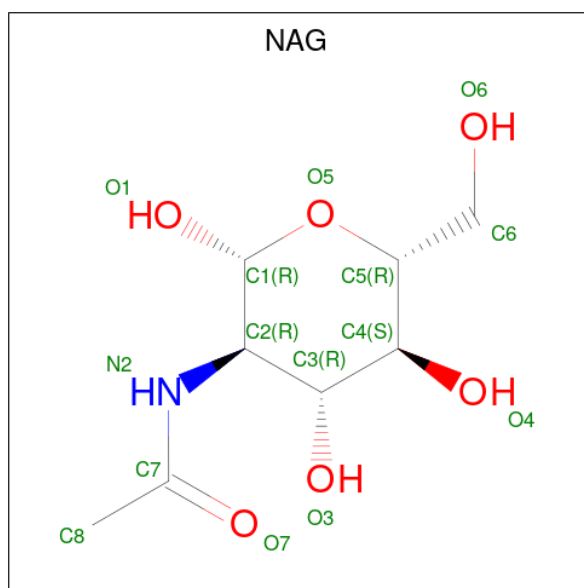
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	S	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

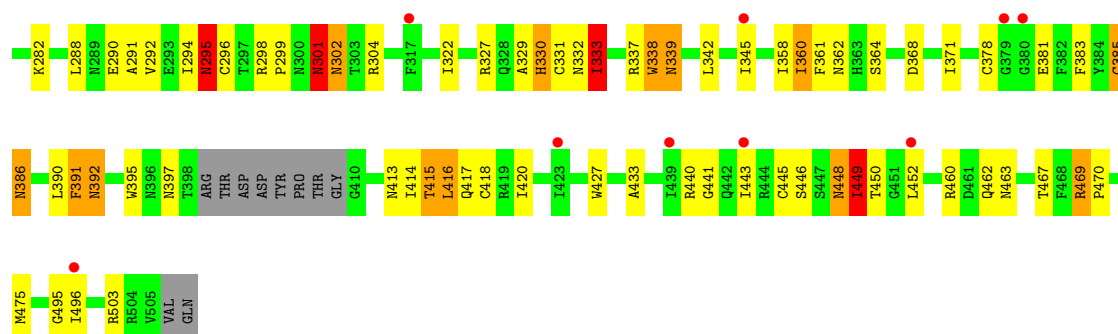
- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



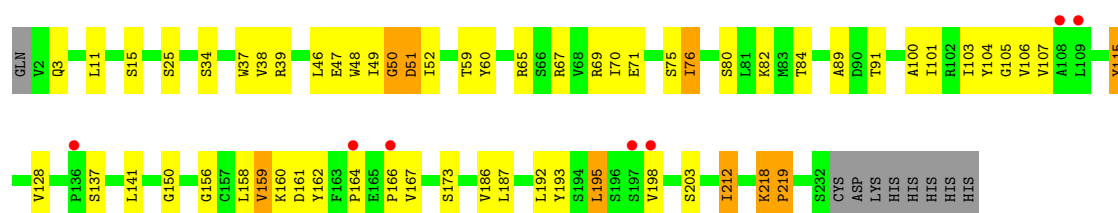
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 1: Envelope glycoprotein gp41

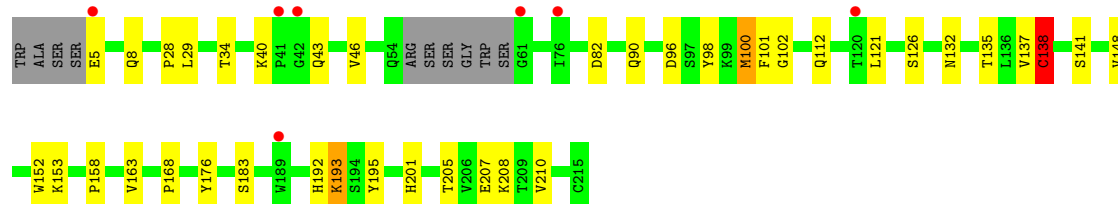
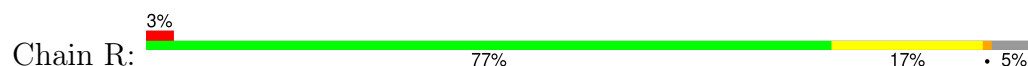




• Molecule 5: BG18 Heavy Chain



• Molecule 6: BG18 Light Chain



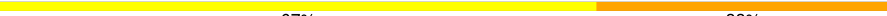
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain H:  67% 33%

MAG1
MAG2
BMA3

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

Chain J:  100%

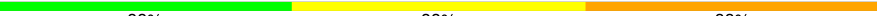
MAG1
MAG2
BMA3

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

Chain O:  33% 67%

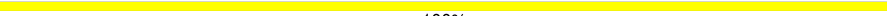
MAG1
MAG2
BMA3

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

Chain P:  33% 33% 33%

MAG1
MAG2
BMA3

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

Chain T:  100%

MAG1
MAG2
BMA3

- Molecule 8: 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 F:  25% 75%

MAG1
MAG2
BMA3
MAN4

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%

MAG1
MAG2

- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 50%

MAG1
MAG2

- Molecule 10: 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 L:  50% 50%

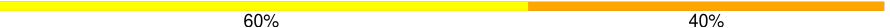
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 11: 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 M:  75% 25%

MAG1
MAG2
BMA3
MAN4

- Molecule 12: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  60% 40%

MAG1
MAG2
BMA3
MAN4
MAN5

- Molecule 13: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  33% 67%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	241.08Å 241.08Å 345.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.90 – 4.85 39.90 – 4.85	Depositor EDS
% Data completeness (in resolution range)	95.3 (39.90-4.85) 95.1 (39.90-4.85)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 4.84Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.285 , 0.292 0.302 , 0.336	Depositor DCC
R_{free} test set	838 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	275.7	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 366.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11974	wwPDB-VP
Average B, all atoms (Å ²)	300.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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: BMA, MAN, 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	B	0.75	0/1113	1.39	2/1509 (0.1%)
2	D	0.77	0/1822	1.15	6/2481 (0.2%)
3	E	0.73	0/1659	1.11	3/2269 (0.1%)
4	G	0.82	5/3572 (0.1%)	1.54	36/4857 (0.7%)
5	Q	0.73	0/1776	1.18	4/2423 (0.2%)
6	R	0.82	0/1577	1.24	6/2153 (0.3%)
All	All	0.78	5/11519 (0.0%)	1.32	57/15692 (0.4%)

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
4	G	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	392	ASN	C-N	11.37	1.49	1.33
4	G	295	ASN	C-N	7.55	1.43	1.33
4	G	385	CYS	C-N	6.87	1.42	1.33
4	G	361	PHE	C-N	6.40	1.42	1.33
4	G	160	ASN	C-N	5.38	1.40	1.33

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	234	ASN	O-C-N	-21.08	95.02	122.43
4	G	295	ASN	CA-C-N	17.03	147.28	121.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	295	ASN	C-N-CA	17.03	147.28	121.40
4	G	275	GLU	O-C-N	16.17	140.59	122.15
4	G	295	ASN	O-C-N	-15.20	105.46	122.79

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	234	ASN	Mainchain

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	B	1094	0	1075	35	0
2	D	1777	0	1755	20	0
3	E	1615	0	1550	10	0
4	G	3499	0	3441	204	0
5	Q	1731	0	1685	45	0
6	R	1540	0	1496	15	0
7	A	39	0	34	1	0
7	C	39	0	34	1	0
7	H	39	0	34	5	0
7	J	39	0	34	0	0
7	O	39	0	34	1	0
7	P	39	0	34	1	0
7	T	39	0	34	0	0
8	F	50	0	43	11	0
9	I	28	0	25	0	0
9	K	28	0	25	10	0
9	N	28	0	25	1	0
10	L	72	0	61	11	0
11	M	50	0	43	5	0
12	S	61	0	52	5	0
13	U	72	0	61	18	0
14	B	14	0	13	4	0
14	G	42	0	39	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11974	0	11627	319	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 14.

The worst 5 of 319 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)
4:G:333:ILE:CD1	4:G:414:ILE:HB	1.30	1.60
4:G:338:TRP:CZ3	4:G:390:LEU:HD22	1.37	1.57
4:G:292:VAL:HB	4:G:449:ILE:CD1	1.30	1.55
4:G:292:VAL:CB	4:G:449:ILE:HD12	1.46	1.44
4:G:292:VAL:O	4:G:449:ILE:CD1	1.68	1.41

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	B	132/153 (86%)	119 (90%)	13 (10%)	0	100	100
2	D	232/243 (96%)	205 (88%)	26 (11%)	1 (0%)	30	67
3	E	211/216 (98%)	192 (91%)	17 (8%)	2 (1%)	14	49
4	G	440/518 (85%)	366 (83%)	69 (16%)	5 (1%)	11	45
5	Q	229/240 (95%)	178 (78%)	44 (19%)	7 (3%)	3	21
6	R	201/215 (94%)	140 (70%)	54 (27%)	7 (4%)	3	20
All	All	1445/1585 (91%)	1200 (83%)	223 (15%)	22 (2%)	8	38

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	53	ASP
4	G	197	ASN
5	Q	51	ASP
5	Q	159	VAL
6	R	29	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	B	119/130 (92%)	116 (98%)	3 (2%)	42	62
2	D	199/206 (97%)	192 (96%)	7 (4%)	32	54
3	E	186/189 (98%)	181 (97%)	5 (3%)	39	60
4	G	393/455 (86%)	360 (92%)	33 (8%)	10	30
5	Q	193/207 (93%)	185 (96%)	8 (4%)	27	49
6	R	174/182 (96%)	164 (94%)	10 (6%)	18	41
All	All	1264/1369 (92%)	1198 (95%)	66 (5%)	21	43

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	R	82	ASP
6	R	137	VAL
6	R	210	VAL
4	G	233	PHE
4	G	231	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
4	G	332	ASN
4	G	463	ASN
4	G	363	HIS
4	G	478	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	197	ASN

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 ⓘ

52 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
7	NAG	A	1	1,7	14,14,15	0.94	0	17,19,21	2.24	4 (23%)
7	NAG	A	2	7	14,14,15	0.85	1 (7%)	17,19,21	1.23	2 (11%)
7	BMA	A	3	7	11,11,12	0.39	0	15,15,17	0.86	0
7	NAG	C	1	1,7	14,14,15	0.78	0	17,19,21	1.95	3 (17%)
7	NAG	C	2	7	14,14,15	0.67	0	17,19,21	2.21	4 (23%)
7	BMA	C	3	7	11,11,12	0.43	0	15,15,17	0.75	0
8	NAG	F	1	8	14,14,15	0.93	0	17,19,21	2.26	6 (35%)
8	NAG	F	2	8	14,14,15	1.11	2 (14%)	17,19,21	2.73	7 (41%)
8	BMA	F	3	8	11,11,12	1.50	2 (18%)	15,15,17	1.95	5 (33%)
8	MAN	F	4	8	11,11,12	2.08	2 (18%)	15,15,17	2.12	6 (40%)
7	NAG	H	1	4,7	14,14,15	0.93	1 (7%)	17,19,21	1.89	7 (41%)
7	NAG	H	2	7	14,14,15	1.24	2 (14%)	17,19,21	2.32	5 (29%)
7	BMA	H	3	7	11,11,12	0.82	0	15,15,17	1.34	2 (13%)
9	NAG	I	1	4,9	14,14,15	1.02	1 (7%)	17,19,21	1.20	1 (5%)
9	NAG	I	2	9	14,14,15	1.18	1 (7%)	17,19,21	1.61	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	J	1	4,7	14,14,15	0.80	0	17,19,21	1.71	5 (29%)
7	NAG	J	2	7	14,14,15	1.41	1 (7%)	17,19,21	1.54	3 (17%)
7	BMA	J	3	7	11,11,12	0.74	0	15,15,17	0.96	1 (6%)
9	NAG	K	1	4,9	14,14,15	0.93	1 (7%)	17,19,21	2.31	6 (35%)
9	NAG	K	2	9	14,14,15	0.69	1 (7%)	17,19,21	0.97	0
10	NAG	L	1	4,10	14,14,15	1.15	1 (7%)	17,19,21	3.06	7 (41%)
10	NAG	L	2	10	14,14,15	0.74	0	17,19,21	2.44	7 (41%)
10	BMA	L	3	10	11,11,12	0.74	0	15,15,17	2.42	5 (33%)
10	MAN	L	4	10	11,11,12	0.42	0	15,15,17	1.75	3 (20%)
10	MAN	L	5	10	11,11,12	0.75	0	15,15,17	1.25	1 (6%)
10	MAN	L	6	10	11,11,12	0.99	1 (9%)	15,15,17	1.41	2 (13%)
11	NAG	M	1	4,11	14,14,15	1.42	2 (14%)	17,19,21	2.55	5 (29%)
11	NAG	M	2	11	14,14,15	0.59	0	17,19,21	1.52	2 (11%)
11	BMA	M	3	11	11,11,12	0.88	0	15,15,17	1.65	4 (26%)
11	MAN	M	4	11	11,11,12	0.65	0	15,15,17	1.33	2 (13%)
9	NAG	N	1	4,9	14,14,15	0.86	1 (7%)	17,19,21	2.34	3 (17%)
9	NAG	N	2	9	14,14,15	0.48	0	17,19,21	1.26	2 (11%)
7	NAG	O	1	4,7	14,14,15	0.38	0	17,19,21	1.26	3 (17%)
7	NAG	O	2	7	14,14,15	0.73	0	17,19,21	1.66	2 (11%)
7	BMA	O	3	7	11,11,12	0.38	0	15,15,17	0.97	0
7	NAG	P	1	4,7	14,14,15	0.62	0	17,19,21	1.38	2 (11%)
7	NAG	P	2	7	14,14,15	0.85	1 (7%)	17,19,21	1.19	1 (5%)
7	BMA	P	3	7	11,11,12	0.46	0	15,15,17	0.86	0
12	NAG	S	1	4,12	14,14,15	1.28	1 (7%)	17,19,21	1.55	4 (23%)
12	NAG	S	2	12	14,14,15	1.38	2 (14%)	17,19,21	2.70	7 (41%)
12	BMA	S	3	12	11,11,12	1.31	1 (9%)	15,15,17	2.21	5 (33%)
12	MAN	S	4	12	11,11,12	0.83	1 (9%)	15,15,17	2.62	7 (46%)
12	MAN	S	5	12	11,11,12	0.72	0	15,15,17	1.14	1 (6%)
7	NAG	T	1	4,7	14,14,15	0.67	0	17,19,21	1.66	3 (17%)
7	NAG	T	2	7	14,14,15	0.82	0	17,19,21	1.44	4 (23%)
7	BMA	T	3	7	11,11,12	0.64	0	15,15,17	1.44	2 (13%)
13	NAG	U	1	13	14,14,15	1.47	3 (21%)	17,19,21	2.20	5 (29%)
13	NAG	U	2	13	14,14,15	0.87	0	17,19,21	2.82	8 (47%)
13	BMA	U	3	13	11,11,12	0.77	0	15,15,17	2.17	5 (33%)
13	MAN	U	4	13	11,11,12	0.63	0	15,15,17	1.85	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	MAN	U	5	13	11,11,12	0.52	0	15,15,17	1.27	1 (6%)
13	MAN	U	6	13	11,11,12	0.83	1 (9%)	15,15,17	2.65	9 (60%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	A	2	7	-	4/6/23/26	0/1/1/1
7	BMA	A	3	7	-	0/2/19/22	0/1/1/1
7	NAG	C	1	1,7	-	6/6/23/26	0/1/1/1
7	NAG	C	2	7	-	2/6/23/26	0/1/1/1
7	BMA	C	3	7	-	1/2/19/22	0/1/1/1
8	NAG	F	1	8	-	4/6/23/26	0/1/1/1
8	NAG	F	2	8	-	4/6/23/26	0/1/1/1
8	BMA	F	3	8	-	2/2/19/22	0/1/1/1
8	MAN	F	4	8	-	2/2/19/22	0/1/1/1
7	NAG	H	1	4,7	-	5/6/23/26	0/1/1/1
7	NAG	H	2	7	-	4/6/23/26	0/1/1/1
7	BMA	H	3	7	-	2/2/19/22	0/1/1/1
9	NAG	I	1	4,9	-	3/6/23/26	0/1/1/1
9	NAG	I	2	9	-	3/6/23/26	0/1/1/1
7	NAG	J	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	J	2	7	-	4/6/23/26	0/1/1/1
7	BMA	J	3	7	-	1/2/19/22	0/1/1/1
9	NAG	K	1	4,9	-	4/6/23/26	0/1/1/1
9	NAG	K	2	9	-	3/6/23/26	0/1/1/1
10	NAG	L	1	4,10	-	5/6/23/26	0/1/1/1
10	NAG	L	2	10	-	1/6/23/26	0/1/1/1
10	BMA	L	3	10	-	2/2/19/22	0/1/1/1
10	MAN	L	4	10	-	2/2/19/22	0/1/1/1
10	MAN	L	5	10	-	1/2/19/22	0/1/1/1
10	MAN	L	6	10	-	1/2/19/22	0/1/1/1
11	NAG	M	1	4,11	-	4/6/23/26	0/1/1/1
11	NAG	M	2	11	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BMA	M	3	11	-	0/2/19/22	0/1/1/1
11	MAN	M	4	11	-	0/2/19/22	0/1/1/1
9	NAG	N	1	4,9	-	5/6/23/26	0/1/1/1
9	NAG	N	2	9	-	4/6/23/26	0/1/1/1
7	NAG	O	1	4,7	-	3/6/23/26	0/1/1/1
7	NAG	O	2	7	-	5/6/23/26	0/1/1/1
7	BMA	O	3	7	-	1/2/19/22	0/1/1/1
7	NAG	P	1	4,7	-	3/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
7	BMA	P	3	7	-	1/2/19/22	0/1/1/1
12	NAG	S	1	4,12	-	2/6/23/26	0/1/1/1
12	NAG	S	2	12	-	2/6/23/26	0/1/1/1
12	BMA	S	3	12	-	2/2/19/22	0/1/1/1
12	MAN	S	4	12	-	2/2/19/22	0/1/1/1
12	MAN	S	5	12	-	1/2/19/22	0/1/1/1
7	NAG	T	1	4,7	-	4/6/23/26	0/1/1/1
7	NAG	T	2	7	-	2/6/23/26	0/1/1/1
7	BMA	T	3	7	-	2/2/19/22	0/1/1/1
13	NAG	U	1	13	-	4/6/23/26	0/1/1/1
13	NAG	U	2	13	-	3/6/23/26	0/1/1/1
13	BMA	U	3	13	-	0/2/19/22	0/1/1/1
13	MAN	U	4	13	-	1/2/19/22	0/1/1/1
13	MAN	U	5	13	-	0/2/19/22	0/1/1/1
13	MAN	U	6	13	-	2/2/19/22	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)
8	F	4	MAN	O5-C1	5.56	1.53	1.43
11	M	1	NAG	C1-C2	3.75	1.57	1.52
7	J	2	NAG	C1-C2	3.64	1.57	1.52
9	I	2	NAG	C1-C2	3.32	1.56	1.52
12	S	3	BMA	C2-C3	3.28	1.57	1.52

The worst 5 of 188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	1	NAG	C2-N2-C7	8.07	133.71	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	1	NAG	C2-N2-C7	7.90	133.49	122.90
12	S	2	NAG	C2-N2-C7	7.16	132.49	122.90
11	M	1	NAG	C2-N2-C7	6.89	132.14	122.90
13	U	2	NAG	O4-C4-C5	-6.75	92.71	109.32

There are no chirality outliers.

5 of 130 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1	NAG	C3-C2-N2-C7
7	A	1	NAG	C8-C7-N2-C2
7	A	1	NAG	O7-C7-N2-C2
7	A	2	NAG	C8-C7-N2-C2
7	A	2	NAG	O7-C7-N2-C2

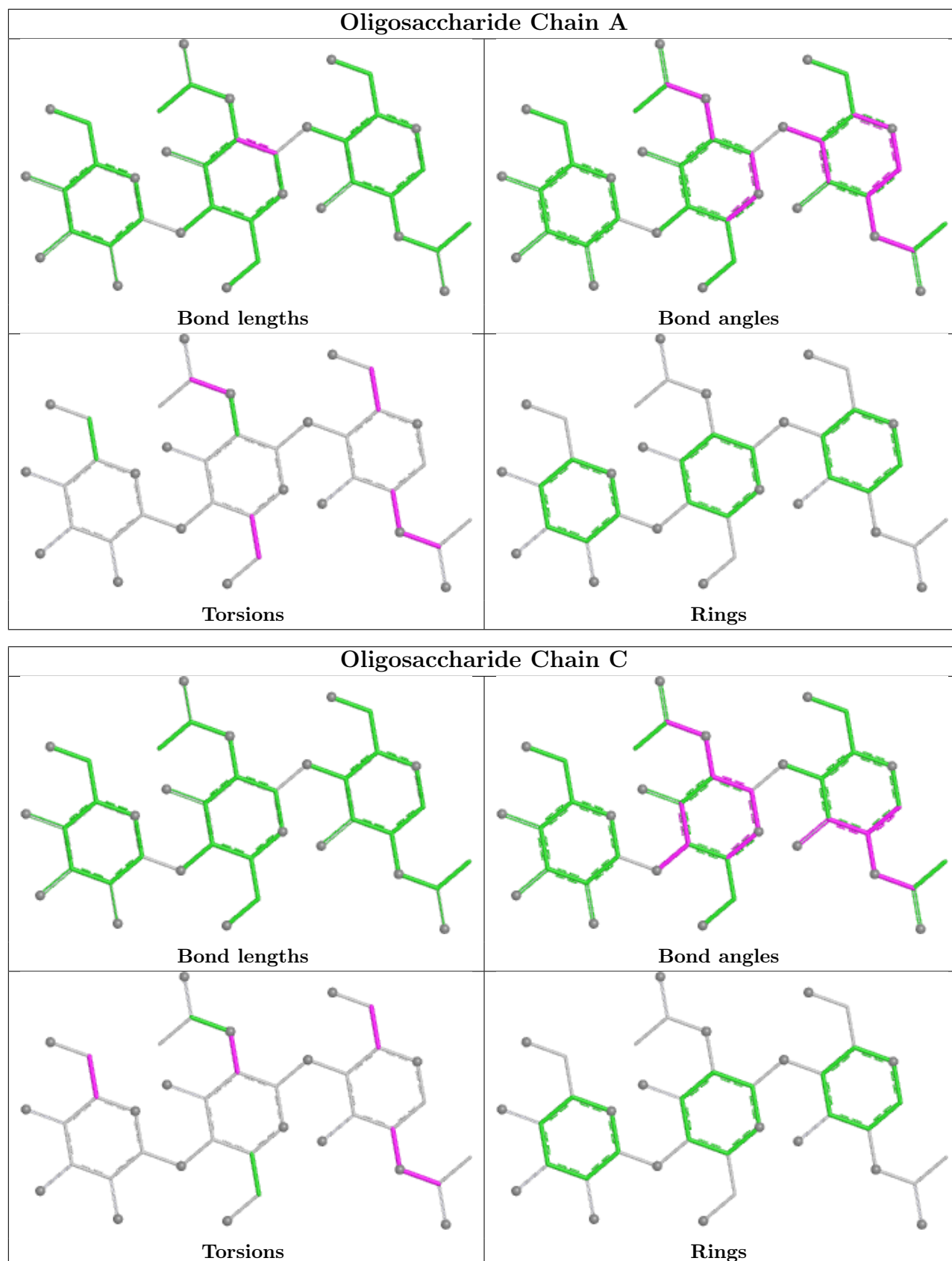
There are no ring outliers.

21 monomers are involved in 70 short contacts:

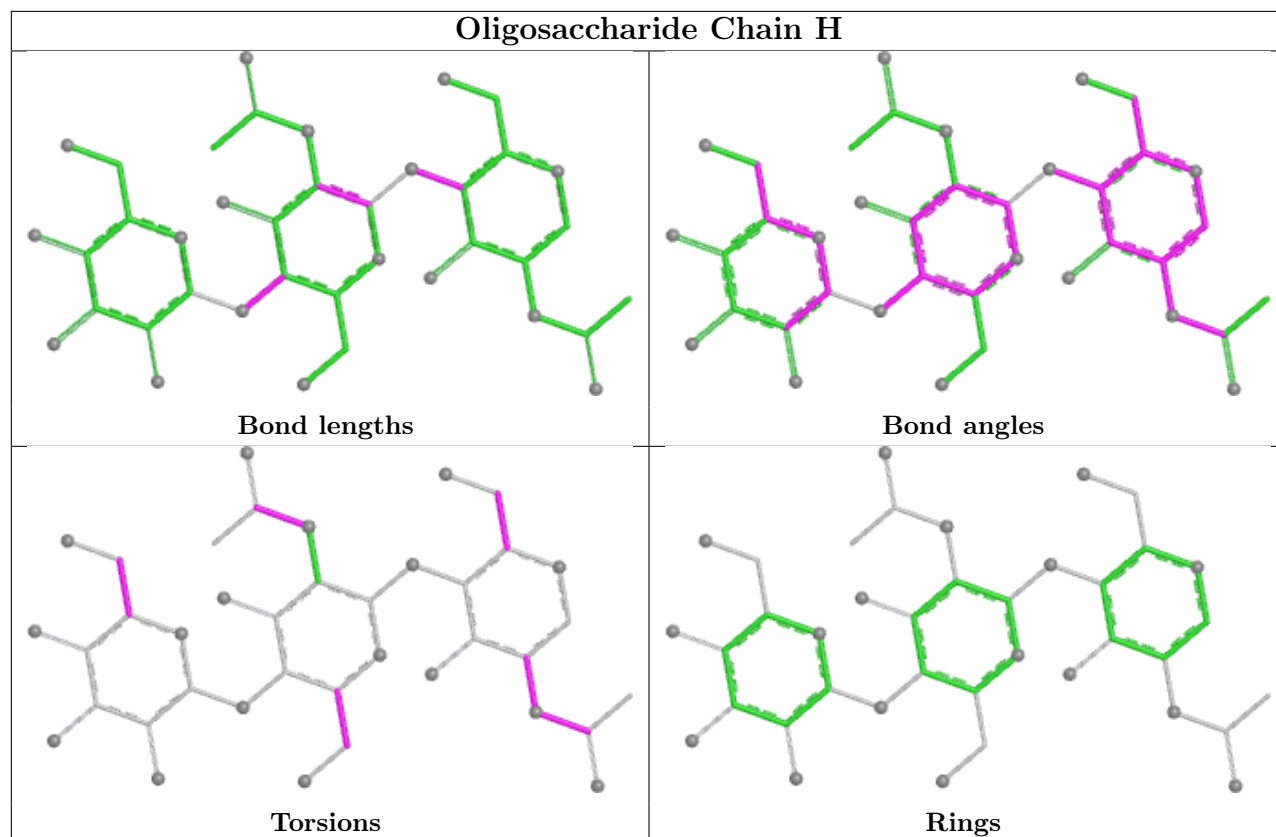
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	U	2	NAG	5	0
13	U	6	MAN	1	0
7	O	2	NAG	1	0
8	F	4	MAN	7	0
12	S	4	MAN	2	0
12	S	1	NAG	3	0
13	U	1	NAG	10	0
7	H	1	NAG	5	0
10	L	2	NAG	1	0
10	L	6	MAN	1	0
11	M	1	NAG	5	0
13	U	3	BMA	2	0
10	L	1	NAG	9	0
7	P	1	NAG	1	0
9	K	1	NAG	10	0
8	F	1	NAG	2	0
7	A	3	BMA	1	0
8	F	2	NAG	2	0
9	N	1	NAG	1	0
7	C	1	NAG	1	0
7	O	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

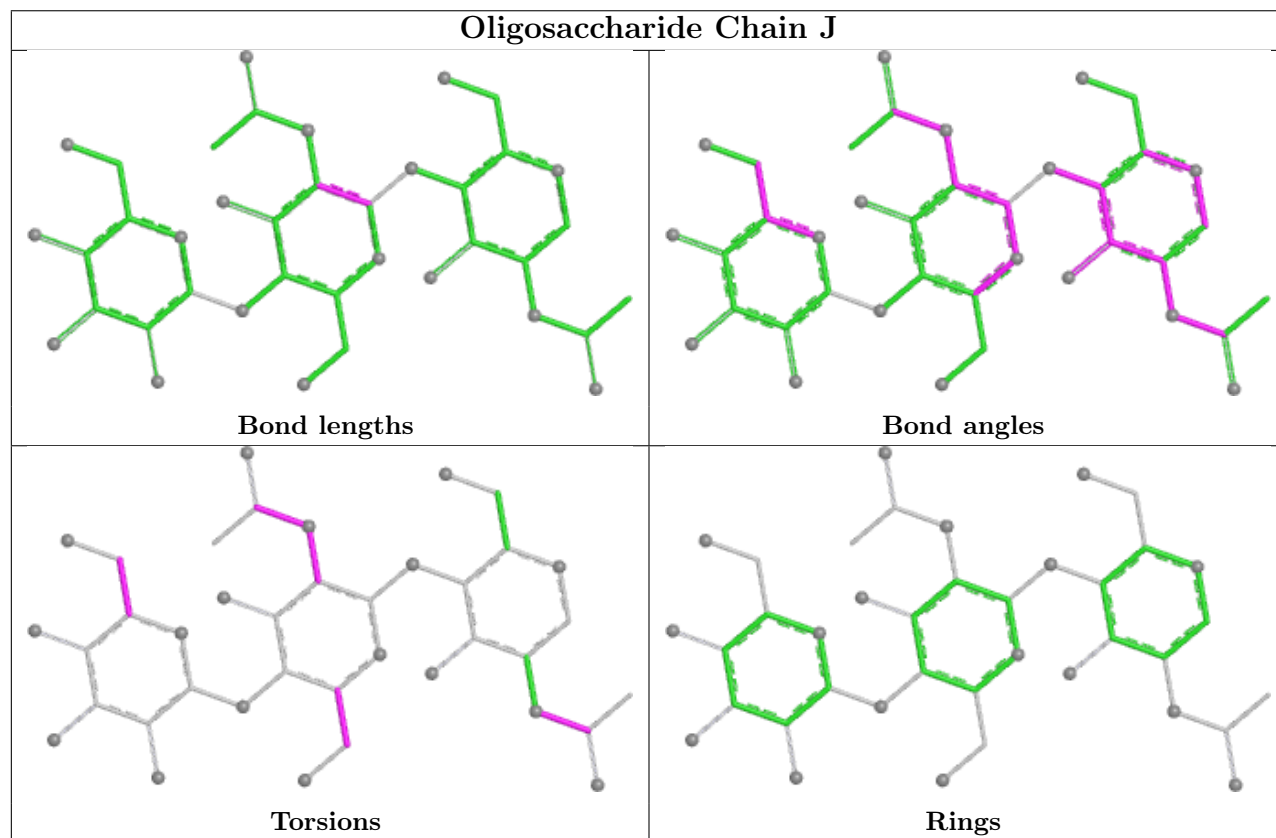
bond angles, torsion angles, and ring geometry for oligosaccharide.

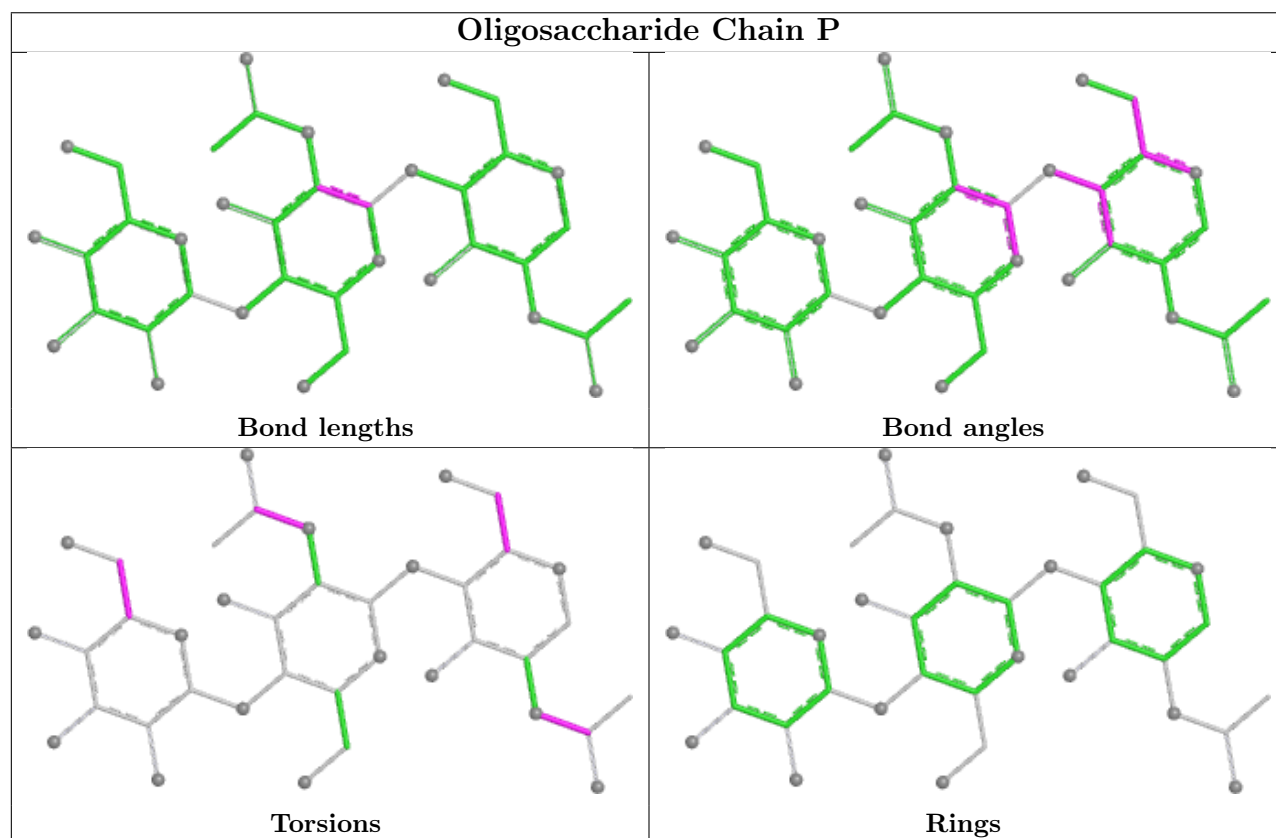
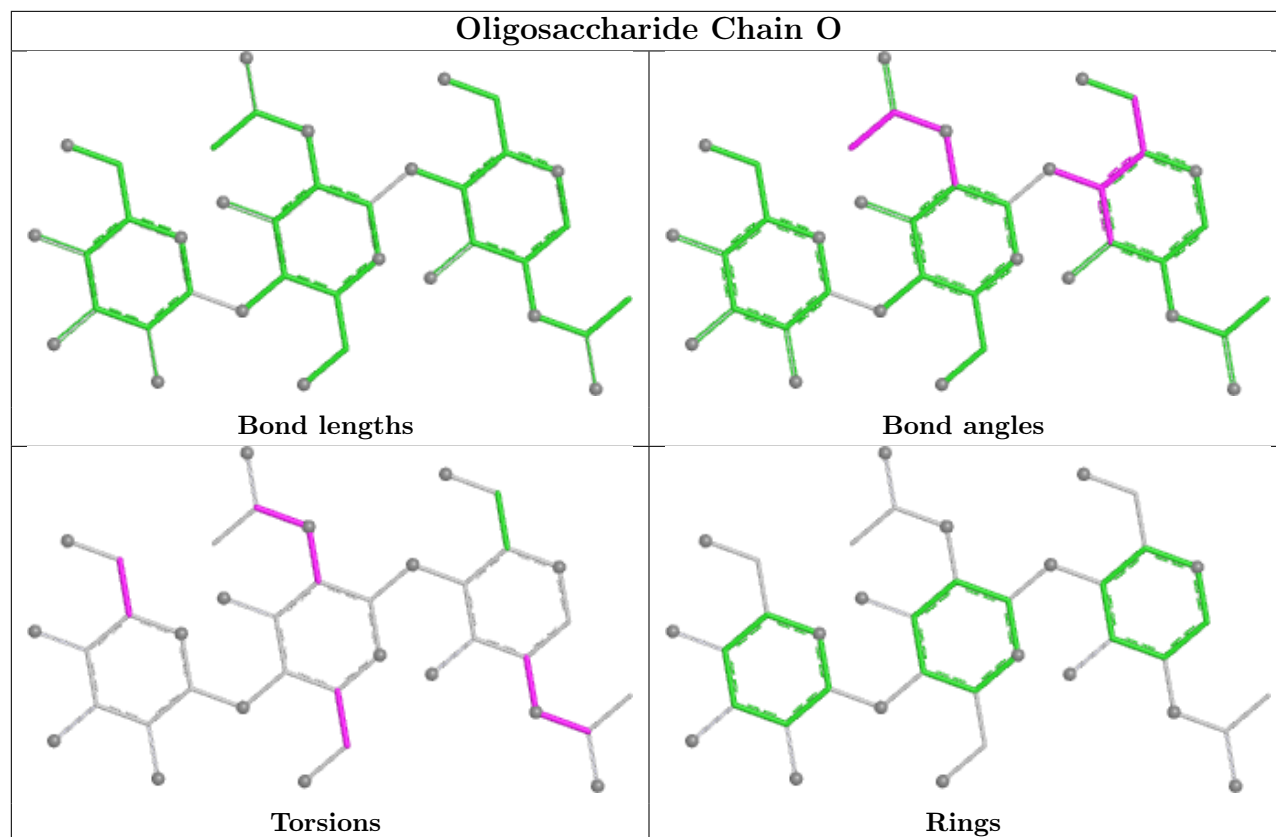


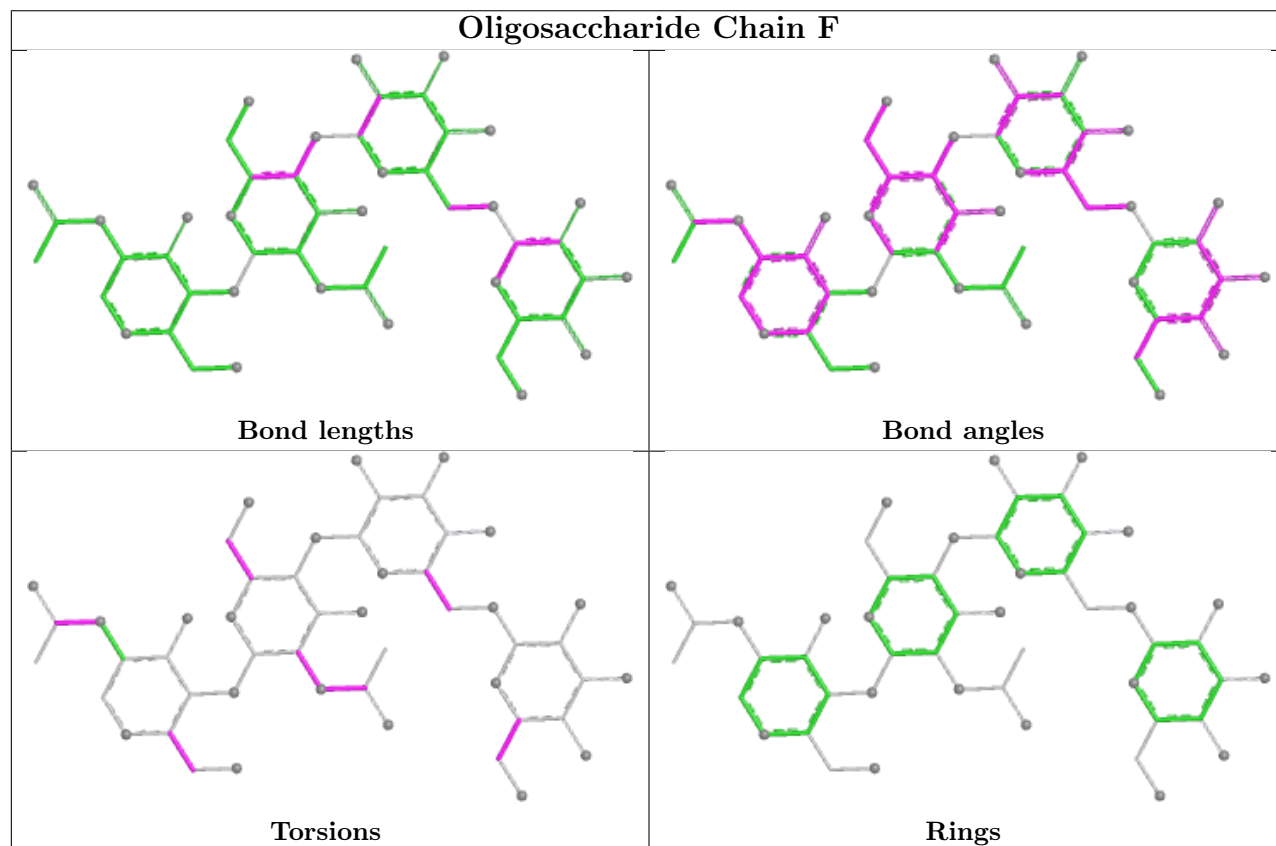
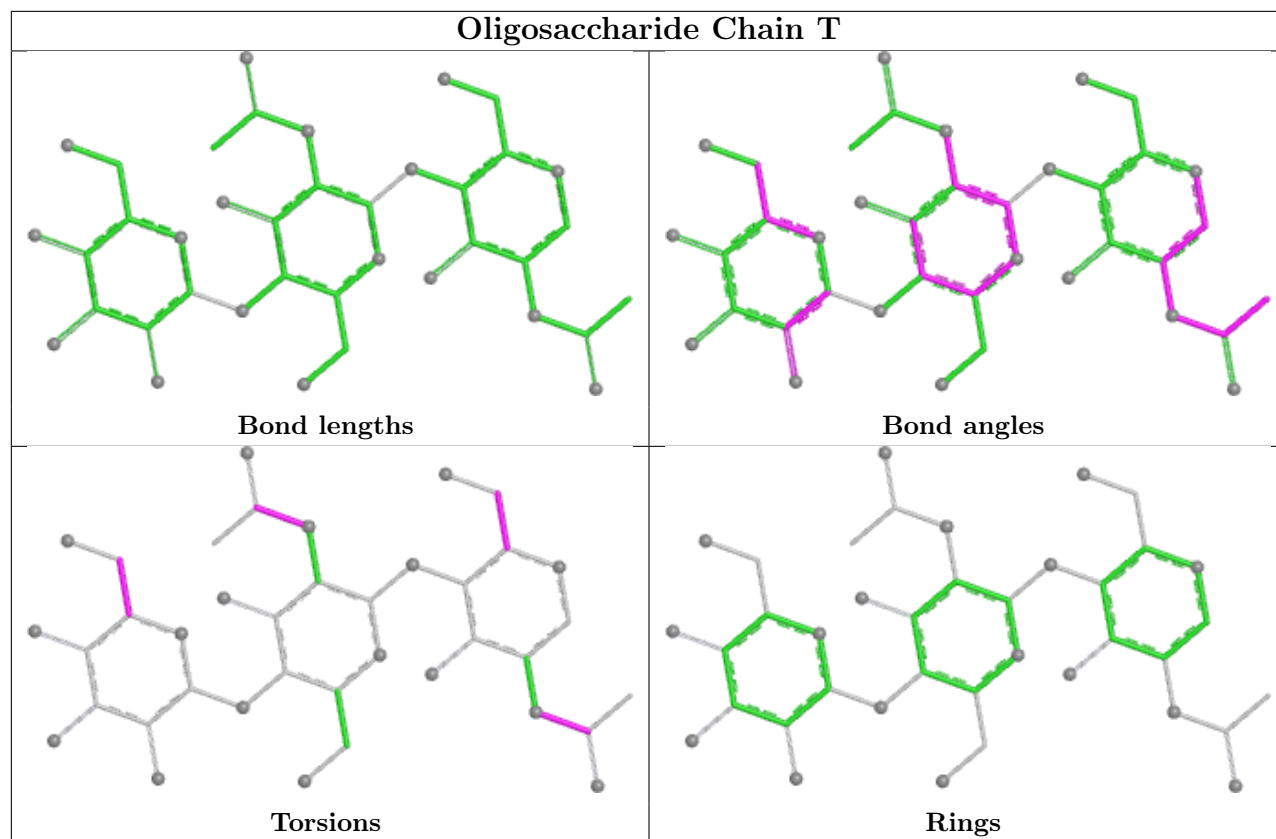
Oligosaccharide Chain H

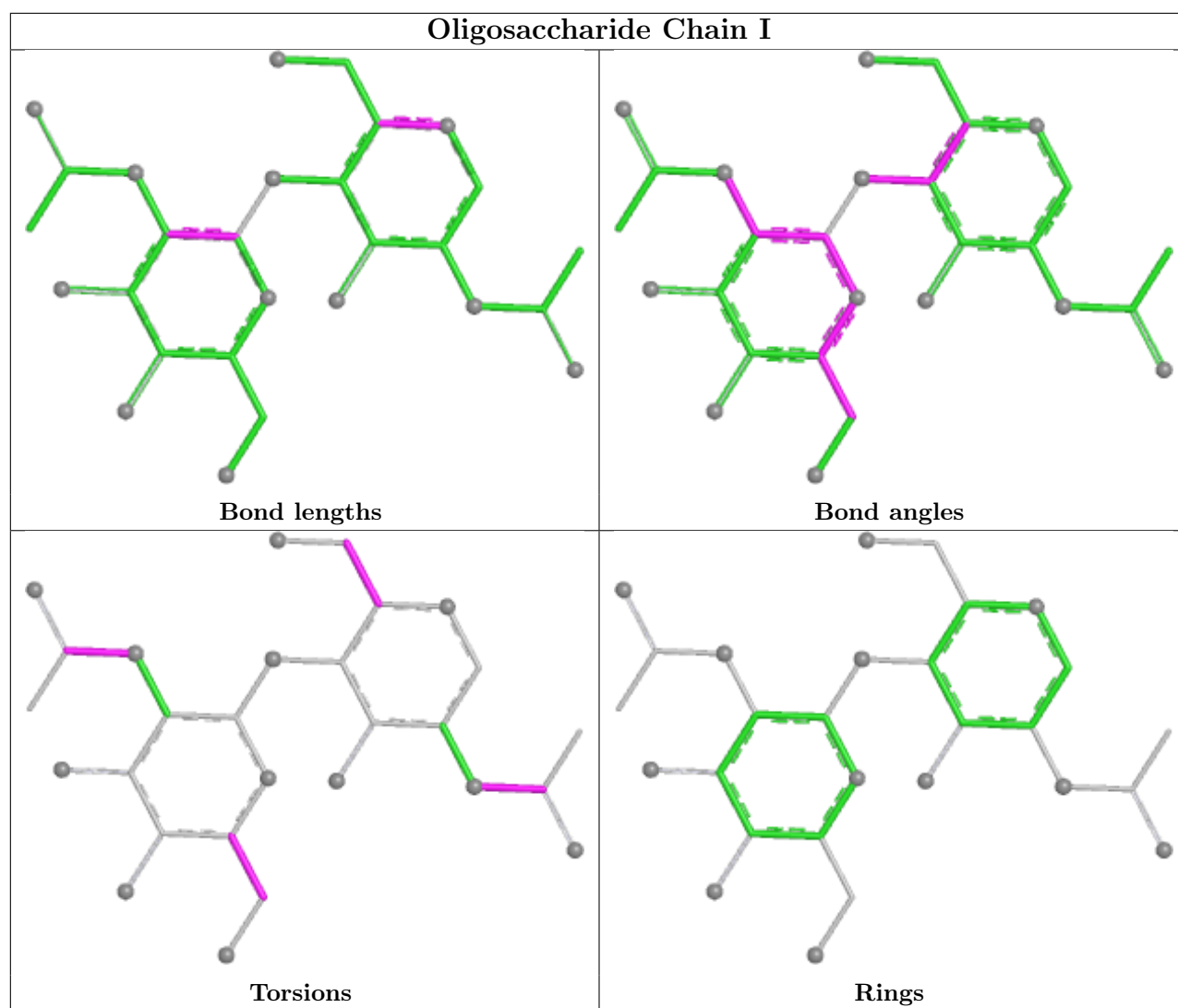


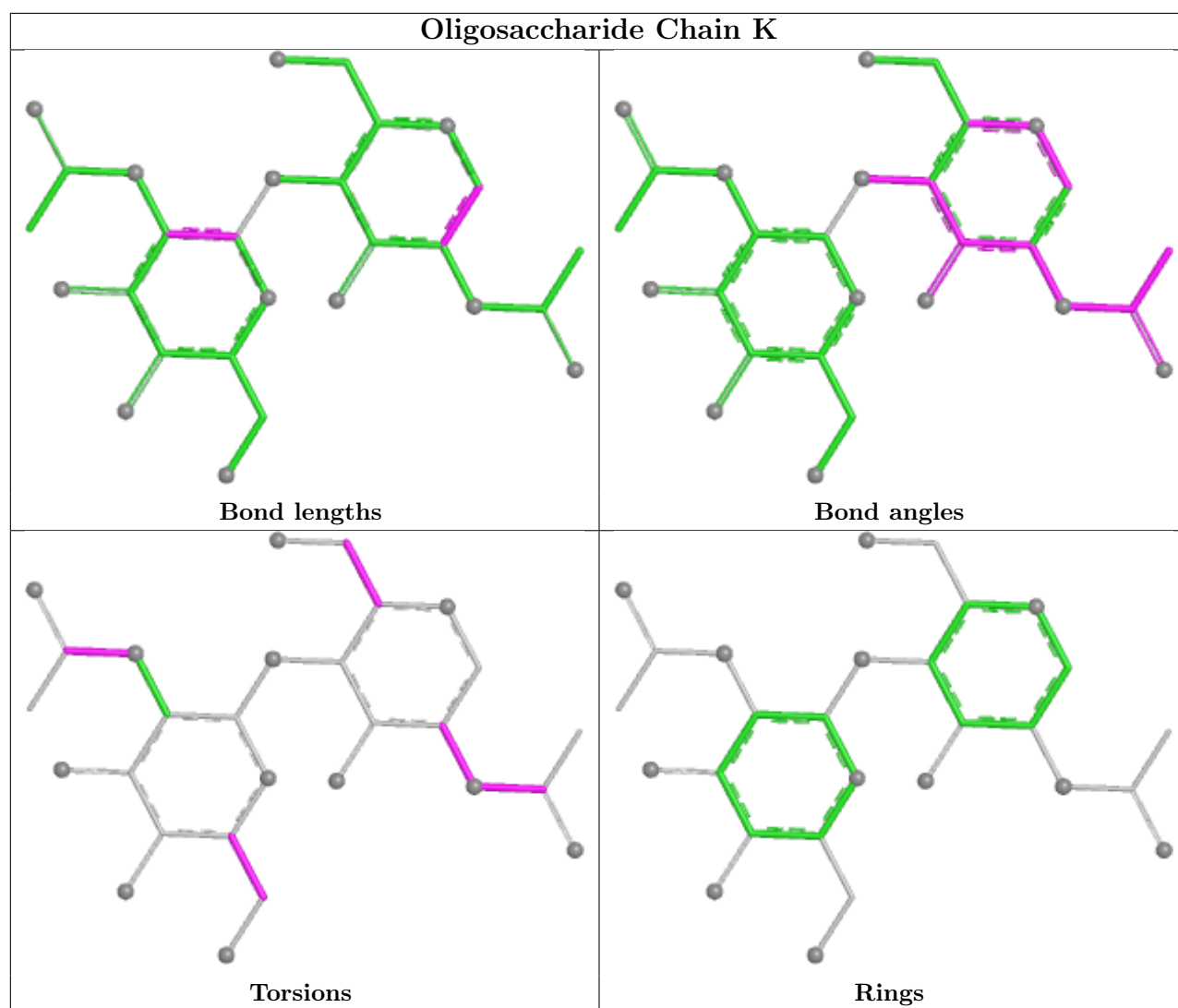
Oligosaccharide Chain J

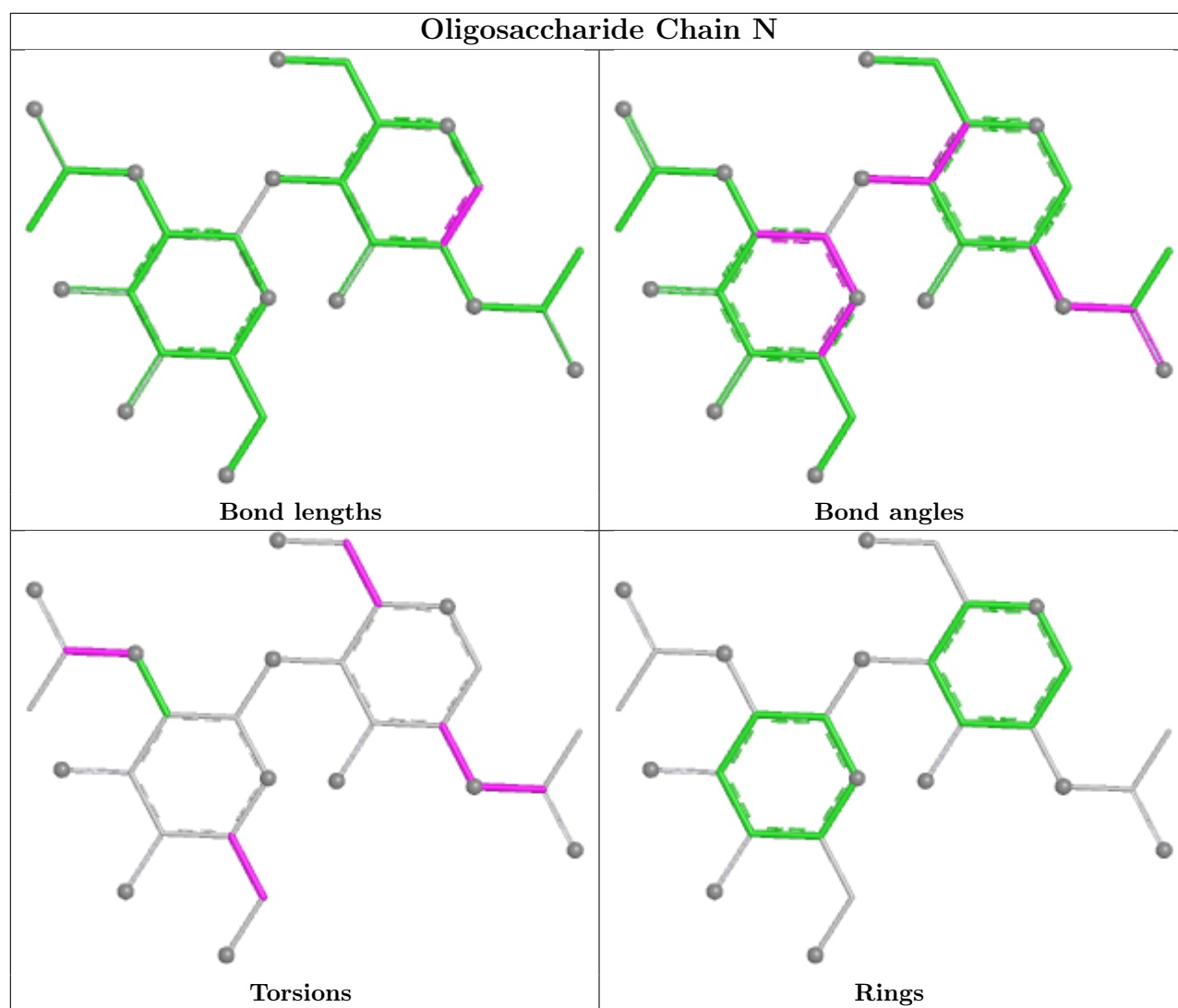


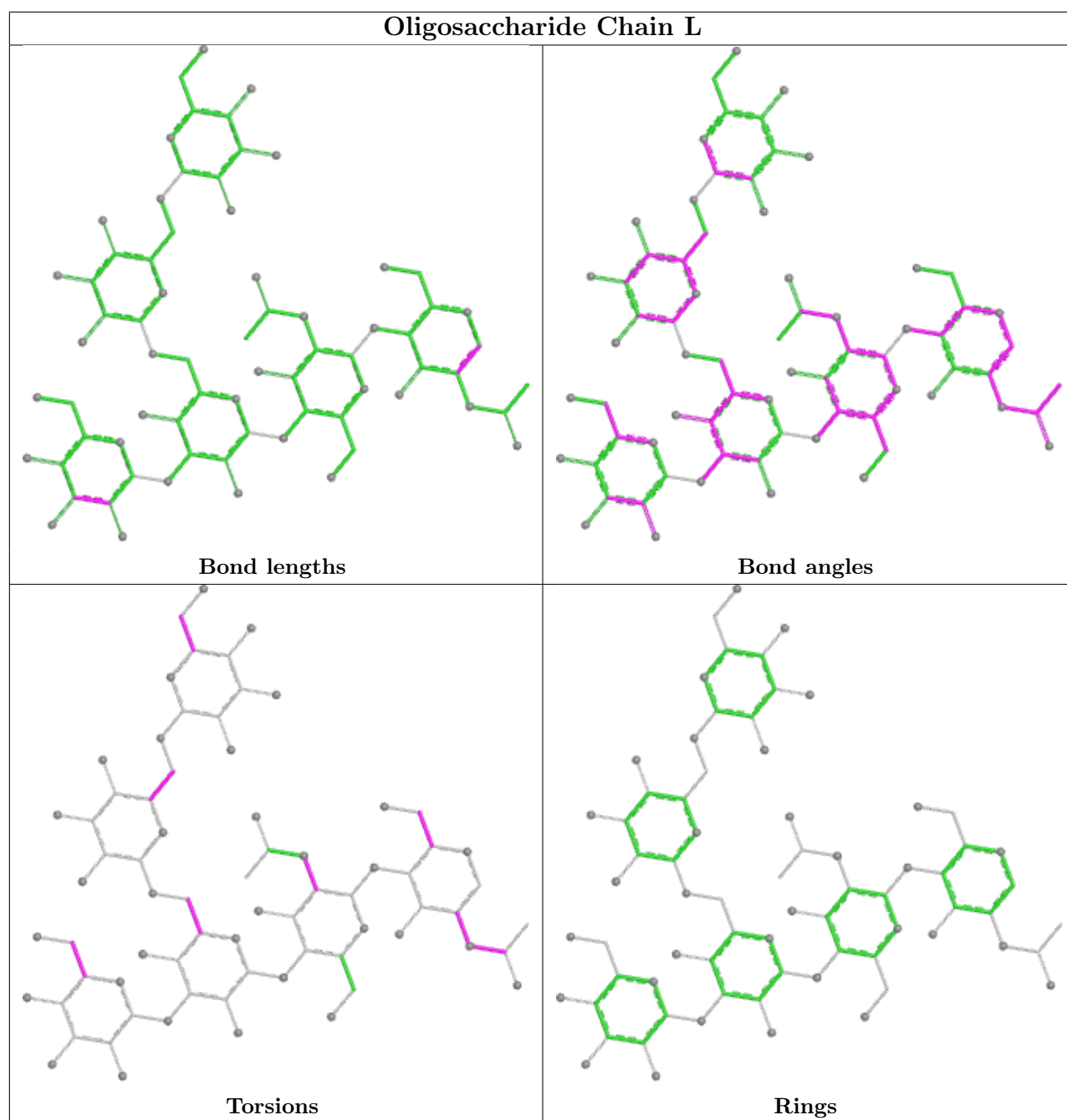




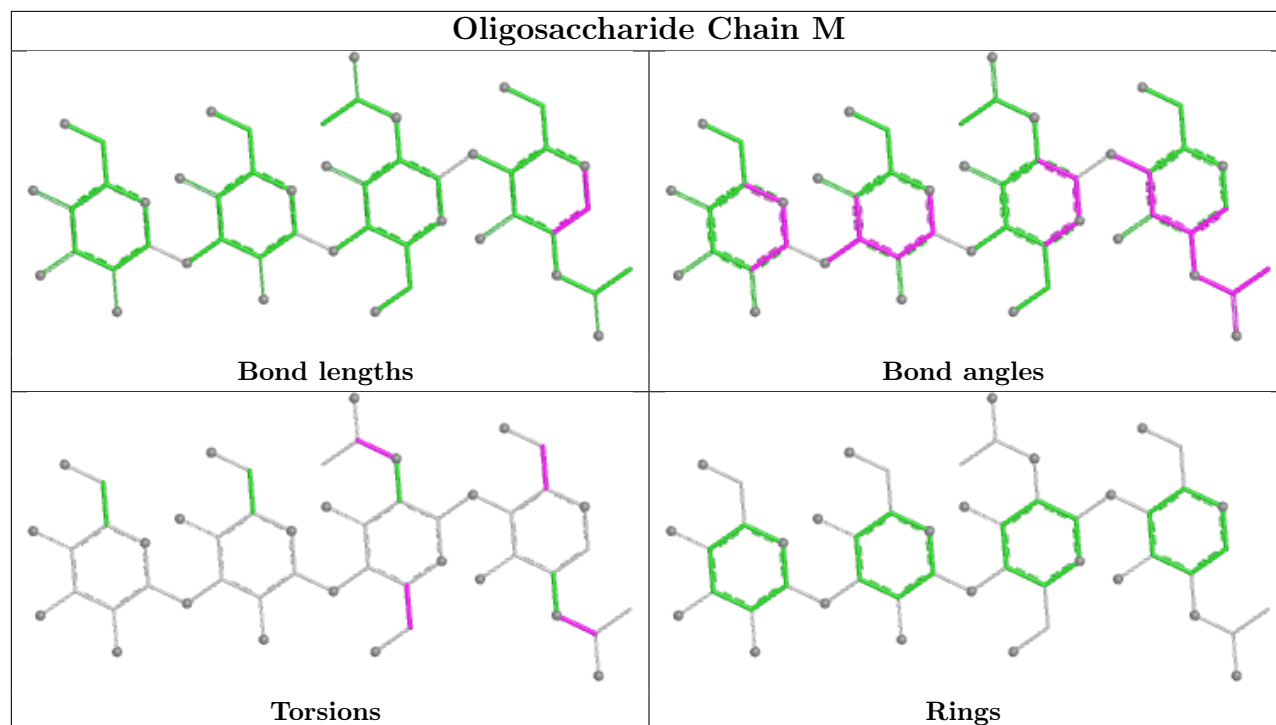




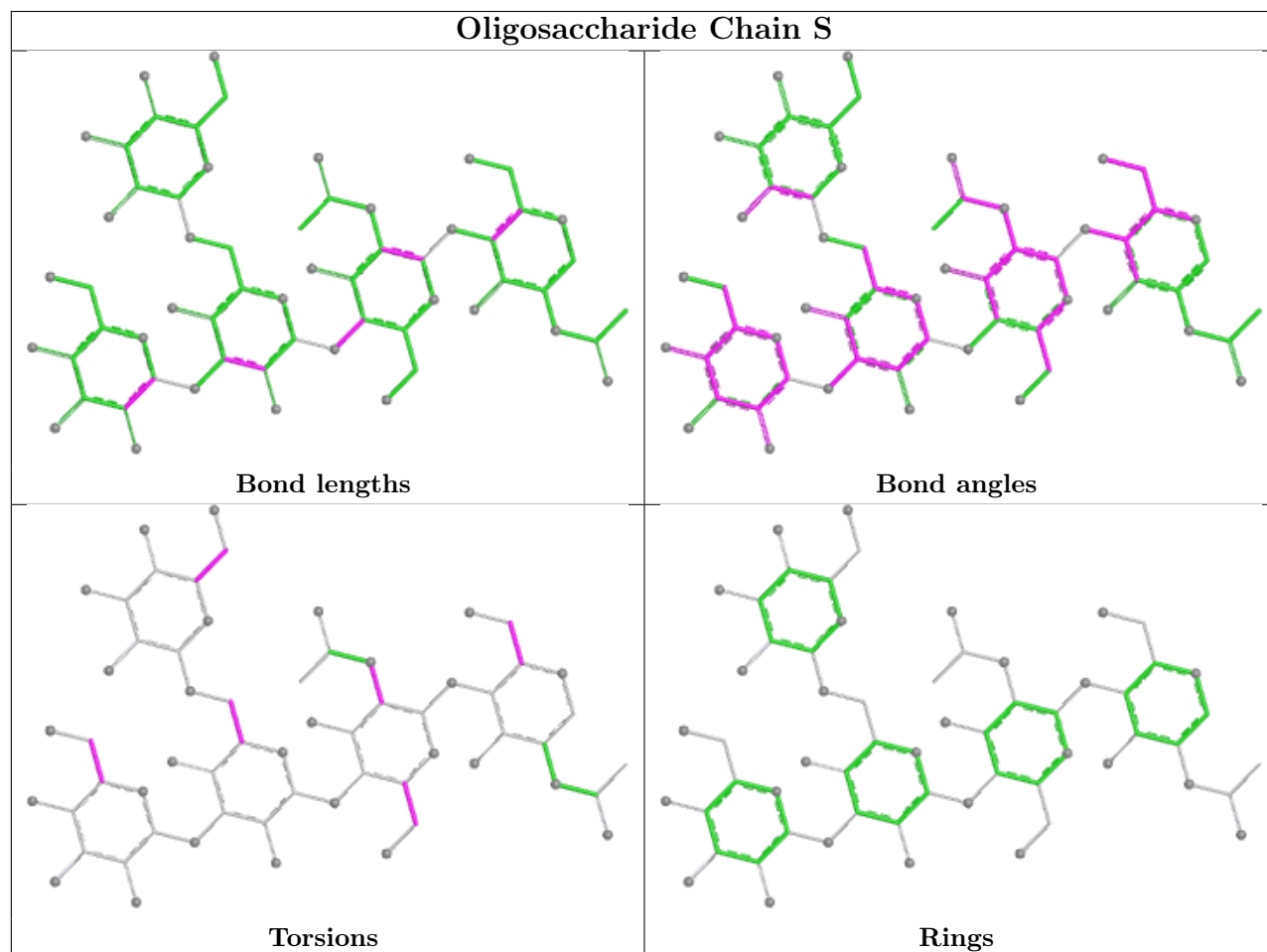


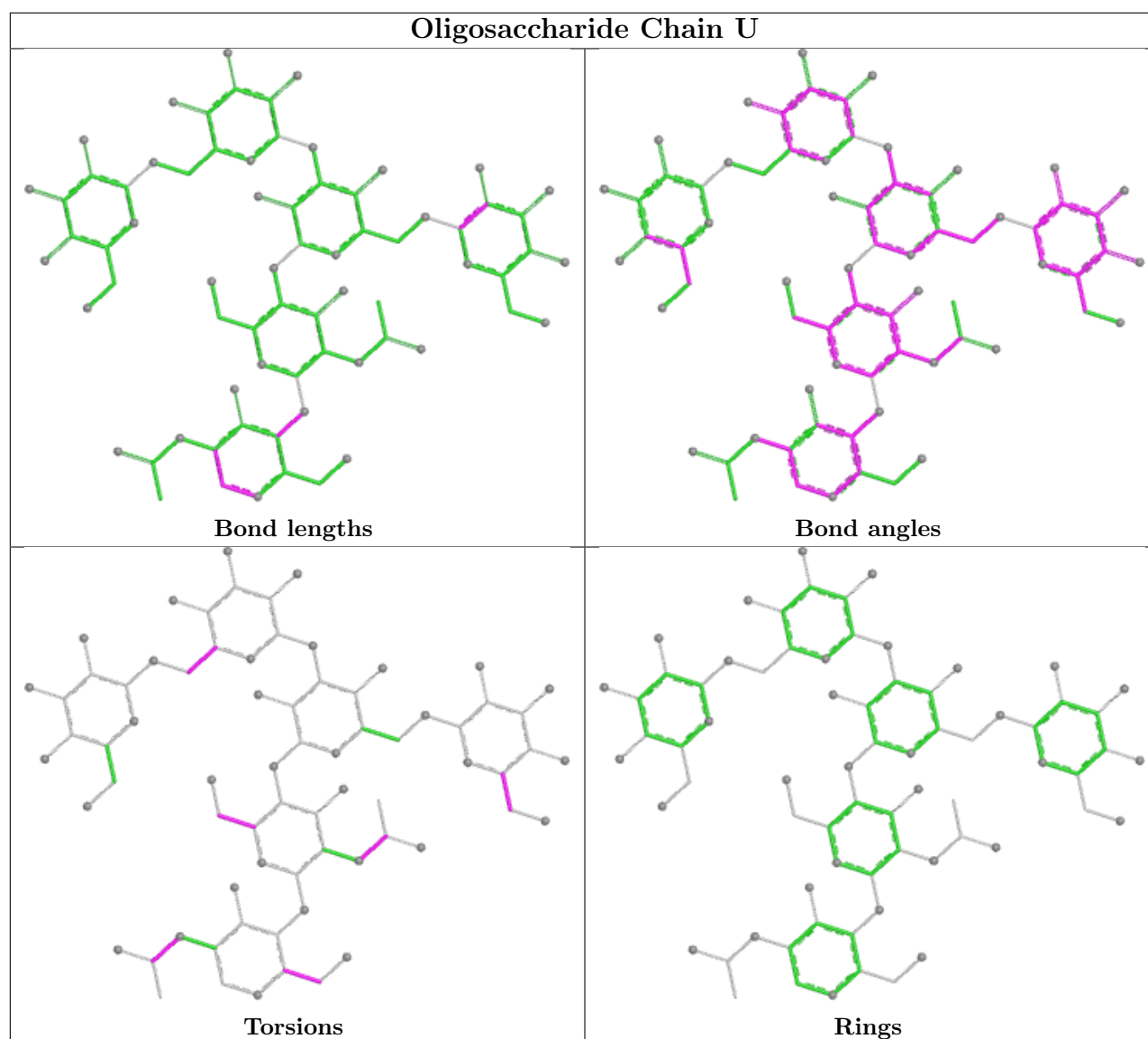


Oligosaccharide Chain M



Oligosaccharide Chain S





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	$\# Z > 2$
14	NAG	G	606	4	14,14,15	1.27	1 (7%)	17,19,21	1.99	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAG	B	704	1	14,14,15	0.30	0	17,19,21	1.12	2 (11%)
14	NAG	G	631	4	14,14,15	0.61	0	17,19,21	1.71	3 (17%)
14	NAG	G	622	4	14,14,15	0.95	1 (7%)	17,19,21	1.93	6 (35%)

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
14	NAG	G	606	4	-	5/6/23/26	0/1/1/1
14	NAG	B	704	1	-	4/6/23/26	0/1/1/1
14	NAG	G	631	4	-	2/6/23/26	0/1/1/1
14	NAG	G	622	4	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	606	NAG	C1-C2	3.86	1.57	1.52
14	G	622	NAG	C1-C2	2.58	1.55	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	606	NAG	C2-N2-C7	5.77	130.64	122.90
14	G	631	NAG	C2-N2-C7	4.42	128.83	122.90
14	G	622	NAG	C2-N2-C7	3.29	127.31	122.90
14	B	704	NAG	C2-N2-C7	-3.23	118.57	122.90
14	G	622	NAG	C6-C5-C4	-2.93	105.82	113.02

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	B	704	NAG	C8-C7-N2-C2
14	B	704	NAG	O7-C7-N2-C2
14	G	606	NAG	C3-C2-N2-C7
14	G	606	NAG	C8-C7-N2-C2
14	G	606	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	704	NAG	4	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	B	136/153 (88%)	0.21	0 100 100	183, 285, 325, 365	0
2	D	236/243 (97%)	-0.05	0 100 100	207, 303, 325, 325	0
3	E	213/216 (98%)	-0.07	1 (0%) 87 75	196, 297, 325, 325	0
4	G	448/518 (86%)	0.10	12 (2%) 56 45	186, 292, 325, 375	0
5	Q	231/240 (96%)	0.13	7 (3%) 52 42	210, 298, 325, 325	0
6	R	205/215 (95%)	-0.01	7 (3%) 48 40	219, 309, 325, 325	0
All	All	1469/1585 (92%)	0.05	27 (1%) 67 54	183, 298, 325, 375	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	439	ILE	5.0
4	G	496	ILE	4.7
4	G	423	ILE	4.1
6	R	76	ILE	3.6
4	G	180	ASP	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 [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.

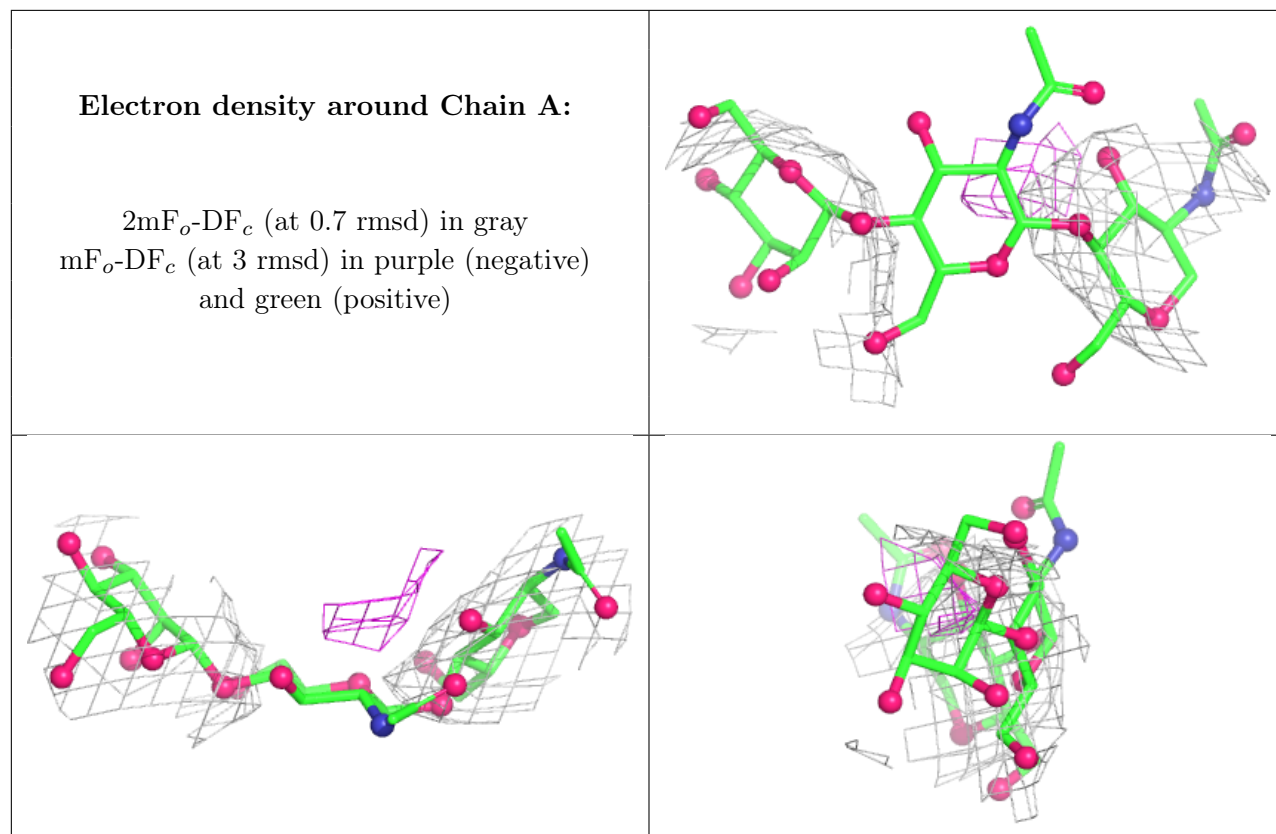
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	A	1	14/15	-	-	411,411,411,411	0
7	NAG	A	2	14/15	-	-	430,430,430,430	0
7	BMA	A	3	11/12	-	-	420,420,420,420	0
7	NAG	C	1	14/15	-	-	428,428,428,428	0
7	NAG	C	2	14/15	-	-	449,449,449,449	0
7	BMA	C	3	11/12	-	-	450,450,450,450	0
7	BMA	O	3	11/12	-0.19	0.13	435,435,435,435	0
7	BMA	H	3	11/12	0.22	0.09	478,478,478,478	0
7	NAG	H	2	14/15	0.25	0.12	449,449,449,449	0
7	BMA	J	3	11/12	0.46	0.08	441,441,441,441	0
7	BMA	T	3	11/12	0.54	0.08	415,415,415,415	0
10	BMA	L	3	11/12	0.55	0.11	386,386,386,386	0
12	MAN	S	4	11/12	0.55	0.15	327,327,327,327	0
12	BMA	S	3	11/12	0.59	0.12	415,415,415,415	0
13	BMA	U	3	11/12	0.63	0.11	334,334,334,334	0
7	NAG	J	2	14/15	0.65	0.10	418,418,418,418	0
9	NAG	K	2	14/15	0.67	0.10	333,333,333,333	0
7	BMA	P	3	11/12	-	-	417,417,417,417	0
7	NAG	O	2	14/15	0.68	0.10	428,428,428,428	0
12	MAN	S	5	11/12	0.73	0.12	397,397,397,397	0
12	NAG	S	2	14/15	0.73	0.10	398,398,398,398	0
8	NAG	F	1	14/15	-	-	343,343,343,343	0
8	NAG	F	2	14/15	-	-	337,337,337,337	0
8	BMA	F	3	11/12	-	-	349,349,349,349	0
8	MAN	F	4	11/12	-	-	360,360,360,360	0
13	MAN	U	6	11/12	0.75	0.09	331,331,331,331	0
13	MAN	U	5	11/12	0.76	0.13	366,366,366,366	0
11	NAG	M	2	14/15	0.77	0.10	405,405,405,405	0
9	NAG	I	1	14/15	0.80	0.13	396,396,396,396	0
7	NAG	T	2	14/15	0.82	0.10	425,425,425,425	0
13	MAN	U	4	11/12	0.82	0.08	373,373,373,373	0
9	NAG	K	1	14/15	0.83	0.11	311,311,311,311	0
7	NAG	P	2	14/15	0.83	0.07	409,409,409,409	0
7	NAG	H	1	14/15	0.84	0.09	383,383,383,383	0
10	MAN	L	4	11/12	-	-	387,387,387,387	0
10	MAN	L	5	11/12	-	-	416,416,416,416	0
10	MAN	L	6	11/12	-	-	369,369,369,369	0
7	NAG	P	1	14/15	0.84	0.11	386,386,386,386	0
9	NAG	I	2	14/15	0.84	0.12	433,433,433,433	0
11	BMA	M	3	11/12	-	-	432,432,432,432	0
11	MAN	M	4	11/12	-	-	456,456,456,456	0
10	NAG	L	2	14/15	0.85	0.10	340,340,340,340	0
11	NAG	M	1	14/15	0.86	0.11	390,390,390,390	0

Continued on next page...

Continued from previous page...

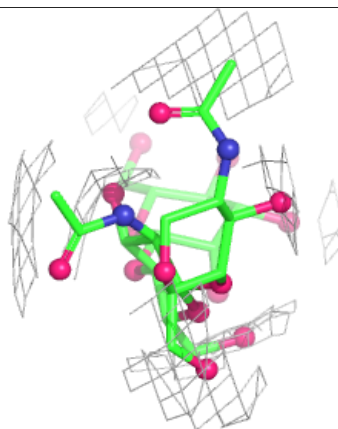
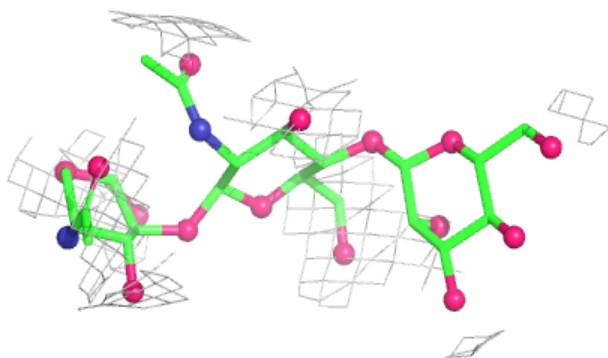
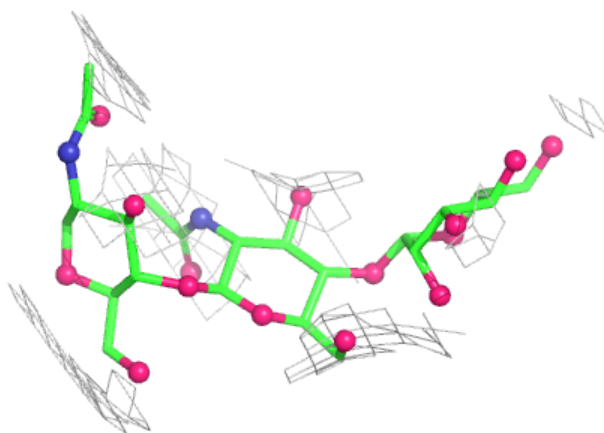
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	J	1	14/15	0.86	0.09	384,384,384,384	0
13	NAG	U	1	14/15	0.88	0.11	352,352,352,352	0
9	NAG	N	2	14/15	0.89	0.12	422,422,422,422	0
7	NAG	T	1	14/15	0.90	0.10	380,380,380,380	0
10	NAG	L	1	14/15	0.90	0.13	396,396,396,396	0
12	NAG	S	1	14/15	0.90	0.10	343,343,343,343	0
9	NAG	N	1	14/15	0.92	0.17	391,391,391,391	0
7	NAG	O	1	14/15	0.93	0.13	394,394,394,394	0
13	NAG	U	2	14/15	0.95	0.14	359,359,359,359	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.

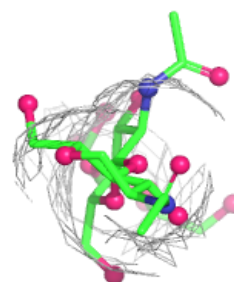
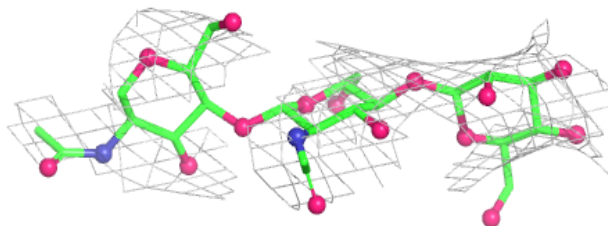
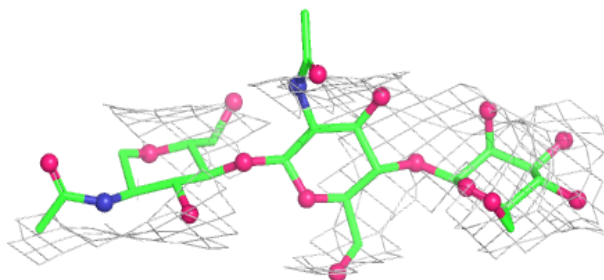


Electron density around Chain C:

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

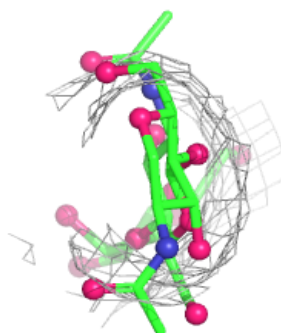
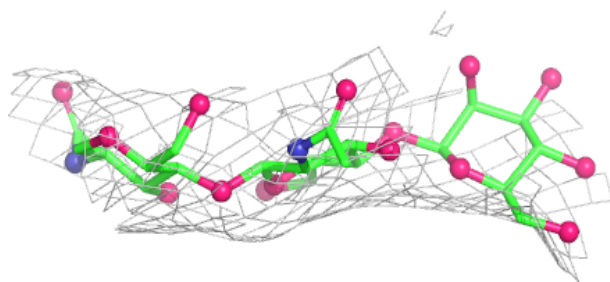
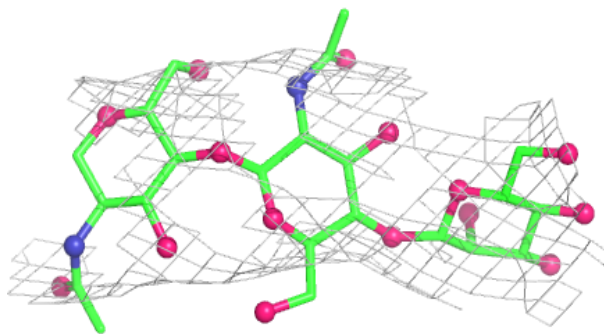
**Electron density around Chain H:**

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

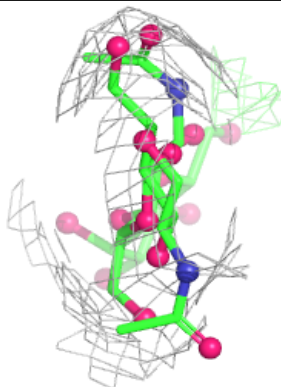
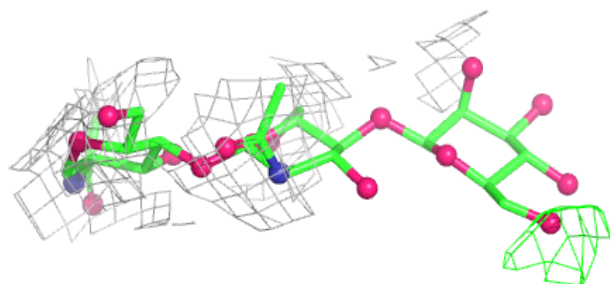
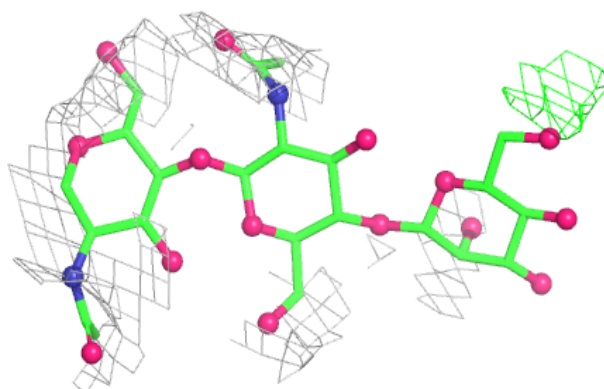


Electron density around Chain J:

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

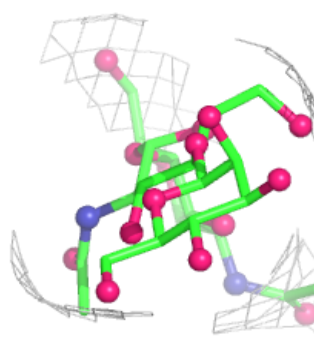
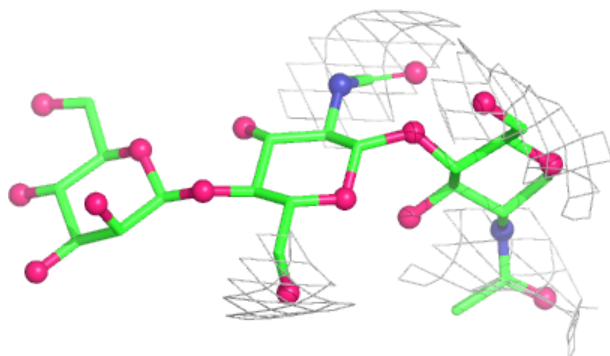
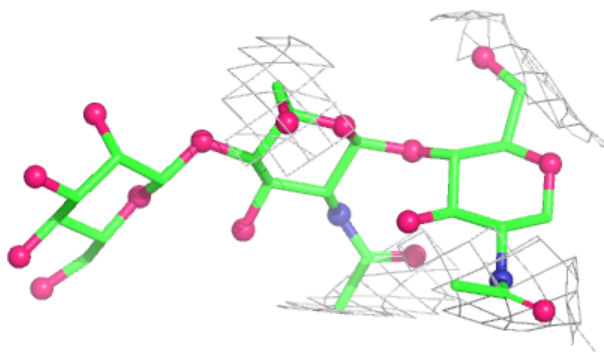
**Electron density around Chain O:**

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

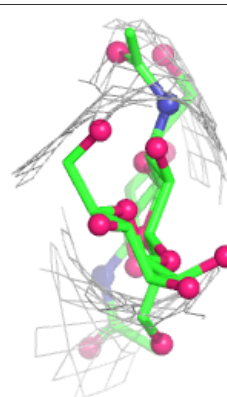
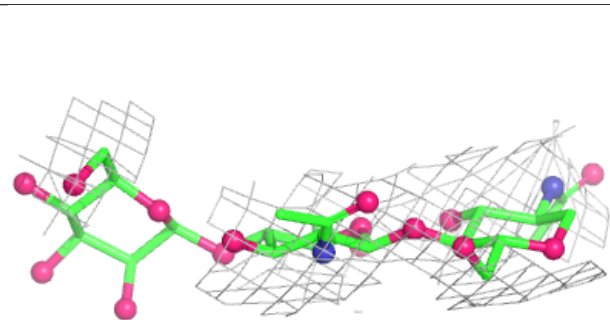
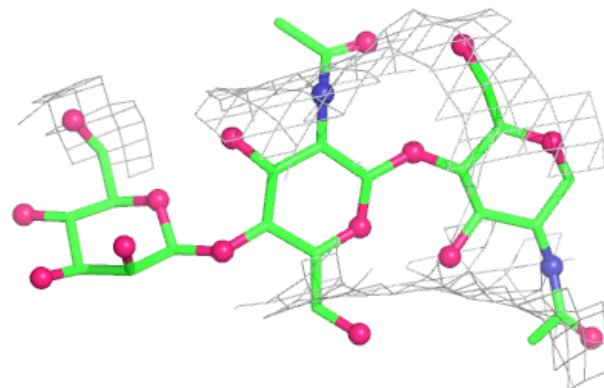


Electron density around Chain P:

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

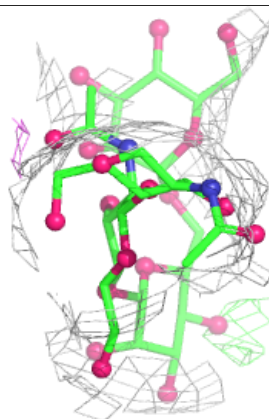
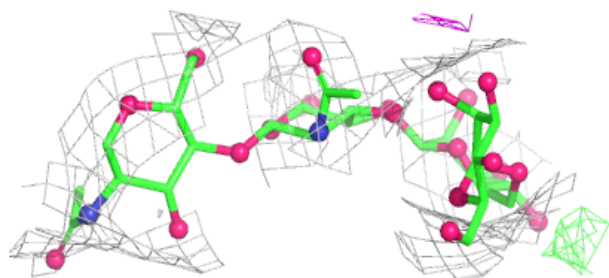
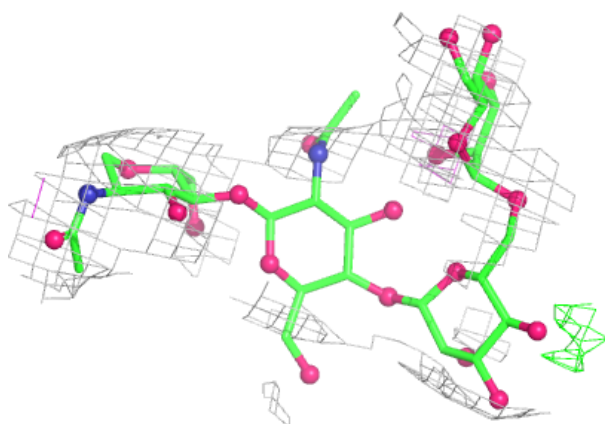
**Electron density around Chain T:**

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



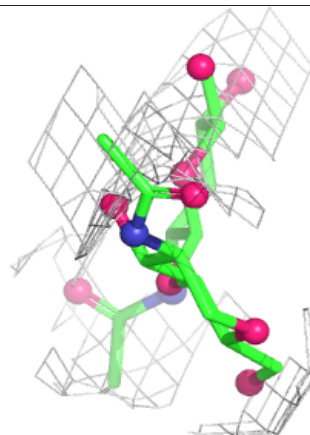
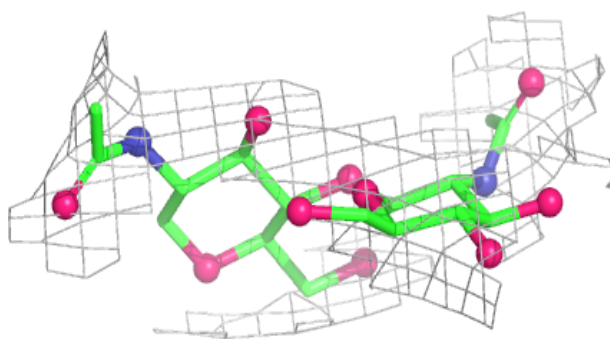
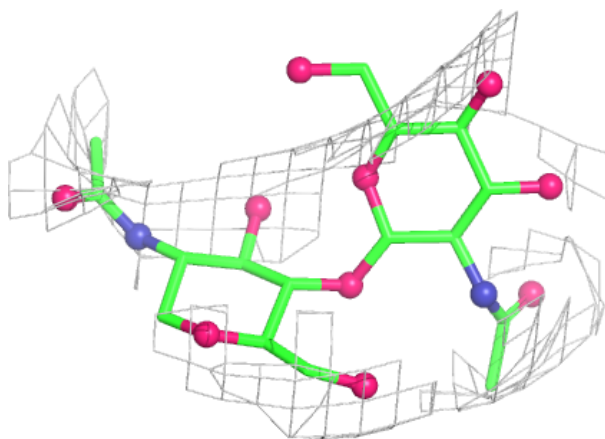
Electron density around Chain F:

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



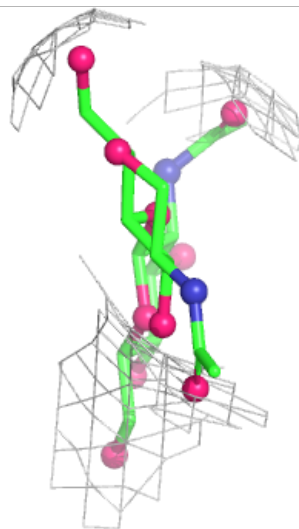
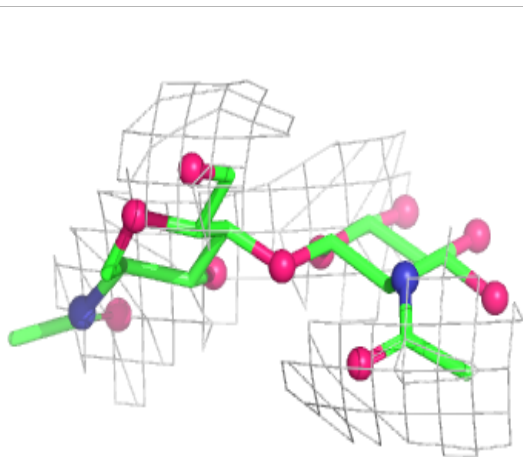
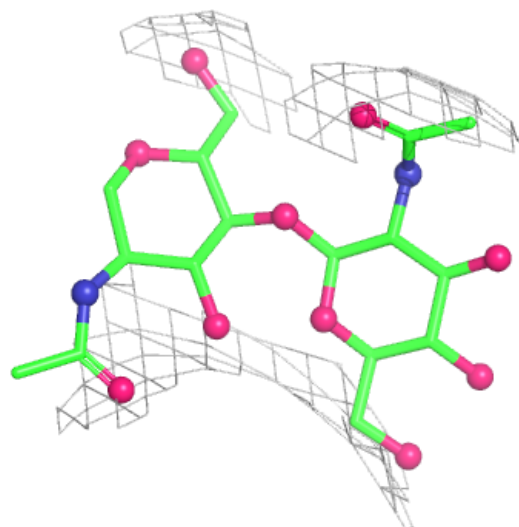
Electron density around Chain I:

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



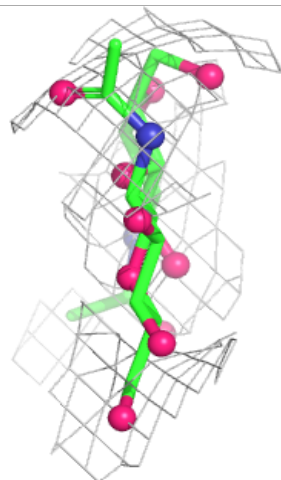
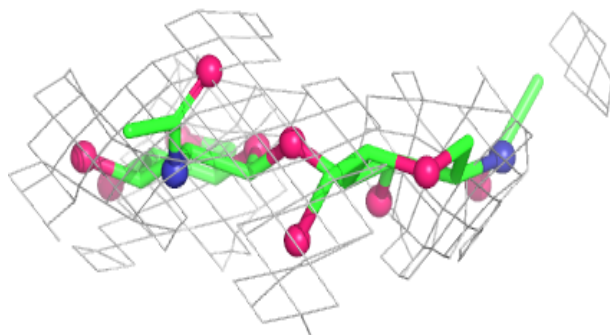
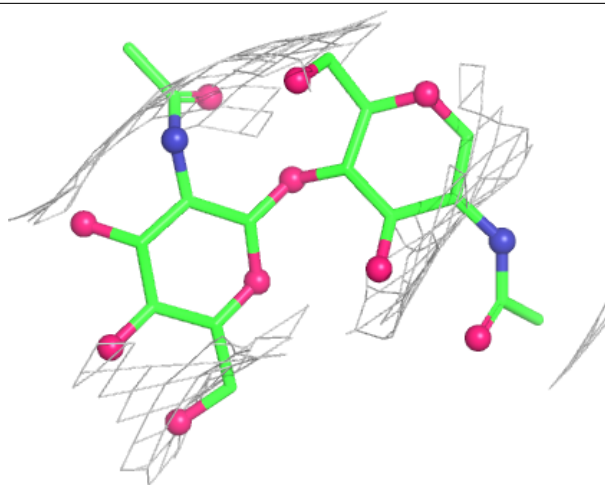
Electron density around Chain K:

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



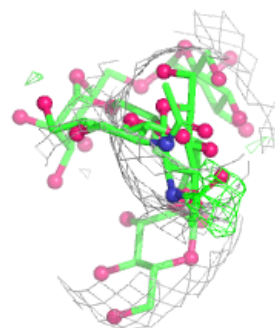
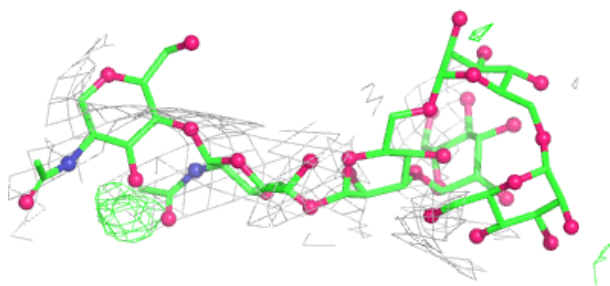
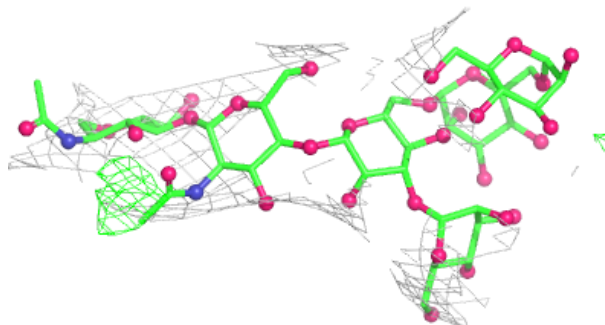
Electron density around Chain N:

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

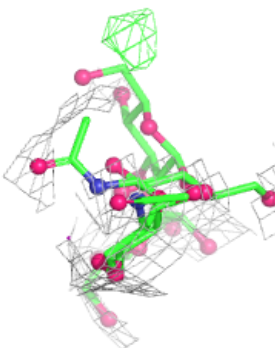
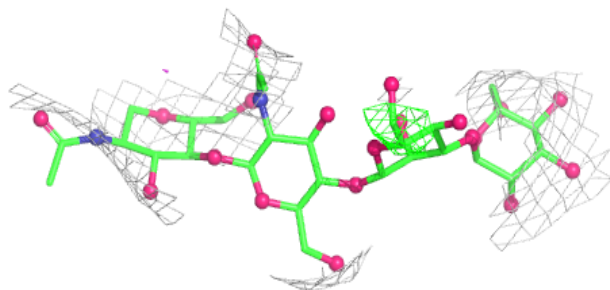
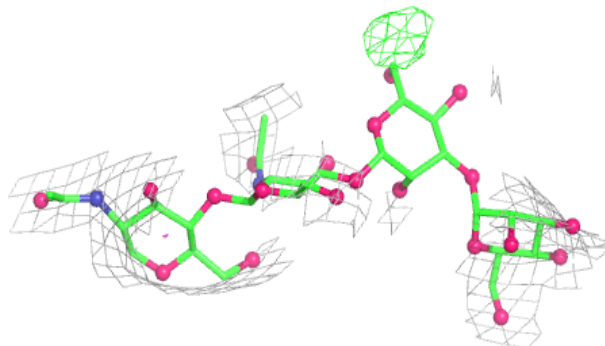


Electron density around Chain L:

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

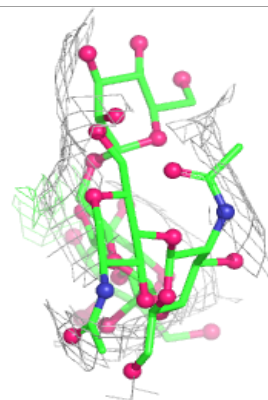
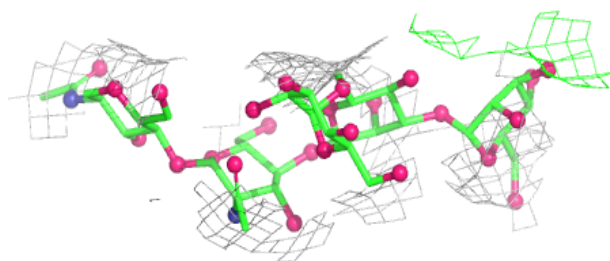
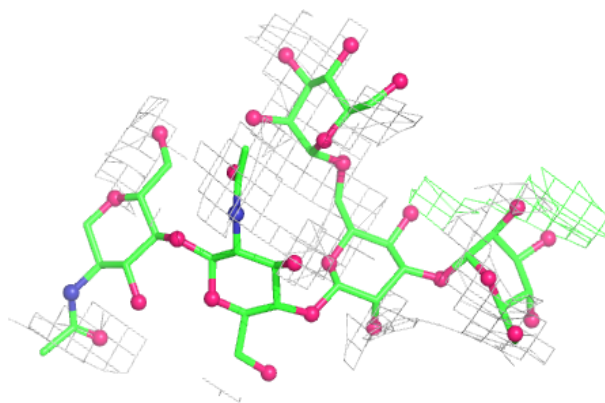
**Electron density around Chain M:**

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

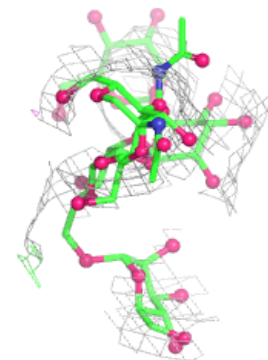
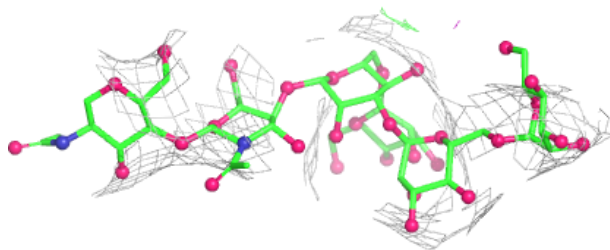
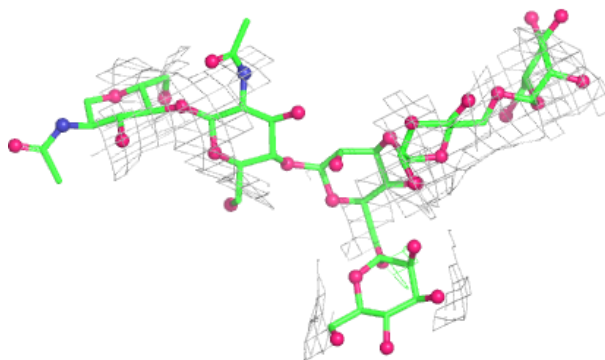


Electron density around Chain S:

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

**Electron density around Chain U:**

$2mF_o-DF_c$ (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
14	NAG	G	606	14/15	0.75	0.14	368,368,368,368	0
14	NAG	G	631	14/15	0.86	0.12	365,365,365,365	0
14	NAG	B	704	14/15	0.90	0.18	326,326,326,326	0
14	NAG	G	622	14/15	0.94	0.10	367,367,367,367	0

6.5 Other polymers [i](#)

There are no such residues in this entry.