



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 02:43 AM UTC

PDB ID : 6DE7 / pdb_00006de7
Title : Crystal Structure at 4.3 Å Resolution of Glycosylated HIV-1 Clade A BG505 SOSIP.664 Prefusion Env Trimer with Interdomain Stabilization 113C-429GCG in Complex with Broadly Neutralizing Antibodies PGT122 and 35O22
Authors : Gorman, J.; Kwong, P.D.
Deposited on : 2018-05-11
Resolution : 4.12 Å (reported)

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

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

A user guide is available at

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

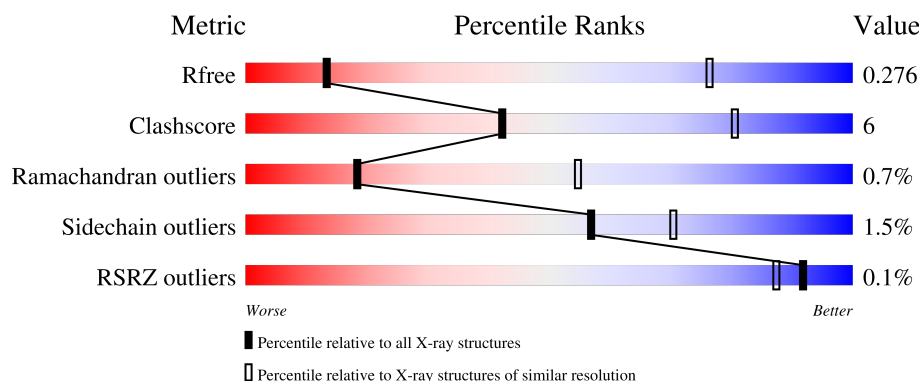
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.12 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.



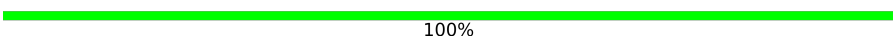
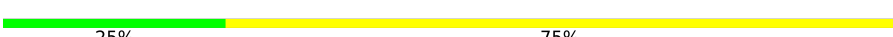
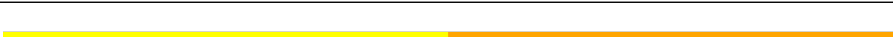
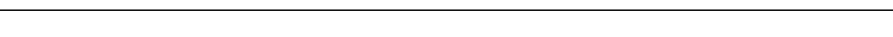
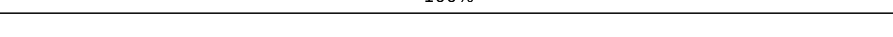
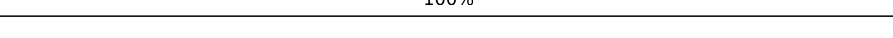
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1249 (4.44-3.80)
Clashscore	190562	1031 (4.42-3.82)
Ramachandran outliers	187476	1211 (4.44-3.80)
Sidechain outliers	187428	1198 (4.44-3.80)
RSRZ outliers	180081	1246 (4.44-3.80)

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	483	

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Mol	Chain	Length	Quality of chain
5	H	235	
6	L	213	
7	A	3	
7	O	3	
8	C	7	
9	F	4	
10	I	2	
10	K	2	
10	M	2	
10	N	2	
10	Q	2	
10	R	2	
10	S	2	
10	T	2	
11	J	6	
12	P	5	
13	U	9	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 11704 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 gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	129	Total	C	N	O	S	0	0	0
			1026	651	176	193	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S7
B	605	CYS	THR	engineered mutation	UNP Q2N0S7

- Molecule 2 is a protein called 35O22 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	205	Total	C	N	O	S	0	0	0
			1571	1005	264	295	7			

- Molecule 3 is a protein called 35O22 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	194	Total	C	N	O	S	0	0	0
			1483	934	243	298	8			

- Molecule 4 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	453	Total	C	N	O	S	0	0	0
			3555	2230	627	668	30			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	113	CYS	ASP	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	engineered mutation	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	429	GLY	-	insertion	UNP Q2N0S6
G	429A	CYS	-	insertion	UNP Q2N0S6
G	429B	GLY	ARG	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	GLU	engineered mutation	UNP Q2N0S6
G	510	ARG	LYS	engineered mutation	UNP Q2N0S6
G	512	ARG	ALA	engineered mutation	UNP Q2N0S6
G	513	ARG	VAL	engineered mutation	UNP Q2N0S6

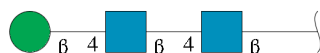
- Molecule 5 is a protein called PGT122 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	226	Total	C	N	O	S	0	0	0
			1730	1103	293	329	5			

- Molecule 6 is a protein called PGT122 Light Chain.

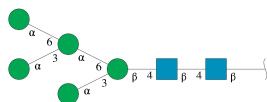
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			

- 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	O	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 9 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
9	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



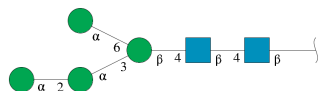
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
10	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

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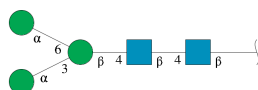
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	T	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



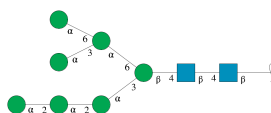
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	J	6	Total	C	N	O	0	0	0
			72	40	2	30			

- 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	P	5	Total	C	N	O	0	0	0
			61	34	2	25			

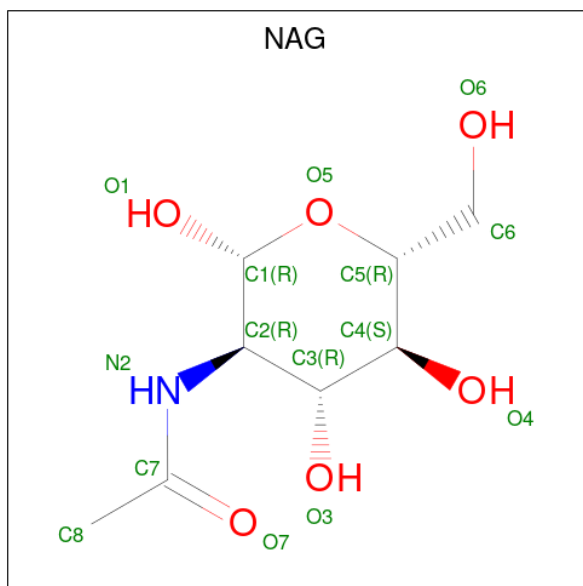
- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	U	9	Total	C	N	O	0	0	0
			105	58	2	45			

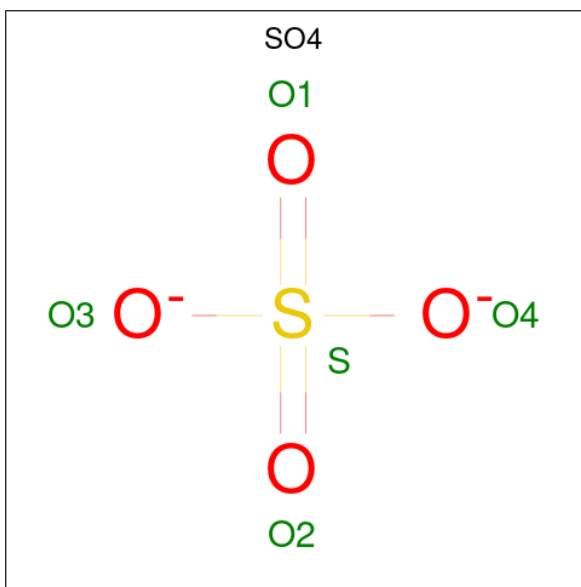
- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



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

- Molecule 15 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

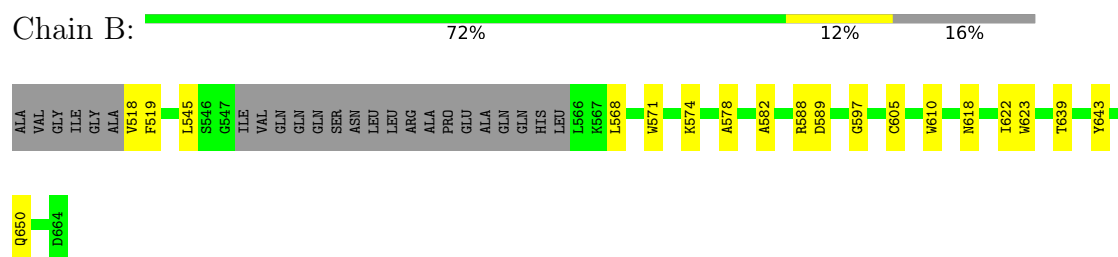


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	G	1	Total	O	S	0	0
			5	4	1		

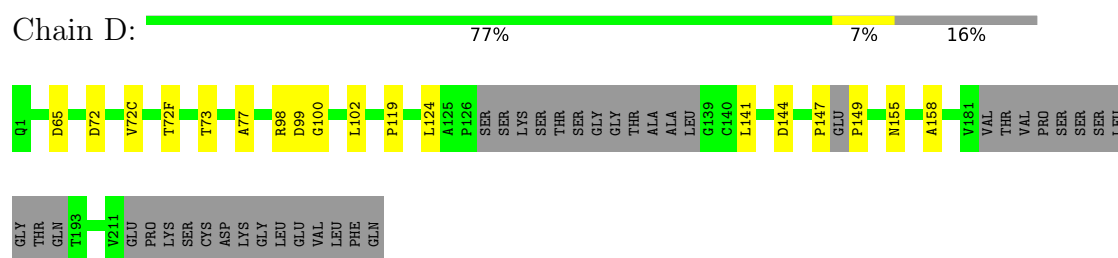
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

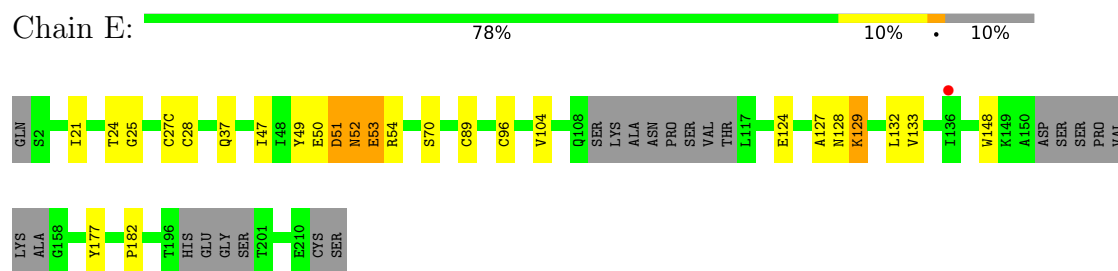
- Molecule 1: Envelope glycoprotein gp160



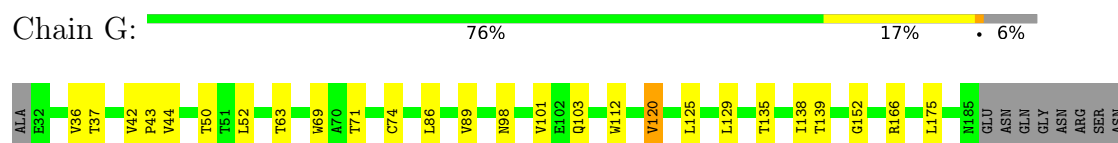
- Molecule 2: 35O22 heavy chain

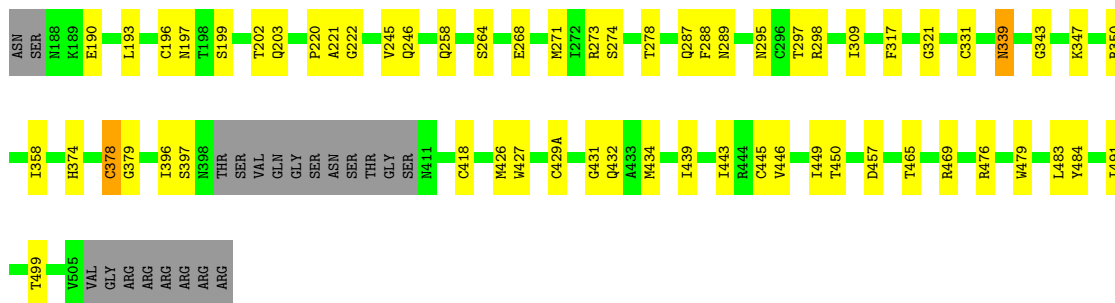


- Molecule 3: 35O22 light chain



- Molecule 4: Envelope glycoprotein gp160





- Molecule 5: PGT122 Heavy chain

Chain H: 86% 10% .



- Molecule 6: PGT122 Light Chain

Chain L: 83% 13% ..



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

Chain A: 100%



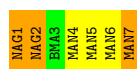
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 33% 67%

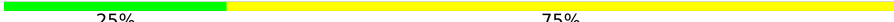


- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 14% 43% 43%



- Molecule 9: 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 F:  25% 75%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  50% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  50% 50%



- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  50% 50%

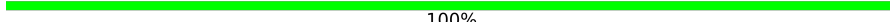


- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  50% 50%

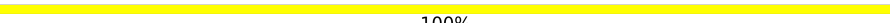
MAG1
MAG2

- Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%

MAG1
MAG2

- Molecule 11: alpha-D-mannopyranose-(1-2)-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 J:  100%

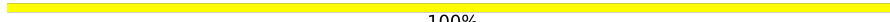
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- 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 P:  20% 80%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain U:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	128.66Å 128.66Å 312.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.11 – 4.12 42.11 – 4.12	Depositor EDS
% Data completeness (in resolution range)	56.6 (42.11-4.12) 62.6 (42.11-4.12)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	351.93 (at 4.13Å)	Xtriage
Refinement program	PHENIX (dev_3126: ???)	Depositor
R, R_{free}	0.248 , 0.258 0.268 , 0.276	Depositor DCC
R_{free} test set	712 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	1.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	-0.04 , 197.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.128 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.160 for h,-h-k,-l	Depositor
Outliers	0 of 14132 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	11704	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, SO4, 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	0.13	0/1044	0.34	0/1415
2	D	0.12	0/1613	0.28	0/2194
3	E	0.12	0/1521	0.33	0/2076
4	G	0.13	0/3629	0.33	0/4927
5	H	0.12	0/1777	0.34	0/2427
6	L	0.12	0/1619	0.31	0/2217
All	All	0.12	0/11203	0.32	0/15256

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1026	0	1010	13	0
2	D	1571	0	1535	11	0
3	E	1483	0	1413	19	0
4	G	3555	0	3482	59	0
5	H	1730	0	1706	18	0
6	L	1577	0	1518	18	0
7	A	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	O	39	0	34	0	0
8	C	83	0	69	6	0
9	F	50	0	43	0	0
10	I	28	0	25	1	0
10	K	28	0	25	0	0
10	M	28	0	25	1	0
10	N	28	0	25	1	0
10	Q	28	0	25	3	0
10	R	28	0	25	1	0
10	S	28	0	25	1	0
10	T	28	0	25	0	0
11	J	72	0	61	3	0
12	P	61	0	52	1	0
13	U	105	0	88	3	0
14	B	28	0	26	1	0
14	G	56	0	52	5	0
15	G	5	0	0	1	0
All	All	11704	0	11323	146	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 6.

All (146) 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:D:98:ARG:NH1	8:C:1:NAG:O6	2.14	0.80
11:J:2:NAG:O7	11:J:2:NAG:O3	1.98	0.79
4:G:378:CYS:SG	4:G:379:GLY:N	2.58	0.76
14:B:702:NAG:O3	3:E:54:ARG:NH2	2.24	0.71
5:H:6:GLU:N	5:H:6:GLU:OE1	2.23	0.71
10:Q:2:NAG:H83	10:Q:2:NAG:H3	1.71	0.71
4:G:264:SER:O	4:G:287:GLN:NE2	2.27	0.67
6:L:109:GLN:NE2	6:L:171:ASN:OD1	2.28	0.67
4:G:166:ARG:NH2	15:G:655:SO4:O2	2.29	0.66
6:L:152:ASP:O	6:L:153:SER:OG	2.07	0.66
4:G:268:GLU:O	4:G:289:ASN:ND2	2.32	0.63
8:C:2:NAG:C1	8:C:2:NAG:H82	2.30	0.62
4:G:347:LYS:HD2	4:G:350:ARG:CZ	2.28	0.61
4:G:339:ASN:OD1	14:G:621:NAG:N2	2.32	0.61
6:L:20:ARG:NH1	6:L:74:THR:OG1	2.33	0.61
3:E:127:ALA:N	3:E:128:ASN:HA	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:37:GLN:HB2	3:E:47:ILE:HD11	1.82	0.60
4:G:37:THR:HG21	4:G:499:THR:CG2	2.32	0.58
4:G:135:THR:OG1	12:P:1:NAG:O7	2.20	0.58
5:H:100(D):VAL:O	5:H:100(D):VAL:HG22	2.04	0.58
4:G:50:THR:O	4:G:103:GLN:NE2	2.33	0.57
5:H:53:ASP:OD1	5:H:54:SER:N	2.37	0.57
1:B:605:CYS:HA	4:G:37:THR:HG22	1.88	0.56
6:L:25:GLU:OE2	6:L:95:ARG:NH2	2.38	0.56
14:G:620:NAG:C1	14:G:620:NAG:H82	2.36	0.55
5:H:136:LEU:HD21	5:H:209:VAL:HG11	1.89	0.55
4:G:278:THR:HG21	14:G:620:NAG:H61	1.89	0.54
2:D:72(C):VAL:HG13	2:D:72(C):VAL:O	2.07	0.54
4:G:298:ARG:NH2	4:G:439:ILE:O	2.41	0.54
4:G:295:ASN:OD1	4:G:446:VAL:HG13	2.07	0.53
6:L:110:PRO:O	6:L:111:LYS:HB3	2.07	0.53
4:G:450:THR:O	4:G:450:THR:HG22	2.09	0.53
14:G:620:NAG:H3	14:G:620:NAG:H83	1.90	0.53
8:C:2:NAG:C1	8:C:2:NAG:C8	2.87	0.53
5:H:66:ARG:NH1	5:H:82(A):THR:O	2.40	0.53
1:B:578:ALA:HB1	4:G:220:PRO:HB3	1.90	0.53
1:B:582:ALA:HB1	4:G:221:ALA:HB3	1.90	0.53
1:B:518:VAL:HG12	1:B:519:PHE:H	1.75	0.52
2:D:98:ARG:O	8:C:2:NAG:H83	2.10	0.52
3:E:52:ASN:O	3:E:53:GLU:HB2	2.08	0.52
11:J:1:NAG:O7	11:J:1:NAG:O3	2.26	0.52
4:G:295:ASN:OD1	4:G:446:VAL:HG22	2.08	0.51
4:G:347:LYS:HD2	4:G:350:ARG:NH2	2.26	0.51
5:H:53:ASP:O	5:H:54:SER:OG	2.21	0.51
4:G:175:LEU:HD12	4:G:321:GLY:O	2.11	0.51
4:G:71:THR:O	4:G:71:THR:HG22	2.11	0.51
4:G:222:GLY:O	4:G:491:ILE:N	2.40	0.51
6:L:12:SER:HB2	6:L:107:LEU:HD11	1.92	0.51
3:E:24:THR:HG22	3:E:25:GLY:H	1.75	0.50
4:G:396:ILE:HG22	4:G:397:SER:N	2.25	0.50
3:E:124:GLU:HG2	3:E:129:LYS:O	2.12	0.50
4:G:358:ILE:O	4:G:465:THR:OG1	2.25	0.50
4:G:457:ASP:OD2	4:G:469:ARG:NH1	2.45	0.49
4:G:86:LEU:HB3	4:G:89:VAL:HG21	1.93	0.49
6:L:51:ASN:OD1	6:L:65:SER:O	2.29	0.49
4:G:199:SER:HB2	4:G:431:GLY:O	2.13	0.49
5:H:100(A):ILE:HG21	5:H:100(E):VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:1:NAG:O7	10:N:1:NAG:O3	2.26	0.49
6:L:196:VAL:O	6:L:196:VAL:HG23	2.13	0.49
2:D:99:ASP:OD1	2:D:100:GLY:N	2.41	0.49
4:G:396:ILE:HG22	4:G:397:SER:H	1.77	0.49
1:B:571:TRP:CZ3	4:G:74:CYS:HB2	2.48	0.49
2:D:100:GLY:C	8:C:7:MAN:O6	2.56	0.49
6:L:51:ASN:O	6:L:52:ASN:CB	2.61	0.49
5:H:148:VAL:HG13	5:H:148:VAL:O	2.13	0.48
4:G:331:CYS:SG	4:G:418:CYS:SG	3.11	0.48
1:B:574:LYS:HE3	4:G:52:LEU:O	2.13	0.48
3:E:52:ASN:O	3:E:53:GLU:CB	2.61	0.48
5:H:100(D):VAL:HA	13:U:2:NAG:H2	1.94	0.48
3:E:49:TYR:OH	3:E:53:GLU:OE1	2.28	0.48
4:G:166:ARG:O	4:G:166:ARG:HG2	2.14	0.48
6:L:188:SER:OG	6:L:189:HIS:N	2.47	0.48
1:B:518:VAL:HG12	1:B:519:PHE:N	2.29	0.48
4:G:297:THR:HG21	13:U:1:NAG:H83	1.95	0.47
4:G:202:THR:O	4:G:434:MET:HA	2.15	0.47
4:G:476:ARG:HA	4:G:479:TRP:CD1	2.49	0.47
6:L:60:ASP:HB2	6:L:61:ARG:HA	1.96	0.47
13:U:2:NAG:H3	13:U:2:NAG:O7	2.14	0.47
4:G:42:VAL:O	4:G:44:VAL:N	2.47	0.47
6:L:110:PRO:O	6:L:111:LYS:HD2	2.15	0.47
3:E:21:ILE:HD11	3:E:104:VAL:HG21	1.97	0.46
6:L:25:GLU:HG2	6:L:26:GLU:N	2.30	0.46
14:G:620:NAG:C1	14:G:620:NAG:C8	2.93	0.46
5:H:100(D):VAL:O	5:H:100(F):ALA:N	2.43	0.46
1:B:545:LEU:C	1:B:545:LEU:HD23	2.41	0.46
4:G:274:SER:O	10:I:1:NAG:H81	2.16	0.46
4:G:120:VAL:HG13	4:G:203:GLN:HB3	1.98	0.46
3:E:129:LYS:HD3	3:E:129:LYS:HA	1.83	0.45
4:G:193:LEU:HB2	4:G:196:CYS:SG	2.55	0.45
4:G:271:MET:HG2	4:G:273:ARG:NH2	2.31	0.45
4:G:309:ILE:HD11	4:G:317:PHE:CB	2.46	0.45
5:H:145:PRO:O	5:H:146:GLU:CB	2.63	0.45
6:L:17:GLN:O	6:L:77:SER:N	2.50	0.45
4:G:112:TRP:CZ3	4:G:429(A):CYS:SG	3.09	0.45
10:Q:2:NAG:H3	10:Q:2:NAG:C8	2.45	0.45
11:J:2:NAG:O7	11:J:2:NAG:C3	2.65	0.45
3:E:132:LEU:HD11	3:E:148:TRP:CZ3	2.53	0.44
4:G:309:ILE:HD11	4:G:317:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:27(C):CYS:HA	3:E:28:CYS:HA	1.81	0.44
1:B:588:ARG:NH2	1:B:589:ASP:OD1	2.47	0.44
4:G:101:VAL:HG22	4:G:483:LEU:HD12	2.00	0.44
4:G:343:GLY:O	4:G:347:LYS:HG2	2.18	0.44
4:G:427:TRP:N	4:G:427:TRP:CD1	2.85	0.43
2:D:119:PRO:HA	2:D:144:ASP:O	2.18	0.43
4:G:69:TRP:CD1	4:G:69:TRP:H	2.35	0.43
1:B:597:GLY:HA2	1:B:650:GLN:CD	2.44	0.43
4:G:288:PHE:HE2	4:G:449:ILE:HG22	1.84	0.43
1:B:622:ILE:HG13	1:B:623:TRP:N	2.32	0.43
1:B:610:TRP:HE3	4:G:36:VAL:HG12	1.84	0.43
4:G:347:LYS:O	4:G:350:ARG:HG2	2.18	0.43
4:G:379:GLY:HA3	4:G:443:ILE:HG21	1.99	0.43
6:L:206:THR:HG22	6:L:207:VAL:N	2.34	0.43
4:G:295:ASN:ND2	10:S:1:NAG:O7	2.48	0.42
4:G:258:GLN:OE1	4:G:374:HIS:N	2.52	0.42
5:H:188:GLY:HA3	5:H:190:GLN:N	2.33	0.42
4:G:197:ASN:HD22	10:R:1:NAG:H83	1.84	0.42
3:E:50:GLU:O	3:E:51:ASP:C	2.63	0.42
3:E:24:THR:HG22	3:E:25:GLY:N	2.35	0.42
4:G:273:ARG:NH2	4:G:484:TYR:CE2	2.87	0.42
5:H:50:TYR:CZ	5:H:58:ASN:HB3	2.55	0.42
5:H:27:THR:HG22	5:H:28:LEU:N	2.35	0.42
2:D:155:ASN:HB2	2:D:158:ALA:HB3	2.01	0.41
3:E:127:ALA:HB3	3:E:128:ASN:HA	2.02	0.41
3:E:128:ASN:ND2	3:E:182:PRO:HG2	2.35	0.41
1:B:639:THR:HG22	1:B:643:TYR:CZ	2.55	0.41
2:D:147:PRO:HG2	2:D:149:PRO:HG2	2.02	0.41
10:M:1:NAG:O7	10:M:1:NAG:H3	2.20	0.41
3:E:133:VAL:HG13	3:E:177:TYR:CE1	2.55	0.41
5:H:58:ASN:OD1	5:H:59:TYR:N	2.53	0.41
5:H:164:PHE:HB3	6:L:176:SER:OG	2.20	0.41
3:E:127:ALA:H	3:E:128:ASN:HA	1.84	0.41
4:G:129:LEU:HD11	4:G:193:LEU:CD1	2.51	0.41
2:D:72(F):THR:HG22	2:D:73:THR:OG1	2.21	0.41
5:H:145:PRO:O	5:H:146:GLU:CG	2.69	0.41
10:Q:2:NAG:C1	10:Q:2:NAG:H82	2.51	0.41
4:G:98:ASN:OD1	4:G:98:ASN:C	2.63	0.40
4:G:138:ILE:HG13	4:G:139:THR:H	1.87	0.40
5:H:181:THR:HG23	5:H:181:THR:O	2.21	0.40
6:L:62:PHE:CZ	6:L:75:ILE:HG23	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:72:ASP:OD2	2:D:77:ALA:HB3	2.21	0.40
4:G:63:THR:HG23	4:G:63:THR:O	2.21	0.40
6:L:48:ILE:CG2	6:L:52:ASN:H	2.33	0.40
2:D:124:LEU:HD21	2:D:141:LEU:HB2	2.04	0.40
3:E:24:THR:HG23	3:E:70:SER:HB2	2.04	0.40
4:G:245:VAL:HG22	4:G:246:GLN:N	2.37	0.40
8:C:2:NAG:H83	8:C:2:NAG:H3	2.03	0.40

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	125/153 (82%)	116 (93%)	9 (7%)	0	100	100
2	D	197/243 (81%)	175 (89%)	22 (11%)	0	100	100
3	E	186/216 (86%)	175 (94%)	8 (4%)	3 (2%)	7	37
4	G	447/483 (92%)	403 (90%)	42 (9%)	2 (0%)	30	65
5	H	222/235 (94%)	208 (94%)	13 (6%)	1 (0%)	24	61
6	L	206/213 (97%)	188 (91%)	14 (7%)	4 (2%)	6	34
All	All	1383/1543 (90%)	1265 (92%)	108 (8%)	10 (1%)	18	55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	52	ASN
3	E	53	GLU
5	H	146	GLU
6	L	52	ASN
3	E	51	ASP

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Mol	Chain	Res	Type
4	G	152	GLY
6	L	111	LYS
6	L	188	SER
4	G	43	PRO
6	L	95(A)	PRO

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	B	111/129 (86%)	109 (98%)	2 (2%)	51	67
2	D	173/206 (84%)	171 (99%)	2 (1%)	63	73
3	E	170/189 (90%)	167 (98%)	3 (2%)	51	67
4	G	403/428 (94%)	395 (98%)	8 (2%)	48	66
5	H	196/205 (96%)	195 (100%)	1 (0%)	81	82
6	L	177/181 (98%)	175 (99%)	2 (1%)	65	74
All	All	1230/1338 (92%)	1212 (98%)	18 (2%)	57	70

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	568	LEU
1	B	618	ASN
2	D	65	ASP
2	D	102	LEU
3	E	89	CYS
3	E	96	CYS
3	E	129	LYS
4	G	120	VAL
4	G	125	LEU
4	G	190	GLU
4	G	339	ASN
4	G	378	CYS
4	G	426	MET

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Mol	Chain	Res	Type
4	G	432	GLN
4	G	445	CYS
5	H	95	THR
6	L	111	LYS
6	L	124	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	575	GLN
1	B	656	ASN
2	D	6	GLN
2	D	164	HIS
3	E	167	GLN
3	E	188	HIS
4	G	85	HIS
4	G	246	GLN
4	G	348	GLN
4	G	432	GLN
5	H	3	HIS
6	L	17	GLN
6	L	37	GLN
6	L	52	ASN
6	L	129	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 ⓘ

53 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	7,1	14,14,15	0.29	0	17,19,21	0.54	0
7	NAG	A	2	7	14,14,15	0.37	0	17,19,21	0.65	0
7	BMA	A	3	7	11,11,12	0.69	0	15,15,17	0.67	0
8	NAG	C	1	8,4	14,14,15	0.60	0	17,19,21	1.86	4 (23%)
8	NAG	C	2	8	14,14,15	0.79	1 (7%)	17,19,21	1.32	3 (17%)
8	BMA	C	3	8	11,11,12	0.71	0	15,15,17	1.07	0
8	MAN	C	4	8	11,11,12	0.73	0	15,15,17	1.14	1 (6%)
8	MAN	C	5	8	11,11,12	0.56	0	15,15,17	0.87	1 (6%)
8	MAN	C	6	8	11,11,12	0.98	1 (9%)	15,15,17	0.95	1 (6%)
8	MAN	C	7	8	11,11,12	1.42	1 (9%)	15,15,17	1.70	3 (20%)
9	NAG	F	1	9,4	14,14,15	0.61	1 (7%)	17,19,21	0.48	0
9	NAG	F	2	9	14,14,15	0.24	0	17,19,21	0.60	0
9	BMA	F	3	9	11,11,12	0.82	0	15,15,17	1.11	1 (6%)
9	MAN	F	4	9	11,11,12	0.70	0	15,15,17	1.07	2 (13%)
10	NAG	I	1	10,4	14,14,15	0.17	0	17,19,21	0.56	0
10	NAG	I	2	10	14,14,15	0.29	0	17,19,21	0.51	0
11	NAG	J	1	4,11	14,14,15	0.35	0	17,19,21	0.55	0
11	NAG	J	2	11	14,14,15	0.61	0	17,19,21	0.63	0
11	BMA	J	3	11	11,11,12	0.76	0	15,15,17	1.10	1 (6%)
11	MAN	J	4	11	11,11,12	0.79	1 (9%)	15,15,17	0.92	1 (6%)
11	MAN	J	5	11	11,11,12	0.77	1 (9%)	15,15,17	2.13	4 (26%)
11	MAN	J	6	11	11,11,12	1.15	2 (18%)	15,15,17	1.45	2 (13%)
10	NAG	K	1	10,4	14,14,15	0.43	0	17,19,21	0.40	0
10	NAG	K	2	10	14,14,15	0.15	0	17,19,21	0.56	0
10	NAG	M	1	10,4	14,14,15	0.41	0	17,19,21	0.88	1 (5%)
10	NAG	M	2	10	14,14,15	0.40	0	17,19,21	0.43	0
10	NAG	N	1	10,4	14,14,15	0.55	0	17,19,21	0.50	0
10	NAG	N	2	10	14,14,15	0.31	0	17,19,21	0.45	0
7	NAG	O	1	7,4	14,14,15	0.17	0	17,19,21	0.85	1 (5%)
7	NAG	O	2	7	14,14,15	0.29	0	17,19,21	0.46	0
7	BMA	O	3	7	11,11,12	0.73	0	15,15,17	1.11	1 (6%)
12	NAG	P	1	12,4	14,14,15	0.19	0	17,19,21	0.50	0
12	NAG	P	2	12	14,14,15	0.23	0	17,19,21	0.47	0
12	BMA	P	3	12	11,11,12	0.67	0	15,15,17	0.86	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	P	4	12	11,11,12	0.70	0	15,15,17	0.94	2 (13%)
12	MAN	P	5	12	11,11,12	1.14	1 (9%)	15,15,17	1.61	3 (20%)
10	NAG	Q	1	10,4	14,14,15	0.68	1 (7%)	17,19,21	0.79	0
10	NAG	Q	2	10	14,14,15	0.31	0	17,19,21	0.95	1 (5%)
10	NAG	R	1	10,4	14,14,15	0.15	0	17,19,21	0.62	0
10	NAG	R	2	10	14,14,15	0.28	0	17,19,21	0.38	0
10	NAG	S	1	10,4	14,14,15	0.30	0	17,19,21	0.71	1 (5%)
10	NAG	S	2	10	14,14,15	0.26	0	17,19,21	0.53	0
10	NAG	T	1	10,4	14,14,15	0.25	0	17,19,21	0.33	0
10	NAG	T	2	10	14,14,15	0.28	0	17,19,21	0.40	0
13	NAG	U	1	13,4	14,14,15	0.54	0	17,19,21	0.49	0
13	NAG	U	2	13	14,14,15	0.17	0	17,19,21	0.82	0
13	BMA	U	3	13	11,11,12	0.79	0	15,15,17	1.20	1 (6%)
13	MAN	U	4	13	11,11,12	0.94	1 (9%)	15,15,17	0.85	0
13	MAN	U	5	13	11,11,12	0.78	0	15,15,17	1.21	2 (13%)
13	MAN	U	6	13	11,11,12	1.15	1 (9%)	15,15,17	0.80	0
13	MAN	U	7	13	11,11,12	0.71	0	15,15,17	0.95	2 (13%)
13	MAN	U	8	13	11,11,12	0.75	0	15,15,17	0.82	1 (6%)
13	MAN	U	9	13	11,11,12	0.68	0	15,15,17	0.92	2 (13%)

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	7,1	-	0/6/23/26	0/1/1/1
7	NAG	A	2	7	-	0/6/23/26	0/1/1/1
7	BMA	A	3	7	-	2/2/19/22	0/1/1/1
8	NAG	C	1	8,4	-	0/6/23/26	0/1/1/1
8	NAG	C	2	8	-	3/6/23/26	0/1/1/1
8	BMA	C	3	8	-	2/2/19/22	0/1/1/1
8	MAN	C	4	8	-	2/2/19/22	0/1/1/1
8	MAN	C	5	8	-	2/2/19/22	0/1/1/1
8	MAN	C	6	8	-	1/2/19/22	0/1/1/1
8	MAN	C	7	8	-	0/2/19/22	0/1/1/1
9	NAG	F	1	9,4	-	0/6/23/26	0/1/1/1
9	NAG	F	2	9	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	F	3	9	-	0/2/19/22	0/1/1/1
9	MAN	F	4	9	-	2/2/19/22	0/1/1/1
10	NAG	I	1	10,4	-	0/6/23/26	0/1/1/1
10	NAG	I	2	10	-	2/6/23/26	0/1/1/1
11	NAG	J	1	4,11	-	1/6/23/26	0/1/1/1
11	NAG	J	2	11	-	1/6/23/26	0/1/1/1
11	BMA	J	3	11	-	2/2/19/22	0/1/1/1
11	MAN	J	4	11	-	2/2/19/22	0/1/1/1
11	MAN	J	5	11	-	0/2/19/22	0/1/1/1
11	MAN	J	6	11	-	2/2/19/22	1/1/1/1
10	NAG	K	1	10,4	-	0/6/23/26	0/1/1/1
10	NAG	K	2	10	-	0/6/23/26	0/1/1/1
10	NAG	M	1	10,4	-	1/6/23/26	0/1/1/1
10	NAG	M	2	10	-	2/6/23/26	0/1/1/1
10	NAG	N	1	10,4	-	3/6/23/26	0/1/1/1
10	NAG	N	2	10	-	2/6/23/26	0/1/1/1
7	NAG	O	1	7,4	-	4/6/23/26	0/1/1/1
7	NAG	O	2	7	-	0/6/23/26	0/1/1/1
7	BMA	O	3	7	-	1/2/19/22	0/1/1/1
12	NAG	P	1	12,4	-	1/6/23/26	0/1/1/1
12	NAG	P	2	12	-	2/6/23/26	0/1/1/1
12	BMA	P	3	12	-	2/2/19/22	0/1/1/1
12	MAN	P	4	12	-	1/2/19/22	0/1/1/1
12	MAN	P	5	12	-	0/2/19/22	0/1/1/1
10	NAG	Q	1	10,4	-	3/6/23/26	0/1/1/1
10	NAG	Q	2	10	-	5/6/23/26	0/1/1/1
10	NAG	R	1	10,4	-	4/6/23/26	0/1/1/1
10	NAG	R	2	10	-	2/6/23/26	0/1/1/1
10	NAG	S	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	S	2	10	-	2/6/23/26	0/1/1/1
10	NAG	T	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	T	2	10	-	2/6/23/26	0/1/1/1
13	NAG	U	1	13,4	-	1/6/23/26	0/1/1/1
13	NAG	U	2	13	-	2/6/23/26	0/1/1/1
13	BMA	U	3	13	-	0/2/19/22	0/1/1/1
13	MAN	U	4	13	-	0/2/19/22	0/1/1/1
13	MAN	U	5	13	-	0/2/19/22	0/1/1/1
13	MAN	U	6	13	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MAN	U	7	13	-	2/2/19/22	0/1/1/1
13	MAN	U	8	13	-	2/2/19/22	0/1/1/1
13	MAN	U	9	13	-	0/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	7	MAN	C1-C2	3.50	1.60	1.52
12	P	5	MAN	C1-C2	3.24	1.59	1.52
13	U	6	MAN	O5-C1	-3.20	1.38	1.43
11	J	6	MAN	O5-C5	2.64	1.48	1.43
11	J	6	MAN	C1-C2	2.29	1.57	1.52
8	C	2	NAG	O5-C1	2.18	1.47	1.43
10	Q	1	NAG	O5-C1	-2.17	1.40	1.43
11	J	5	MAN	C1-C2	2.14	1.57	1.52
9	F	1	NAG	O5-C1	-2.11	1.40	1.43
11	J	4	MAN	O5-C1	-2.07	1.40	1.43
13	U	4	MAN	O5-C1	-2.07	1.40	1.43
8	C	6	MAN	O5-C1	-2.07	1.40	1.43

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	J	5	MAN	C1-O5-C5	6.67	121.13	112.19
8	C	1	NAG	C1-O5-C5	5.58	119.67	112.19
11	J	6	MAN	C1-O5-C5	4.49	118.20	112.19
12	P	5	MAN	C1-O5-C5	4.47	118.18	112.19
8	C	7	MAN	O2-C2-C3	-4.05	101.76	110.15
8	C	7	MAN	C1-C2-C3	3.78	115.14	109.64
13	U	5	MAN	O2-C2-C3	-3.08	103.77	110.15
8	C	6	MAN	O2-C2-C3	-2.96	104.03	110.15
8	C	1	NAG	O5-C5-C6	-2.87	102.07	107.66
11	J	5	MAN	O5-C1-C2	2.85	117.58	110.79
13	U	5	MAN	C1-O5-C5	2.84	115.99	112.19
10	Q	2	NAG	C2-N2-C7	2.77	126.61	122.90
8	C	5	MAN	O2-C2-C3	-2.75	104.47	110.15
8	C	2	NAG	O3-C3-C2	2.70	115.01	109.40
10	M	1	NAG	C1-O5-C5	2.70	115.80	112.19
9	F	4	MAN	C1-O5-C5	2.69	115.79	112.19
8	C	1	NAG	O4-C4-C5	-2.68	102.72	109.32
8	C	2	NAG	C2-N2-C7	2.64	126.44	122.90
13	U	3	BMA	C1-C2-C3	2.63	113.47	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	5	MAN	C1-C2-C3	2.62	113.47	109.64
7	O	1	NAG	C1-O5-C5	2.61	115.68	112.19
11	J	5	MAN	O2-C2-C3	-2.51	104.96	110.15
8	C	4	MAN	O2-C2-C3	-2.47	105.04	110.15
11	J	4	MAN	O2-C2-C3	-2.45	105.08	110.15
11	J	5	MAN	C1-C2-C3	2.41	113.15	109.64
12	P	5	MAN	O2-C2-C3	-2.38	105.22	110.15
9	F	4	MAN	O2-C2-C3	-2.37	105.24	110.15
8	C	7	MAN	C1-O5-C5	2.34	115.33	112.19
9	F	3	BMA	C1-O5-C5	2.34	115.32	112.19
11	J	6	MAN	O2-C2-C3	-2.33	105.33	110.15
11	J	3	BMA	C3-C4-C5	2.32	114.43	110.23
7	O	3	BMA	C1-O5-C5	2.32	115.29	112.19
8	C	2	NAG	C4-C3-C2	-2.27	107.69	111.02
10	S	1	NAG	C1-O5-C5	2.22	115.16	112.19
12	P	4	MAN	O2-C2-C3	-2.19	105.61	110.15
12	P	4	MAN	C1-O5-C5	2.16	115.08	112.19
13	U	7	MAN	O2-C2-C3	-2.15	105.70	110.15
13	U	8	MAN	O2-C2-C3	-2.14	105.71	110.15
12	P	3	BMA	C1-O5-C5	2.14	115.05	112.19
8	C	1	NAG	O4-C4-C3	-2.05	105.55	110.38
13	U	9	MAN	C1-O5-C5	2.04	114.92	112.19
13	U	7	MAN	C1-O5-C5	2.02	114.89	112.19
13	U	9	MAN	O2-C2-C3	-2.01	105.98	110.15

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	2	NAG	C1-C2-N2-C7
11	J	2	NAG	C3-C2-N2-C7
13	U	2	NAG	C3-C2-N2-C7
7	A	3	BMA	C4-C5-C6-O6
9	F	4	MAN	O5-C5-C6-O6
11	J	3	BMA	O5-C5-C6-O6
8	C	3	BMA	O5-C5-C6-O6
7	A	3	BMA	O5-C5-C6-O6
9	F	2	NAG	O5-C5-C6-O6
7	O	1	NAG	O5-C5-C6-O6
10	T	2	NAG	O5-C5-C6-O6
10	I	2	NAG	O5-C5-C6-O6
8	C	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	S	1	NAG	O5-C5-C6-O6
11	J	4	MAN	O5-C5-C6-O6
9	F	2	NAG	C4-C5-C6-O6
9	F	4	MAN	C4-C5-C6-O6
11	J	3	BMA	C4-C5-C6-O6
8	C	4	MAN	O5-C5-C6-O6
10	R	2	NAG	O5-C5-C6-O6
10	N	2	NAG	O5-C5-C6-O6
8	C	4	MAN	C4-C5-C6-O6
10	I	2	NAG	C4-C5-C6-O6
10	R	2	NAG	C4-C5-C6-O6
10	S	1	NAG	C4-C5-C6-O6
10	T	2	NAG	C4-C5-C6-O6
11	J	4	MAN	C4-C5-C6-O6
10	N	2	NAG	C4-C5-C6-O6
7	O	1	NAG	C8-C7-N2-C2
7	O	1	NAG	O7-C7-N2-C2
8	C	2	NAG	C8-C7-N2-C2
8	C	2	NAG	O7-C7-N2-C2
10	Q	1	NAG	C8-C7-N2-C2
10	Q	1	NAG	O7-C7-N2-C2
10	Q	2	NAG	C8-C7-N2-C2
10	Q	2	NAG	O7-C7-N2-C2
10	R	1	NAG	C8-C7-N2-C2
10	R	1	NAG	O7-C7-N2-C2
10	S	2	NAG	O5-C5-C6-O6
11	J	6	MAN	O5-C5-C6-O6
12	P	2	NAG	O5-C5-C6-O6
13	U	8	MAN	O5-C5-C6-O6
12	P	3	BMA	C4-C5-C6-O6
10	R	1	NAG	O5-C5-C6-O6
13	U	6	MAN	O5-C5-C6-O6
10	M	2	NAG	C4-C5-C6-O6
7	O	1	NAG	C4-C5-C6-O6
10	N	1	NAG	C4-C5-C6-O6
10	S	2	NAG	C4-C5-C6-O6
10	R	1	NAG	C4-C5-C6-O6
8	C	5	MAN	O5-C5-C6-O6
10	M	2	NAG	O5-C5-C6-O6
13	U	1	NAG	O5-C5-C6-O6
12	P	3	BMA	O5-C5-C6-O6
8	C	6	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	N	1	NAG	O5-C5-C6-O6
10	Q	2	NAG	O5-C5-C6-O6
12	P	4	MAN	O5-C5-C6-O6
7	O	3	BMA	O5-C5-C6-O6
10	M	1	NAG	C3-C2-N2-C7
10	Q	1	NAG	O5-C5-C6-O6
10	T	1	NAG	O5-C5-C6-O6
12	P	1	NAG	O5-C5-C6-O6
12	P	2	NAG	C4-C5-C6-O6
13	U	8	MAN	C4-C5-C6-O6
10	Q	2	NAG	C1-C2-N2-C7
11	J	6	MAN	C4-C5-C6-O6
13	U	7	MAN	C4-C5-C6-O6
13	U	7	MAN	O5-C5-C6-O6
8	C	5	MAN	C4-C5-C6-O6
10	N	1	NAG	C3-C2-N2-C7
10	Q	2	NAG	C3-C2-N2-C7
10	T	1	NAG	C3-C2-N2-C7
11	J	1	NAG	C3-C2-N2-C7
13	U	2	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	J	6	MAN	C1-C2-C3-C4-C5-O5

14 monomers are involved in 21 short contacts:

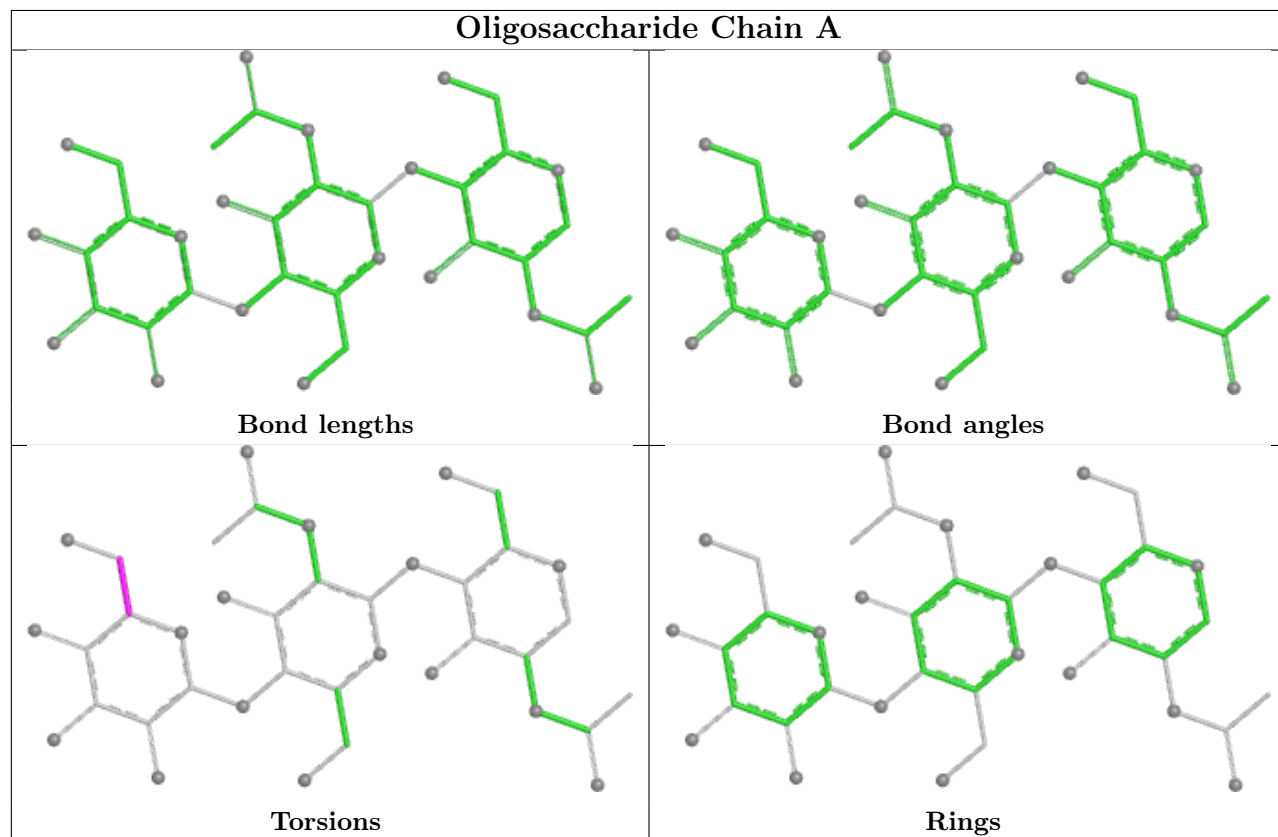
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	J	2	NAG	2	0
8	C	1	NAG	1	0
10	Q	2	NAG	3	0
8	C	2	NAG	4	0
10	I	1	NAG	1	0
13	U	2	NAG	2	0
12	P	1	NAG	1	0
8	C	7	MAN	1	0
10	M	1	NAG	1	0
10	N	1	NAG	1	0
10	R	1	NAG	1	0
11	J	1	NAG	1	0
10	S	1	NAG	1	0

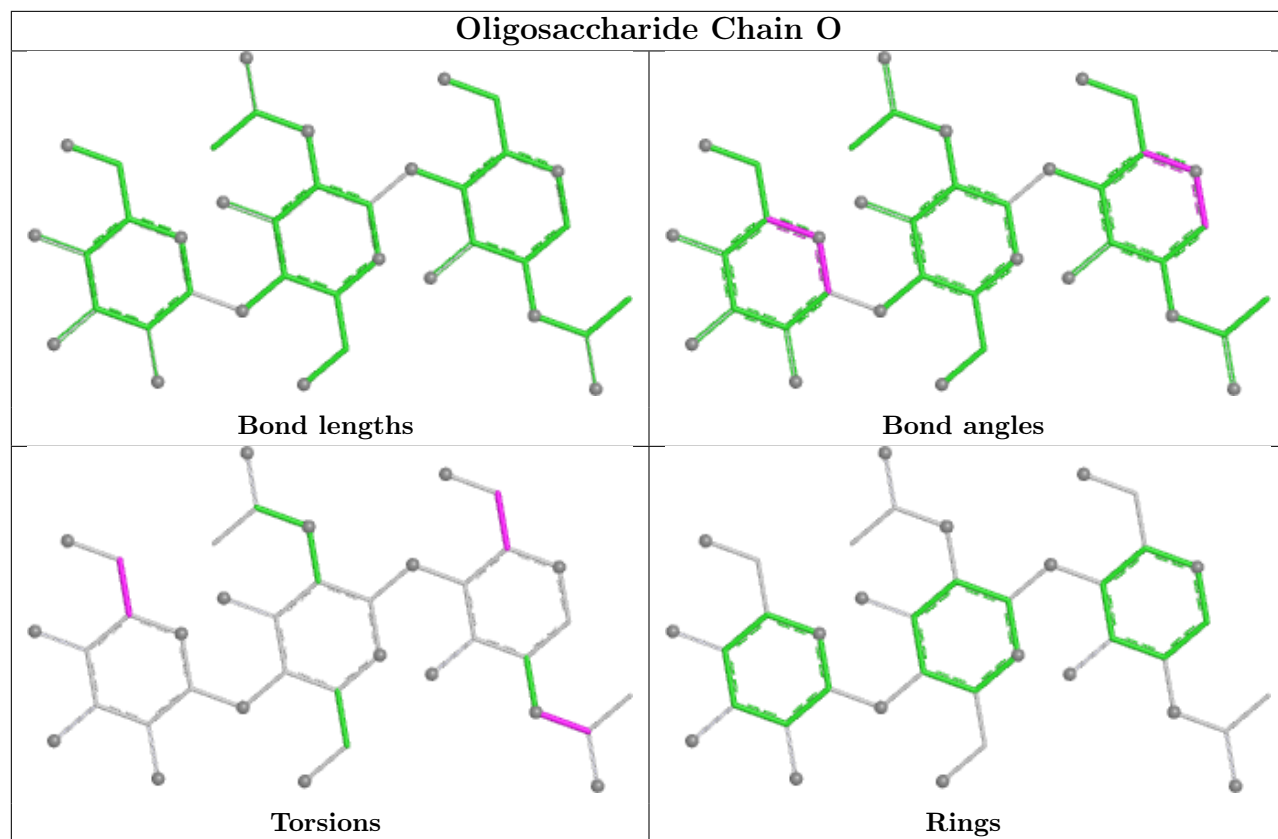
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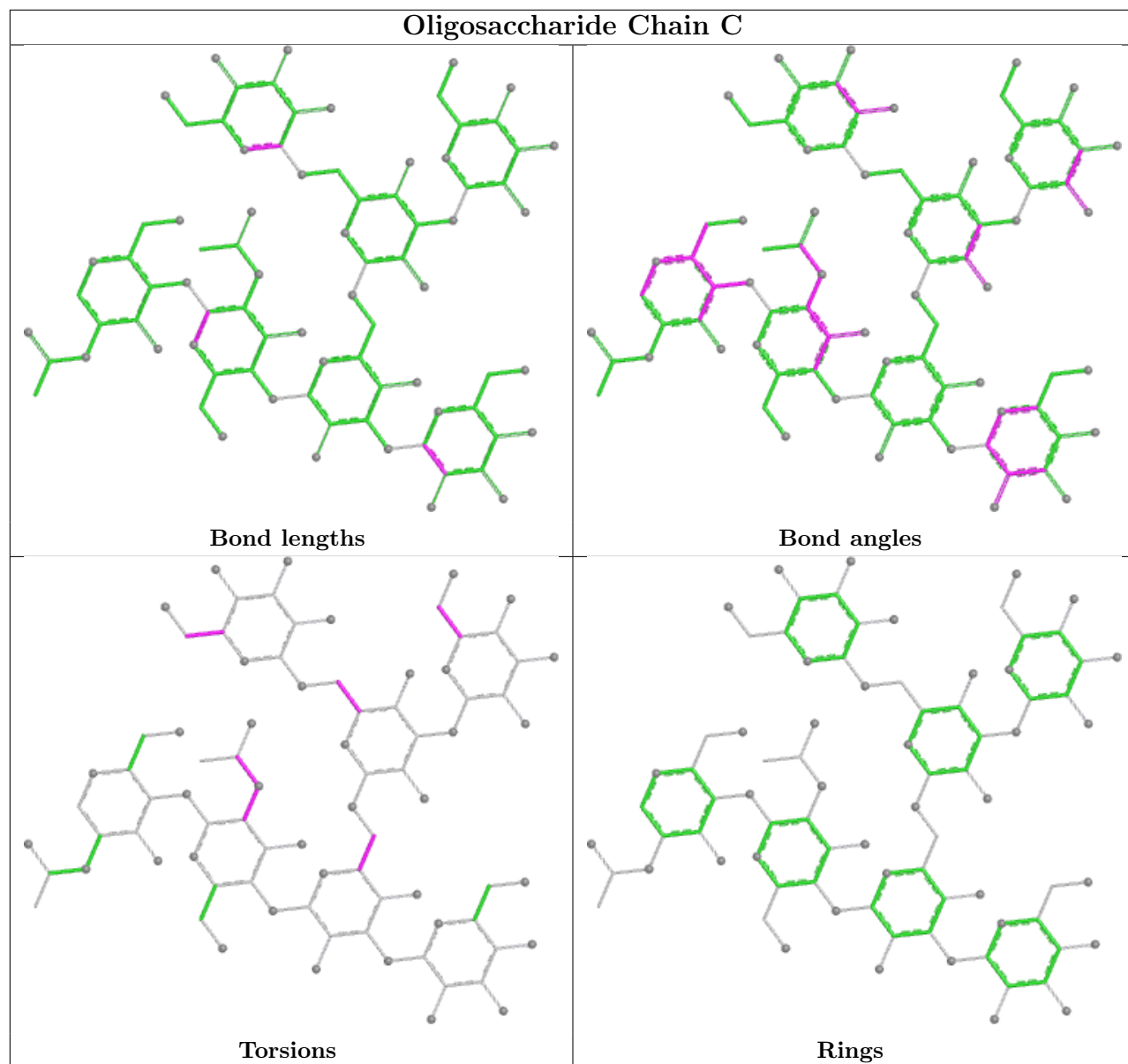
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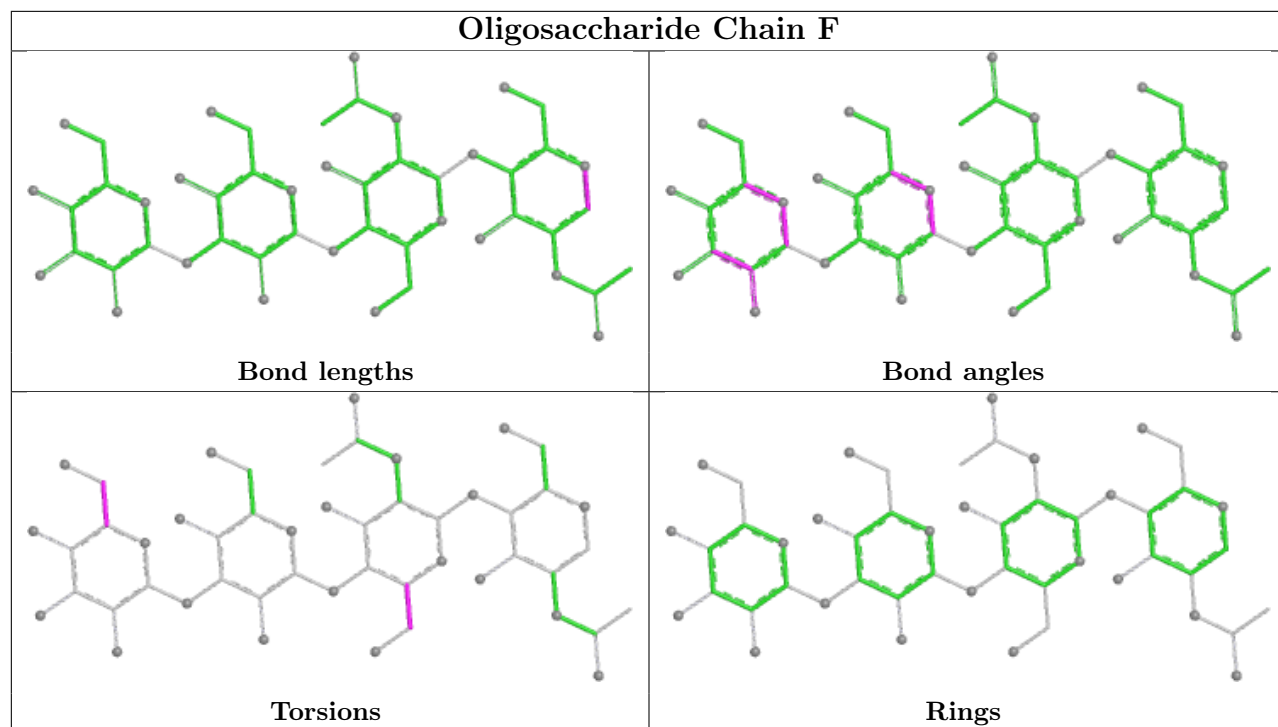
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	U	1	NAG	1	0

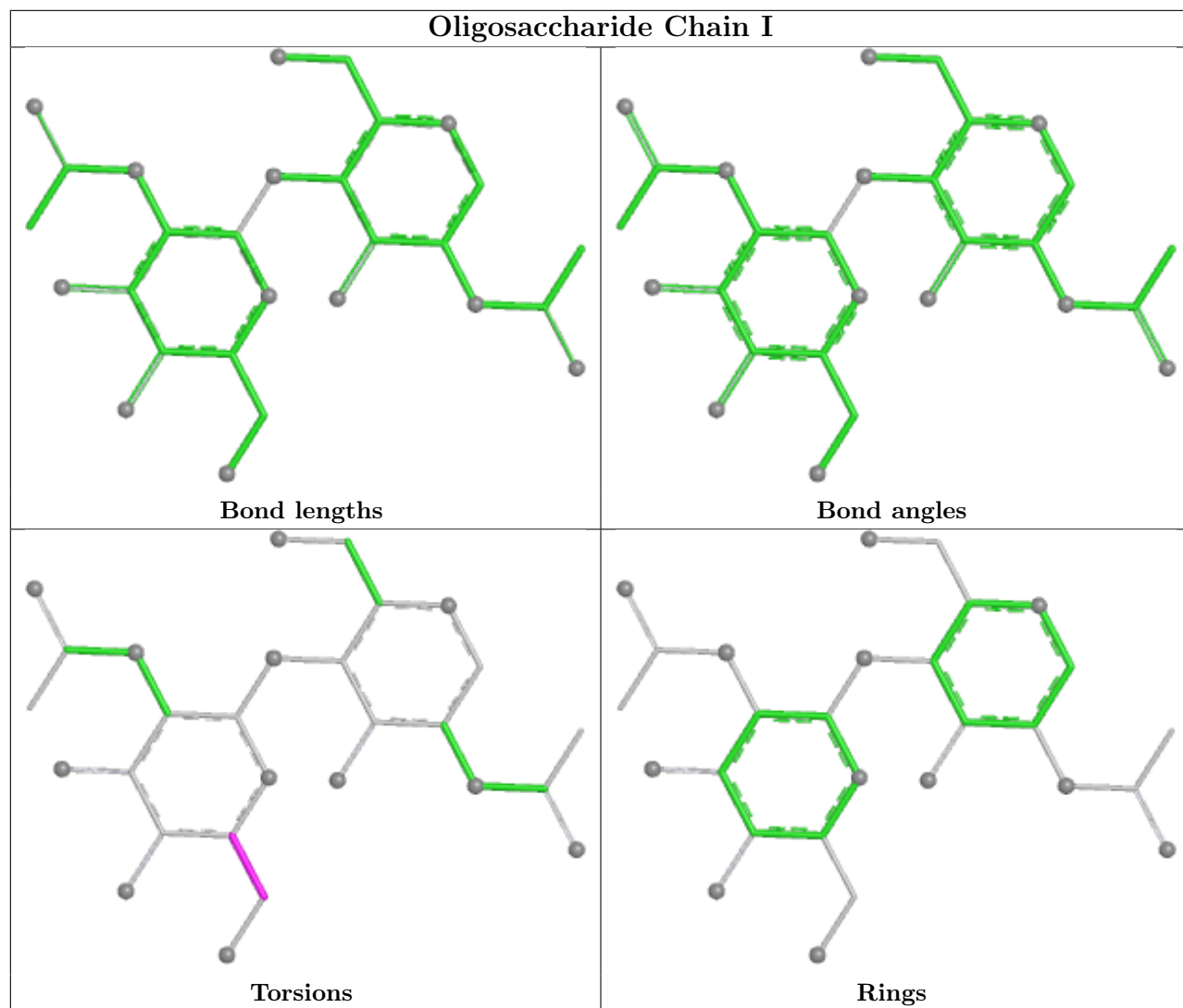
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

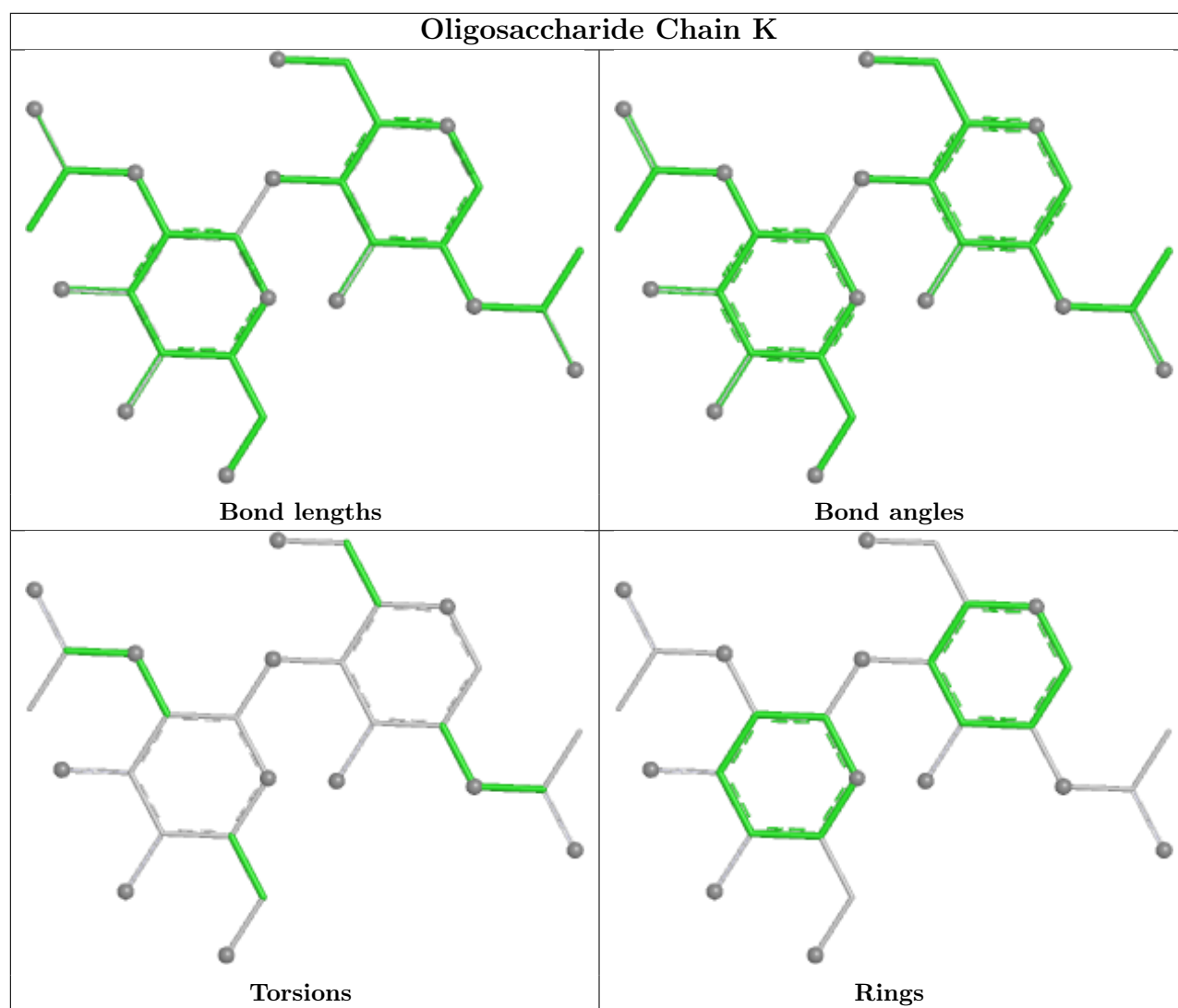


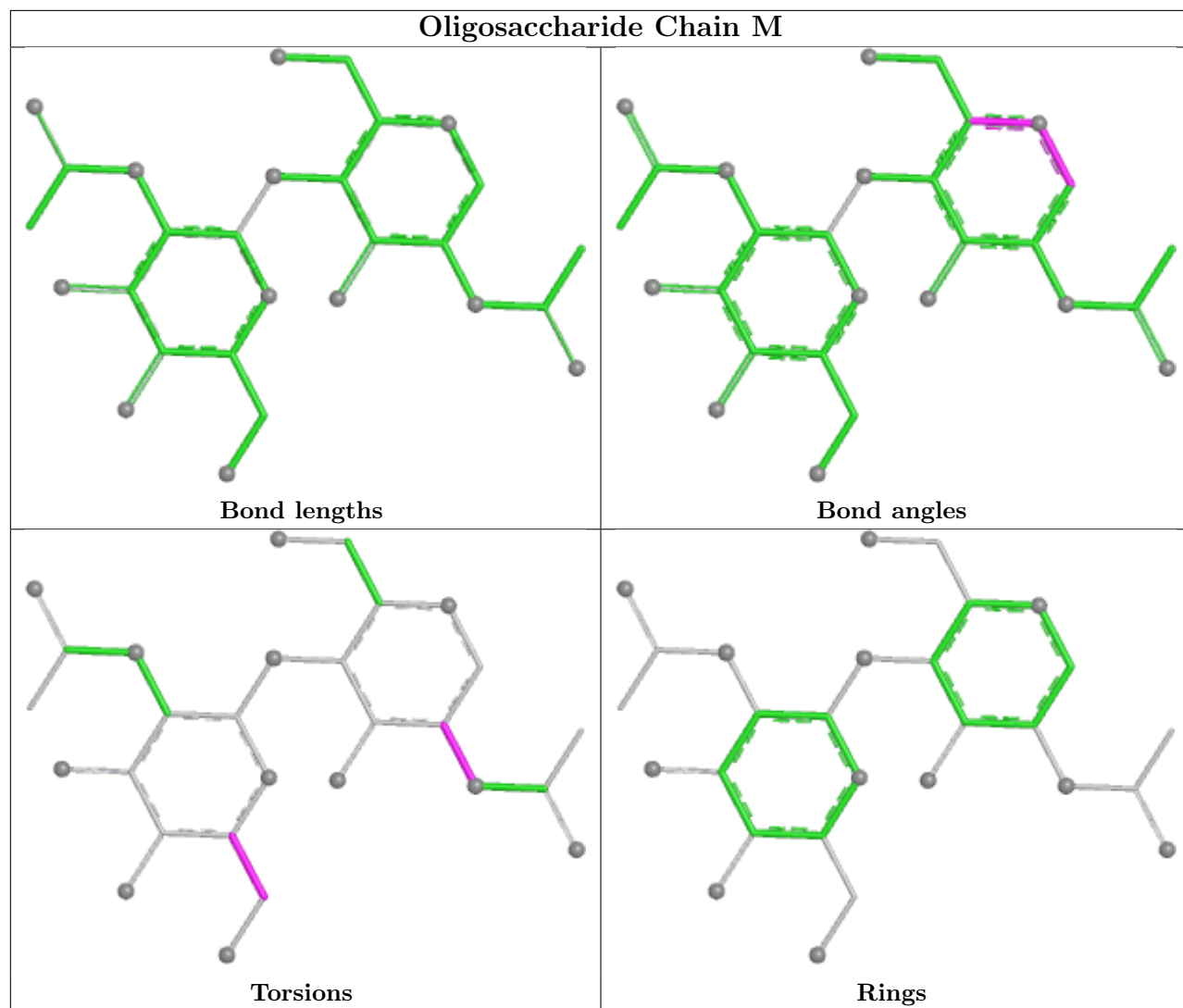


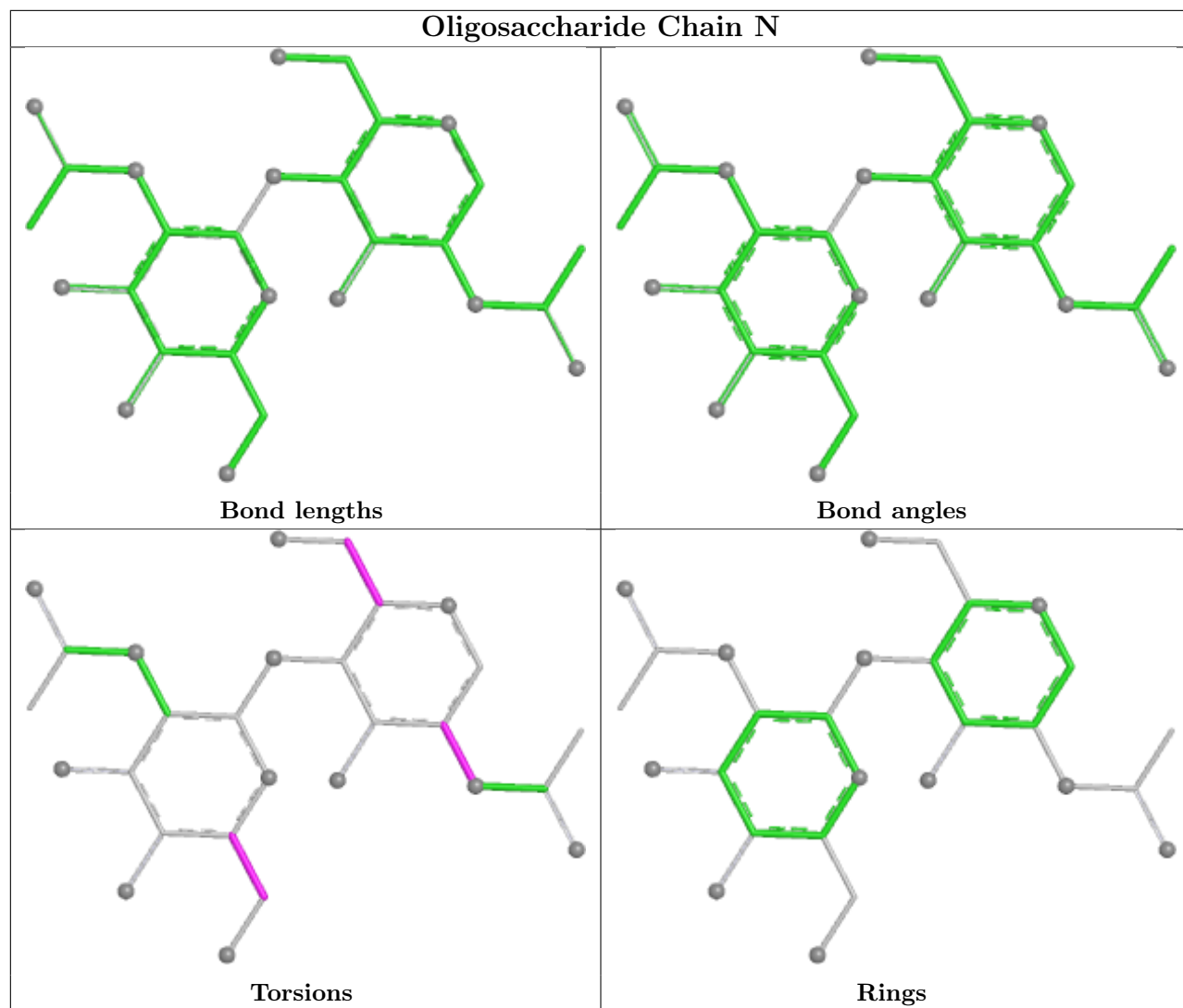


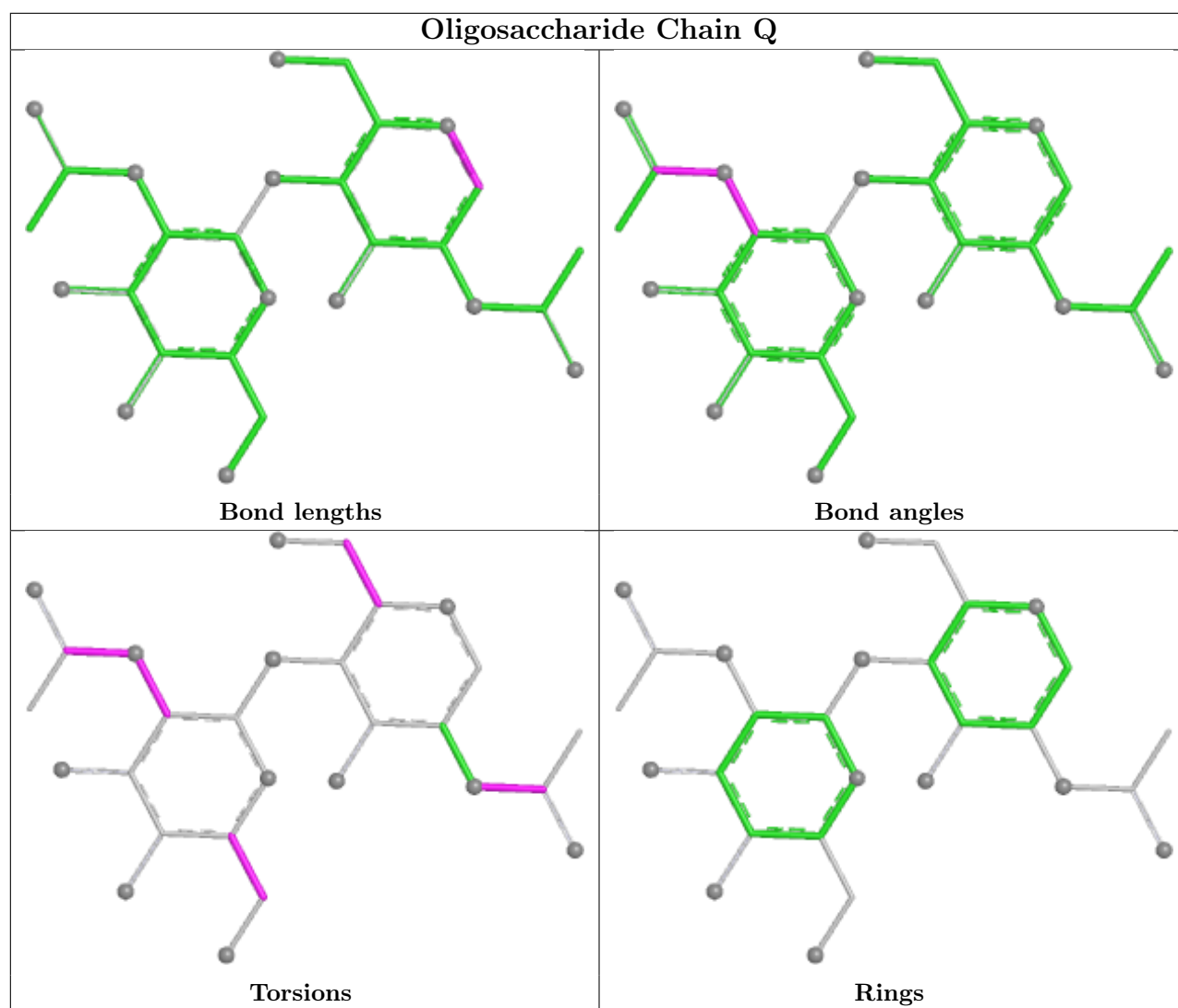


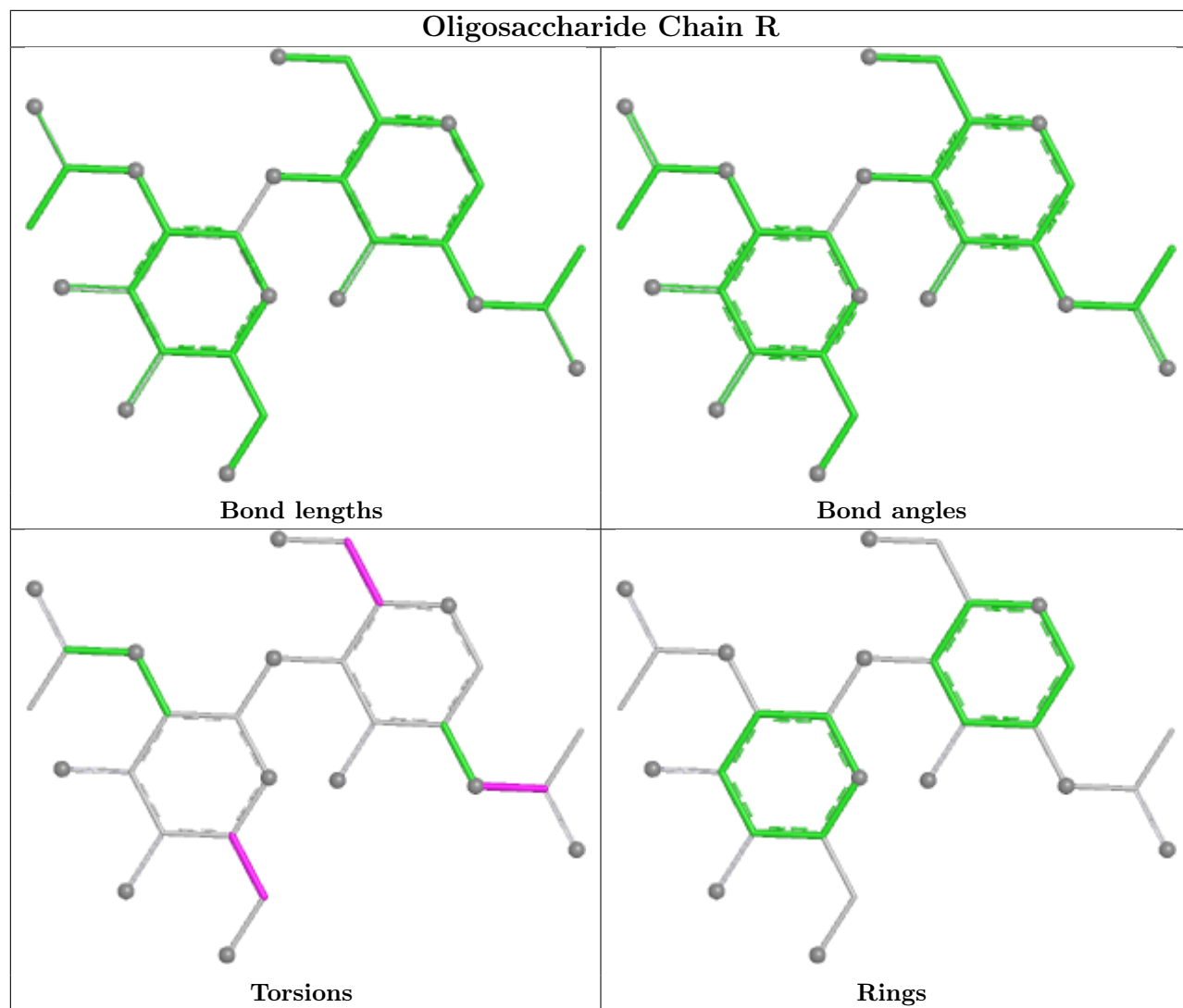


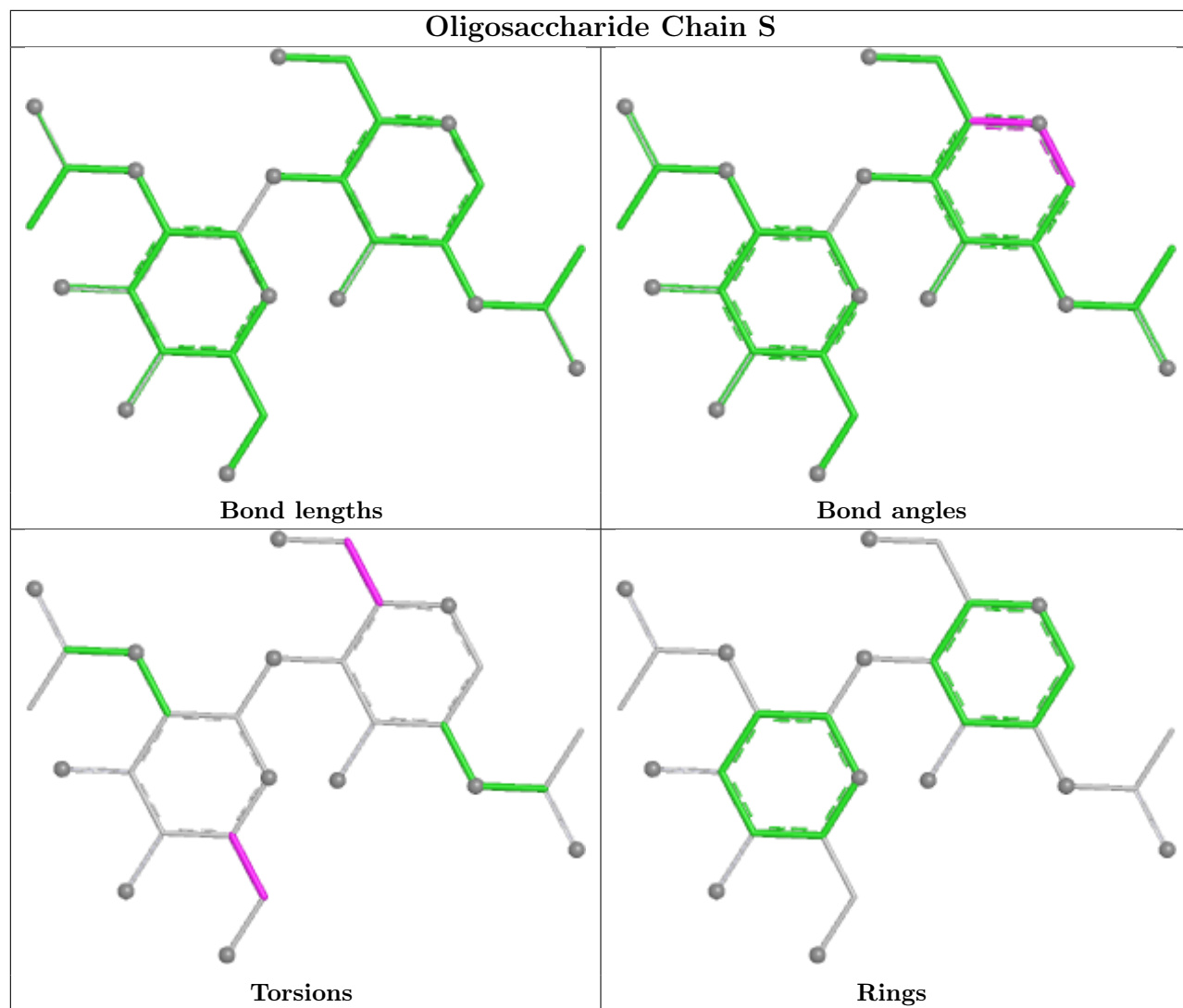


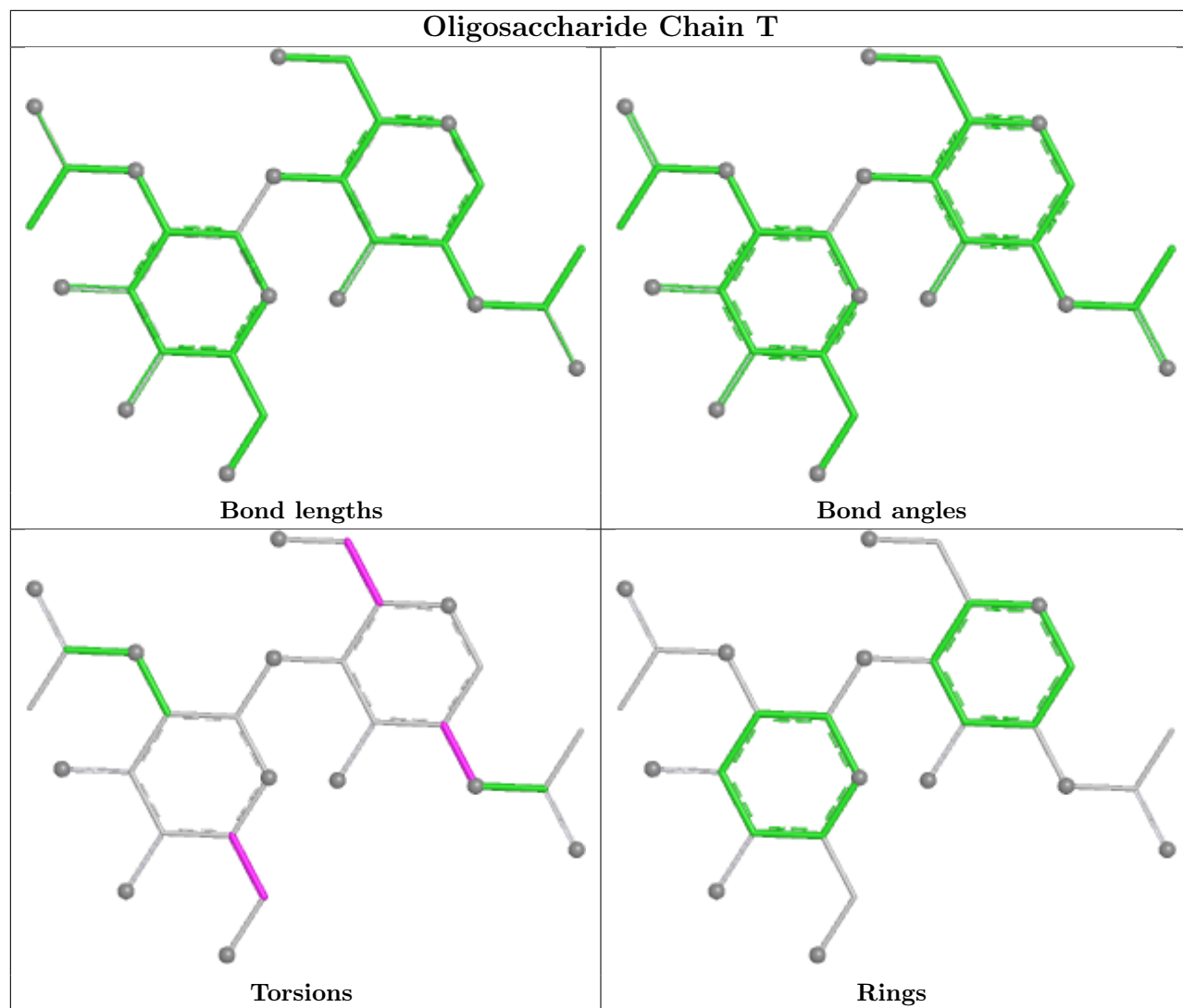




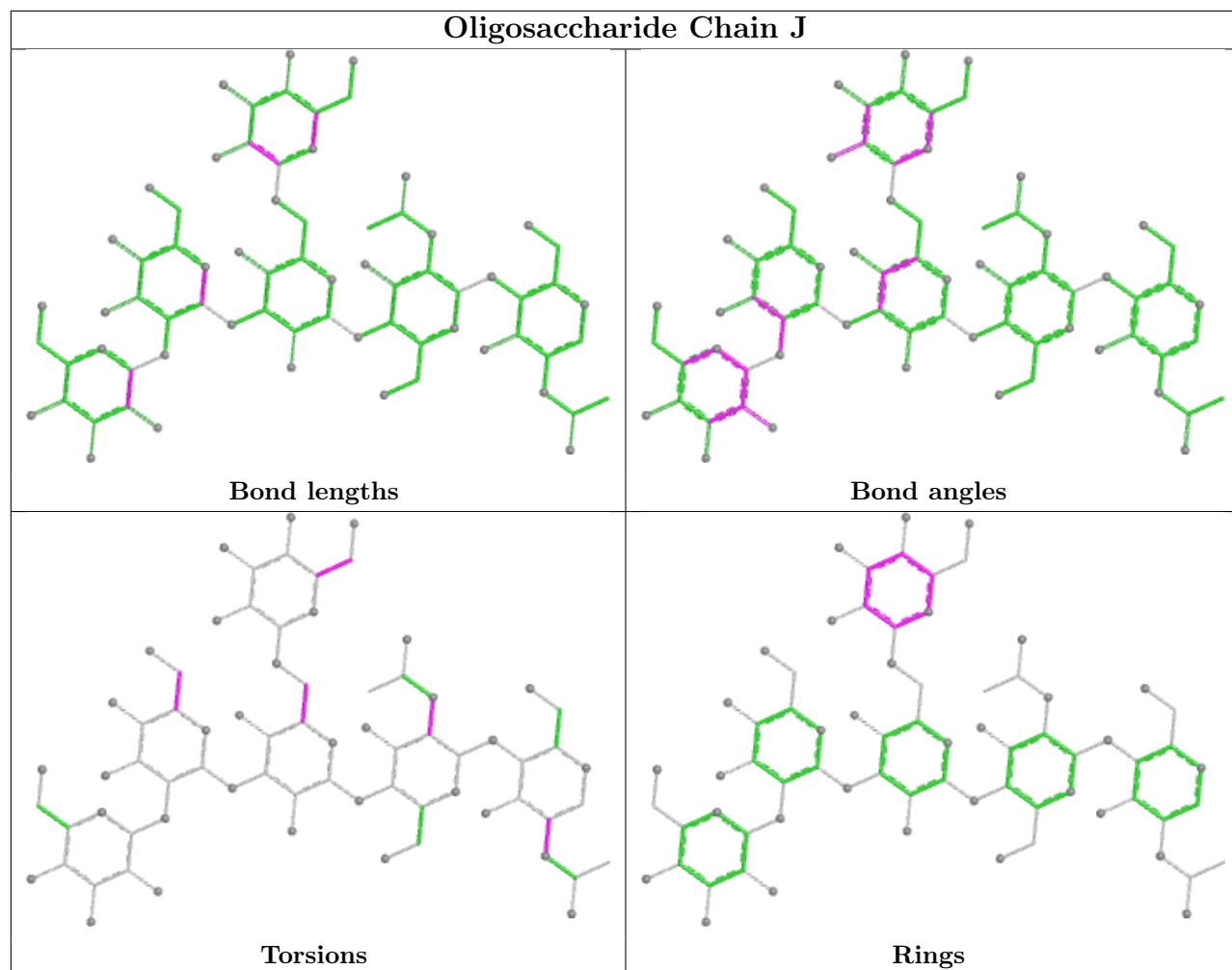


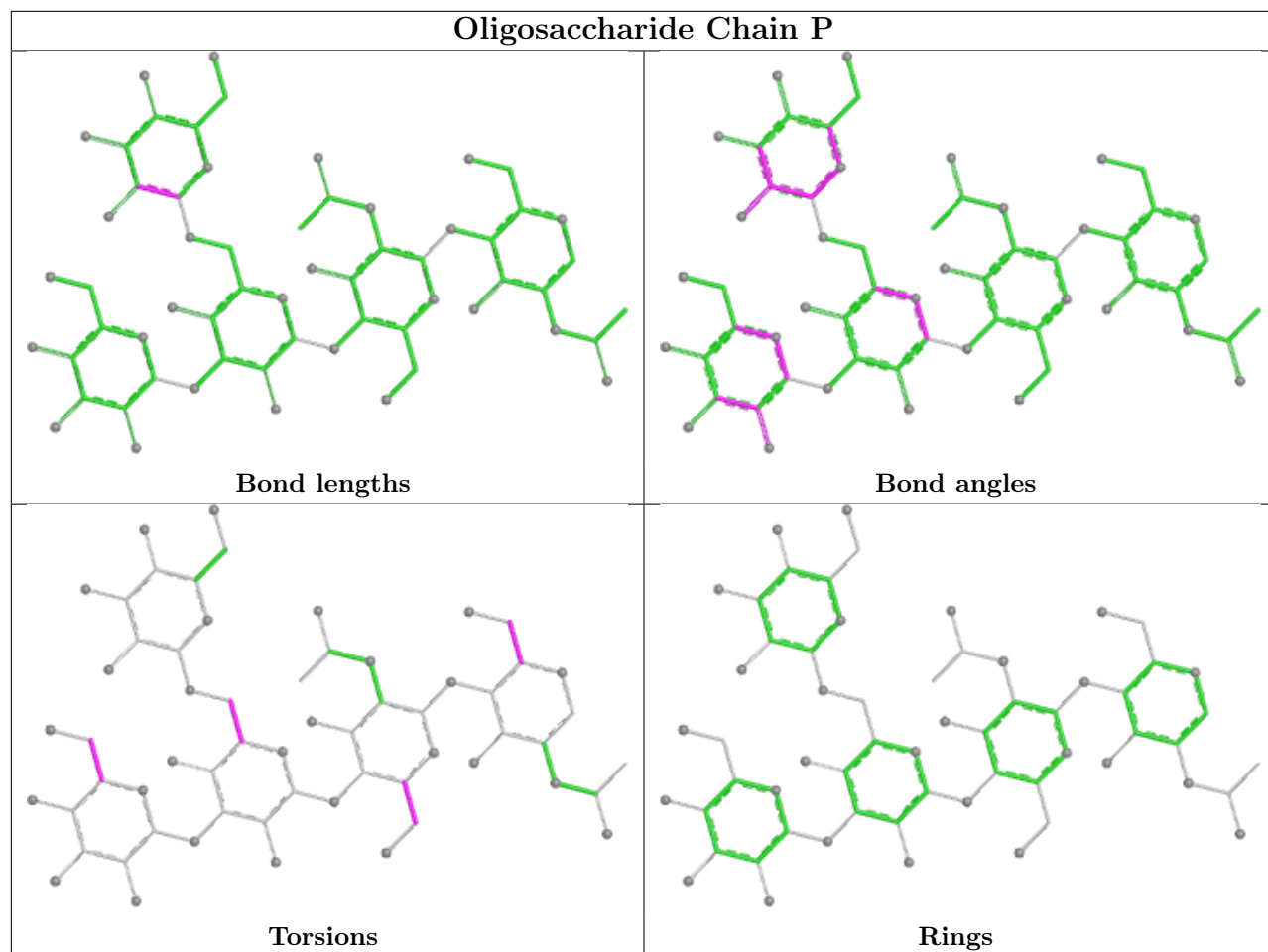


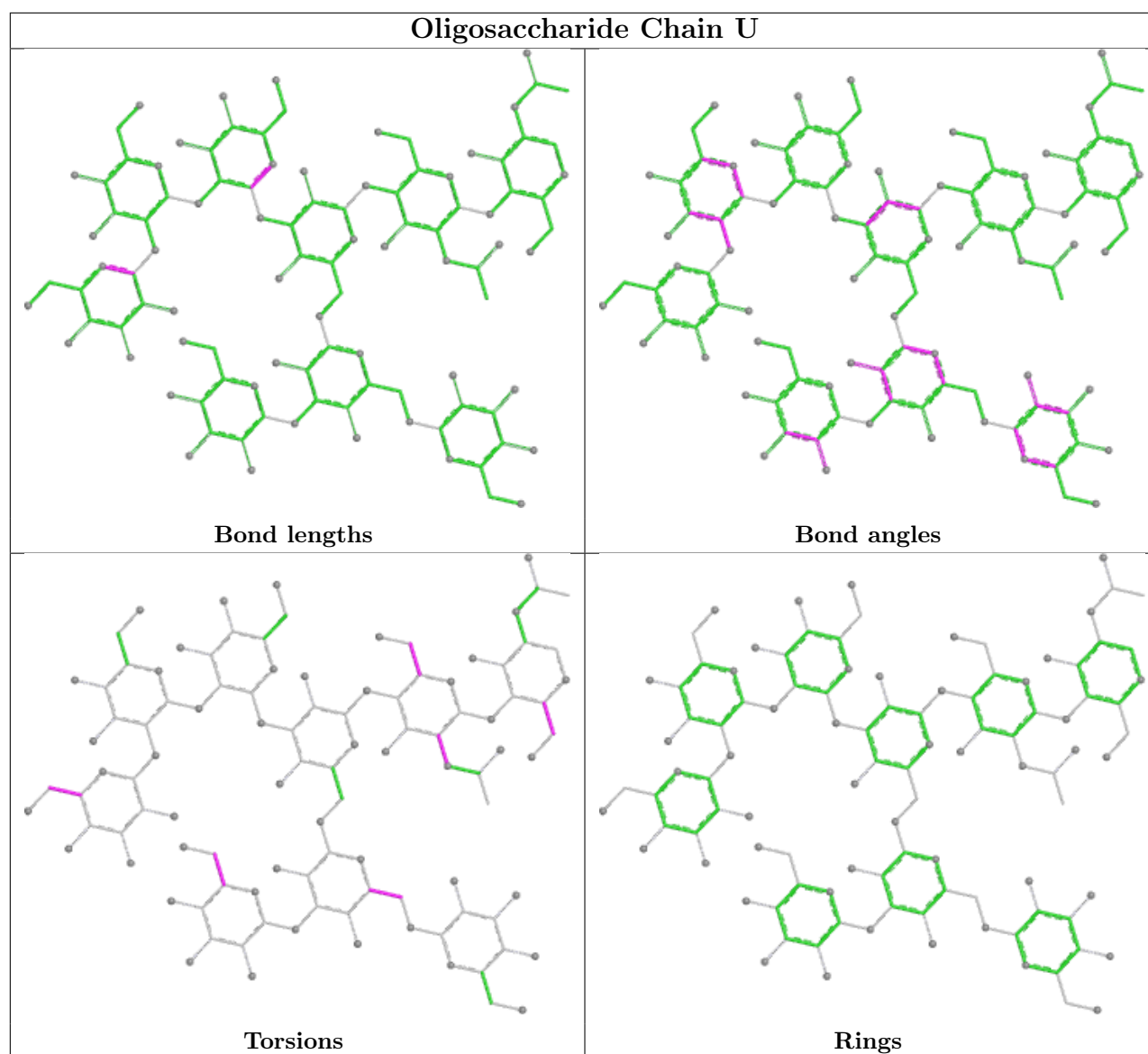




Oligosaccharide Chain J







5.6 Ligand geometry [i](#)

7 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	622	4	14,14,15	0.45	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAG	G	621	4	14,14,15	0.46	0	17,19,21	0.45	0
14	NAG	G	620	4	14,14,15	0.39	0	17,19,21	0.83	1 (5%)
14	NAG	B	702	1	14,14,15	0.41	0	17,19,21	0.41	0
14	NAG	G	632	4	14,14,15	0.42	0	17,19,21	0.61	1 (5%)
15	SO4	G	655	-	4,4,4	0.23	0	6,6,6	0.09	0
14	NAG	B	701	1	14,14,15	1.08	1 (7%)	17,19,21	1.08	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	G	622	4	-	2/6/23/26	0/1/1/1
14	NAG	G	621	4	-	2/6/23/26	0/1/1/1
14	NAG	G	620	4	-	4/6/23/26	0/1/1/1
14	NAG	B	702	1	-	2/6/23/26	0/1/1/1
14	NAG	G	632	4	-	2/6/23/26	0/1/1/1
14	NAG	B	701	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	701	NAG	O5-C1	3.40	1.49	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	620	NAG	C2-N2-C7	2.65	126.45	122.90
14	B	701	NAG	C2-N2-C7	2.08	125.68	122.90
14	G	632	NAG	C1-O5-C5	2.07	114.96	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	G	620	NAG	C1-C2-N2-C7
14	G	621	NAG	C4-C5-C6-O6
14	G	621	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
14	B	701	NAG	O5-C5-C6-O6
14	B	702	NAG	O5-C5-C6-O6
14	G	632	NAG	O5-C5-C6-O6
14	B	702	NAG	C4-C5-C6-O6
14	B	701	NAG	C4-C5-C6-O6
14	G	632	NAG	C4-C5-C6-O6
14	G	620	NAG	C8-C7-N2-C2
14	G	620	NAG	O7-C7-N2-C2
14	G	622	NAG	C8-C7-N2-C2
14	G	622	NAG	O7-C7-N2-C2
14	G	620	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	621	NAG	1	0
14	G	620	NAG	4	0
14	B	702	NAG	1	0
15	G	655	SO4	1	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	129/153 (84%)	-0.29	0	100	100	45, 67, 113, 123	0
2	D	205/243 (84%)	-0.34	0	100	100	94, 126, 161, 165	0
3	E	194/216 (89%)	-0.31	1 (0%)	87	74	96, 136, 164, 172	0
4	G	453/483 (93%)	-0.25	0	100	100	52, 75, 119, 143	0
5	H	226/235 (96%)	-0.30	0	100	100	92, 117, 148, 157	0
6	L	208/213 (97%)	-0.38	0	100	100	85, 114, 126, 133	0
All	All	1415/1543 (91%)	-0.30	1 (0%)	92	87	45, 106, 156, 172	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	136	ILE	2.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	A	1	14/15	-	-	110,110,110,110	0
7	NAG	A	2	14/15	-	-	128,128,128,128	0
7	BMA	A	3	11/12	-	-	135,135,135,135	0

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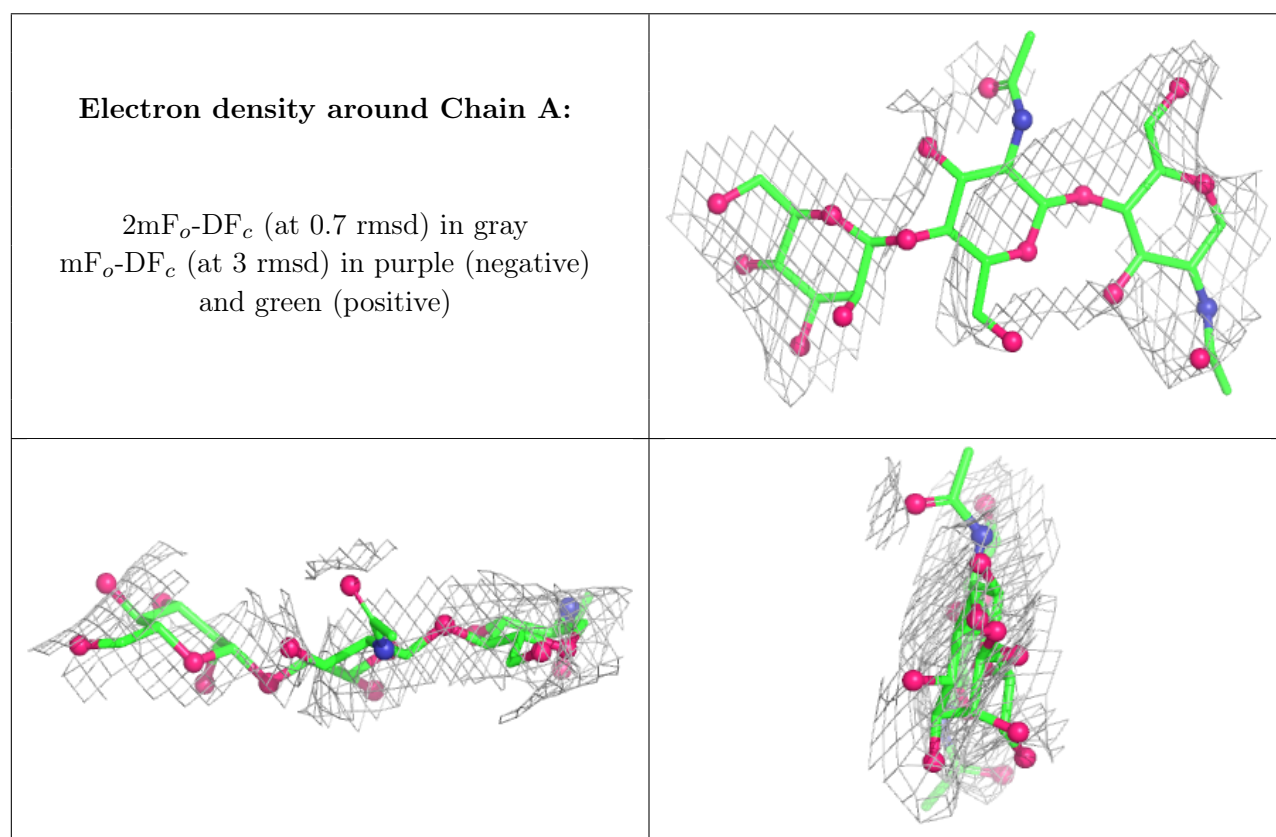
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	MAN	P	4	11/12	0.91	0.07	120,120,120,120	0
10	NAG	R	2	14/15	0.94	0.07	83,83,83,83	0
12	BMA	P	3	11/12	0.95	0.06	111,111,111,111	0
8	NAG	C	1	14/15	-	-	76,76,76,76	0
8	NAG	C	2	14/15	-	-	82,82,82,82	0
8	BMA	C	3	11/12	-	-	90,90,90,90	0
8	MAN	C	4	11/12	-	-	101,101,101,101	0
8	MAN	C	5	11/12	-	-	104,104,104,104	0
8	MAN	C	6	11/12	-	-	107,107,107,107	0
8	MAN	C	7	11/12	-	-	92,92,92,92	0
9	NAG	F	1	14/15	-	-	87,87,87,87	0
9	NAG	F	2	14/15	-	-	92,92,92,92	0
9	BMA	F	3	11/12	-	-	97,97,97,97	0
9	MAN	F	4	11/12	-	-	101,101,101,101	0
11	NAG	J	2	14/15	0.95	0.07	88,88,88,88	0
10	NAG	N	1	14/15	0.96	0.09	113,113,113,113	0
10	NAG	Q	2	14/15	0.96	0.07	91,91,91,91	0
10	NAG	I	2	14/15	0.96	0.09	85,85,85,85	0
13	MAN	U	6	11/12	0.96	0.13	106,106,106,106	0
7	BMA	O	3	11/12	0.97	0.06	95,95,95,95	0
10	NAG	R	1	14/15	0.97	0.09	79,79,79,79	0
7	NAG	O	1	14/15	0.97	0.07	81,81,81,81	0
10	NAG	S	2	14/15	0.97	0.09	86,86,86,86	0
10	NAG	T	2	14/15	0.97	0.09	100,100,100,100	0
10	NAG	M	2	14/15	0.97	0.06	96,96,96,96	0
12	NAG	P	2	14/15	0.97	0.10	98,98,98,98	0
7	NAG	O	2	14/15	0.97	0.06	89,89,89,89	0
10	NAG	N	2	14/15	0.97	0.07	111,111,111,111	0
12	MAN	P	5	11/12	0.97	0.07	111,111,111,111	0
13	NAG	U	1	14/15	0.97	0.09	84,84,84,84	0
13	NAG	U	2	14/15	0.97	0.06	87,87,87,87	0
10	NAG	Q	1	14/15	0.97	0.09	85,85,85,85	0
11	BMA	J	3	11/12	-	-	99,99,99,99	0
11	MAN	J	4	11/12	-	-	105,105,105,105	0
11	MAN	J	5	11/12	-	-	106,106,106,106	0
11	MAN	J	6	11/12	-	-	106,106,106,106	0
13	MAN	U	8	11/12	0.97	0.06	99,99,99,99	0
10	NAG	K	2	14/15	0.98	0.10	100,100,100,100	0
10	NAG	S	1	14/15	0.98	0.06	79,79,79,79	0
10	NAG	M	1	14/15	0.98	0.09	89,89,89,89	0
10	NAG	T	1	14/15	0.98	0.08	91,91,91,91	0
10	NAG	I	1	14/15	0.98	0.08	81,81,81,81	0

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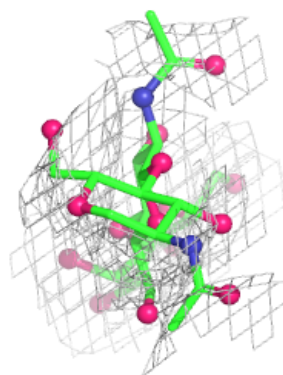
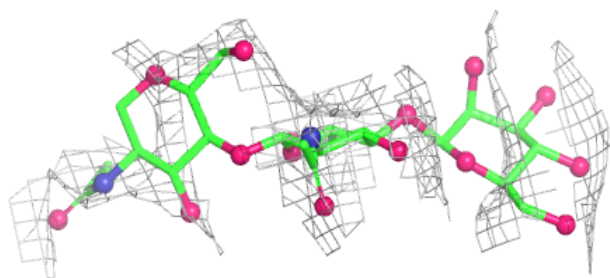
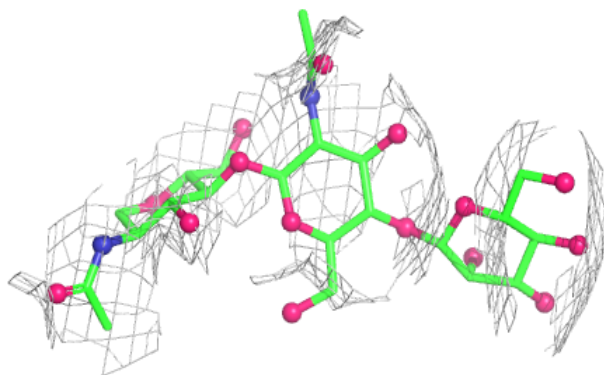
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	NAG	J	1	14/15	0.98	0.07	77,77,77,77	0
13	MAN	U	4	11/12	0.98	0.06	95,95,95,95	0
13	MAN	U	5	11/12	0.98	0.07	99,99,99,99	0
10	NAG	K	1	14/15	0.98	0.08	94,94,94,94	0
13	MAN	U	7	11/12	0.98	0.08	98,98,98,98	0
12	NAG	P	1	14/15	0.98	0.09	88,88,88,88	0
13	MAN	U	9	11/12	0.98	0.08	96,96,96,96	0
13	BMA	U	3	11/12	0.99	0.05	96,96,96,96	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.

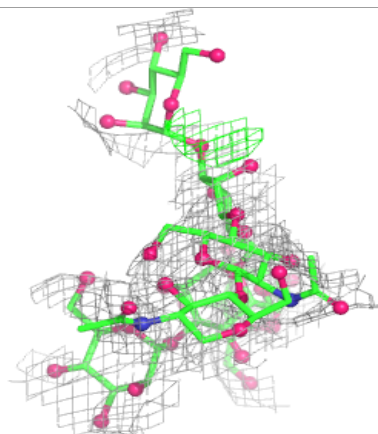
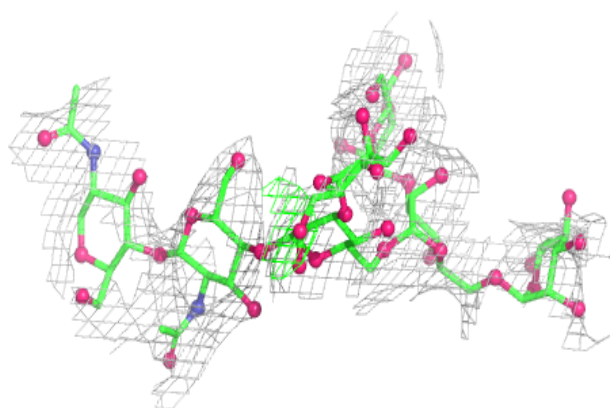
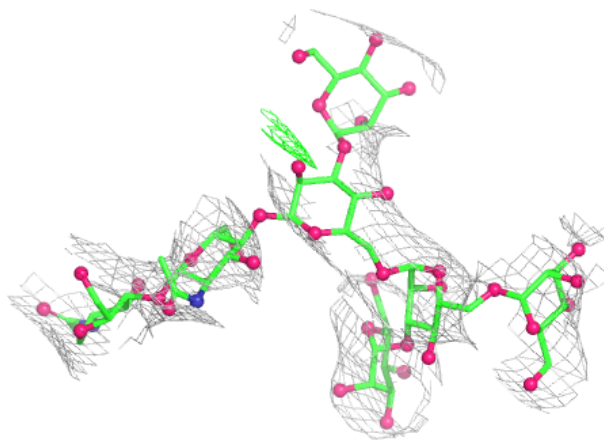


Electron density around Chain O:

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

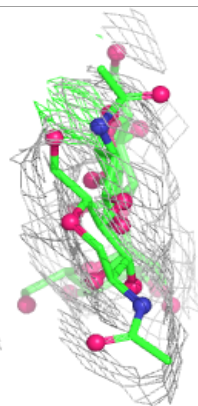
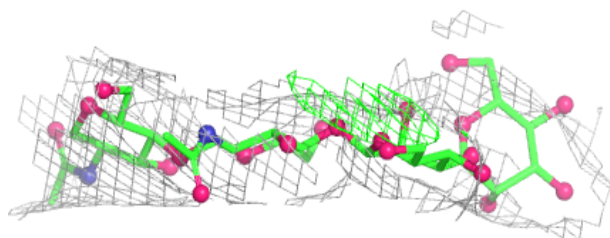
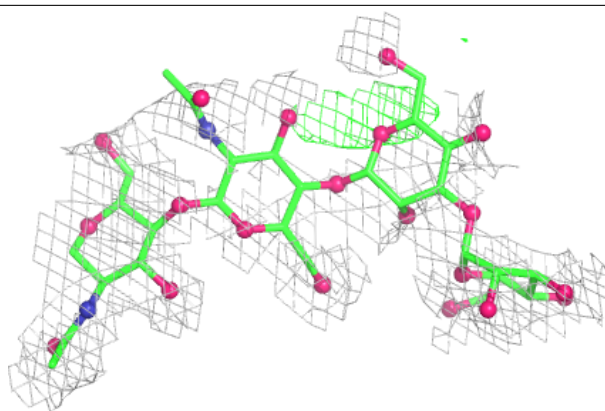
**Electron density around Chain C:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

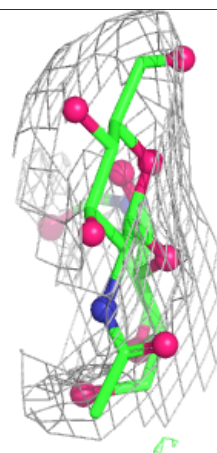
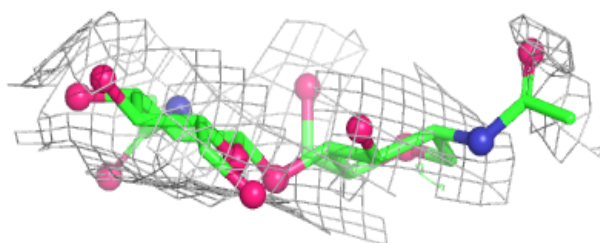
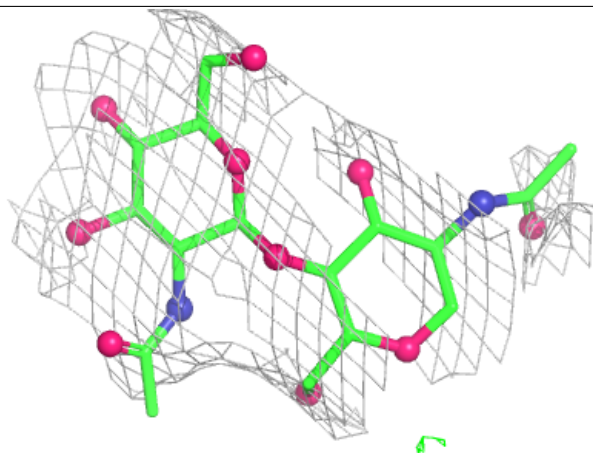


Electron density around Chain F:

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

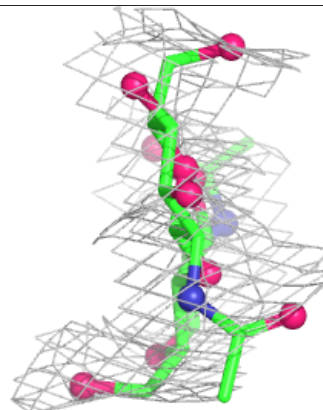
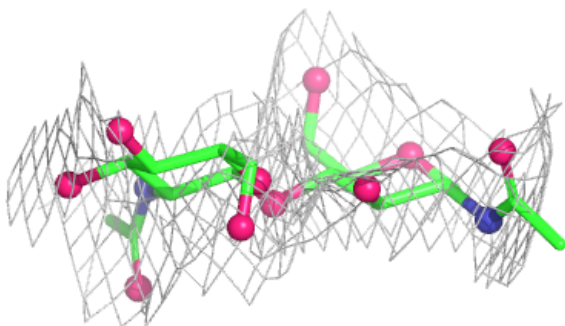
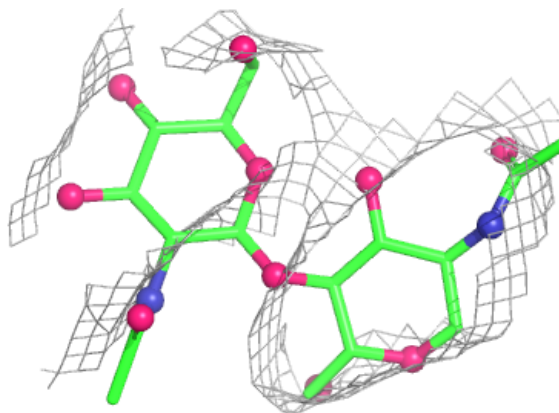
**Electron density around Chain I:**

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



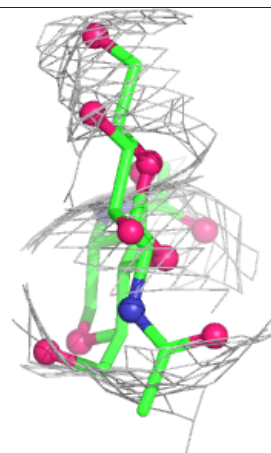
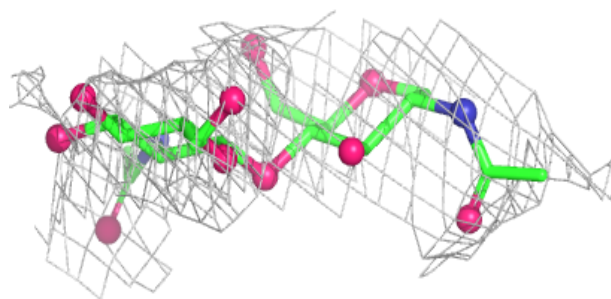
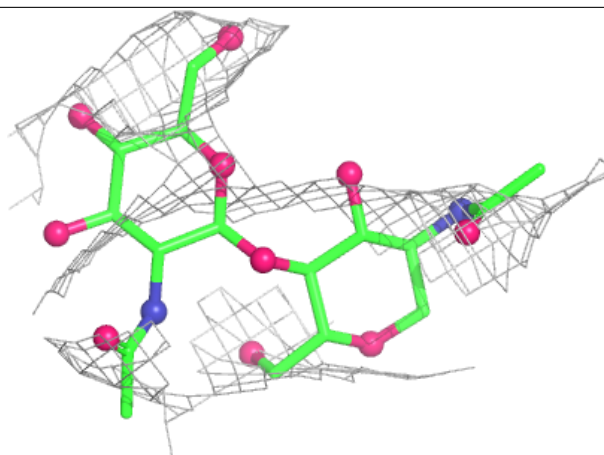
Electron density around Chain K:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



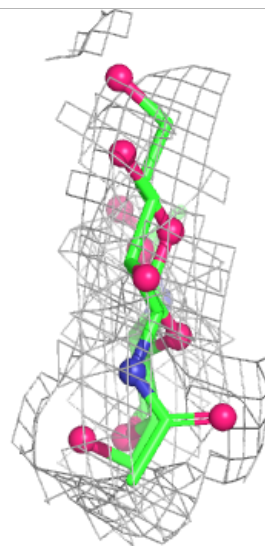
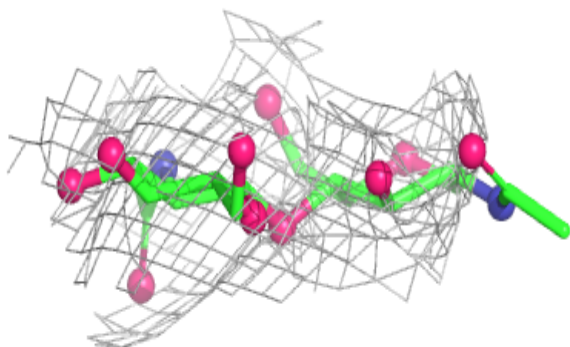
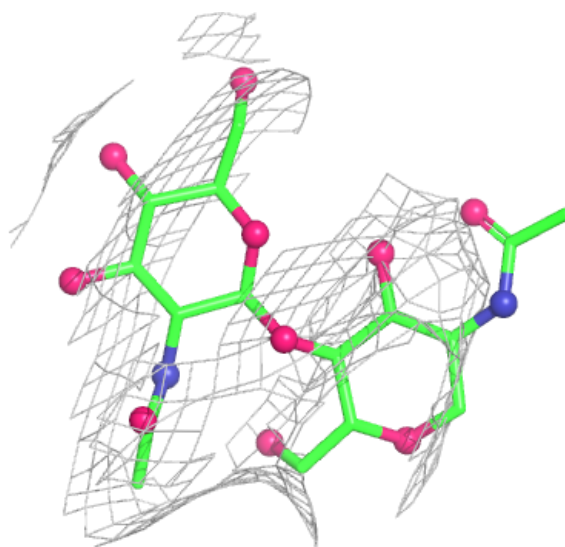
Electron density around Chain M:

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



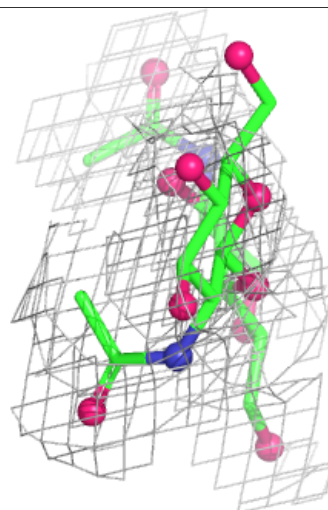
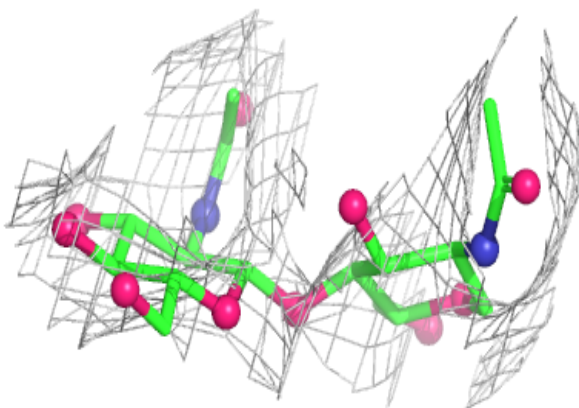
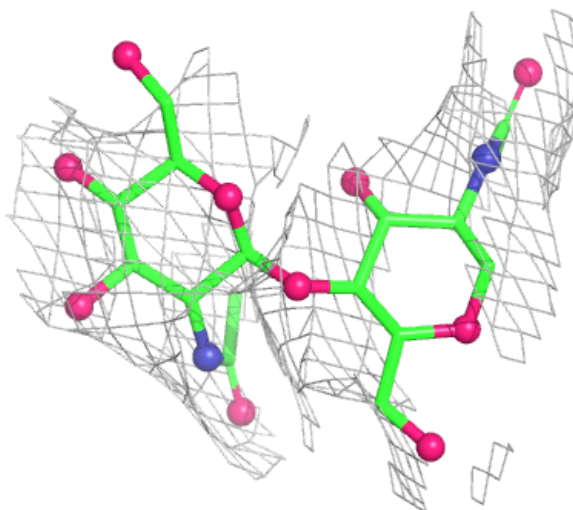
Electron density around Chain N:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



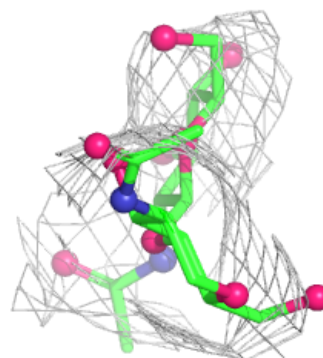
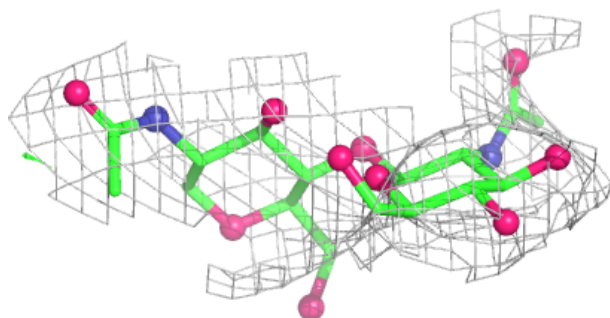
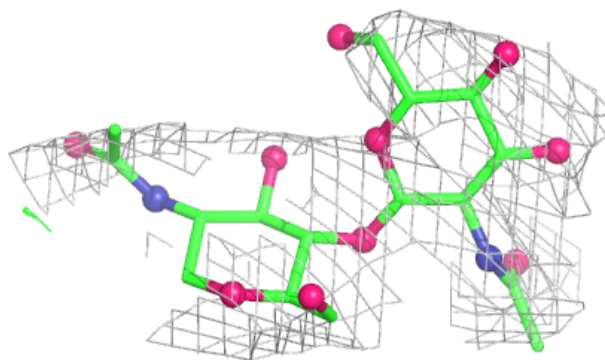
Electron density around Chain Q:

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and green (positive)

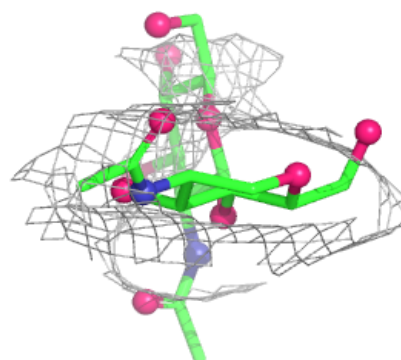
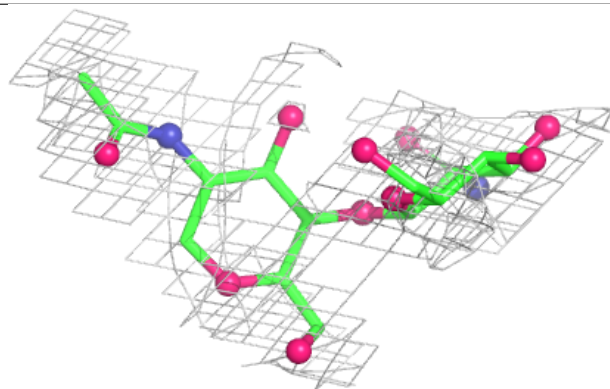
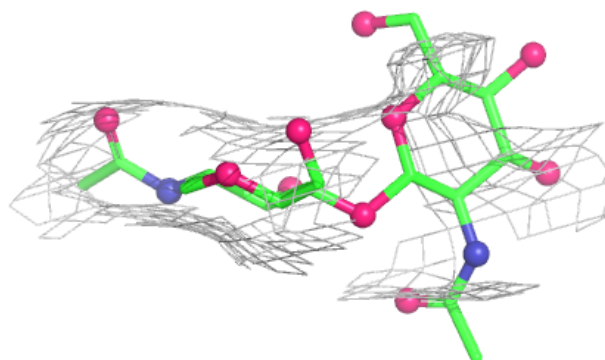


Electron density around Chain R:

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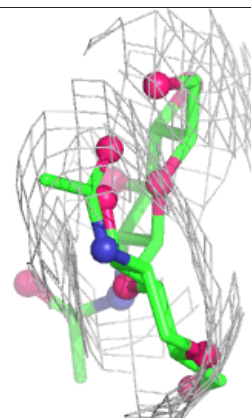
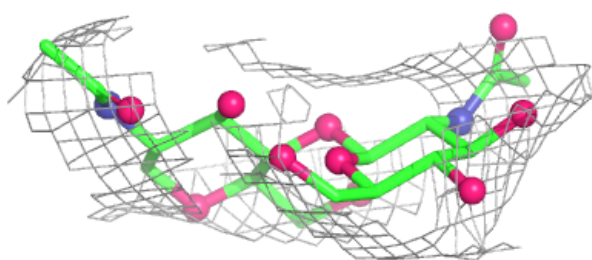
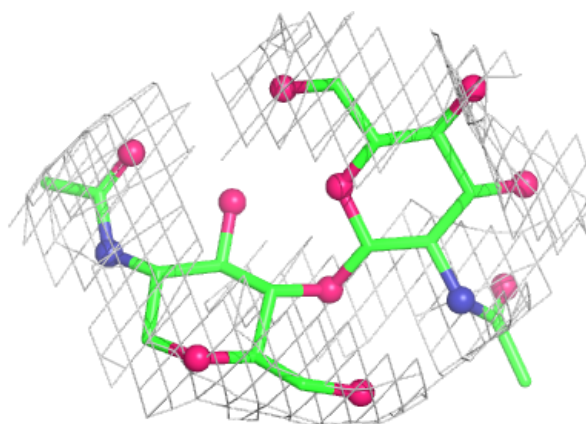
**Electron density around Chain S:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



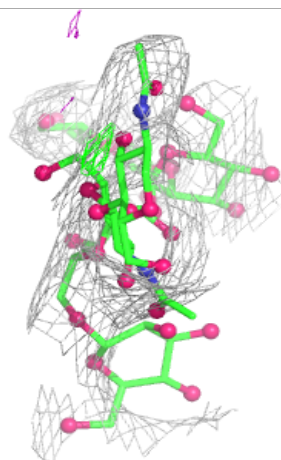
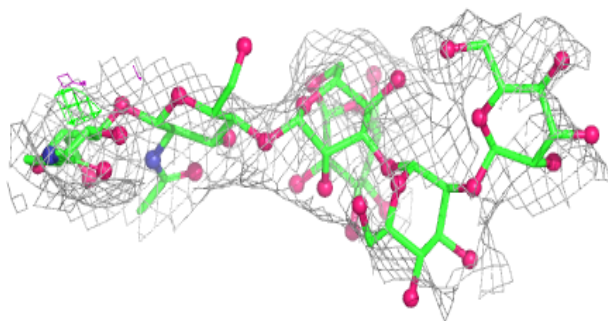
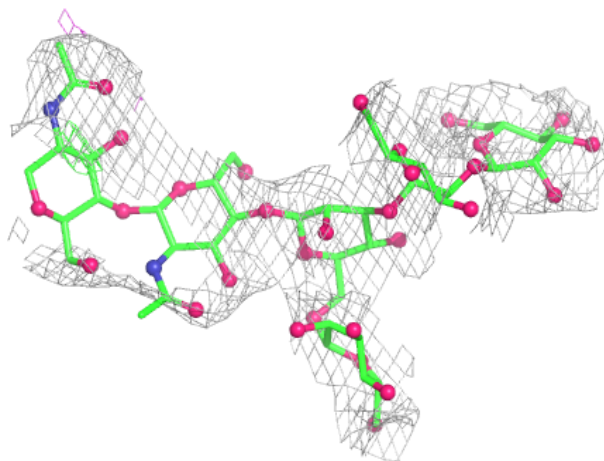
Electron density around Chain T:

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and green (positive)



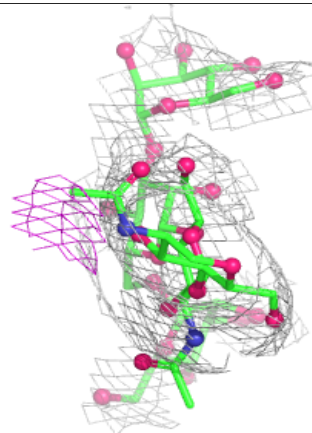
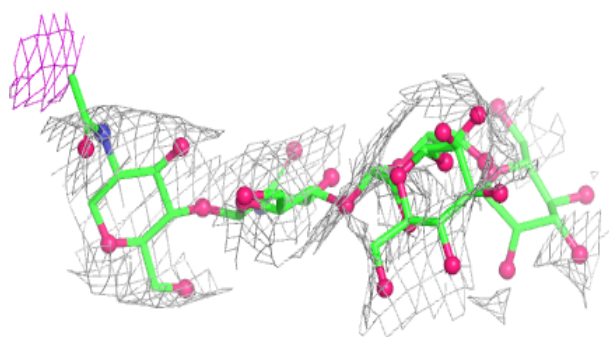
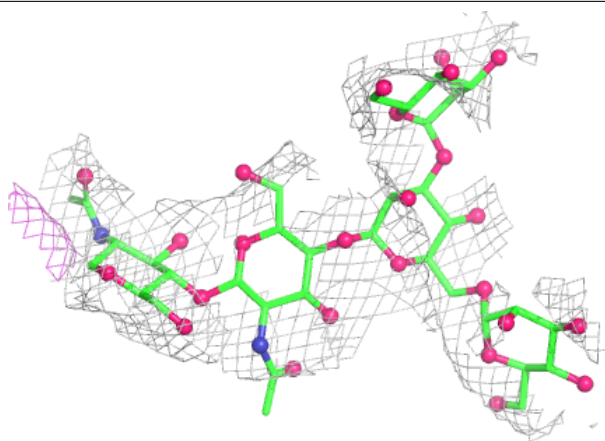
Electron density around Chain J:

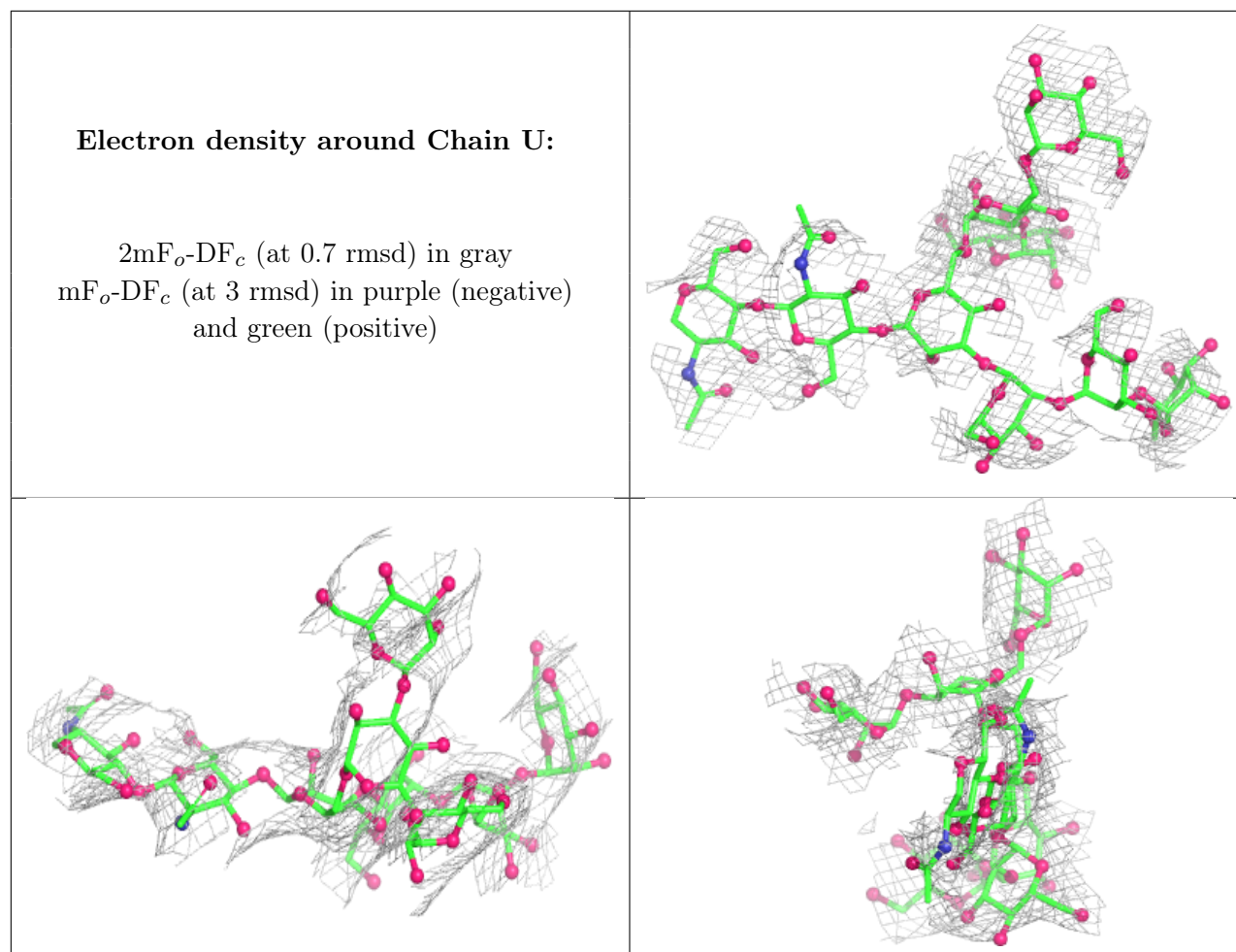
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain P:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	SO4	G	655	5/5	0.93	0.09	65,65,65,65	5
14	NAG	B	702	14/15	0.95	0.07	97,97,97,97	0
14	NAG	G	621	14/15	0.96	0.09	108,108,108,108	0
14	NAG	G	622	14/15	0.96	0.06	123,123,123,123	0
14	NAG	B	701	14/15	0.96	0.09	104,104,104,104	0
14	NAG	G	620	14/15	0.97	0.07	98,98,98,98	0
14	NAG	G	632	14/15	0.98	0.10	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.