



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:55 PM UTC

PDB ID : 4TVP / pdb_00004tvp
Title : Crystal Structure of the HIV-1 BG505 SOSIP.664 Env Trimer Ectodomain, Comprising Atomic-Level Definition of Pre-Fusion gp120 and gp41, in Complex with Human Antibodies PGT122 and 35O22
Authors : Pancera, M.; Zhou, T.; Kwong, P.D.
Deposited on : 2014-06-27
Resolution : 3.10 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

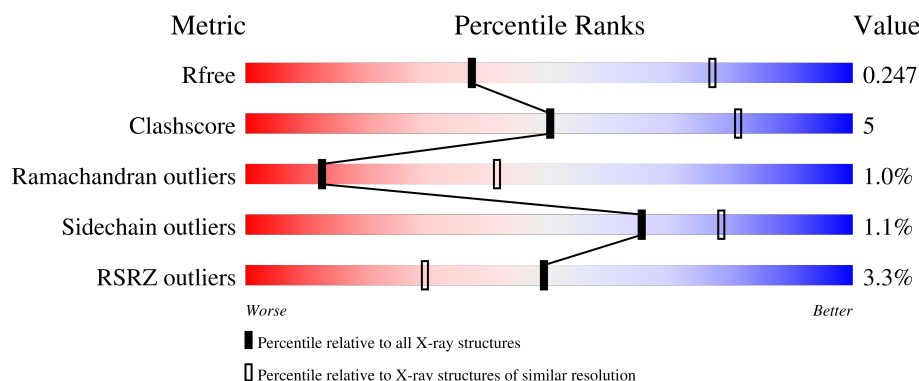
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	G	481	
2	B	153	
3	L	213	
4	H	235	
5	D	243	

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Mol	Chain	Length	Quality of chain
6	E	216	 6% 86% 12%
7	A	7	 14% 29% 57%
8	C	4	 50% 25% 25%
9	F	2	 100%
9	J	2	 100%
9	K	2	 100%
9	M	2	 100%
9	P	2	 50% 50%
9	Q	2	 100%
9	R	2	 100%
9	S	2	 100%
10	I	6	 50% 50%
11	N	3	 100%
12	O	5	 60% 40%
13	T	10	 10% 70% 20%

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 12188 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	G	453	Total	C	N	O	S	0	0	0
			3565	2236	630	671	28			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S5
G	501	CYS	ALA	engineered mutation	UNP Q2N0S5
G	509	ARG	-	expression tag	UNP Q2N0S5
G	510	ARG	-	expression tag	UNP Q2N0S5
G	511	ARG	-	expression tag	UNP Q2N0S5
G	512	ARG	-	expression tag	UNP Q2N0S5
G	513	ARG	-	expression tag	UNP Q2N0S5

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	126	Total	C	N	O	S	0	0	0
			1001	633	172	190	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S5
B	605	CYS	THR	engineered mutation	UNP Q2N0S5

- Molecule 3 is a protein called PGT122 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1589	998	267	320	4			

- Molecule 4 is a protein called PGT122 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			

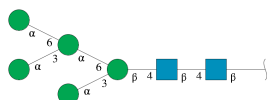
- Molecule 5 is a protein called 35O22 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	242	Total	C	N	O	S	0	0	0
			1832	1165	306	353	8			

- Molecule 6 is a protein called 35O22 Light chain.

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

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



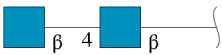
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	A	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 8 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.



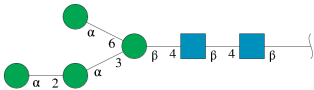
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	C	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



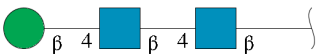
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	R	2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

- Molecule 10 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.



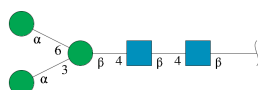
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 11 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.



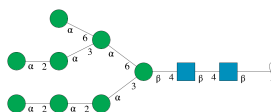
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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.



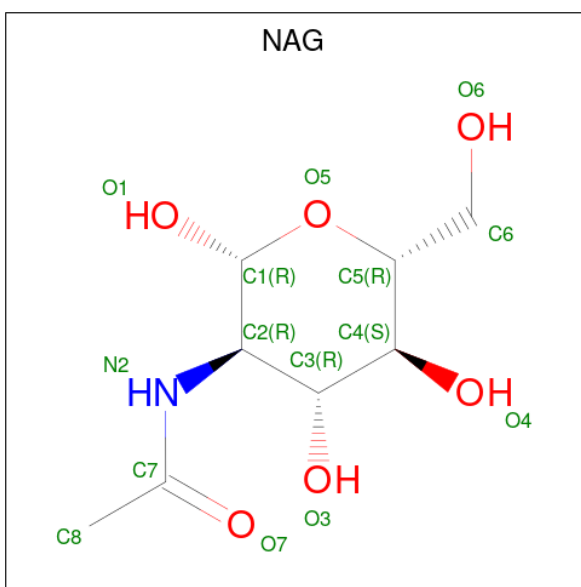
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	O	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-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	T	10	Total	C	N	O	0	0	0
			116	64	2	50			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		
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	B	1	Total	C	N	O	0	0
			14	8	1	5		
14	H	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		
15	G	1	Total	O	S	0	0
			5	4	1		
15	G	1	Total	O	S	0	0
			5	4	1		
15	G	1	Total	O	S	0	0
			5	4	1		
15	G	1	Total	O	S	0	0
			5	4	1		
15	G	1	Total	O	S	0	0
			5	4	1		
15	B	1	Total	O	S	0	0
			5	4	1		
15	B	1	Total	O	S	0	0
			5	4	1		
15	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	17	Total	O	0	0
			17	17		
16	B	2	Total	O	0	0
			2	2		

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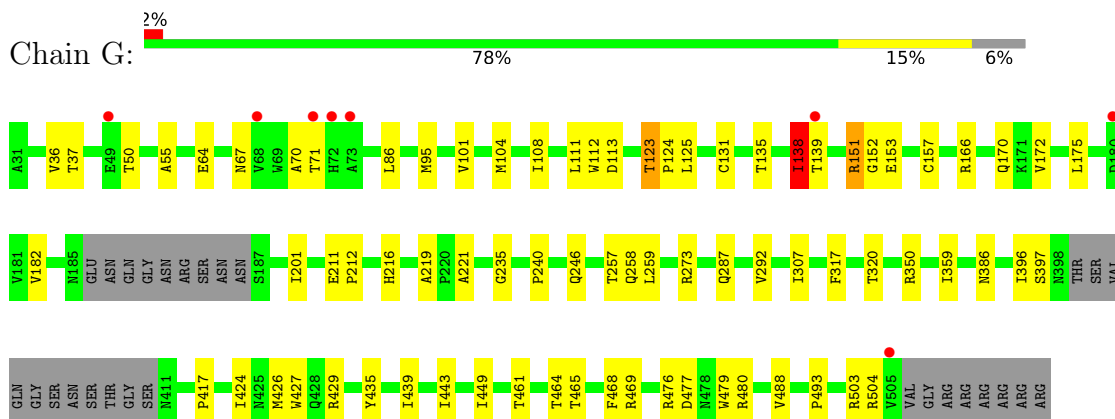
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	L	3	Total 3	O 3	0	0
16	H	2	Total 2	O 2	0	0
16	D	11	Total 11	O 11	0	0
16	E	2	Total 2	O 2	0	0

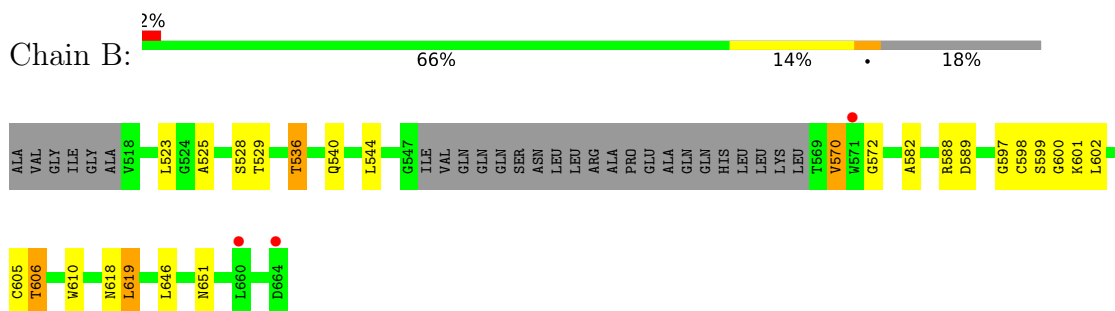
3 Residue-property plots [i](#)

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

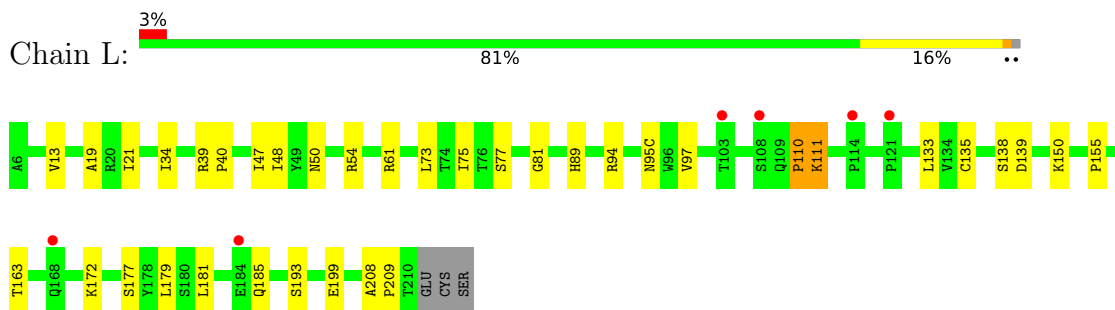
- Molecule 1: Envelope glycoprotein gp160



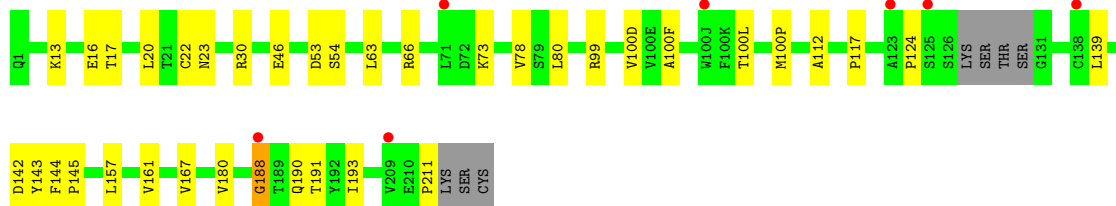
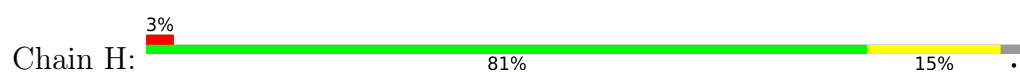
- Molecule 2: Envelope glycoprotein gp160



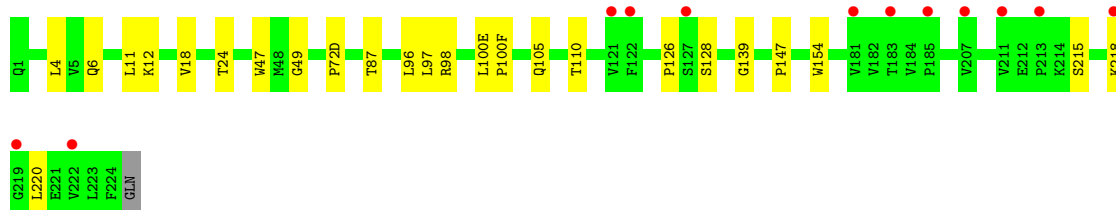
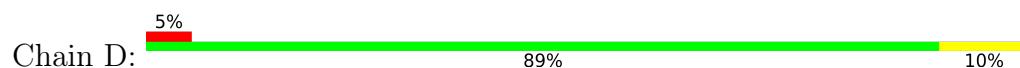
- Molecule 3: PGT122 Light chain



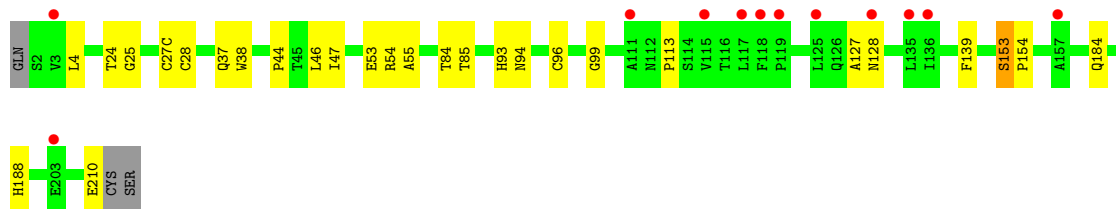
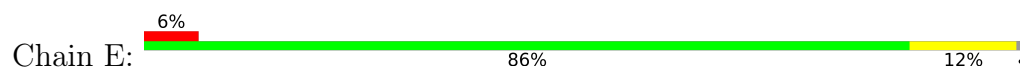
- Molecule 4: PGT122 Heavy chain



- Molecule 5: 35O22 Heavy chain



- Molecule 6: 35O22 Light chain



- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 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



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

Chain F:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2

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

Chain K:  100%

MAG1
MAG2

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

Chain M:  100%

MAG1
MAG2

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

Chain P:  50%  50%

MAG1
MAG2

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

Chain Q:  100%

MAG1
MAG2

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

Chain R:  100%

MAG1
MAG2

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

Chain S:  100%

MAG1
MAG2

- Molecule 10: 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 I:  50% 50%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

- Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1
MAG2
BMA3

- 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 O:  60% 40%

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-(1-2)-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 T:  10% 70% 20%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	128.89Å 128.89Å 313.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.74 – 3.10 40.74 – 3.10	Depositor EDS
% Data completeness (in resolution range)	55.0 (40.74-3.10) 55.1 (40.74-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.213 , 0.248 0.217 , 0.247	Depositor DCC
R_{free} test set	1451 reflections (2.69%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 62.8	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12188	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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: MAN, SO4, BMA, 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	G	0.27	0/3639	0.71	0/4941
2	B	0.24	0/1019	0.62	0/1382
3	L	0.26	0/1632	0.73	0/2236
4	H	0.25	0/1789	0.69	0/2443
5	D	0.24	0/1880	0.67	0/2560
6	E	0.26	0/1659	0.71	2/2269 (0.1%)
All	All	0.26	0/11618	0.69	2/15831 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	153	SER	CA-C-N	6.17	127.56	119.84
6	E	153	SER	C-N-CA	6.17	127.56	119.84

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	G	3565	0	3495	44	0
2	B	1001	0	975	15	0
3	L	1589	0	1530	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1742	0	1715	21	0
5	D	1832	0	1806	15	0
6	E	1615	0	1542	16	0
7	A	83	0	70	4	0
8	C	50	0	43	2	0
9	F	28	0	25	0	0
9	J	28	0	25	0	0
9	K	28	0	25	0	0
9	M	28	0	25	0	0
9	P	28	0	25	2	0
9	Q	28	0	25	0	0
9	R	28	0	25	0	0
9	S	28	0	25	0	0
10	I	72	0	61	0	0
11	N	39	0	34	0	0
12	O	61	0	52	0	0
13	T	116	0	97	2	0
14	B	42	0	39	2	0
14	G	56	0	52	1	0
14	H	14	0	13	0	0
15	B	10	0	0	1	0
15	G	35	0	0	2	0
15	L	5	0	0	0	0
16	B	2	0	0	0	0
16	D	11	0	0	0	0
16	E	2	0	0	0	0
16	G	17	0	0	0	0
16	H	2	0	0	0	0
16	L	3	0	0	0	0
All	All	12188	0	11724	127	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 5.

All (127) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:ALA:HB2	1:G:111:LEU:HD11	1.69	0.75
1:G:55:ALA:HB3	1:G:216:HIS:HB2	1.71	0.71
6:E:37:GLN:HB2	6:E:47:ILE:HD11	1.74	0.68
1:G:350:ARG:NH2	1:G:396:ILE:O	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:6:GLN:H	5:D:105:GLN:HE22	1.43	0.66
2:B:536:THR:O	2:B:540:GLN:NE2	2.29	0.66
3:L:110:PRO:HG2	3:L:111:LYS:HD2	1.79	0.64
5:D:12:LYS:HG3	5:D:18:VAL:HB	1.80	0.63
1:G:219:ALA:O	1:G:246:GLN:NE2	2.31	0.63
3:L:47:ILE:HG22	3:L:48:ILE:HG13	1.80	0.62
3:L:163:THR:HG22	4:H:167:VAL:HB	1.81	0.62
1:G:37:THR:HG22	2:B:605:CYS:HA	1.81	0.62
3:L:181:LEU:HD22	3:L:185:GLN:HG2	1.83	0.60
4:H:99:ARG:HG2	4:H:100(L):THR:HG22	1.83	0.60
1:G:201:ILE:HD11	1:G:435:TYR:HB2	1.82	0.60
3:L:139:ASP:H	3:L:172:LYS:HG3	1.67	0.59
3:L:39:ARG:NH1	3:L:81:GLY:O	2.35	0.59
1:G:166:ARG:NH2	15:G:606:SO4:O2	2.34	0.59
1:G:464:THR:OG1	1:G:465:THR:N	2.34	0.58
4:H:100(D):VAL:HA	13:T:2:NAG:H2	1.86	0.58
1:G:113:ASP:OD1	1:G:429:ARG:NH1	2.37	0.58
2:B:588:ARG:NH2	15:B:701:SO4:O3	2.37	0.57
1:G:292:VAL:HB	1:G:449:ILE:HB	1.85	0.57
9:P:2:NAG:H83	9:P:2:NAG:H3	1.87	0.57
5:D:100(E):LEU:HD12	5:D:100(F):PRO:HD2	1.87	0.57
3:L:39:ARG:HG3	3:L:40:PRO:HD2	1.87	0.56
7:A:2:NAG:H3	7:A:2:NAG:H83	1.87	0.56
14:G:1276:NAG:H3	14:G:1276:NAG:H83	1.88	0.55
1:G:469:ARG:NH2	15:G:602:SO4:O4	2.40	0.55
5:D:128:SER:HB2	5:D:220:LEU:HB2	1.89	0.55
5:D:4:LEU:HG	5:D:24:THR:HG22	1.90	0.54
1:G:36:VAL:HG12	2:B:610:TRP:HE3	1.74	0.53
6:E:127:ALA:N	6:E:128:ASN:HA	2.22	0.53
5:D:126:PRO:HB2	5:D:215:SER:HB2	1.91	0.53
1:G:257:THR:O	1:G:259:LEU:N	2.40	0.52
4:H:30:ARG:HD3	4:H:73:LYS:HD2	1.91	0.52
5:D:218:LYS:NZ	6:E:210:GLU:OE1	2.42	0.52
6:E:84:THR:OG1	6:E:85:THR:N	2.41	0.52
5:D:87:THR:HG23	5:D:110:THR:HA	1.92	0.52
3:L:97:VAL:HG22	4:H:46:GLU:HG3	1.93	0.51
1:G:175:LEU:HB3	1:G:320:THR:HB	1.92	0.51
4:H:188:GLY:HA3	4:H:190:GLN:N	2.26	0.51
1:G:359:ILE:HD12	1:G:468:PHE:HE2	1.76	0.50
2:B:529:THR:HG23	5:D:98:ARG:HD2	1.93	0.50
5:D:11:LEU:HD13	5:D:147:PRO:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:618:ASN:OD1	2:B:619:LEU:N	2.43	0.50
9:P:1:NAG:H62	9:P:2:NAG:H82	1.94	0.49
6:E:113:PRO:HB3	6:E:139:PHE:HB3	1.93	0.49
4:H:63:LEU:HD22	4:H:66:ARG:HH21	1.78	0.49
1:G:240:PRO:HG3	5:D:72(D):PRO:HG2	1.93	0.49
1:G:477:ASP:OD1	1:G:480:ARG:NH1	2.46	0.49
1:G:439:ILE:HB	1:G:443:ILE:HD11	1.95	0.49
14:B:1618:NAG:H83	6:E:54:ARG:HH21	1.78	0.49
3:L:150:LYS:HB2	3:L:193:SER:HB2	1.95	0.49
3:L:133:LEU:HD12	3:L:179:LEU:HD23	1.95	0.49
6:E:24:THR:OG1	6:E:25:GLY:N	2.45	0.49
2:B:588:ARG:NH1	2:B:589:ASP:OD1	2.46	0.48
4:H:117:PRO:HB3	4:H:143:TYR:HB3	1.94	0.48
3:L:61:ARG:HD2	3:L:77:SER:HB2	1.95	0.48
2:B:570:VAL:C	2:B:572:GLY:H	2.22	0.47
2:B:598:CYS:O	2:B:600:GLY:N	2.45	0.47
4:H:191:THR:HG22	4:H:193:ILE:HG13	1.96	0.47
1:G:221:ALA:HB3	2:B:582:ALA:HB1	1.96	0.47
1:G:476:ARG:HA	1:G:479:TRP:CD1	2.49	0.47
1:G:95:MET:SD	1:G:273:ARG:HD3	2.55	0.47
1:G:170:GLN:HG2	1:G:172:VAL:HG13	1.96	0.47
4:H:100(D):VAL:O	4:H:100(F):ALA:N	2.43	0.47
4:H:53:ASP:OD1	4:H:54:SER:N	2.42	0.46
5:D:47:TRP:CZ2	5:D:49:GLY:HA2	2.51	0.46
1:G:386:ASN:HB3	1:G:417:PRO:HD2	1.97	0.46
1:G:123:THR:HG23	1:G:124:PRO:HD3	1.97	0.46
1:G:138:ILE:CB	1:G:139:THR:HA	2.46	0.46
1:G:424:ILE:HD12	1:G:426:MET:HE3	1.97	0.46
1:G:138:ILE:HB	1:G:139:THR:HA	1.98	0.45
2:B:525:ALA:HB1	2:B:528:SER:HB2	1.97	0.45
5:D:96:LEU:HG	5:D:97:LEU:HG	1.98	0.45
3:L:138:SER:HB2	3:L:172:LYS:HE2	1.99	0.45
1:G:101:VAL:HG13	1:G:479:TRP:HB2	1.99	0.45
1:G:101:VAL:HG21	1:G:480:ARG:HG2	1.98	0.45
4:H:20:LEU:HD12	4:H:80:LEU:HD22	1.98	0.45
3:L:150:LYS:HD3	3:L:155:PRO:HA	1.99	0.45
4:H:144:PHE:HA	4:H:145:PRO:HA	1.78	0.44
6:E:153:SER:HA	6:E:154:PRO:HD2	1.76	0.44
2:B:606:THR:HG21	2:B:646:LEU:HD22	1.98	0.44
4:H:100(L):THR:HG21	8:C:4:MAN:H62	1.99	0.44
1:G:135:THR:O	3:L:94:ARG:NE	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:21:ILE:HB	3:L:73:LEU:HB3	1.98	0.44
4:H:161:VAL:HG22	4:H:180:VAL:HG22	2.00	0.43
6:E:4:LEU:HB3	6:E:99:GLY:HA2	1.99	0.43
4:H:16:GLU:HG2	4:H:17:THR:H	1.82	0.43
6:E:38:TRP:CG	6:E:44:PRO:HB3	2.53	0.43
4:H:22:CYS:HB3	4:H:78:VAL:HB	2.01	0.43
3:L:19:ALA:HB3	3:L:75:ILE:HB	1.99	0.43
4:H:157:LEU:HD21	4:H:180:VAL:HG11	2.00	0.43
6:E:184:GLN:O	6:E:188:HIS:ND1	2.47	0.43
5:D:126:PRO:O	5:D:215:SER:OG	2.31	0.42
6:E:27(C):CYS:HA	6:E:28:CYS:HA	1.58	0.42
1:G:493:PRO:HG3	2:B:544:LEU:HD21	2.00	0.42
4:H:13:LYS:NZ	4:H:112:ALA:O	2.52	0.42
3:L:13:VAL:HG21	3:L:19:ALA:HA	2.01	0.42
6:E:94:ASN:HD21	7:A:6:MAN:H2	1.85	0.42
7:A:3:BMA:H61	7:A:4:MAN:H2	1.29	0.42
1:G:396:ILE:HG22	1:G:397:SER:H	1.84	0.42
6:E:93:HIS:CG	7:A:7:MAN:H2	2.55	0.42
1:G:86:LEU:HD22	2:B:523:LEU:O	2.20	0.41
3:L:135:CYS:HB3	3:L:177:SER:HB3	2.01	0.41
1:G:503:ARG:HB3	1:G:504:ARG:H	1.76	0.41
3:L:208:ALA:HA	3:L:209:PRO:HD3	1.88	0.41
13:T:8:MAN:H2	13:T:9:MAN:H2	1.86	0.41
1:G:131:CYS:HA	1:G:157:CYS:HA	2.02	0.41
1:G:211:GLU:HA	1:G:212:PRO:HD3	1.90	0.41
1:G:273:ARG:NH1	1:G:287:GLN:OE1	2.52	0.41
1:G:138:ILE:HB	8:C:1:NAG:H61	2.03	0.41
3:L:34:ILE:HD13	3:L:50:ASN:H	1.86	0.41
1:G:50:THR:HG22	1:G:488:VAL:HG11	2.03	0.41
1:G:151:ARG:O	1:G:153:GLU:N	2.54	0.41
1:G:307:ILE:HD11	1:G:317:PHE:HD2	1.86	0.41
3:L:89:HIS:NE2	3:L:95(C):ASN:O	2.38	0.41
4:H:124:PRO:HD2	4:H:211:PRO:HA	2.02	0.41
6:E:46:LEU:HG	6:E:55:ALA:HB2	2.03	0.41
1:G:112:TRP:CG	1:G:427:TRP:HZ3	2.39	0.40
14:B:1618:NAG:H4	6:E:53:GLU:HG2	2.04	0.40
4:H:100(P):MET:N	4:H:100(P):MET:SD	2.94	0.40
5:D:139:GLY:HA2	5:D:154:TRP:CZ2	2.56	0.40
1:G:95:MET:SD	1:G:235:GLY:HA3	2.61	0.40
2:B:597:GLY:HA2	2:B:651:ASN:HD21	1.87	0.40
1:G:104:MET:O	1:G:108:ILE:HG12	2.21	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	G	447/481 (93%)	405 (91%)	35 (8%)	7 (2%)	7	30
2	B	122/153 (80%)	108 (88%)	11 (9%)	3 (2%)	4	21
3	L	208/213 (98%)	196 (94%)	10 (5%)	2 (1%)	12	41
4	H	224/235 (95%)	211 (94%)	11 (5%)	2 (1%)	14	44
5	D	240/243 (99%)	228 (95%)	12 (5%)	0	100	100
6	E	211/216 (98%)	197 (93%)	14 (7%)	0	100	100
All	All	1452/1541 (94%)	1345 (93%)	93 (6%)	14 (1%)	12	41

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	138	ILE
3	L	110	PRO
1	G	71	THR
1	G	152	GLY
2	B	602	LEU
1	G	151	ARG
1	G	258	GLN
3	L	199	GLU
4	H	142	ASP
1	G	64	GLU
1	G	67	ASN
2	B	599	SER
2	B	601	LYS
4	H	188	GLY

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	G	404/428 (94%)	399 (99%)	5 (1%)	63	78
2	B	108/129 (84%)	104 (96%)	4 (4%)	30	61
3	L	178/181 (98%)	176 (99%)	2 (1%)	65	78
4	H	198/205 (97%)	196 (99%)	2 (1%)	68	79
5	D	205/206 (100%)	205 (100%)	0	100	100
6	E	186/189 (98%)	185 (100%)	1 (0%)	81	85
All	All	1279/1338 (96%)	1265 (99%)	14 (1%)	65	78

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	123	THR
1	G	125	LEU
1	G	138	ILE
1	G	182	VAL
1	G	461	THR
2	B	536	THR
2	B	570	VAL
2	B	606	THR
2	B	619	LEU
3	L	54	ARG
3	L	111	LYS
4	H	23	ASN
4	H	139	LEU
6	E	96	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	67	ASN
1	G	462	ASN
3	L	109	GLN

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Mol	Chain	Res	Type
3	L	189	HIS
4	H	32	ASN
5	D	192	GLN
5	D	199	ASN
6	E	167	GLN
6	E	184	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

51 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	0.33	0	17,19,21	0.43	0
7	NAG	A	2	7	14,14,15	0.45	0	17,19,21	1.36	2 (11%)
7	BMA	A	3	7	11,11,12	0.66	0	15,15,17	0.71	0
7	MAN	A	4	7	11,11,12	0.81	1 (9%)	15,15,17	1.20	2 (13%)
7	MAN	A	5	7	11,11,12	0.69	0	15,15,17	0.96	2 (13%)
7	MAN	A	6	7	11,11,12	0.61	0	15,15,17	1.03	2 (13%)
7	MAN	A	7	7	11,11,12	0.65	0	15,15,17	1.13	2 (13%)
8	NAG	C	1	1,8	14,14,15	0.42	0	17,19,21	0.49	0
8	NAG	C	2	8	14,14,15	0.39	0	17,19,21	0.39	0
8	BMA	C	3	8	11,11,12	0.53	0	15,15,17	0.76	0
8	MAN	C	4	8	11,11,12	0.67	0	15,15,17	1.00	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	F	1	1,9	14,14,15	0.18	0	17,19,21	0.43	0
9	NAG	F	2	9	14,14,15	0.22	0	17,19,21	0.40	0
10	NAG	I	1	1,10	14,14,15	0.26	0	17,19,21	0.49	0
10	NAG	I	2	10	14,14,15	0.33	0	17,19,21	0.44	0
10	BMA	I	3	10	11,11,12	0.66	0	15,15,17	0.66	0
10	MAN	I	4	10	11,11,12	0.68	0	15,15,17	1.03	2 (13%)
10	MAN	I	5	10	11,11,12	0.79	0	15,15,17	1.15	2 (13%)
10	MAN	I	6	10	11,11,12	0.63	0	15,15,17	1.04	2 (13%)
9	NAG	J	1	1,9	14,14,15	0.22	0	17,19,21	0.39	0
9	NAG	J	2	9	14,14,15	0.21	0	17,19,21	0.45	0
9	NAG	K	1	1,9	14,14,15	0.24	0	17,19,21	0.64	0
9	NAG	K	2	9	14,14,15	0.23	0	17,19,21	0.42	0
9	NAG	M	1	1,9	14,14,15	0.24	0	17,19,21	0.46	0
9	NAG	M	2	9	14,14,15	0.32	0	17,19,21	0.48	0
11	NAG	N	1	1,11	14,14,15	0.20	0	17,19,21	0.51	0
11	NAG	N	2	11	14,14,15	0.25	0	17,19,21	0.37	0
11	BMA	N	3	11	11,11,12	0.55	0	15,15,17	0.81	0
12	NAG	O	1	1,12	14,14,15	0.26	0	17,19,21	0.38	0
12	NAG	O	2	12	14,14,15	0.23	0	17,19,21	0.39	0
12	BMA	O	3	12	11,11,12	0.59	0	15,15,17	0.73	0
12	MAN	O	4	12	11,11,12	0.69	0	15,15,17	0.99	2 (13%)
12	MAN	O	5	12	11,11,12	0.68	0	15,15,17	1.04	2 (13%)
9	NAG	P	1	1,9	14,14,15	0.29	0	17,19,21	0.46	0
9	NAG	P	2	9	14,14,15	0.47	0	17,19,21	1.33	2 (11%)
9	NAG	Q	1	1,9	14,14,15	0.22	0	17,19,21	0.43	0
9	NAG	Q	2	9	14,14,15	0.22	0	17,19,21	0.42	0
9	NAG	R	1	1,9	14,14,15	0.27	0	17,19,21	0.48	0
9	NAG	R	2	9	14,14,15	0.20	0	17,19,21	0.42	0
9	NAG	S	1	1,9	14,14,15	0.20	0	17,19,21	0.40	0
9	NAG	S	2	9	14,14,15	0.24	0	17,19,21	0.44	0
13	NAG	T	1	1,13	14,14,15	0.25	0	17,19,21	0.40	0
13	MAN	T	10	13	11,11,12	0.70	0	15,15,17	0.96	2 (13%)
13	NAG	T	2	13	14,14,15	0.30	0	17,19,21	0.55	0
13	BMA	T	3	13	11,11,12	0.74	0	15,15,17	1.19	1 (6%)
13	MAN	T	4	13	11,11,12	0.63	0	15,15,17	1.05	1 (6%)
13	MAN	T	5	13	11,11,12	0.58	0	15,15,17	1.00	1 (6%)
13	MAN	T	6	13	11,11,12	0.60	0	15,15,17	1.32	2 (13%)
13	MAN	T	7	13	11,11,12	0.78	0	15,15,17	0.95	2 (13%)
13	MAN	T	8	13	11,11,12	0.69	0	15,15,17	0.97	2 (13%)
13	MAN	T	9	13	11,11,12	0.81	0	15,15,17	1.13	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	1,7	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	4/6/23/26	0/1/1/1
7	BMA	A	3	7	-	2/2/19/22	0/1/1/1
7	MAN	A	4	7	-	0/2/19/22	0/1/1/1
7	MAN	A	5	7	-	0/2/19/22	0/1/1/1
7	MAN	A	6	7	-	0/2/19/22	0/1/1/1
7	MAN	A	7	7	-	0/2/19/22	0/1/1/1
8	NAG	C	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1
8	BMA	C	3	8	-	0/2/19/22	0/1/1/1
8	MAN	C	4	8	-	1/2/19/22	0/1/1/1
9	NAG	F	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	F	2	9	-	1/6/23/26	0/1/1/1
10	NAG	I	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	I	2	10	-	2/6/23/26	0/1/1/1
10	BMA	I	3	10	-	0/2/19/22	0/1/1/1
10	MAN	I	4	10	-	2/2/19/22	0/1/1/1
10	MAN	I	5	10	-	0/2/19/22	1/1/1/1
10	MAN	I	6	10	-	0/2/19/22	0/1/1/1
9	NAG	J	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	J	2	9	-	2/6/23/26	0/1/1/1
9	NAG	K	1	1,9	-	4/6/23/26	0/1/1/1
9	NAG	K	2	9	-	0/6/23/26	0/1/1/1
9	NAG	M	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	M	2	9	-	2/6/23/26	0/1/1/1
11	NAG	N	1	1,11	-	4/6/23/26	0/1/1/1
11	NAG	N	2	11	-	0/6/23/26	0/1/1/1
11	BMA	N	3	11	-	2/2/19/22	0/1/1/1
12	NAG	O	1	1,12	-	2/6/23/26	0/1/1/1
12	NAG	O	2	12	-	2/6/23/26	0/1/1/1
12	BMA	O	3	12	-	2/2/19/22	0/1/1/1
12	MAN	O	4	12	-	1/2/19/22	0/1/1/1
12	MAN	O	5	12	-	0/2/19/22	0/1/1/1
9	NAG	P	1	1,9	-	4/6/23/26	0/1/1/1
9	NAG	P	2	9	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	Q	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	2/6/23/26	0/1/1/1
9	NAG	R	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	R	2	9	-	2/6/23/26	0/1/1/1
9	NAG	S	1	1,9	-	1/6/23/26	0/1/1/1
9	NAG	S	2	9	-	2/6/23/26	0/1/1/1
13	NAG	T	1	1,13	-	2/6/23/26	0/1/1/1
13	MAN	T	10	13	-	0/2/19/22	0/1/1/1
13	NAG	T	2	13	-	4/6/23/26	0/1/1/1
13	BMA	T	3	13	-	0/2/19/22	0/1/1/1
13	MAN	T	4	13	-	0/2/19/22	0/1/1/1
13	MAN	T	5	13	-	0/2/19/22	0/1/1/1
13	MAN	T	6	13	-	1/2/19/22	0/1/1/1
13	MAN	T	7	13	-	2/2/19/22	0/1/1/1
13	MAN	T	8	13	-	0/2/19/22	0/1/1/1
13	MAN	T	9	13	-	0/2/19/22	1/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	4	MAN	C1-C2	2.23	1.57	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2	NAG	C2-N2-C7	4.63	129.10	122.90
9	P	2	NAG	C2-N2-C7	4.56	129.01	122.90
13	T	6	MAN	C1-O5-C5	3.92	117.44	112.19
10	I	5	MAN	C1-O5-C5	3.36	116.69	112.19
13	T	9	MAN	C1-O5-C5	3.31	116.62	112.19
7	A	4	MAN	C1-O5-C5	2.91	116.08	112.19
13	T	4	MAN	C1-O5-C5	2.87	116.03	112.19
7	A	7	MAN	C1-O5-C5	2.81	115.95	112.19
13	T	3	BMA	C1-O5-C5	2.72	115.83	112.19
13	T	5	MAN	C1-O5-C5	2.67	115.76	112.19
10	I	4	MAN	O2-C2-C3	-2.63	104.71	110.15
7	A	6	MAN	C1-O5-C5	2.55	115.60	112.19
10	I	6	MAN	C1-O5-C5	2.53	115.58	112.19
10	I	4	MAN	C1-O5-C5	2.43	115.44	112.19
12	O	5	MAN	C1-O5-C5	2.41	115.42	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	8	MAN	C1-O5-C5	2.39	115.39	112.19
8	C	4	MAN	C1-O5-C5	2.26	115.22	112.19
7	A	7	MAN	O2-C2-C3	-2.24	105.50	110.15
12	O	4	MAN	C1-O5-C5	2.24	115.19	112.19
10	I	6	MAN	O2-C2-C3	-2.22	105.55	110.15
7	A	6	MAN	O2-C2-C3	-2.22	105.55	110.15
12	O	5	MAN	O2-C2-C3	-2.20	105.59	110.15
8	C	4	MAN	O2-C2-C3	-2.20	105.60	110.15
9	P	2	NAG	C1-C2-N2	2.19	113.89	110.43
12	O	4	MAN	O2-C2-C3	-2.19	105.62	110.15
13	T	10	MAN	C1-O5-C5	2.18	115.11	112.19
7	A	2	NAG	C1-C2-N2	2.17	113.86	110.43
7	A	5	MAN	O2-C2-C3	-2.16	105.68	110.15
7	A	5	MAN	C1-O5-C5	2.16	115.08	112.19
13	T	6	MAN	O2-C2-C3	-2.15	105.69	110.15
10	I	5	MAN	O2-C2-C3	-2.15	105.70	110.15
7	A	4	MAN	O2-C2-C3	-2.13	105.73	110.15
13	T	10	MAN	O2-C2-C3	-2.12	105.75	110.15
13	T	9	MAN	O2-C2-C3	-2.12	105.77	110.15
13	T	7	MAN	O2-C2-C3	-2.07	105.86	110.15
13	T	7	MAN	C1-O5-C5	2.06	114.95	112.19
13	T	8	MAN	O2-C2-C3	-2.02	105.96	110.15

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	O	3	BMA	C4-C5-C6-O6
9	R	1	NAG	O5-C5-C6-O6
12	O	2	NAG	O5-C5-C6-O6
7	A	3	BMA	C4-C5-C6-O6
13	T	2	NAG	O5-C5-C6-O6
12	O	2	NAG	C4-C5-C6-O6
9	J	2	NAG	O5-C5-C6-O6
10	I	4	MAN	O5-C5-C6-O6
9	R	1	NAG	C4-C5-C6-O6
11	N	3	BMA	O5-C5-C6-O6
9	P	1	NAG	C4-C5-C6-O6
12	O	3	BMA	O5-C5-C6-O6
9	J	2	NAG	C4-C5-C6-O6
9	K	1	NAG	O5-C5-C6-O6
9	F	1	NAG	C4-C5-C6-O6

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

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Mol	Chain	Res	Type	Atoms
7	A	1	NAG	C4-C5-C6-O6
9	K	1	NAG	C3-C2-N2-C7
13	T	2	NAG	C3-C2-N2-C7
7	A	1	NAG	O5-C5-C6-O6
9	S	1	NAG	O5-C5-C6-O6
7	A	2	NAG	C1-C2-N2-C7
9	J	1	NAG	C1-C2-N2-C7
9	K	1	NAG	C1-C2-N2-C7
9	P	2	NAG	C1-C2-N2-C7
13	T	2	NAG	C1-C2-N2-C7
7	A	2	NAG	C3-C2-N2-C7
9	P	2	NAG	C3-C2-N2-C7

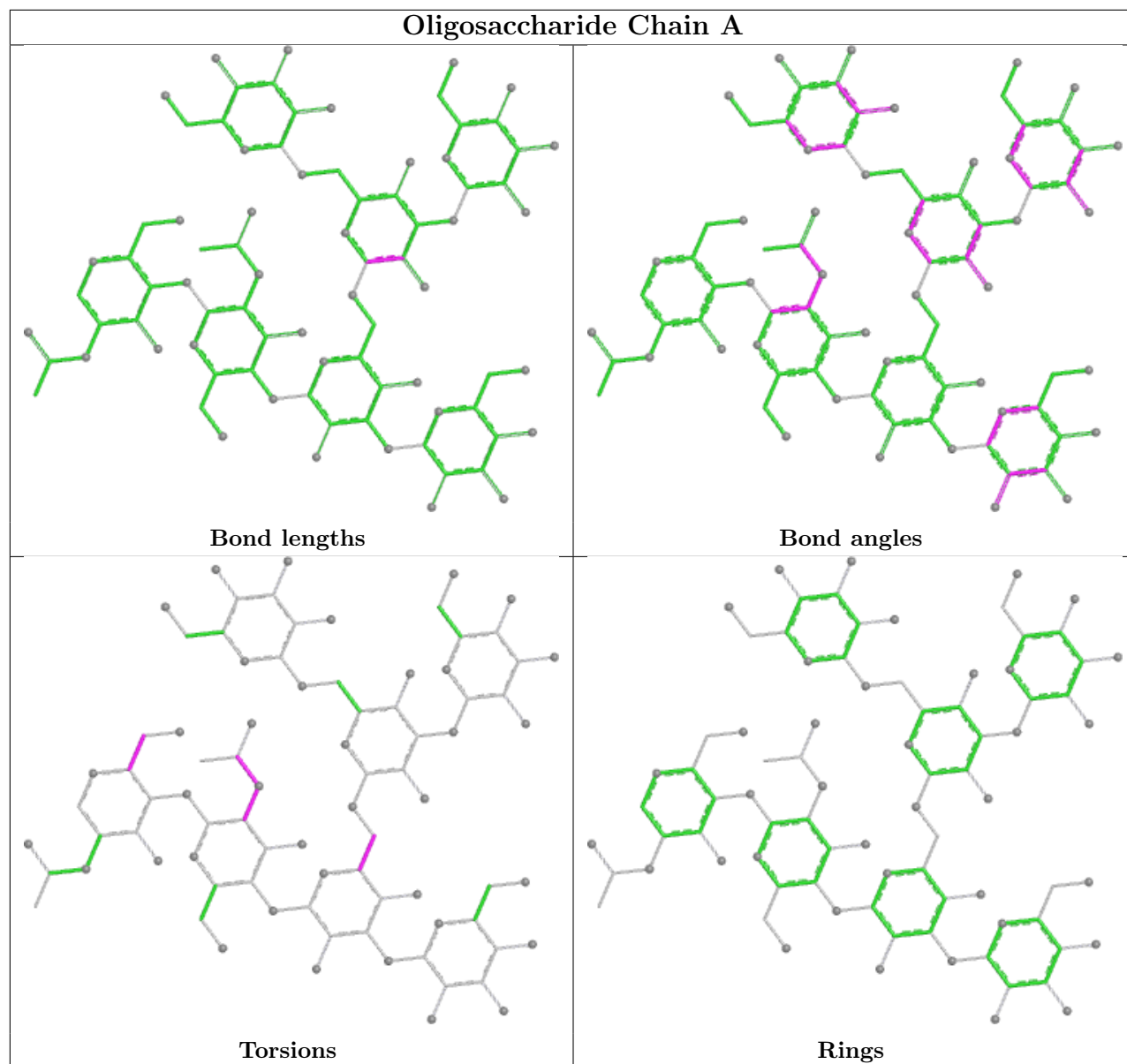
All (2) ring outliers are listed below:

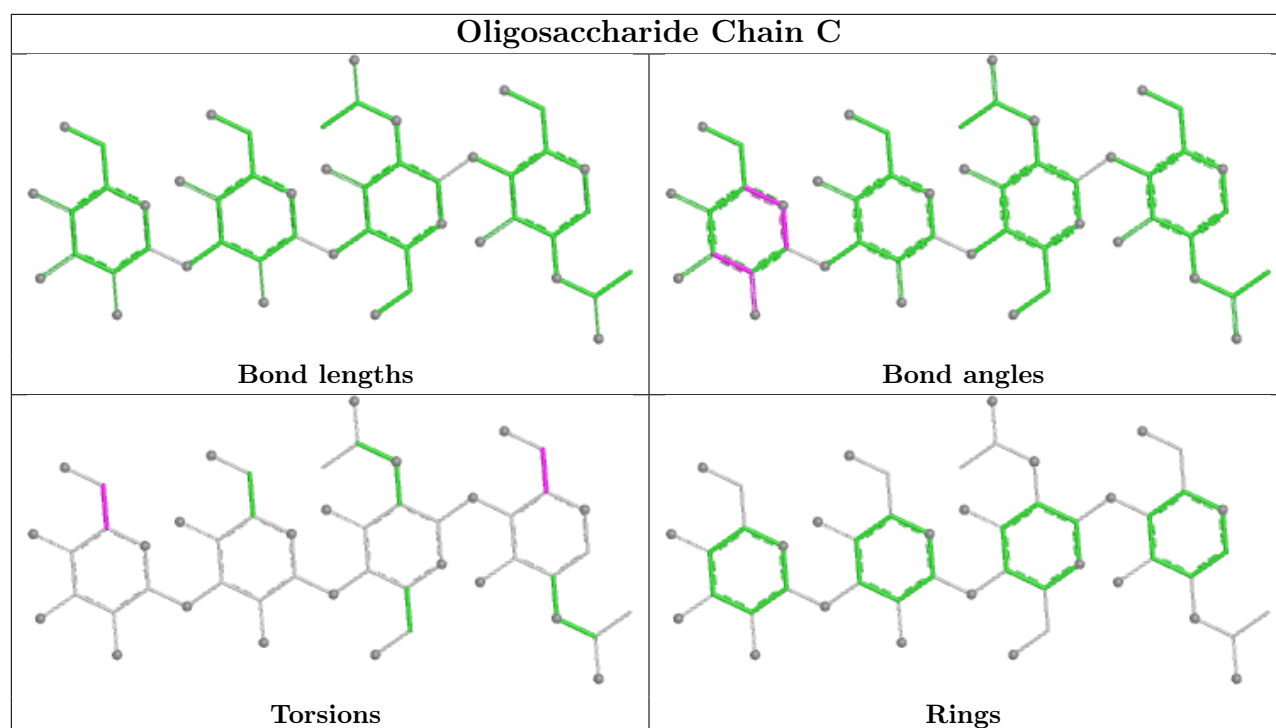
Mol	Chain	Res	Type	Atoms
13	T	9	MAN	C1-C2-C3-C4-C5-O5
10	I	5	MAN	C1-C2-C3-C4-C5-O5

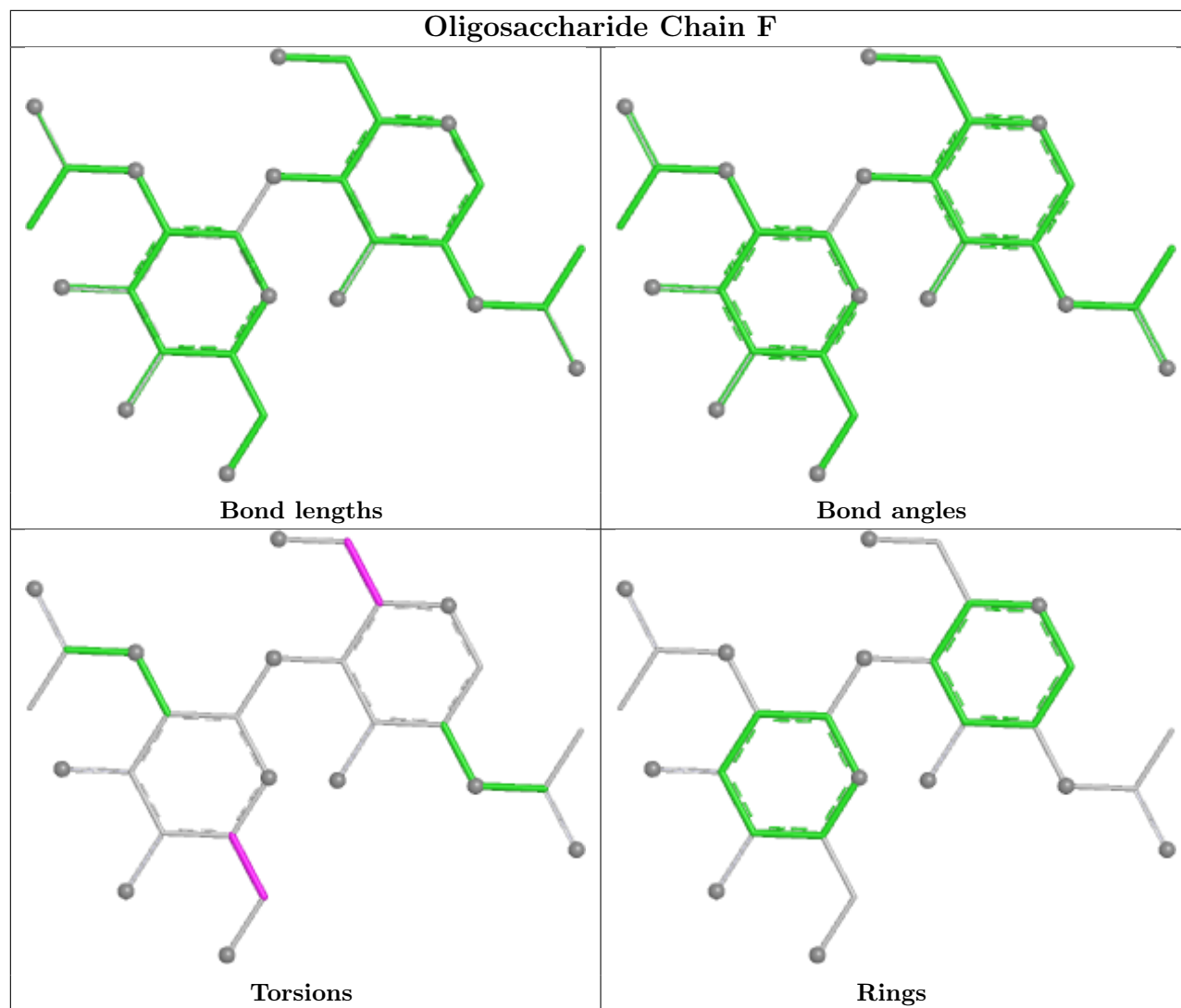
12 monomers are involved in 10 short contacts:

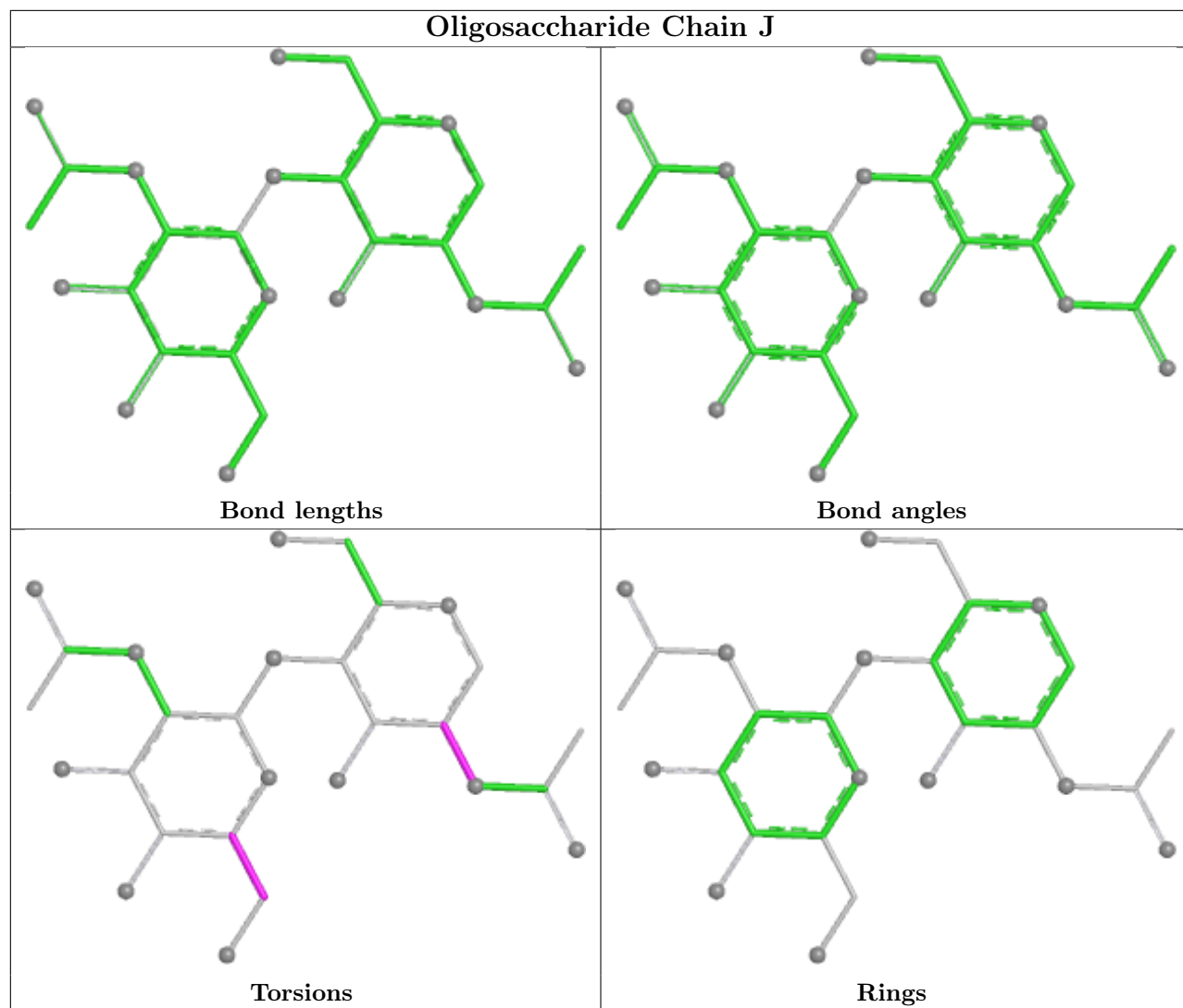
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1	NAG	1	0
13	T	2	NAG	1	0
7	A	6	MAN	1	0
9	P	1	NAG	1	0
7	A	2	NAG	1	0
7	A	7	MAN	1	0
8	C	4	MAN	1	0
9	P	2	NAG	2	0
13	T	8	MAN	1	0
7	A	3	BMA	1	0
7	A	4	MAN	1	0
13	T	9	MAN	1	0

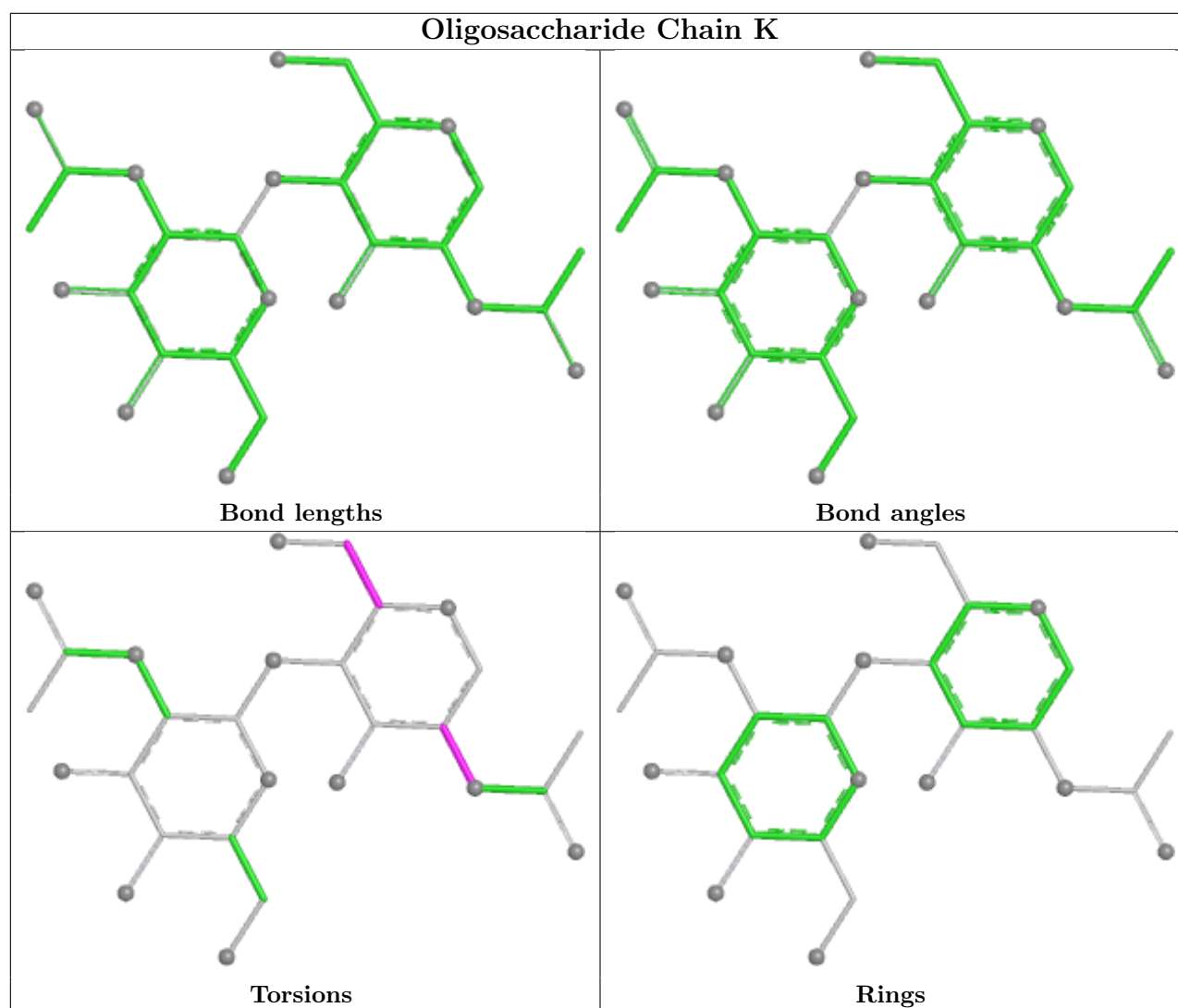
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

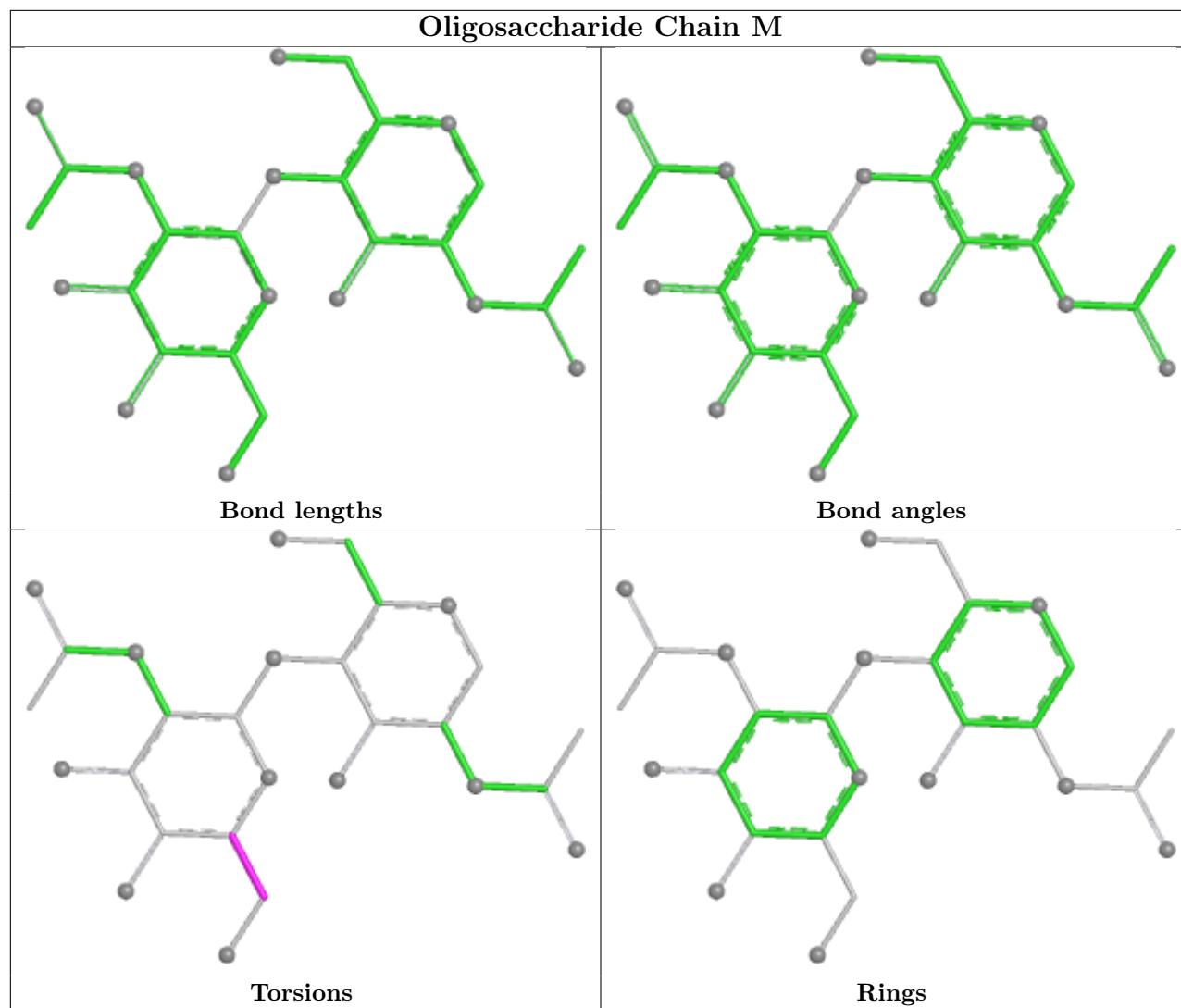


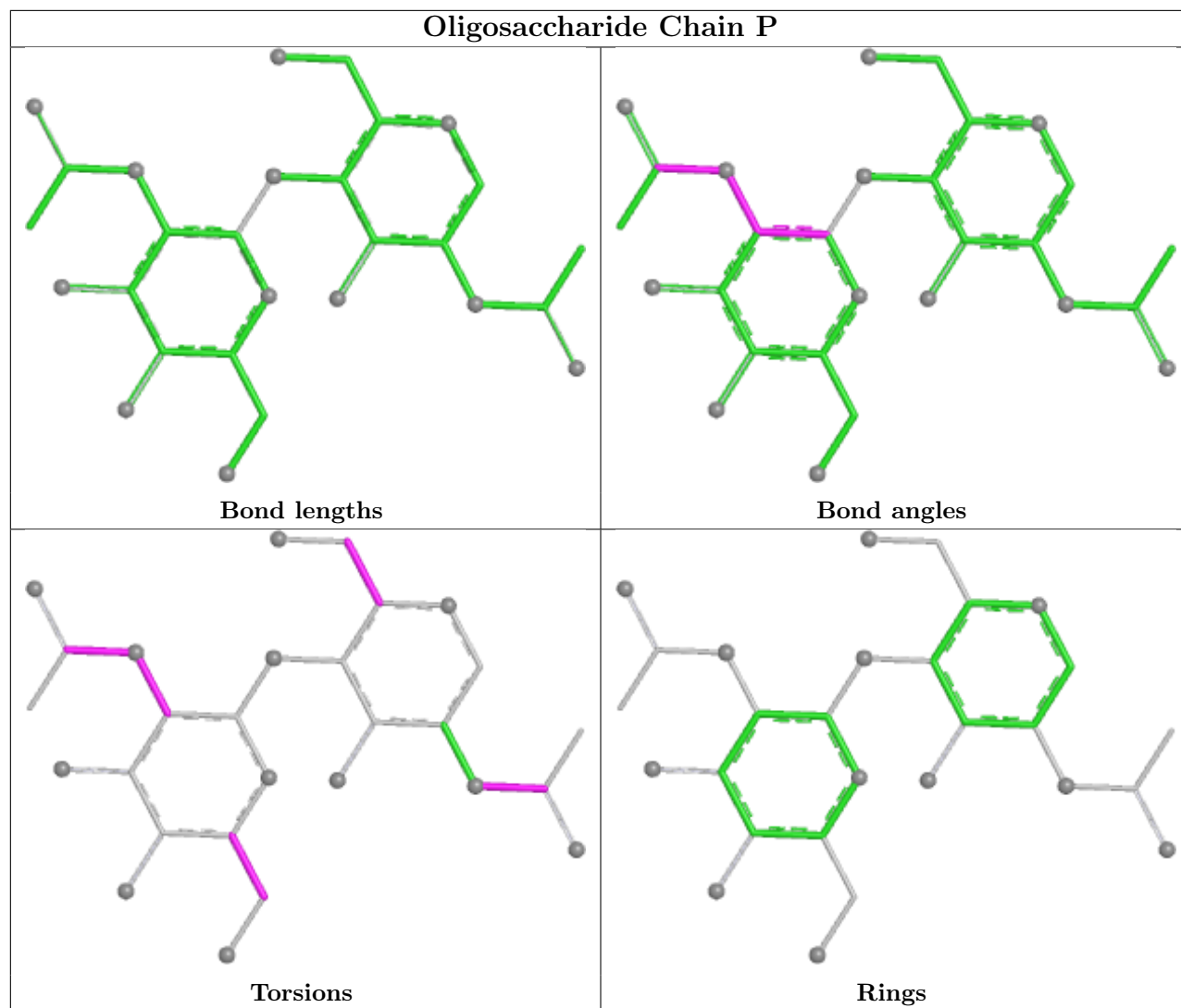


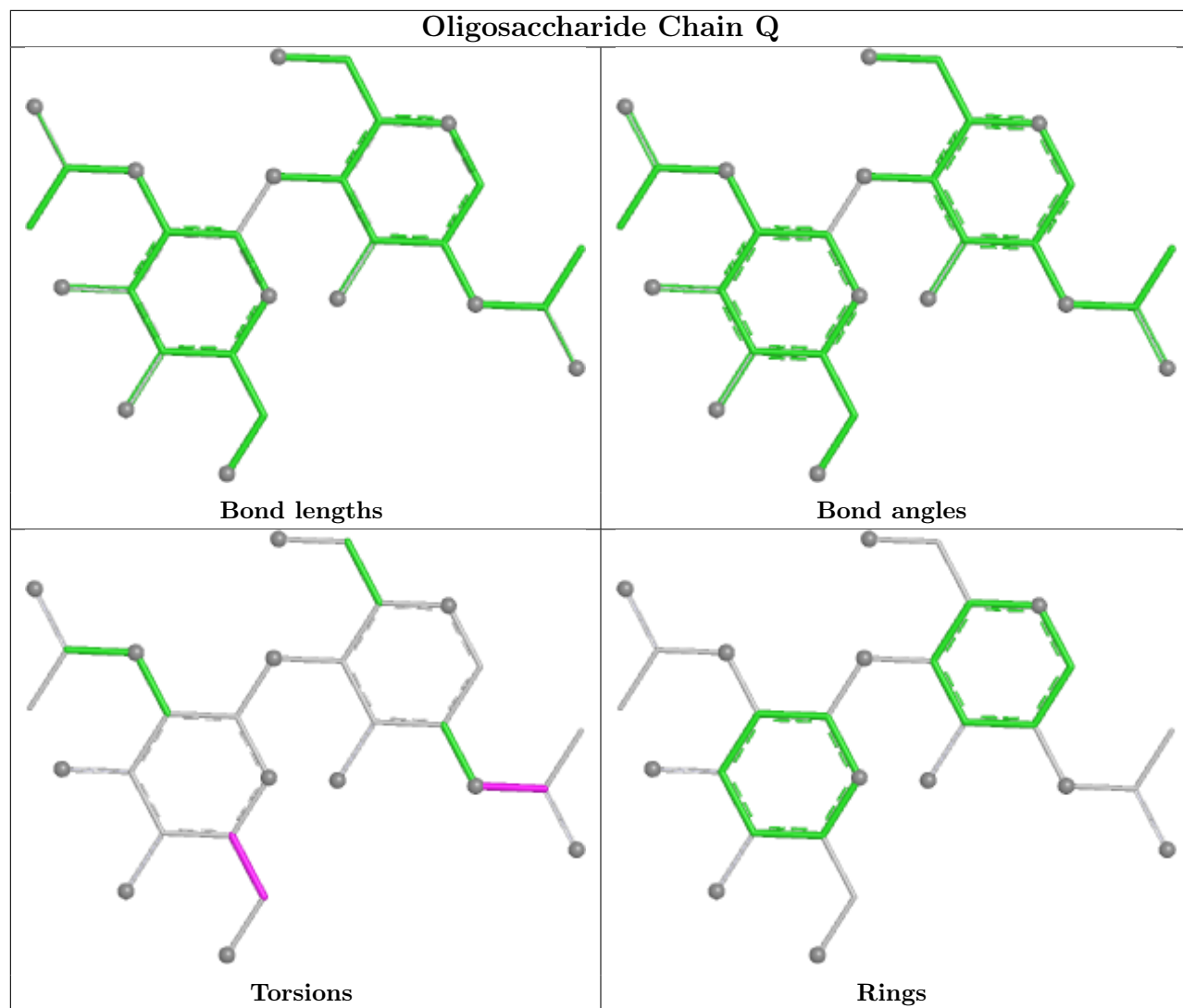


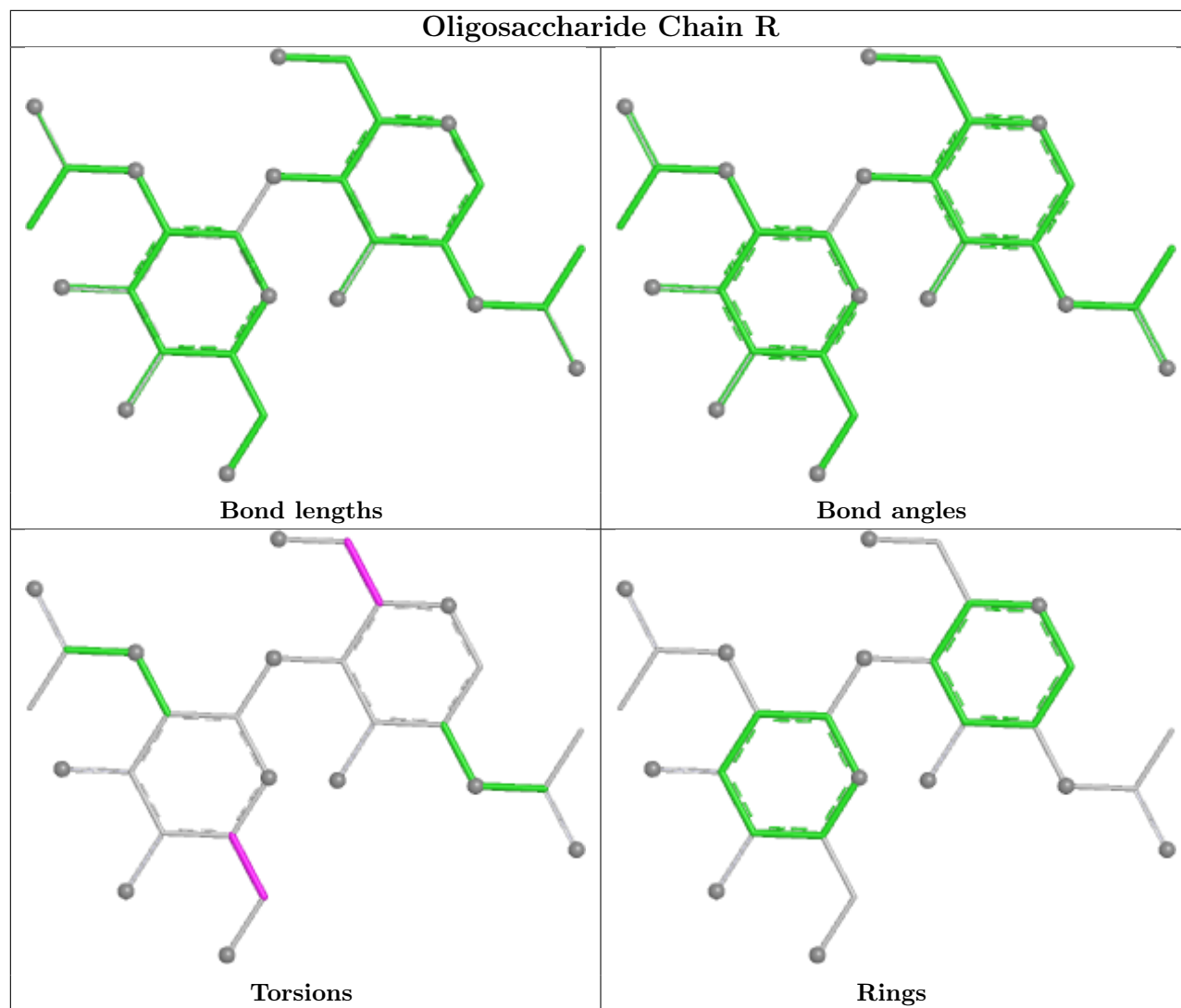


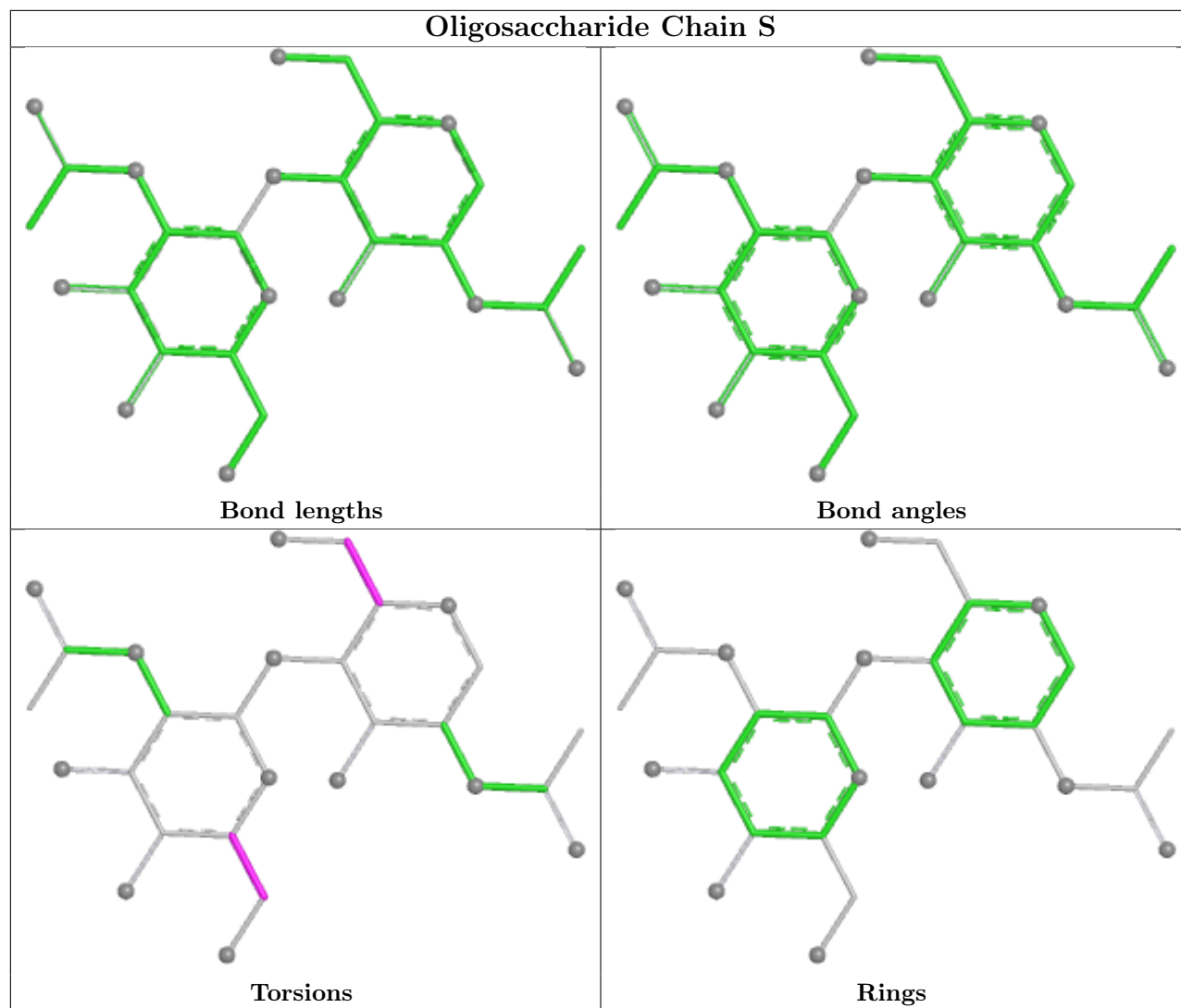


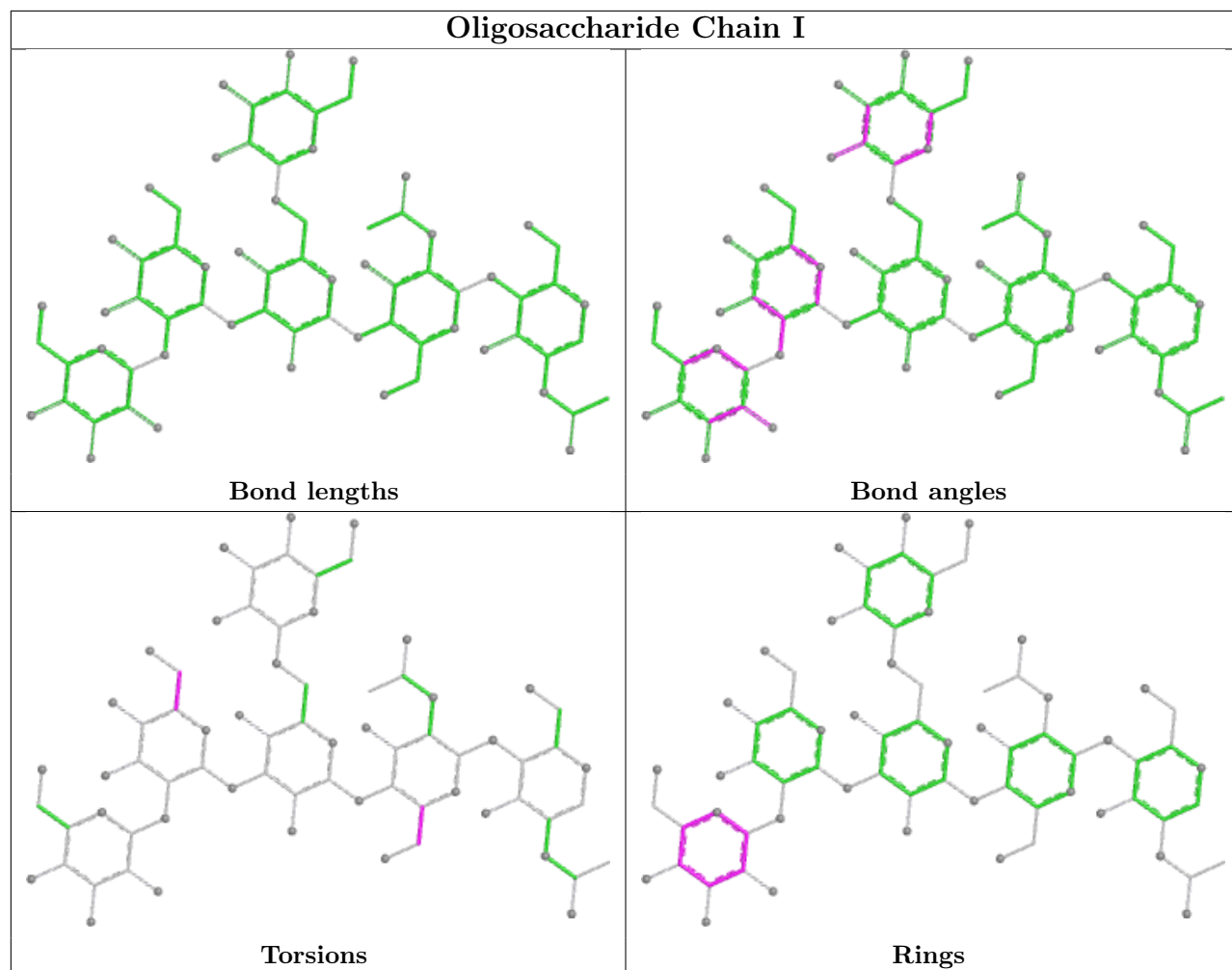


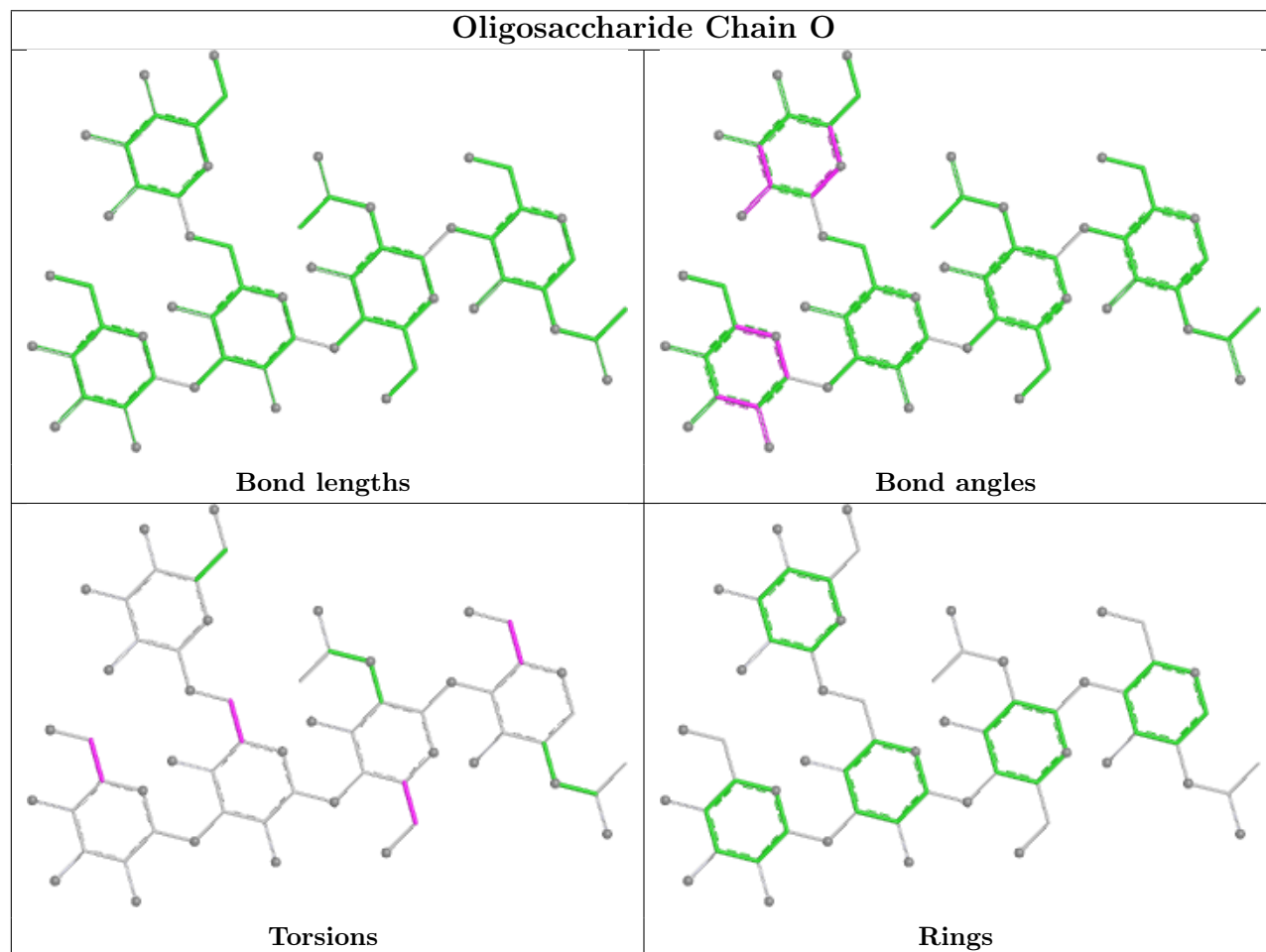
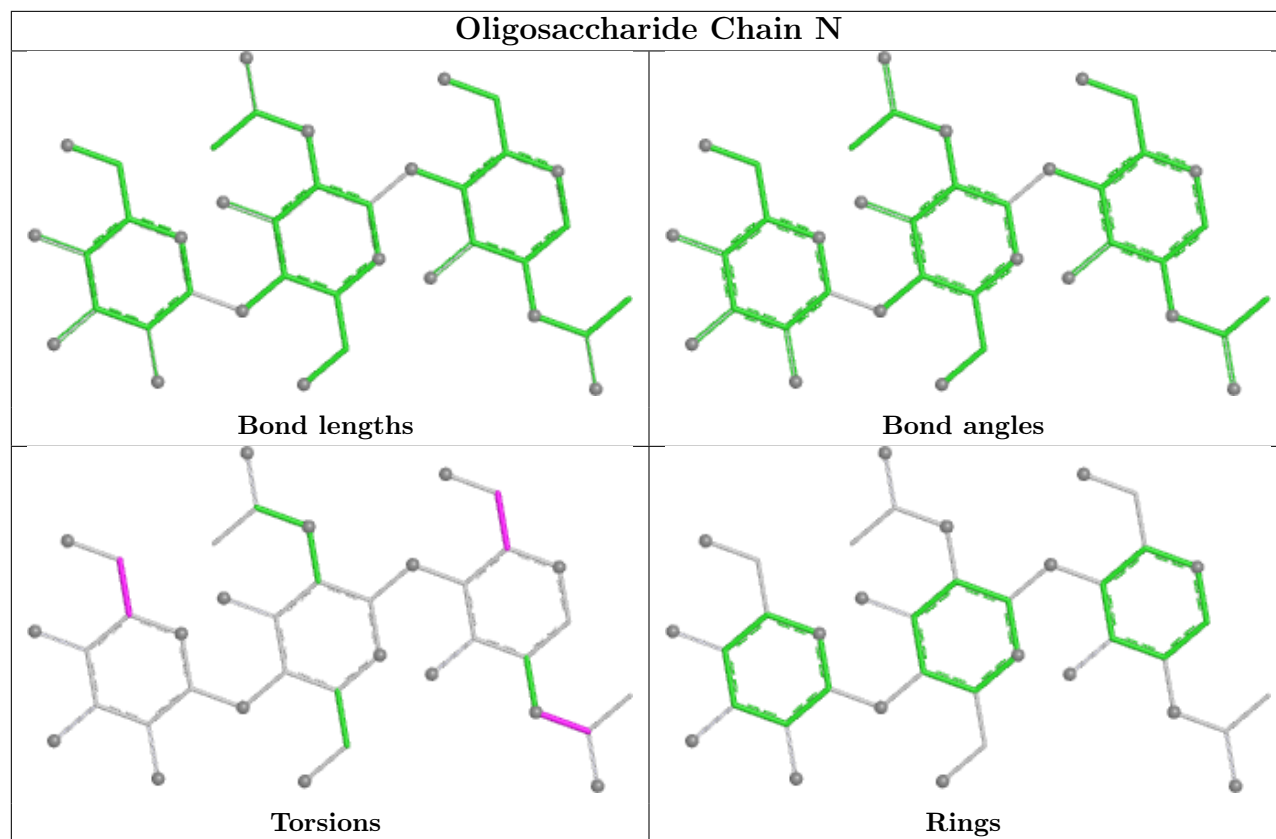


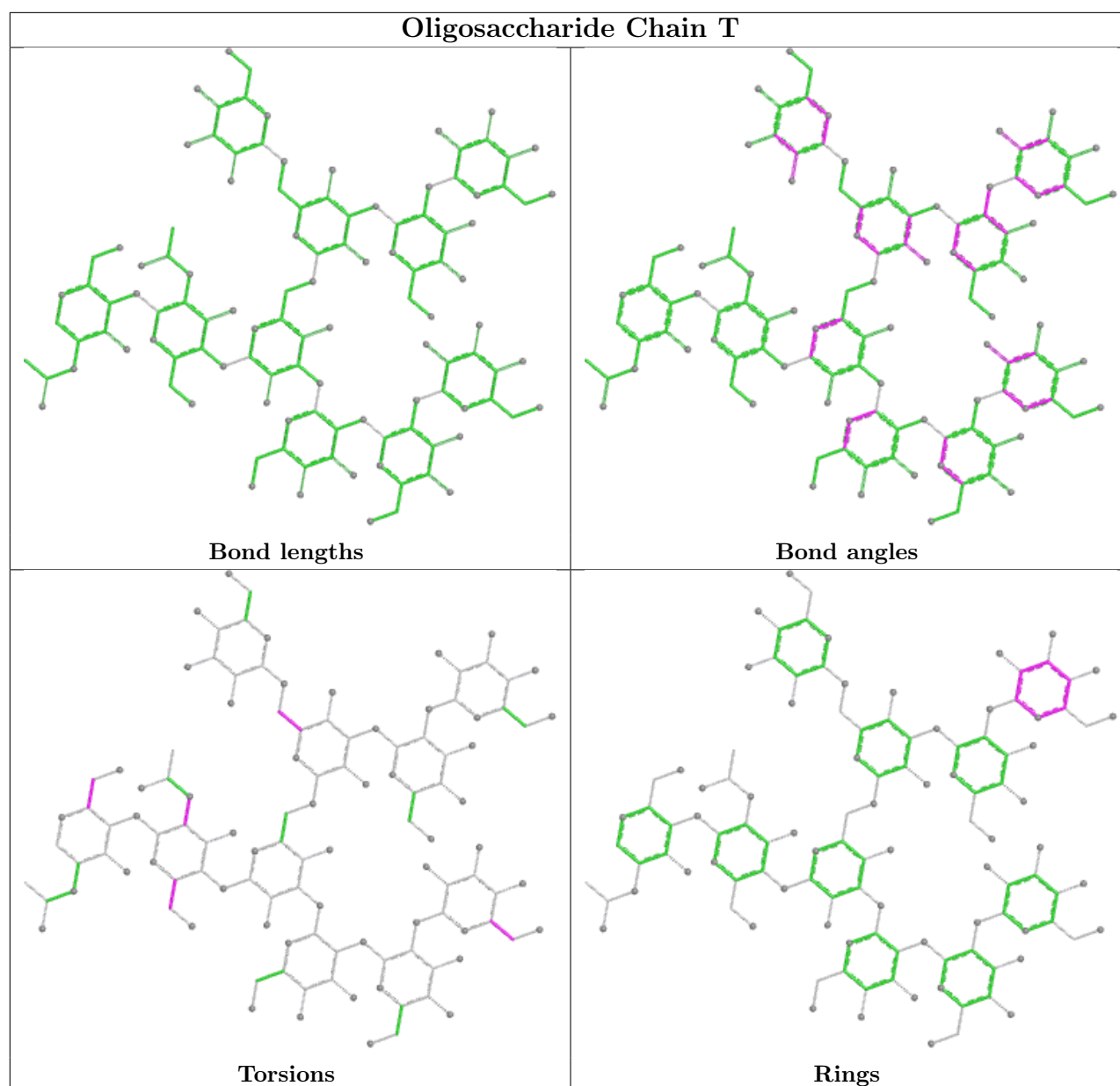












5.6 Ligand geometry [i](#)

18 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	1276	1	14,14,15	0.46	0	17,19,21	1.34	2 (11%)
15	SO4	G	602	-	4,4,4	0.23	0	6,6,6	0.08	0
14	NAG	G	1839	1	14,14,15	0.27	0	17,19,21	0.41	0
15	SO4	G	601	-	4,4,4	0.24	0	6,6,6	0.08	0
15	SO4	G	604	-	4,4,4	0.23	0	6,6,6	0.08	0
14	NAG	B	1618	2	14,14,15	0.22	0	17,19,21	0.37	0
14	NAG	G	1355	1	14,14,15	0.23	0	17,19,21	0.39	0
15	SO4	L	301	-	4,4,4	0.22	0	6,6,6	0.08	0
15	SO4	B	702	-	4,4,4	0.24	0	6,6,6	0.08	0
15	SO4	G	603	-	4,4,4	0.23	0	6,6,6	0.07	0
14	NAG	G	1133	1	14,14,15	0.25	0	17,19,21	0.41	0
14	NAG	H	523	4	14,14,15	0.24	0	17,19,21	0.41	0
15	SO4	G	605	-	4,4,4	0.24	0	6,6,6	0.07	0
15	SO4	G	607	-	4,4,4	0.24	0	6,6,6	0.07	0
15	SO4	B	701	-	4,4,4	0.23	0	6,6,6	0.07	0
15	SO4	G	606	-	4,4,4	0.26	0	6,6,6	0.20	0
14	NAG	B	1611	2	14,14,15	0.24	0	17,19,21	0.43	0
14	NAG	B	1637	2	14,14,15	0.26	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	G	1276	1	-	6/6/23/26	0/1/1/1
14	NAG	G	1839	1	-	1/6/23/26	0/1/1/1
14	NAG	B	1618	2	-	3/6/23/26	0/1/1/1
14	NAG	G	1355	1	-	2/6/23/26	0/1/1/1
14	NAG	G	1133	1	-	1/6/23/26	0/1/1/1
14	NAG	H	523	4	-	2/6/23/26	0/1/1/1
14	NAG	B	1611	2	-	2/6/23/26	0/1/1/1
14	NAG	B	1637	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	1276	NAG	C2-N2-C7	4.62	129.09	122.90
14	G	1276	NAG	C1-C2-N2	2.21	113.91	110.43

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	G	1276	NAG	O5-C5-C6-O6
14	G	1276	NAG	C4-C5-C6-O6
14	B	1618	NAG	O5-C5-C6-O6
14	B	1618	NAG	C4-C5-C6-O6
14	B	1637	NAG	O5-C5-C6-O6
14	G	1276	NAG	C8-C7-N2-C2
14	G	1276	NAG	O7-C7-N2-C2
14	G	1355	NAG	C8-C7-N2-C2
14	G	1355	NAG	O7-C7-N2-C2
14	H	523	NAG	O5-C5-C6-O6
14	B	1637	NAG	C4-C5-C6-O6
14	B	1611	NAG	C4-C5-C6-O6
14	G	1133	NAG	O5-C5-C6-O6
14	B	1611	NAG	O5-C5-C6-O6
14	H	523	NAG	C4-C5-C6-O6
14	G	1839	NAG	O5-C5-C6-O6
14	G	1276	NAG	C1-C2-N2-C7
14	B	1618	NAG	C1-C2-N2-C7
14	G	1276	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	G	1276	NAG	1	0
15	G	602	SO4	1	0
14	B	1618	NAG	2	0
15	B	701	SO4	1	0
15	G	606	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	G	453/481 (94%)	0.01	8 (1%) 67 47	33, 72, 145, 193	0
2	B	126/153 (82%)	0.24	3 (2%) 59 38	38, 77, 145, 176	0
3	L	210/213 (98%)	0.23	6 (2%) 53 32	60, 96, 142, 172	0
4	H	228/235 (97%)	0.20	7 (3%) 51 30	65, 111, 160, 199	0
5	D	242/243 (99%)	0.36	12 (4%) 34 18	51, 123, 284, 386	0
6	E	213/216 (98%)	0.43	12 (5%) 30 16	82, 146, 238, 257	0
All	All	1472/1541 (95%)	0.21	48 (3%) 49 29	33, 97, 220, 386	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	E	117	LEU	4.2
4	H	138	CYS	3.9
3	L	108	SER	3.6
2	B	571	TRP	3.3
1	G	71	THR	3.0
4	H	100(J)	TRP	3.0
1	G	505	VAL	2.9
6	E	115	VAL	2.9
6	E	136	ILE	2.9
4	H	125	SER	2.8
4	H	123	ALA	2.8
4	H	188	GLY	2.7
5	D	219	GLY	2.7
3	L	184	GLU	2.7
5	D	222	VAL	2.7
5	D	122	PHE	2.6
6	E	157	ALA	2.6
4	H	209	VAL	2.5
1	G	68	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
5	D	121	VAL	2.5
6	E	125	LEU	2.4
6	E	135	LEU	2.4
6	E	119	PRO	2.4
6	E	3	VAL	2.4
1	G	73	ALA	2.3
2	B	664	ASP	2.3
5	D	127	SER	2.3
5	D	183	THR	2.3
3	L	168	GLN	2.3
1	G	180	ASP	2.3
5	D	181	VAL	2.3
2	B	660	LEU	2.2
6	E	118	PHE	2.2
3	L	121	PRO	2.2
5	D	207	VAL	2.2
5	D	185	PRO	2.2
1	G	72	HIS	2.2
3	L	103	THR	2.2
6	E	111	ALA	2.2
5	D	213	PRO	2.1
3	L	114	PRO	2.1
6	E	203	GLU	2.1
5	D	211	VAL	2.1
5	D	218	LYS	2.1
6	E	128	ASN	2.0
4	H	71	LEU	2.0
1	G	139	THR	2.0
1	G	49	GLU	2.0

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.

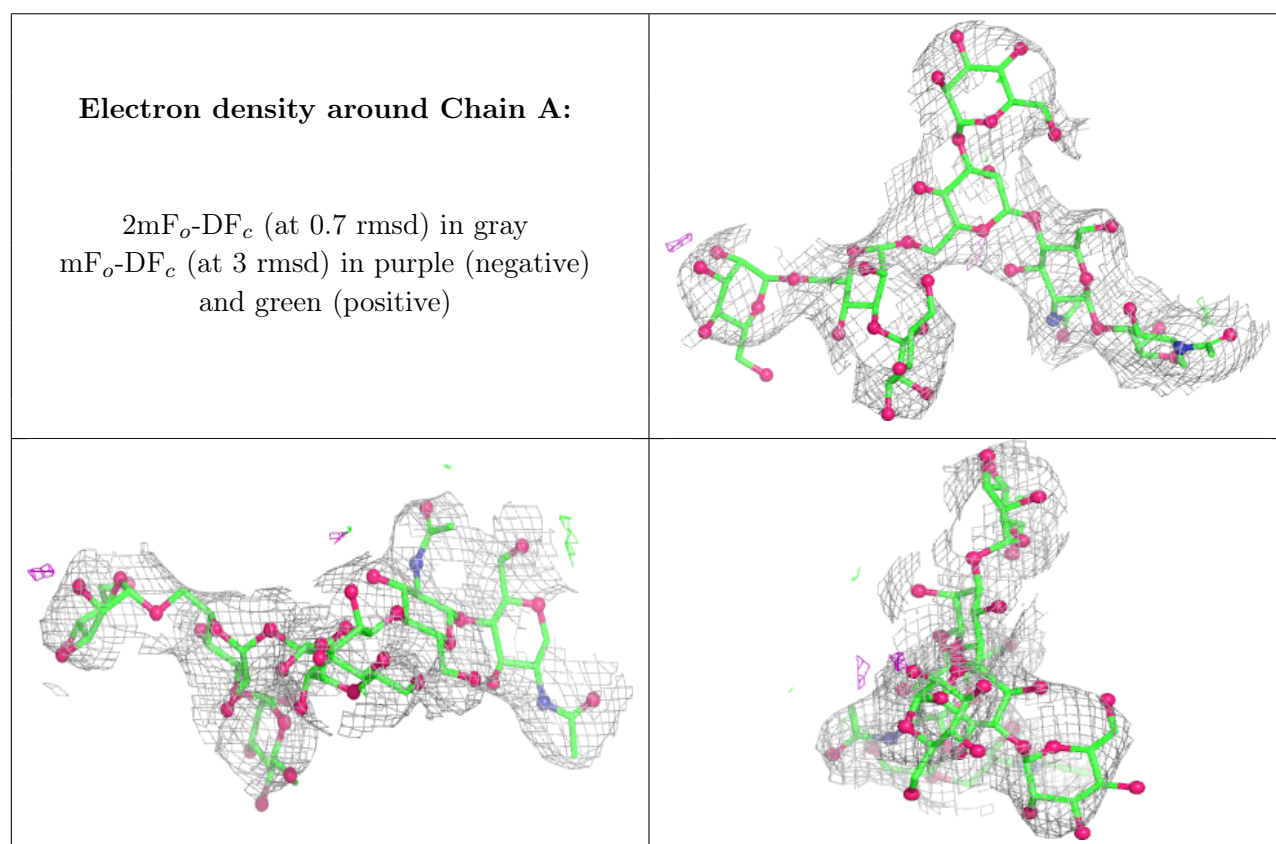
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	A	1	14/15	-	-	35,43,56,57	0
7	NAG	A	2	14/15	-	-	44,56,72,76	0
7	BMA	A	3	11/12	-	-	66,77,101,104	0
7	MAN	A	4	11/12	-	-	107,114,122,123	0
7	MAN	A	5	11/12	-	-	116,133,144,153	0
7	MAN	A	6	11/12	-	-	97,104,117,118	0
7	MAN	A	7	11/12	-	-	68,74,91,105	0
8	NAG	C	1	14/15	-	-	72,98,116,118	0
8	NAG	C	2	14/15	-	-	109,118,126,127	0
8	BMA	C	3	11/12	-	-	123,133,142,149	0
8	MAN	C	4	11/12	-	-	139,156,166,167	0
9	NAG	F	1	14/15	-	-	85,99,116,124	0
9	NAG	F	2	14/15	-	-	135,137,140,141	0
9	NAG	K	2	14/15	0.40	0.14	131,149,156,158	0
9	NAG	M	2	14/15	0.50	0.11	121,142,144,145	0
12	MAN	O	4	11/12	0.53	0.11	110,122,126,127	0
12	MAN	O	5	11/12	0.55	0.10	153,155,158,160	0
13	MAN	T	9	11/12	0.56	0.12	142,149,153,154	0
13	MAN	T	6	11/12	0.63	0.20	115,120,125,126	0
11	BMA	N	3	11/12	0.64	0.11	161,197,227,281	0
9	NAG	P	2	14/15	0.65	0.10	93,107,118,125	0
13	MAN	T	7	11/12	0.66	0.10	100,117,123,132	0
9	NAG	R	2	14/15	0.71	0.12	117,131,142,150	0
12	BMA	O	3	11/12	0.73	0.09	126,135,145,155	0
9	NAG	S	2	14/15	0.74	0.11	117,131,141,146	0
13	MAN	T	8	11/12	0.78	0.09	135,138,146,152	0
11	NAG	N	2	14/15	0.81	0.11	102,124,150,177	0
9	NAG	Q	1	14/15	0.82	0.11	75,106,125,140	0
13	MAN	T	10	11/12	0.82	0.09	94,109,115,117	0
10	BMA	I	3	11/12	-	-	123,129,144,150	0
10	MAN	I	4	11/12	-	-	117,128,138,144	0
10	MAN	I	5	11/12	-	-	131,135,139,140	0
10	MAN	I	6	11/12	-	-	122,141,149,150	0
12	NAG	O	2	14/15	0.83	0.09	91,105,116,127	0
9	NAG	M	1	14/15	0.83	0.10	110,120,137,140	0
11	NAG	N	1	14/15	0.83	0.11	73,91,103,106	0
13	MAN	T	5	11/12	0.84	0.14	76,80,93,100	0
10	NAG	I	2	14/15	0.85	0.11	77,92,102,112	0
9	NAG	J	2	14/15	0.88	0.09	142,148,156,161	0
10	NAG	I	1	14/15	0.88	0.12	34,54,70,80	0
13	NAG	T	2	14/15	0.88	0.12	71,88,108,114	0
9	NAG	K	1	14/15	0.89	0.10	74,111,130,137	0
9	NAG	Q	2	14/15	0.89	0.12	143,152,162,166	0

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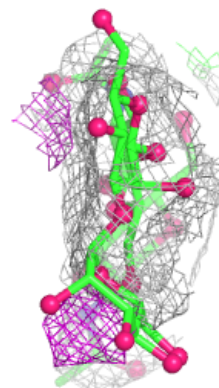
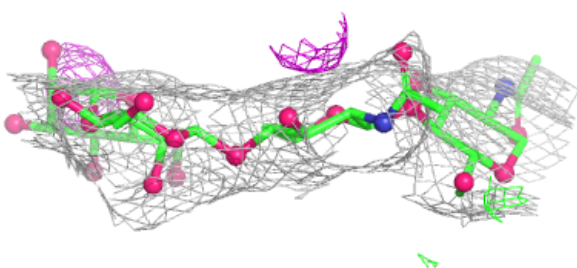
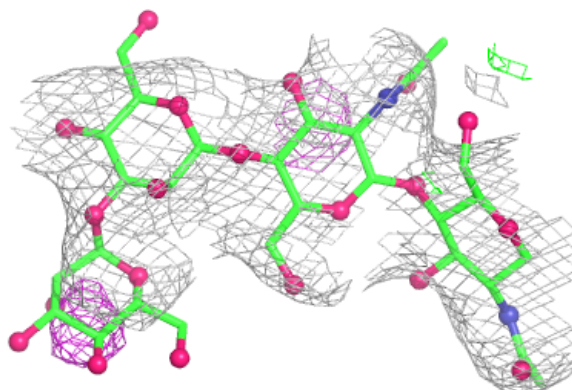
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	NAG	P	1	14/15	0.90	0.08	66,90,98,111	0
13	BMA	T	3	11/12	0.90	0.10	65,82,97,99	0
9	NAG	R	1	14/15	0.91	0.09	59,75,100,110	0
9	NAG	S	1	14/15	0.92	0.08	62,77,90,104	0
12	NAG	O	1	14/15	0.92	0.08	27,73,91,94	0
13	NAG	T	1	14/15	0.94	0.08	51,62,79,84	0
13	MAN	T	4	11/12	0.94	0.09	49,55,72,92	0
9	NAG	J	1	14/15	0.97	0.06	81,90,114,132	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.

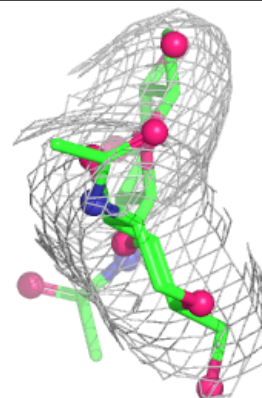
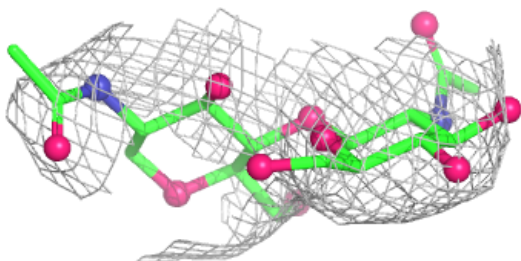
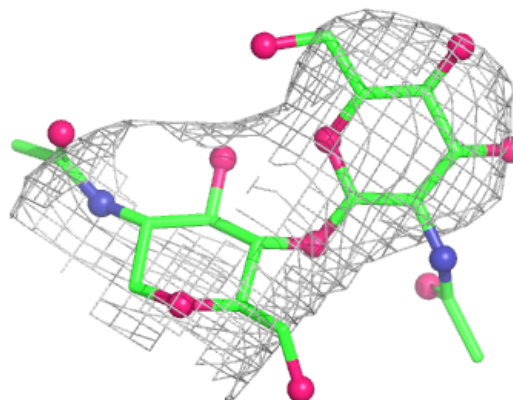


Electron density around Chain C:

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

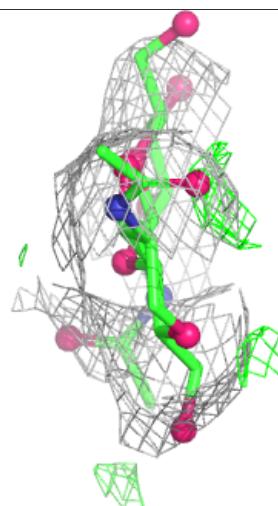
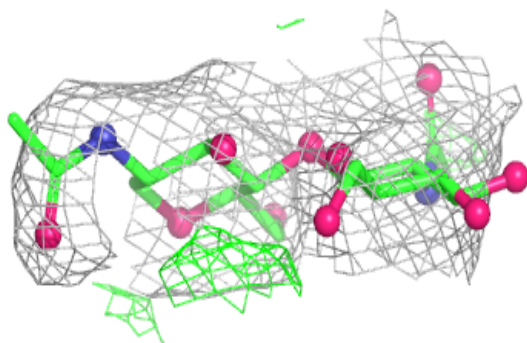
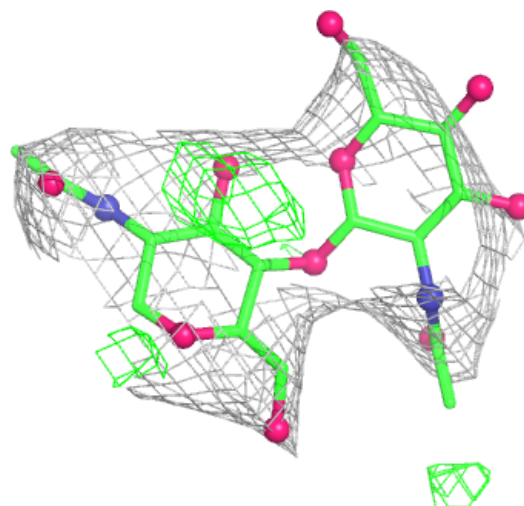
**Electron density around Chain F:**

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



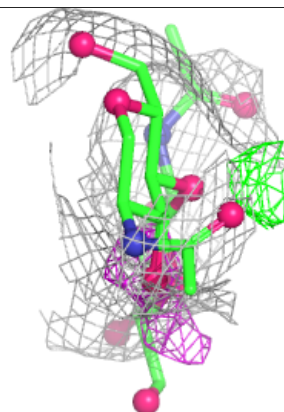
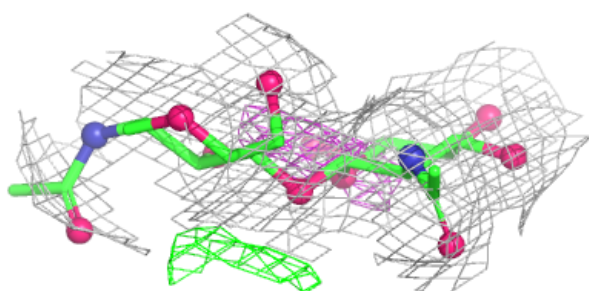
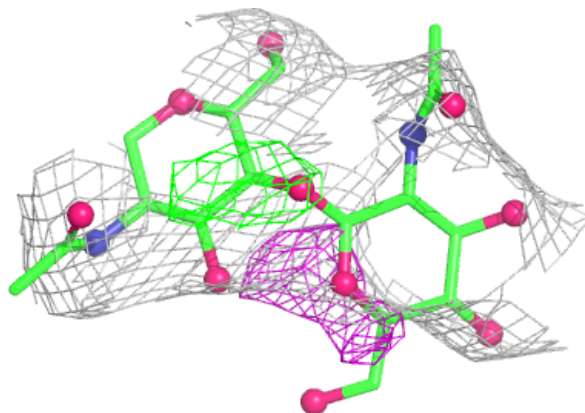
Electron density around Chain J:

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

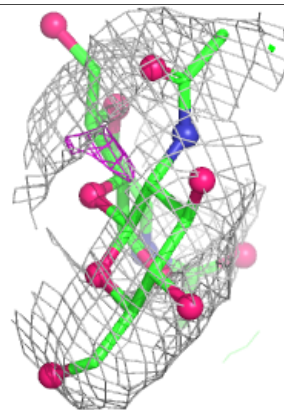
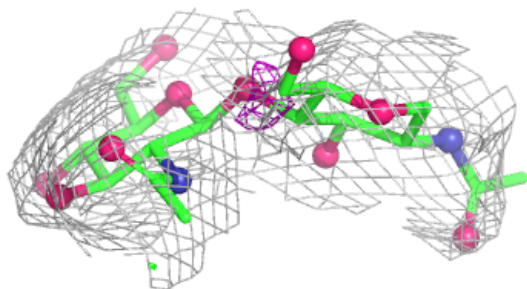
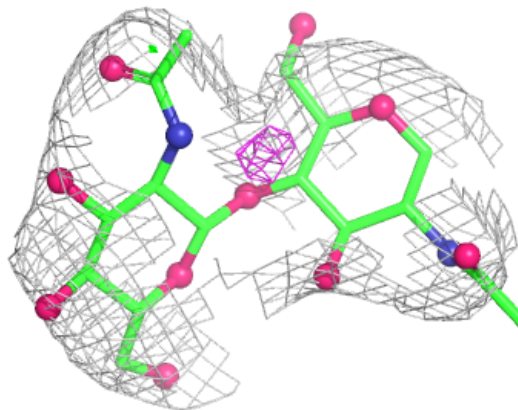


Electron density around Chain K:

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

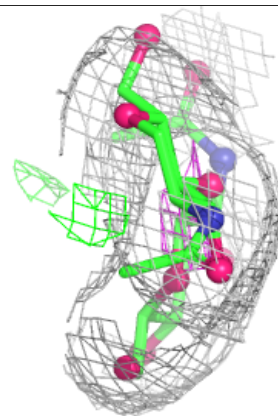
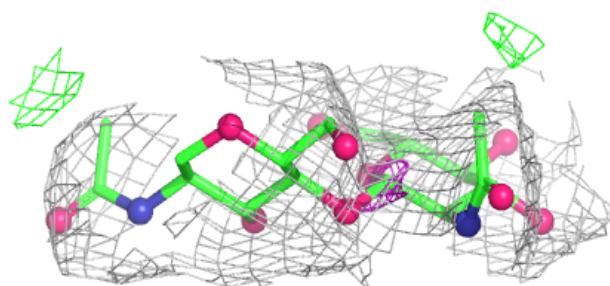
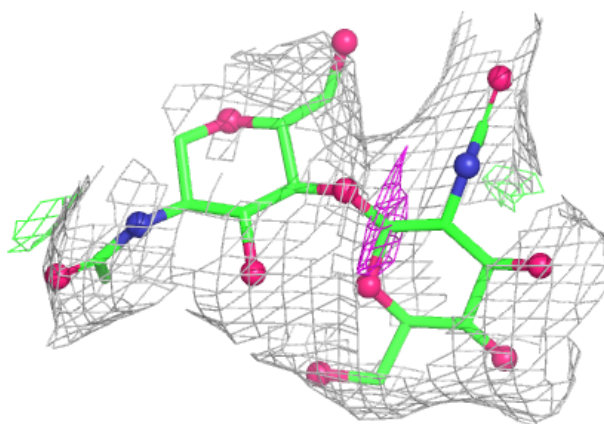
**Electron density around Chain M:**

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

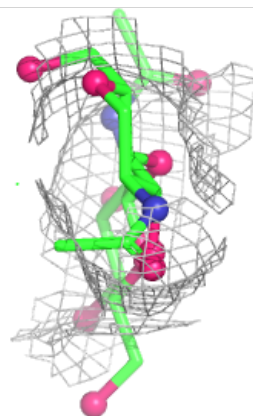
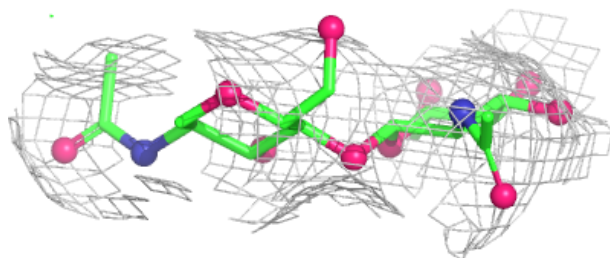
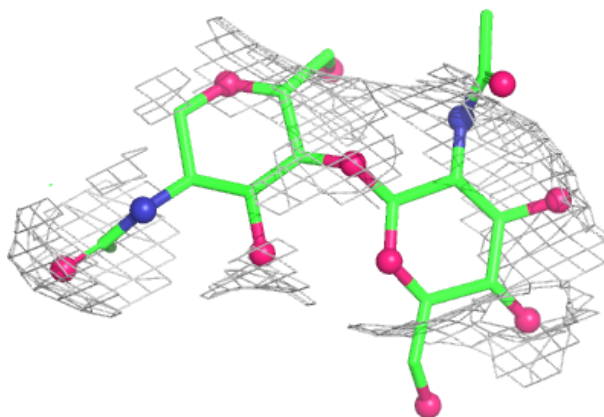


Electron density around Chain P:

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

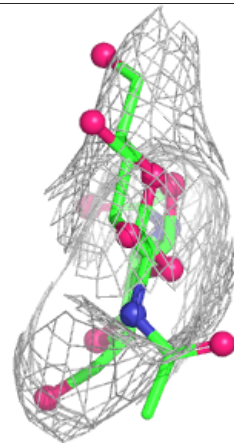
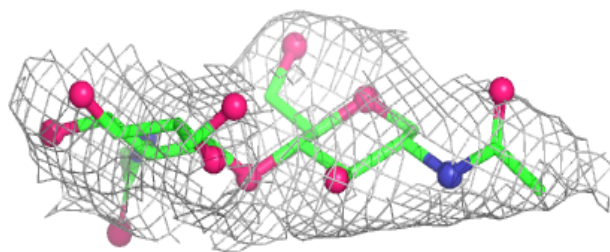
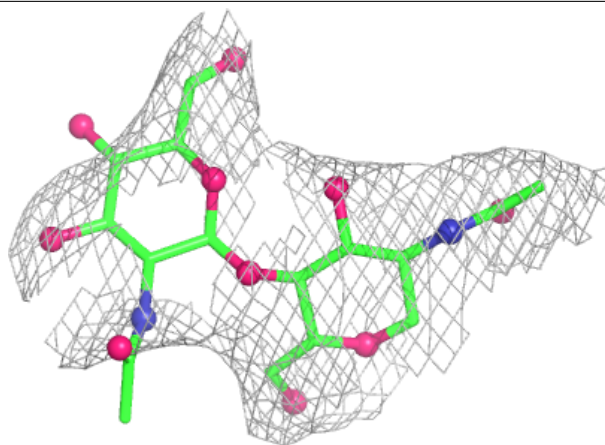
**Electron density around Chain Q:**

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



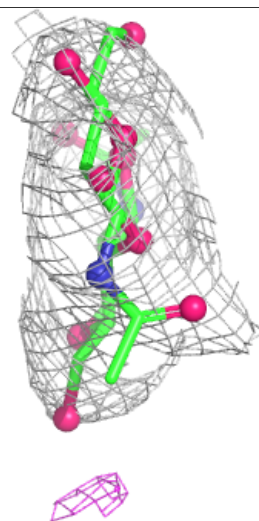
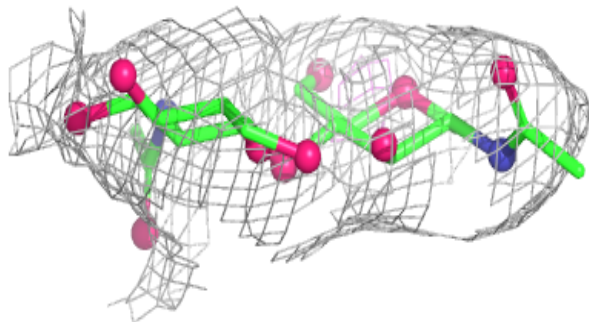
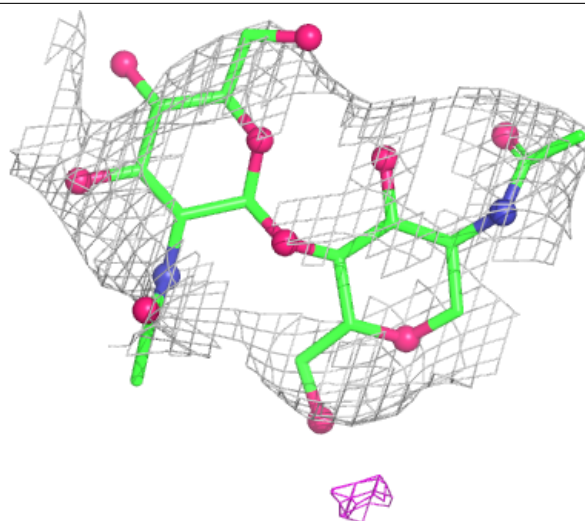
Electron density around Chain R:

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



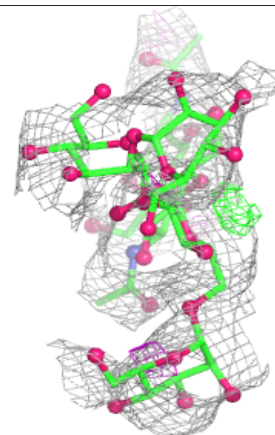
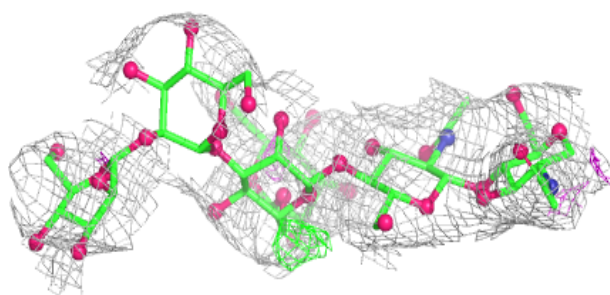
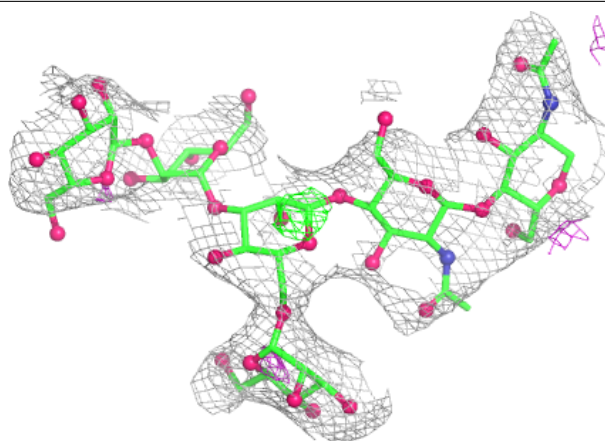
Electron density around Chain S:

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

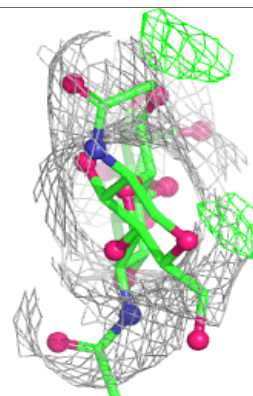
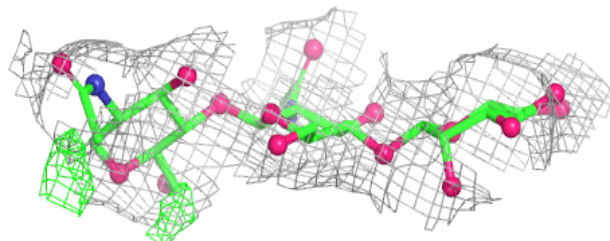
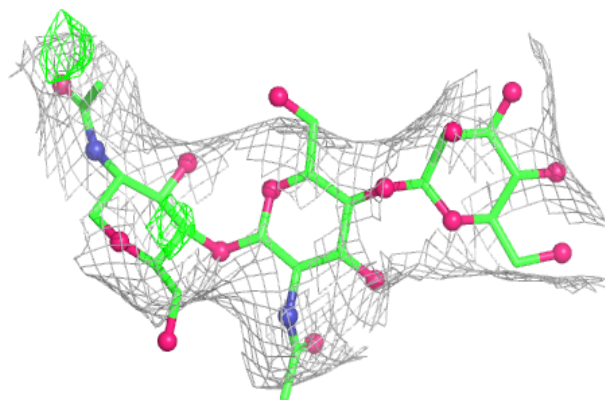


Electron density around Chain I:

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

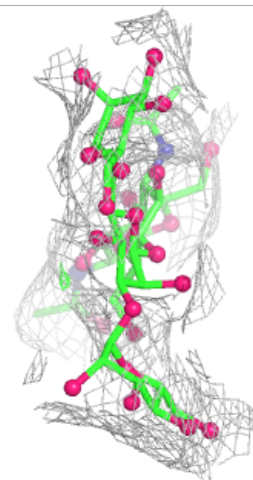
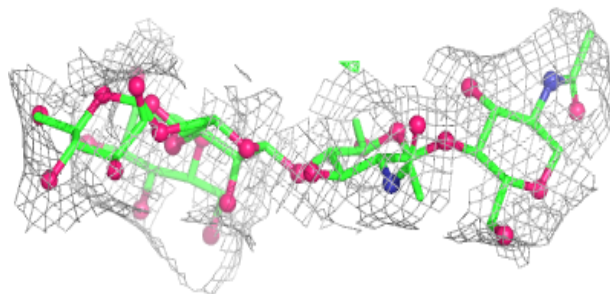
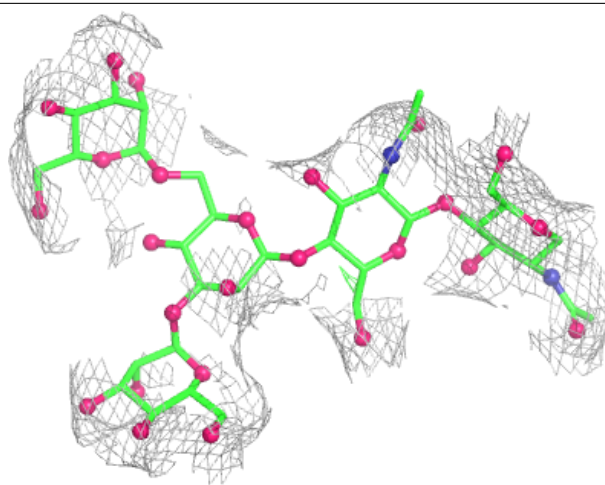
**Electron density around Chain N:**

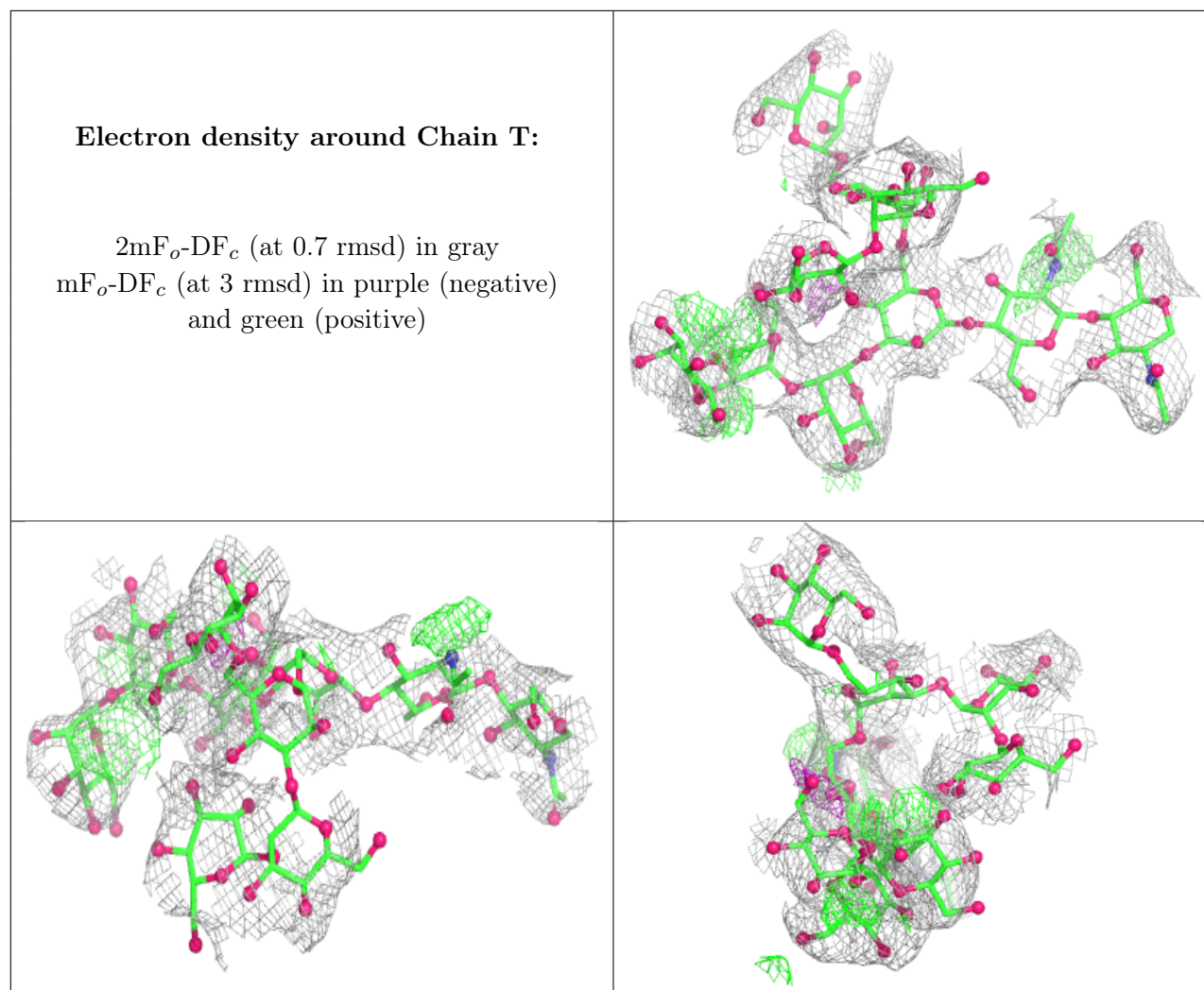
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain O:

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





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
14	NAG	G	1839	14/15	0.33	0.15	107,125,132,137	0
14	NAG	B	1611	14/15	0.51	0.14	110,127,140,144	0
14	NAG	H	523	14/15	0.60	0.12	113,124,132,136	0
15	SO4	G	603	5/5	0.64	0.14	147,147,152,153	0
14	NAG	G	1276	14/15	0.65	0.12	113,122,128,128	0
15	SO4	G	607	5/5	0.65	0.13	155,157,158,160	0
15	SO4	B	702	5/5	0.67	0.09	154,155,156,156	0
14	NAG	B	1618	14/15	0.71	0.12	95,108,114,122	0
15	SO4	G	601	5/5	0.76	0.12	123,126,128,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	SO4	G	606	5/5	0.76	0.10	229,229,230,246	5
15	SO4	G	602	5/5	0.79	0.20	107,114,116,121	0
14	NAG	B	1637	14/15	0.81	0.07	99,117,130,131	0
14	NAG	G	1355	14/15	0.82	0.10	121,137,144,146	0
14	NAG	G	1133	14/15	0.84	0.11	104,119,131,133	0
15	SO4	G	604	5/5	0.86	0.10	135,139,141,142	0
15	SO4	G	605	5/5	0.92	0.11	147,147,151,157	0
15	SO4	B	701	5/5	0.95	0.04	81,82,86,101	0
15	SO4	L	301	5/5	0.95	0.05	90,90,92,93	5

6.5 Other polymers [i](#)

There are no such residues in this entry.