



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:50 PM UTC

PDB ID : 6J11 / pdb_00006j11
Title : MERS-CoV spike N-terminal domain and 7D10 scFv complex
Authors : Zhou, H.; Zhang, S.; Zhang, S.; Tang, W.; Wang, X.
Deposited on : 2018-12-27
Resolution : 3.00 Å(reported)

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

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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:

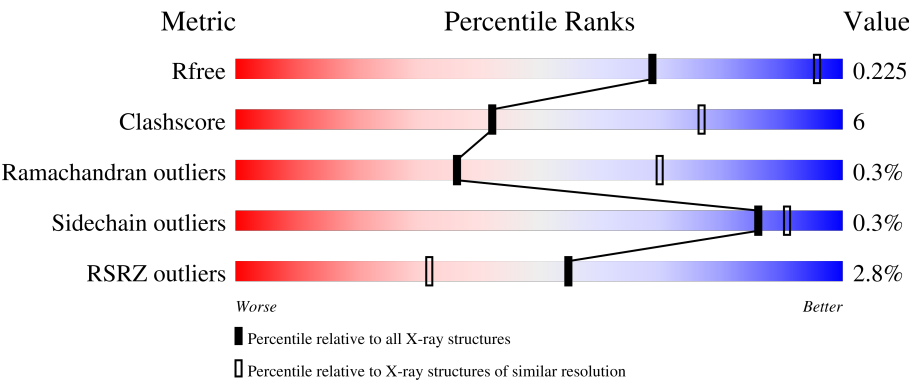
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



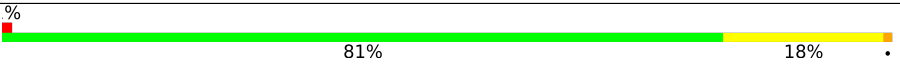
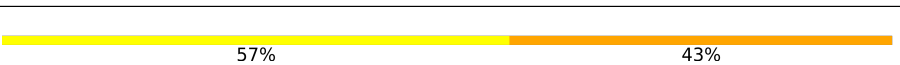
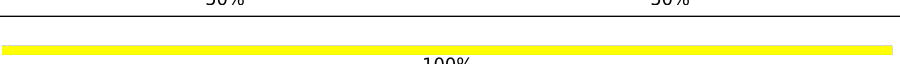
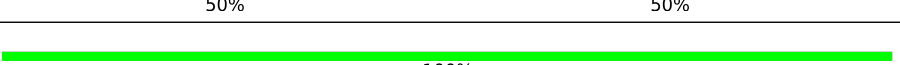
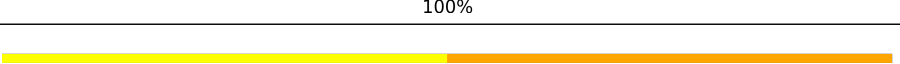
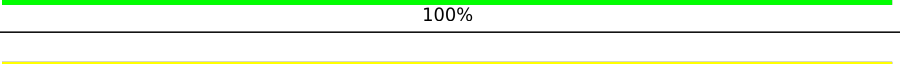
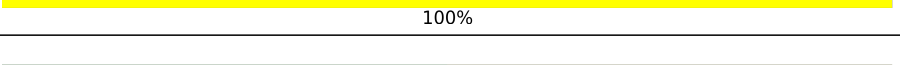
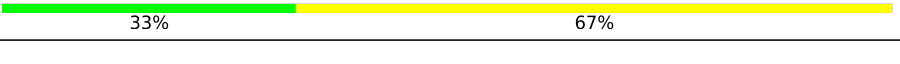
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	336	88%12%
1	B	336	2% 89%11%
1	C	336	3% 83%16%
2	D	132	8% 67%24%9%
2	F	132	5% 76%15%9%

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Mol	Chain	Length	Quality of chain
2	H	132	
3	E	111	
3	G	111	
3	L	111	
4	I	7	
4	O	7	
4	X	7	
5	J	4	
6	K	2	
6	M	2	
6	P	2	
6	R	2	
6	S	2	
6	T	2	
6	U	2	
6	V	2	
7	N	3	
7	W	3	
8	Q	5	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14135 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 N-terminal domain of Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2662	1707	439	503	13			
1	B	336	Total	C	N	O	S	0	0	0
			2662	1707	439	503	13			
1	C	336	Total	C	N	O	S	0	0	0
			2662	1707	439	503	13			

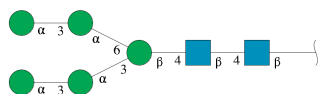
- Molecule 2 is a protein called VH of 7D10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	128	Total	C	N	O	S	0	0	0
			952	599	153	195	5			
2	D	120	Total	C	N	O	S	0	0	0
			916	581	145	185	5			
2	F	120	Total	C	N	O	S	0	0	0
			916	581	145	185	5			

- Molecule 3 is a protein called VL of 7D10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	111	Total	C	N	O	S	0	0	0
			859	543	147	166	3			
3	E	111	Total	C	N	O	S	0	0	0
			859	543	147	166	3			
3	G	111	Total	C	N	O	S	0	0	0
			859	543	147	166	3			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[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
4	I	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	O	7	Total	C	N	O	0	0	0
			83	46	2	35			
4	X	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 5 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
5	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



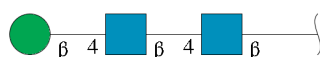
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

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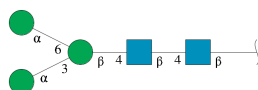
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	V	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



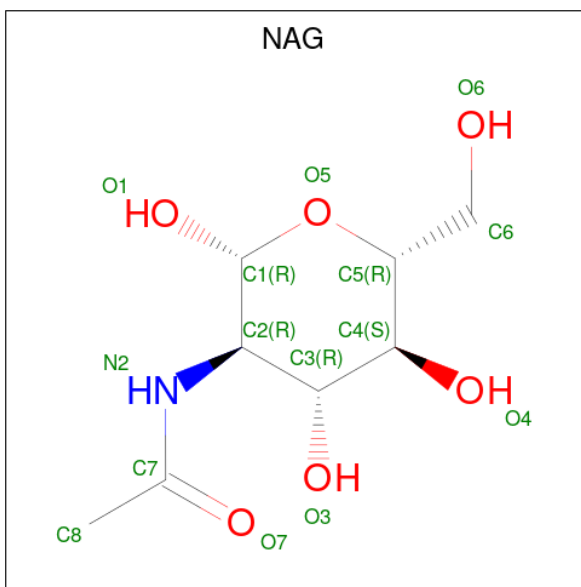
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	W	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



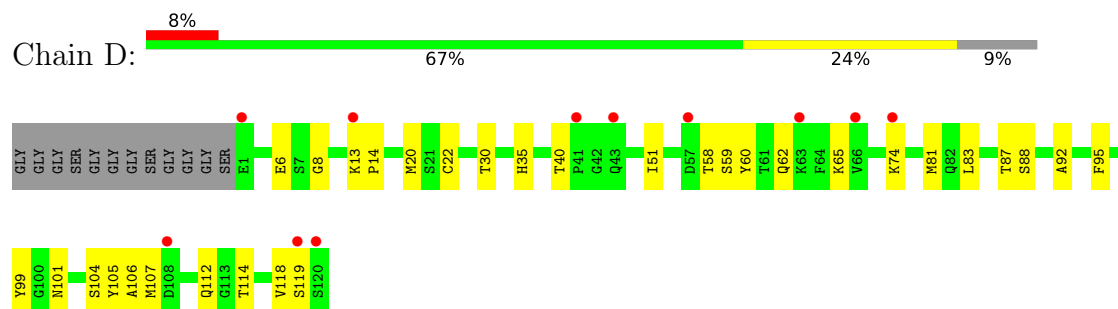
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	Q	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

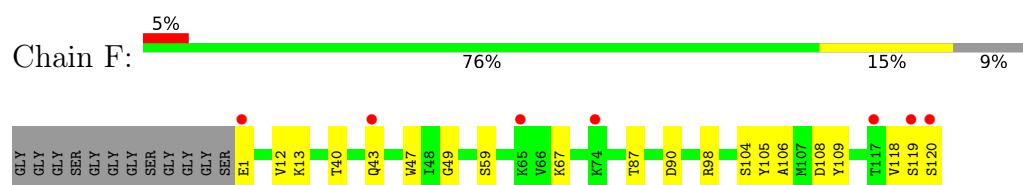


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1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

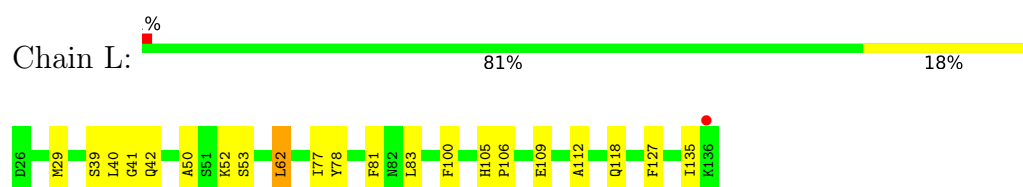
- Molecule 2: VH of 7D10



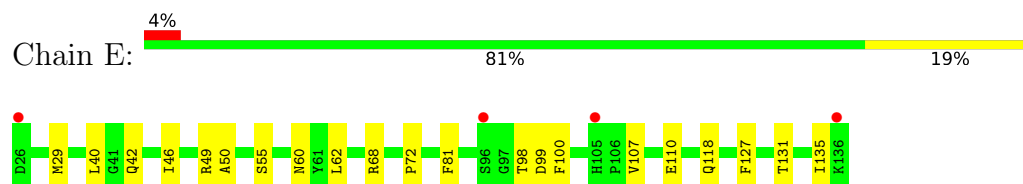
- Molecule 2: VH of 7D10



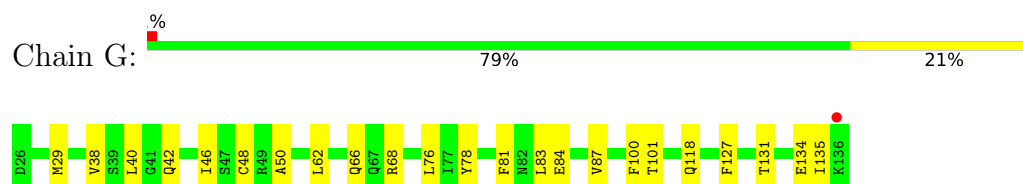
- Molecule 3: VL of 7D10



- Molecule 3: VL of 7D10



- Molecule 3: VL of 7D10



- Molecule 4: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[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



- Molecule 4: α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain O:  29% 71%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 4: α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain X:  14% 86%

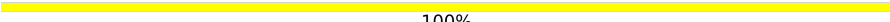
MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 5: α -D-mannopyranose-(1-3)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain J:  50% 50%

MAG1
MAG2
BMA3
MAN4

- Molecule 6: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain K:  100%

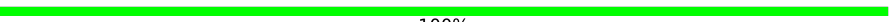
MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain M:  50% 50%

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain P:  100%

MAG1
MAG2

- Molecule 6: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain R:  50% 50%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  50% 50%

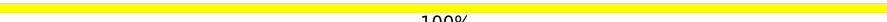


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%

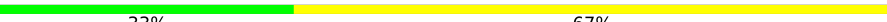


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  50% 50%

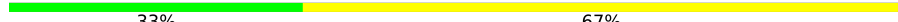


- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  33% 67%



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

Chain W:  33% 67%



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

Chain Q:

100%

NAG1
NAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.57Å 180.35Å 245.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.31 – 3.00 47.31 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.31-3.00) 99.9 (47.31-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155: ???	Depositor
R, R_{free}	0.188 , 0.225 0.190 , 0.225	Depositor DCC
R_{free} test set	4781 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14135	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/2738	0.71	0/3725
1	B	0.41	0/2738	0.66	1/3725 (0.0%)
1	C	0.41	0/2738	0.64	0/3725
2	D	0.46	0/940	0.74	0/1277
2	F	0.50	0/940	0.78	0/1277
2	H	0.57	0/976	0.77	0/1323
3	E	0.46	0/881	0.65	0/1197
3	G	0.49	0/881	0.69	0/1197
3	L	0.57	0/881	0.74	0/1197
All	All	0.47	0/13713	0.70	1/18643 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	CYS	CA-CB-SG	5.34	126.69	114.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	62	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2662	0	2519	26	0
1	B	2662	0	2517	24	0
1	C	2662	0	2517	33	0
2	D	916	0	871	27	0
2	F	916	0	873	15	0
2	H	952	0	901	9	0
3	E	859	0	828	13	0
3	G	859	0	828	15	0
3	L	859	0	828	14	0
4	I	83	0	69	2	0
4	O	83	0	70	6	0
4	X	83	0	69	4	0
5	J	50	0	43	0	0
6	K	28	0	25	2	0
6	M	28	0	25	0	0
6	P	28	0	25	0	0
6	R	28	0	25	2	0
6	S	28	0	25	0	0
6	T	28	0	25	0	0
6	U	28	0	25	2	0
6	V	28	0	25	0	0
7	N	39	0	34	0	0
7	W	39	0	34	0	0
8	Q	61	0	52	0	0
9	A	42	0	39	0	0
9	B	42	0	39	0	0
9	C	42	0	39	0	0
All	All	14135	0	13370	174	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 (174) 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:B:181:ARG:NH2	1:B:221:ARG:O	2.07	0.88
2:F:104:SER:O	2:F:106:ALA:N	2.15	0.79
2:D:81:MET:HE3	2:D:83:LEU:HD21	1.66	0.74
3:G:84:GLU:O	3:G:87:VAL:HG12	1.91	0.70
1:A:93:THR:HG23	1:A:94:GLY:H	1.56	0.70
2:D:6:GLU:O	2:D:112:GLN:NE2	2.25	0.69
2:D:104:SER:O	2:D:106:ALA:N	2.24	0.68
2:F:13:LYS:NZ	2:F:120:SER:O	2.19	0.68
1:C:257:THR:HG22	1:C:266:PHE:HE1	1.58	0.67
1:C:26:VAL:O	2:D:59:SER:HB2	1.94	0.67
1:C:19:VAL:HG11	4:X:7:MAN:H61	1.76	0.67
2:F:40:THR:HG23	2:F:43:GLN:HB2	1.77	0.67
3:E:81:PHE:HZ	6:U:2:NAG:H82	1.59	0.67
1:A:181:ARG:NH2	1:A:221:ARG:O	2.28	0.67
1:B:19:VAL:HG21	4:O:7:MAN:H61	1.77	0.67
3:E:68:ARG:NH1	3:E:110:GLU:O	2.26	0.66
1:B:174:ASP:HB3	1:B:179:LEU:HD22	1.76	0.66
2:D:20:MET:SD	2:D:114:THR:OG1	2.53	0.66
3:L:81:PHE:HZ	6:K:2:NAG:H82	1.59	0.66
3:G:81:PHE:HZ	6:R:2:NAG:H82	1.61	0.65
1:A:196:PRO:HA	1:A:201:TYR:CD1	2.33	0.64
1:A:26:VAL:O	2:H:59:SER:HB2	1.96	0.64
1:A:84:MET:HG3	1:A:314:TYR:CE2	2.33	0.64
1:A:19:VAL:HG21	4:I:7:MAN:H61	1.80	0.63
2:F:108:ASP:HB3	2:F:109:TYR:CD2	2.35	0.62
2:F:98:ARG:NH2	4:O:4:MAN:O6	2.33	0.61
4:O:4:MAN:H4	4:O:5:MAN:H2	1.81	0.61
1:C:33:VAL:HG11	1:C:203:SER:O	2.00	0.61
2:F:87:THR:O	2:F:118:VAL:HG21	2.01	0.61
1:A:24:ASP:OD2	1:A:235:ARG:NH2	2.34	0.61
1:C:93:THR:OG1	1:C:94:GLY:N	2.35	0.60
4:X:4:MAN:H4	4:X:5:MAN:H2	1.82	0.60
1:B:179:LEU:HD12	1:B:221:ARG:CZ	2.32	0.59
3:G:118:GLN:HB2	3:G:127:PHE:CD2	2.37	0.59
2:D:62:GLN:HG3	2:D:65:LYS:NZ	2.17	0.59
2:F:104:SER:O	2:F:104:SER:OG	2.16	0.59
3:E:118:GLN:HB2	3:E:127:PHE:CD2	2.37	0.59
3:L:52:LYS:HD3	3:L:53:SER:N	2.17	0.59
3:L:40:LEU:HD11	3:L:109:GLU:HG2	1.85	0.59
2:D:74:LYS:H	2:D:74:LYS:HD2	1.66	0.59
1:C:33:VAL:HG23	1:C:100:LEU:HB2	1.85	0.58
3:L:81:PHE:CZ	6:K:2:NAG:H82	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:104:SER:HA	3:L:78:TYR:CD1	2.39	0.57
3:L:29:MET:HE1	3:L:50:ALA:HB2	1.86	0.57
2:D:87:THR:O	2:D:118:VAL:HG21	2.03	0.57
1:A:185:CYS:HB3	1:A:237:CYS:SG	2.45	0.56
1:B:84:MET:HG3	1:B:314:TYR:CE2	2.40	0.56
2:F:1:GLU:OE1	4:O:5:MAN:O3	2.20	0.56
2:D:13:LYS:HG3	2:D:14:PRO:HD2	1.88	0.56
3:E:81:PHE:CZ	6:U:2:NAG:H82	2.40	0.55
3:E:49:ARG:NH1	3:E:99:ASP:OD1	2.37	0.55
2:F:12:VAL:O	2:F:118:VAL:HA	2.07	0.55
1:C:214:CYS:HB3	1:C:219:TYR:HD1	1.71	0.55
3:G:29:MET:HE1	3:G:50:ALA:HB2	1.87	0.55
1:B:179:LEU:HD12	1:B:221:ARG:NH2	2.22	0.55
1:C:84:MET:HG3	1:C:314:TYR:CE2	2.42	0.55
3:L:77:ILE:HG12	3:L:83:LEU:HD23	1.89	0.54
2:F:104:SER:C	2:F:106:ALA:H	2.11	0.54
3:G:81:PHE:CZ	6:R:2:NAG:H82	2.42	0.54
1:A:174:ASP:HB3	1:A:179:LEU:HD22	1.89	0.54
3:L:62:LEU:HD22	3:L:100:PHE:CG	2.44	0.53
1:A:179:LEU:HD12	1:A:221:ARG:CZ	2.38	0.52
1:C:181:ARG:HD3	1:C:240:MET:SD	2.50	0.52
2:D:14:PRO:HD3	2:D:119:SER:O	2.10	0.52
1:C:85:TYR:HB2	1:C:313:PHE:CE1	2.45	0.52
3:L:118:GLN:HB2	3:L:127:PHE:CD2	2.45	0.52
3:E:29:MET:HE1	3:E:50:ALA:HB2	1.92	0.52
3:G:66:GLN:HB2	3:G:76:LEU:HD22	1.91	0.52
3:L:52:LYS:HD3	3:L:53:SER:H	1.74	0.51
1:A:154:GLY:HA3	1:A:165:PHE:HE2	1.75	0.51
2:D:104:SER:C	2:D:106:ALA:H	2.14	0.51
1:A:93:THR:HG23	1:A:94:GLY:N	2.24	0.51
1:B:154:GLY:HA3	1:B:165:PHE:HE2	1.76	0.51
2:D:60:TYR:HB2	2:D:65:LYS:HG3	1.93	0.51
1:C:46:ARG:HH12	1:C:123:ALA:CA	2.24	0.51
1:A:320:PRO:O	1:A:321:LEU:HD23	2.11	0.50
2:D:87:THR:HG22	2:D:88:SER:H	1.76	0.50
1:C:206:THR:HG23	1:C:298:HIS:ND1	2.26	0.50
3:E:42:GLN:O	3:E:107:VAL:HG23	2.10	0.50
1:A:23:PRO:HA	2:H:101:ASN:OD1	2.11	0.50
1:A:324:LEU:HD12	1:A:337:ILE:HD12	1.93	0.50
1:A:141:ARG:HE	1:A:308:LYS:HD3	1.77	0.50
1:B:93:THR:OG1	1:B:94:GLY:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:HD11	1:A:284:LEU:HD11	1.94	0.49
1:C:85:TYR:CZ	1:C:295:ILE:HG13	2.47	0.49
1:C:257:THR:HG22	1:C:266:PHE:CE1	2.44	0.49
1:C:117:VAL:HG11	1:C:278:MET:HE1	1.95	0.49
1:C:100:LEU:HD22	1:C:299:SER:HB3	1.94	0.49
1:C:59:PRO:HB3	1:C:71:TYR:CZ	2.47	0.48
3:E:40:LEU:N	3:E:135:ILE:HD11	2.29	0.48
2:D:99:TYR:HD2	2:D:107:MET:HE1	1.78	0.48
1:C:46:ARG:HH12	1:C:123:ALA:HA	1.79	0.48
2:F:104:SER:HB2	3:G:78:TYR:CG	2.49	0.48
1:A:69:ILE:HG12	1:A:327:PHE:HE1	1.79	0.48
1:C:49:ASP:OD1	1:C:51:SER:OG	2.30	0.48
2:D:104:SER:O	2:D:104:SER:OG	2.25	0.48
2:F:119:SER:OG	2:F:120:SER:N	2.46	0.48
1:A:40:PHE:CG	1:A:103:ALA:HB2	2.49	0.47
2:D:30:THR:HG23	4:X:1:NAG:H83	1.96	0.47
1:B:100:LEU:HD22	1:B:299:SER:HB3	1.96	0.47
1:B:325:LEU:HD22	1:B:333:ILE:HD13	1.97	0.47
2:H:14:PRO:HD3	2:H:119:SER:O	2.16	0.46
1:B:181:ARG:NH1	4:O:1:NAG:O6	2.48	0.46
3:L:41:GLY:HA2	3:L:106:PRO:HB2	1.97	0.46
2:D:74:LYS:H	2:D:74:LYS:CD	2.25	0.46
2:F:67:LYS:NZ	2:F:90:ASP:OD2	2.48	0.46
3:E:55:SER:HB3	3:E:60:ASN:OD1	2.16	0.46
3:G:38:VAL:HG13	3:G:42:GLN:HG3	1.98	0.46
4:X:3:BMA:H61	4:X:6:MAN:O2	2.16	0.46
1:A:33:VAL:HG22	1:A:100:LEU:HD12	1.97	0.46
3:G:29:MET:HE2	3:G:48:CYS:SG	2.56	0.46
1:A:117:VAL:HG13	1:A:318:LEU:HD21	1.98	0.45
1:B:335:ARG:NH2	1:B:352:GLU:OE2	2.42	0.45
3:G:62:LEU:HD22	3:G:100:PHE:CG	2.51	0.45
1:C:250:ILE:HD12	1:C:273:LEU:HD21	1.98	0.45
2:D:95:PHE:HE2	3:E:72:PRO:HB3	1.80	0.45
2:F:47:TRP:CH2	2:F:49:GLY:HA2	2.51	0.45
1:B:209:THR:HG22	1:B:301:ARG:HB2	1.99	0.45
1:C:325:LEU:HD22	1:C:333:ILE:HD13	1.98	0.45
3:E:46:ILE:HG12	3:E:131:THR:HG21	1.99	0.45
3:G:134:GLU:C	3:G:135:ILE:HD13	2.42	0.45
1:B:36:GLN:HG3	1:B:101:PHE:HE1	1.82	0.44
1:C:221:ARG:NH2	1:C:244:ASN:OD1	2.50	0.44
1:C:300:ILE:HD13	1:C:310:TRP:NE1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:62:GLN:HG3	2:D:65:LYS:HZ2	1.81	0.44
3:G:83:LEU:HB3	3:G:87:VAL:CG1	2.47	0.44
1:B:62:ARG:N	1:B:62:ARG:HD3	2.32	0.44
3:G:46:ILE:HG12	3:G:131:THR:HG21	2.00	0.44
2:H:51:ILE:HD13	2:H:72:SER:HB3	1.99	0.44
1:C:343:ASP:O	1:C:347:LEU:HD22	2.17	0.44
2:H:74:LYS:HE3	2:H:74:LYS:HB2	1.69	0.44
1:C:154:GLY:HA3	1:C:165:PHE:HE2	1.83	0.44
1:B:271:VAL:HB	1:B:279:PHE:CD1	2.52	0.43
3:E:62:LEU:HD13	3:E:100:PHE:CD1	2.53	0.43
1:C:161:MET:HE3	1:C:161:MET:HB2	1.88	0.43
3:L:112:ALA:HB2	3:L:135:ILE:HD13	2.00	0.43
2:D:51:ILE:HD12	2:D:58:THR:HG22	2.00	0.43
3:E:49:ARG:HA	3:E:98:THR:O	2.18	0.43
1:B:40:PHE:HD2	1:B:86:VAL:HG13	1.83	0.43
1:B:67:ILE:HG13	1:B:68:THR:N	2.34	0.43
4:I:3:BMA:H61	4:I:6:MAN:O2	2.19	0.43
2:D:87:THR:HG22	2:D:88:SER:N	2.33	0.43
3:G:40:LEU:HD23	3:G:40:LEU:HA	1.69	0.43
2:D:40:THR:HG22	2:D:92:ALA:HB2	2.01	0.43
1:A:152:SER:HB2	1:A:165:PHE:HB2	2.01	0.42
2:D:65:LYS:HB2	2:D:65:LYS:HE2	1.63	0.42
1:B:62:ARG:HD3	1:B:62:ARG:H	1.83	0.42
1:C:69:ILE:HG12	1:C:327:PHE:HE1	1.84	0.42
2:D:104:SER:C	2:D:106:ALA:N	2.77	0.42
4:O:3:BMA:H61	4:O:6:MAN:O2	2.19	0.42
1:B:330:ASP:N	1:B:330:ASP:OD1	2.52	0.42
1:C:67:ILE:HG13	1:C:68:THR:N	2.35	0.42
1:C:189:PRO:HB2	1:C:197:ALA:HB2	2.02	0.42
1:C:190:ARG:NH1	1:C:233:ASN:OD1	2.51	0.42
2:H:67:LYS:NZ	2:H:90:ASP:OD2	2.40	0.42
1:B:37:GLN:OE1	1:B:103:ALA:HB1	2.21	0.41
2:D:35:HIS:CD2	2:D:99:TYR:HB2	2.55	0.41
1:B:124:ALA:O	1:B:125:ASN:HB2	2.20	0.41
2:D:6:GLU:HA	2:D:22:CYS:HA	2.01	0.41
3:L:105:HIS:HA	3:L:106:PRO:HA	1.77	0.41
1:A:59:PRO:HB3	1:A:71:TYR:CZ	2.55	0.41
1:A:67:ILE:HG12	1:A:68:THR:N	2.36	0.41
1:B:26:VAL:O	2:F:59:SER:HB2	2.21	0.41
1:A:78:GLN:HG2	1:A:341:PHE:CD2	2.56	0.41
1:C:59:PRO:HB3	1:C:71:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:68:ARG:HH11	3:G:68:ARG:HD3	1.75	0.41
1:C:124:ALA:C	1:C:126:SER:H	2.29	0.41
3:L:39:SER:HB2	3:L:42:GLN:HG3	2.03	0.41
1:A:235:ARG:HD3	1:A:235:ARG:HA	1.89	0.40
1:B:324:LEU:O	1:B:336:ALA:HA	2.21	0.40
1:C:39:PHE:O	1:C:131:ILE:HG23	2.21	0.40
2:H:91:SER:HA	2:H:116:VAL:O	2.22	0.40
2:D:8:GLY:O	2:D:114:THR:HB	2.22	0.40
2:H:2:VAL:HB	2:H:109:TYR:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/336 (99%)	317 (95%)	17 (5%)	0	100	100
1	B	334/336 (99%)	316 (95%)	18 (5%)	0	100	100
1	C	334/336 (99%)	313 (94%)	20 (6%)	1 (0%)	36	70
2	D	118/132 (89%)	109 (92%)	7 (6%)	2 (2%)	7	32
2	F	118/132 (89%)	108 (92%)	9 (8%)	1 (1%)	16	50
2	H	126/132 (96%)	117 (93%)	8 (6%)	1 (1%)	16	50
3	E	109/111 (98%)	105 (96%)	4 (4%)	0	100	100
3	G	109/111 (98%)	105 (96%)	4 (4%)	0	100	100
3	L	109/111 (98%)	106 (97%)	3 (3%)	0	100	100
All	All	1691/1737 (97%)	1596 (94%)	90 (5%)	5 (0%)	36	70

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	-5	GLY
2	D	105	TYR
2	F	105	TYR
2	D	101	ASN
1	C	216	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	288/288 (100%)	288 (100%)	0	100	100
1	B	288/288 (100%)	288 (100%)	0	100	100
1	C	288/288 (100%)	286 (99%)	2 (1%)	76	86
2	D	100/103 (97%)	100 (100%)	0	100	100
2	F	100/103 (97%)	100 (100%)	0	100	100
2	H	102/103 (99%)	102 (100%)	0	100	100
3	E	94/94 (100%)	94 (100%)	0	100	100
3	G	94/94 (100%)	93 (99%)	1 (1%)	65	83
3	L	94/94 (100%)	93 (99%)	1 (1%)	65	83
All	All	1448/1455 (100%)	1444 (100%)	4 (0%)	86	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	109	VAL
1	C	214	CYS
3	L	62	LEU
3	G	101	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN

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Mol	Chain	Res	Type
1	A	194	HIS
1	A	346	GLN
1	B	199	ASN
1	C	60	GLN
1	C	72	GLN
1	C	114	ASN
2	H	33	ASN
3	L	66	GLN
3	L	103	ASN
3	L	105	HIS
2	D	43	GLN
2	F	33	ASN
2	F	82	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 ⓘ

52 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	I	1	1,4	14,14,15	0.88	1 (7%)	17,19,21	0.51	0
4	NAG	I	2	4	14,14,15	1.12	1 (7%)	17,19,21	1.99	2 (11%)
4	BMA	I	3	4	11,11,12	2.05	4 (36%)	15,15,17	1.59	3 (20%)
4	MAN	I	4	4	11,11,12	1.55	2 (18%)	15,15,17	1.51	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	I	5	4	11,11,12	1.85	4 (36%)	15,15,17	1.32	1 (6%)
4	MAN	I	6	4	11,11,12	2.76	7 (63%)	15,15,17	1.86	5 (33%)
4	MAN	I	7	4	11,11,12	2.20	4 (36%)	15,15,17	1.49	4 (26%)
5	NAG	J	1	5,1	14,14,15	0.52	0	17,19,21	0.82	0
5	NAG	J	2	5	14,14,15	0.25	0	17,19,21	0.50	0
5	BMA	J	3	5	11,11,12	1.72	3 (27%)	15,15,17	1.53	4 (26%)
5	MAN	J	4	5	11,11,12	1.00	1 (9%)	15,15,17	1.48	1 (6%)
6	NAG	K	1	6,1	14,14,15	0.68	0	17,19,21	1.64	2 (11%)
6	NAG	K	2	6	14,14,15	0.33	0	17,19,21	0.52	0
6	NAG	M	1	6,1	14,14,15	1.44	1 (7%)	17,19,21	2.58	3 (17%)
6	NAG	M	2	6	14,14,15	0.27	0	17,19,21	0.54	0
7	NAG	N	1	7,1	14,14,15	0.26	0	17,19,21	0.70	0
7	NAG	N	2	7	14,14,15	1.03	1 (7%)	17,19,21	0.66	0
7	BMA	N	3	7	11,11,12	1.88	4 (36%)	15,15,17	1.87	7 (46%)
4	NAG	O	1	1,4	14,14,15	0.46	0	17,19,21	0.60	0
4	NAG	O	2	4	14,14,15	0.68	0	17,19,21	1.69	1 (5%)
4	BMA	O	3	4	11,11,12	0.97	1 (9%)	15,15,17	1.43	2 (13%)
4	MAN	O	4	4	11,11,12	1.53	2 (18%)	15,15,17	1.40	2 (13%)
4	MAN	O	5	4	11,11,12	1.48	3 (27%)	15,15,17	1.30	1 (6%)
4	MAN	O	6	4	11,11,12	2.64	7 (63%)	15,15,17	1.69	3 (20%)
4	MAN	O	7	4	11,11,12	2.20	5 (45%)	15,15,17	1.51	3 (20%)
6	NAG	P	1	6,1	14,14,15	0.46	0	17,19,21	0.47	0
6	NAG	P	2	6	14,14,15	0.62	0	17,19,21	0.67	0
8	NAG	Q	1	8,1	14,14,15	0.44	0	17,19,21	1.00	2 (11%)
8	NAG	Q	2	8	14,14,15	0.55	0	17,19,21	0.77	1 (5%)
8	BMA	Q	3	8	11,11,12	2.37	4 (36%)	15,15,17	2.17	5 (33%)
8	MAN	Q	4	8	11,11,12	1.73	3 (27%)	15,15,17	2.25	1 (6%)
8	MAN	Q	5	8	11,11,12	2.11	5 (45%)	15,15,17	1.11	1 (6%)
6	NAG	R	1	6,1	14,14,15	0.47	0	17,19,21	1.86	2 (11%)
6	NAG	R	2	6	14,14,15	0.27	0	17,19,21	1.07	1 (5%)
6	NAG	S	1	6,1	14,14,15	0.68	0	17,19,21	1.88	2 (11%)
6	NAG	S	2	6	14,14,15	0.29	0	17,19,21	0.55	0
6	NAG	T	1	6,1	14,14,15	0.53	0	17,19,21	0.51	0
6	NAG	T	2	6	14,14,15	0.19	0	17,19,21	0.60	0
6	NAG	U	1	6,1	14,14,15	0.54	0	17,19,21	1.81	2 (11%)
6	NAG	U	2	6	14,14,15	0.33	0	17,19,21	0.56	0
6	NAG	V	1	6,1	14,14,15	0.86	1 (7%)	17,19,21	2.04	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	V	2	6	14,14,15	0.48	0	17,19,21	0.52	0
7	NAG	W	1	7,1	14,14,15	0.38	0	17,19,21	0.68	1 (5%)
7	NAG	W	2	7	14,14,15	0.50	0	17,19,21	0.60	0
7	BMA	W	3	7	11,11,12	2.04	4 (36%)	15,15,17	1.54	5 (33%)
4	NAG	X	1	1,4	14,14,15	0.60	0	17,19,21	1.15	2 (11%)
4	NAG	X	2	4	14,14,15	0.55	0	17,19,21	1.53	1 (5%)
4	BMA	X	3	4	11,11,12	1.14	0	15,15,17	1.28	1 (6%)
4	MAN	X	4	4	11,11,12	1.34	1 (9%)	15,15,17	1.57	3 (20%)
4	MAN	X	5	4	11,11,12	1.14	1 (9%)	15,15,17	1.16	1 (6%)
4	MAN	X	6	4	11,11,12	2.63	6 (54%)	15,15,17	1.86	3 (20%)
4	MAN	X	7	4	11,11,12	1.53	2 (18%)	15,15,17	1.49	3 (20%)

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
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	BMA	I	3	4	-	2/2/19/22	0/1/1/1
4	MAN	I	4	4	-	2/2/19/22	1/1/1/1
4	MAN	I	5	4	-	0/2/19/22	0/1/1/1
4	MAN	I	6	4	-	0/2/19/22	1/1/1/1
4	MAN	I	7	4	-	2/2/19/22	0/1/1/1
5	NAG	J	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1
5	BMA	J	3	5	-	2/2/19/22	0/1/1/1
5	MAN	J	4	5	-	0/2/19/22	0/1/1/1
6	NAG	K	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	4/6/23/26	0/1/1/1
6	NAG	M	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	M	2	6	-	3/6/23/26	0/1/1/1
7	NAG	N	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1
7	BMA	N	3	7	-	1/2/19/22	0/1/1/1
4	NAG	O	1	1,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	BMA	O	3	4	-	2/2/19/22	0/1/1/1
4	MAN	O	4	4	-	2/2/19/22	1/1/1/1
4	MAN	O	5	4	-	1/2/19/22	1/1/1/1
4	MAN	O	6	4	-	0/2/19/22	1/1/1/1
4	MAN	O	7	4	-	2/2/19/22	0/1/1/1
6	NAG	P	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
8	NAG	Q	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	2/6/23/26	0/1/1/1
8	BMA	Q	3	8	-	1/2/19/22	0/1/1/1
8	MAN	Q	4	8	-	1/2/19/22	0/1/1/1
8	MAN	Q	5	8	-	1/2/19/22	1/1/1/1
6	NAG	R	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	R	2	6	-	4/6/23/26	0/1/1/1
6	NAG	S	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	S	2	6	-	4/6/23/26	0/1/1/1
6	NAG	T	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1
6	NAG	U	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	U	2	6	-	4/6/23/26	0/1/1/1
6	NAG	V	1	6,1	-	3/6/23/26	0/1/1/1
6	NAG	V	2	6	-	4/6/23/26	0/1/1/1
7	NAG	W	1	7,1	-	1/6/23/26	0/1/1/1
7	NAG	W	2	7	-	2/6/23/26	0/1/1/1
7	BMA	W	3	7	-	0/2/19/22	0/1/1/1
4	NAG	X	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	BMA	X	3	4	-	2/2/19/22	0/1/1/1
4	MAN	X	4	4	-	2/2/19/22	1/1/1/1
4	MAN	X	5	4	-	0/2/19/22	1/1/1/1
4	MAN	X	6	4	-	0/2/19/22	1/1/1/1
4	MAN	X	7	4	-	2/2/19/22	0/1/1/1

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1	NAG	O5-C1	5.08	1.52	1.43
8	Q	3	BMA	C4-C5	4.87	1.63	1.53
4	I	7	MAN	O5-C1	-4.86	1.35	1.43
4	X	6	MAN	O5-C1	4.82	1.51	1.43
4	I	6	MAN	O5-C5	4.70	1.52	1.43
8	Q	3	BMA	C6-C5	4.03	1.65	1.51
8	Q	5	MAN	O5-C5	4.01	1.51	1.43
8	Q	4	MAN	O5-C1	3.86	1.50	1.43
4	O	7	MAN	O2-C2	3.82	1.51	1.43
4	O	7	MAN	O5-C1	-3.78	1.37	1.43
4	I	2	NAG	O5-C1	-3.77	1.37	1.43
7	W	3	BMA	C2-C3	3.76	1.58	1.52
4	I	5	MAN	C4-C5	3.75	1.61	1.53
4	X	6	MAN	O5-C5	3.75	1.50	1.43
4	I	6	MAN	O5-C1	3.73	1.50	1.43
4	I	6	MAN	C6-C5	3.64	1.64	1.51
7	W	3	BMA	C1-C2	3.64	1.60	1.52
7	N	3	BMA	C4-C3	3.61	1.61	1.52
7	N	2	NAG	O5-C1	-3.55	1.37	1.43
4	O	6	MAN	C4-C3	3.55	1.61	1.52
4	X	4	MAN	O3-C3	3.46	1.51	1.43
8	Q	5	MAN	O5-C1	3.40	1.49	1.43
4	O	6	MAN	O5-C1	3.38	1.49	1.43
4	O	6	MAN	O3-C3	3.37	1.51	1.43
4	O	4	MAN	O3-C3	3.30	1.51	1.43
4	I	3	BMA	O6-C6	3.28	1.56	1.42
4	I	7	MAN	C4-C5	3.26	1.60	1.53
4	X	6	MAN	C1-C2	3.25	1.60	1.52
4	I	3	BMA	C6-C5	3.23	1.62	1.51
4	X	6	MAN	C6-C5	3.14	1.62	1.51
4	I	1	NAG	O5-C1	-3.11	1.38	1.43
4	O	6	MAN	C2-C3	-3.11	1.47	1.52
5	J	3	BMA	C2-C3	-3.08	1.47	1.52
4	O	6	MAN	C1-C2	3.07	1.59	1.52
4	O	6	MAN	C6-C5	3.03	1.62	1.51
4	I	7	MAN	O5-C5	3.01	1.49	1.43
4	I	6	MAN	O2-C2	-2.99	1.37	1.43
4	O	7	MAN	O5-C5	2.97	1.49	1.43
4	I	5	MAN	C1-C2	2.93	1.59	1.52
8	Q	4	MAN	O5-C5	2.89	1.49	1.43
7	W	3	BMA	C4-C3	2.88	1.59	1.52
4	I	4	MAN	O3-C3	2.86	1.50	1.43
4	I	3	BMA	O5-C5	2.82	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	7	MAN	O5-C1	-2.82	1.39	1.43
8	Q	3	BMA	C2-C3	2.74	1.56	1.52
8	Q	4	MAN	C1-C2	2.71	1.58	1.52
4	X	6	MAN	C4-C3	2.69	1.59	1.52
4	X	5	MAN	C1-C2	2.69	1.58	1.52
5	J	3	BMA	C4-C3	2.68	1.59	1.52
4	O	7	MAN	C4-C5	2.60	1.58	1.53
4	X	7	MAN	O5-C5	2.58	1.48	1.43
7	N	3	BMA	C6-C5	2.58	1.60	1.51
7	N	3	BMA	C2-C3	2.53	1.56	1.52
8	Q	5	MAN	C1-C2	2.51	1.58	1.52
4	I	5	MAN	O5-C5	2.49	1.48	1.43
5	J	3	BMA	C1-C2	-2.48	1.46	1.52
4	O	5	MAN	C1-C2	2.48	1.58	1.52
4	I	6	MAN	C4-C3	2.47	1.58	1.52
4	I	7	MAN	O2-C2	2.45	1.48	1.43
4	O	6	MAN	O2-C2	-2.45	1.38	1.43
4	O	5	MAN	O5-C1	2.40	1.47	1.43
4	O	7	MAN	C1-C2	2.40	1.57	1.52
6	V	1	NAG	O5-C1	2.38	1.47	1.43
7	N	3	BMA	C1-C2	2.37	1.57	1.52
8	Q	5	MAN	C4-C5	2.36	1.58	1.53
4	I	6	MAN	C2-C3	-2.30	1.49	1.52
4	I	6	MAN	O3-C3	2.28	1.48	1.43
8	Q	5	MAN	C4-C3	2.25	1.58	1.52
4	O	5	MAN	O5-C5	2.20	1.47	1.43
4	X	6	MAN	O3-C3	2.19	1.48	1.43
7	W	3	BMA	C6-C5	2.18	1.59	1.51
4	I	3	BMA	O2-C2	-2.17	1.38	1.43
4	O	4	MAN	C1-C2	-2.12	1.47	1.52
5	J	4	MAN	O5-C5	2.11	1.47	1.43
4	I	5	MAN	C2-C3	2.10	1.55	1.52
8	Q	3	BMA	O3-C3	2.07	1.48	1.43
4	O	3	BMA	C2-C3	-2.06	1.49	1.52
4	I	4	MAN	C2-C3	2.05	1.55	1.52

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	1	NAG	C1-O5-C5	8.49	123.56	112.19
8	Q	4	MAN	C1-O5-C5	7.76	122.59	112.19
6	V	1	NAG	C1-O5-C5	7.42	122.13	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2	NAG	C1-O5-C5	7.18	121.81	112.19
6	R	1	NAG	C1-O5-C5	6.86	121.37	112.19
6	U	1	NAG	C1-O5-C5	6.28	120.61	112.19
4	O	2	NAG	C1-O5-C5	6.28	120.60	112.19
6	K	1	NAG	C1-O5-C5	5.74	119.88	112.19
6	S	1	NAG	C1-O5-C5	5.69	119.81	112.19
4	X	2	NAG	C1-O5-C5	5.38	119.40	112.19
4	I	6	MAN	O5-C5-C6	4.50	116.43	107.66
4	O	5	MAN	C1-O5-C5	4.50	118.21	112.19
8	Q	3	BMA	C6-C5-C4	4.47	123.98	113.02
6	M	1	NAG	C3-C4-C5	4.41	118.24	110.23
4	X	4	MAN	C1-O5-C5	4.14	117.73	112.19
4	I	3	BMA	C1-O5-C5	4.10	117.68	112.19
4	X	6	MAN	O5-C5-C6	3.99	115.43	107.66
5	J	4	MAN	C1-O5-C5	3.95	117.49	112.19
4	O	4	MAN	C1-O5-C5	3.95	117.48	112.19
4	O	3	BMA	C1-O5-C5	3.87	117.37	112.19
4	O	6	MAN	O2-C2-C3	-3.85	102.17	110.15
4	X	6	MAN	C1-O5-C5	3.81	117.29	112.19
4	I	4	MAN	C1-O5-C5	3.73	117.19	112.19
4	X	5	MAN	C1-O5-C5	3.68	117.11	112.19
6	S	1	NAG	C3-C4-C5	3.67	116.89	110.23
6	R	2	NAG	C1-O5-C5	3.65	117.08	112.19
4	X	1	NAG	C2-N2-C7	3.61	127.74	122.90
8	Q	3	BMA	C1-O5-C5	3.61	117.02	112.19
4	O	7	MAN	O5-C1-C2	-3.51	102.42	110.79
4	X	3	BMA	C1-O5-C5	3.39	116.72	112.19
8	Q	3	BMA	O3-C3-C2	3.37	116.94	110.05
5	J	3	BMA	O3-C3-C2	-3.36	103.19	110.05
4	I	6	MAN	O2-C2-C3	-3.25	103.42	110.15
4	X	7	MAN	O5-C1-C2	-3.25	103.03	110.79
7	N	3	BMA	O5-C5-C6	3.05	113.60	107.66
4	O	6	MAN	O5-C5-C6	3.00	113.51	107.66
7	N	3	BMA	C1-C2-C3	2.95	113.94	109.64
4	I	4	MAN	O3-C3-C2	2.92	116.02	110.05
4	X	4	MAN	O3-C3-C2	2.91	115.99	110.05
8	Q	3	BMA	O6-C6-C5	2.90	121.20	111.33
4	I	7	MAN	O5-C1-C2	-2.86	103.97	110.79
4	X	7	MAN	O2-C2-C3	-2.79	104.37	110.15
4	X	6	MAN	O2-C2-C3	-2.76	104.43	110.15
4	I	7	MAN	O2-C2-C3	-2.72	104.51	110.15
4	O	6	MAN	C1-O5-C5	2.69	115.80	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	1	NAG	C3-C4-C5	2.65	115.04	110.23
8	Q	1	NAG	C1-O5-C5	2.64	115.72	112.19
4	O	3	BMA	O2-C2-C3	-2.62	104.72	110.15
4	I	3	BMA	C3-C4-C5	2.61	114.97	110.23
7	N	3	BMA	O5-C5-C4	-2.61	104.48	110.83
4	I	5	MAN	C1-O5-C5	-2.60	108.70	112.19
4	I	2	NAG	O5-C5-C6	-2.57	102.66	107.66
6	M	1	NAG	O6-C6-C5	2.53	119.96	111.33
7	N	3	BMA	C6-C5-C4	2.52	119.21	113.02
7	W	3	BMA	C2-C3-C4	2.51	115.28	110.86
4	I	6	MAN	C1-O5-C5	2.49	115.52	112.19
7	W	3	BMA	C1-C2-C3	2.49	113.27	109.64
7	N	3	BMA	C2-C3-C4	2.45	115.17	110.86
4	O	7	MAN	O2-C2-C3	-2.45	105.07	110.15
4	O	4	MAN	O3-C3-C2	2.45	115.06	110.05
7	W	3	BMA	O2-C2-C1	2.44	114.81	109.22
5	J	3	BMA	C1-O5-C5	2.43	115.45	112.19
6	U	1	NAG	C3-C4-C5	2.42	114.62	110.23
5	J	3	BMA	O2-C2-C3	-2.41	105.16	110.15
5	J	3	BMA	C3-C4-C5	2.39	114.57	110.23
7	N	3	BMA	C1-O5-C5	-2.39	108.98	112.19
7	W	3	BMA	O5-C5-C6	2.38	112.30	107.66
4	I	6	MAN	O5-C5-C4	-2.26	105.34	110.83
4	I	7	MAN	O6-C6-C5	-2.23	103.73	111.33
4	O	7	MAN	C3-C4-C5	2.23	114.27	110.23
8	Q	3	BMA	C3-C4-C5	2.22	114.25	110.23
4	X	7	MAN	C3-C4-C5	2.20	114.22	110.23
7	N	3	BMA	O3-C3-C4	2.20	115.56	110.38
4	I	7	MAN	O2-C2-C1	2.18	114.21	109.22
8	Q	5	MAN	C1-C2-C3	-2.16	106.50	109.64
7	W	1	NAG	C1-O5-C5	2.15	115.07	112.19
4	I	3	BMA	O5-C5-C6	2.15	111.84	107.66
7	W	3	BMA	O5-C5-C4	-2.11	105.70	110.83
8	Q	1	NAG	O6-C6-C5	2.10	118.47	111.33
4	X	1	NAG	O4-C4-C5	-2.09	104.19	109.32
8	Q	2	NAG	O4-C4-C5	-2.08	104.21	109.32
4	X	4	MAN	O5-C5-C4	-2.07	105.79	110.83
4	I	6	MAN	O3-C3-C2	2.05	114.25	110.05
6	R	1	NAG	C3-C4-C5	2.01	113.88	110.23
6	K	1	NAG	C3-C4-C5	2.00	113.86	110.23

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	W	2	NAG	O5-C5-C6-O6
7	N	2	NAG	O5-C5-C6-O6
8	Q	2	NAG	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	T	1	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	X	4	MAN	C4-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	I	4	MAN	O5-C5-C6-O6
4	X	4	MAN	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	O	7	MAN	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	I	4	MAN	C4-C5-C6-O6
7	N	2	NAG	C4-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
4	O	4	MAN	C4-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	S	1	NAG	C4-C5-C6-O6
4	O	4	MAN	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
7	W	2	NAG	C4-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	X	7	MAN	O5-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
4	I	7	MAN	O5-C5-C6-O6
5	J	3	BMA	C4-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
6	M	1	NAG	C4-C5-C6-O6
6	U	1	NAG	C4-C5-C6-O6
8	Q	2	NAG	C4-C5-C6-O6
6	T	1	NAG	C4-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
6	V	2	NAG	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
6	M	2	NAG	C8-C7-N2-C2
6	M	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	R	2	NAG	C8-C7-N2-C2
6	R	2	NAG	O7-C7-N2-C2
6	S	2	NAG	C8-C7-N2-C2
6	S	2	NAG	O7-C7-N2-C2
6	U	2	NAG	C8-C7-N2-C2
6	U	2	NAG	O7-C7-N2-C2
6	V	2	NAG	C8-C7-N2-C2
6	V	2	NAG	O7-C7-N2-C2
4	I	7	MAN	C4-C5-C6-O6
6	S	1	NAG	O5-C5-C6-O6
4	X	7	MAN	C4-C5-C6-O6
8	Q	3	BMA	O5-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
6	R	2	NAG	C4-C5-C6-O6
4	O	7	MAN	C4-C5-C6-O6
6	U	1	NAG	O5-C5-C6-O6
6	M	1	NAG	O5-C5-C6-O6
6	S	2	NAG	C4-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
5	J	3	BMA	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
4	I	3	BMA	C4-C5-C6-O6
4	O	3	BMA	C4-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
6	R	1	NAG	C4-C5-C6-O6
6	U	2	NAG	C4-C5-C6-O6
4	O	3	BMA	O5-C5-C6-O6
4	X	3	BMA	C4-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
6	P	1	NAG	C4-C5-C6-O6
4	I	3	BMA	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
8	Q	4	MAN	O5-C5-C6-O6
6	P	1	NAG	O5-C5-C6-O6
6	R	1	NAG	O5-C5-C6-O6
6	M	2	NAG	O5-C5-C6-O6
7	N	3	BMA	C4-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
4	X	3	BMA	O5-C5-C6-O6
8	Q	5	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	X	1	NAG	C1-C2-N2-C7
6	M	1	NAG	C1-C2-N2-C7
6	S	1	NAG	C1-C2-N2-C7
6	V	1	NAG	C1-C2-N2-C7
7	W	1	NAG	C1-C2-N2-C7
8	Q	1	NAG	O5-C5-C6-O6
8	Q	1	NAG	C4-C5-C6-O6
4	O	5	MAN	O5-C5-C6-O6

All (9) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	Q	5	MAN	C1-C2-C3-C4-C5-O5
4	O	5	MAN	C1-C2-C3-C4-C5-O5
4	O	4	MAN	C1-C2-C3-C4-C5-O5
4	X	4	MAN	C1-C2-C3-C4-C5-O5
4	O	6	MAN	C1-C2-C3-C4-C5-O5
4	X	5	MAN	C1-C2-C3-C4-C5-O5
4	X	6	MAN	C1-C2-C3-C4-C5-O5
4	I	4	MAN	C1-C2-C3-C4-C5-O5
4	I	6	MAN	C1-C2-C3-C4-C5-O5

18 monomers are involved in 18 short contacts:

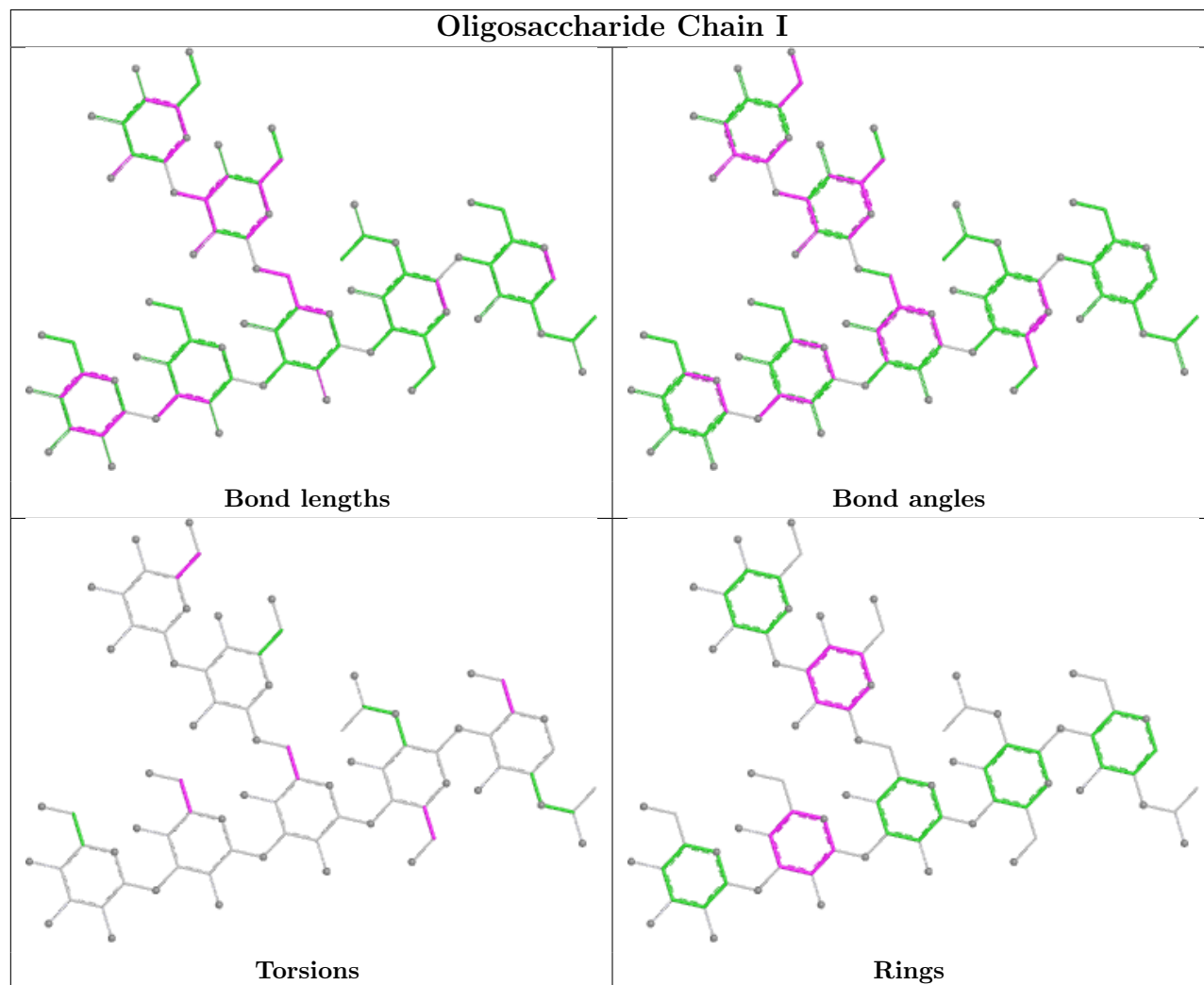
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	7	MAN	1	0
4	X	4	MAN	1	0
4	O	4	MAN	2	0
4	X	3	BMA	1	0
6	U	2	NAG	2	0
4	X	7	MAN	1	0
4	O	3	BMA	1	0
4	I	6	MAN	1	0
4	O	7	MAN	1	0
4	X	5	MAN	1	0
4	X	1	NAG	1	0
4	O	1	NAG	1	0
6	K	2	NAG	2	0
4	X	6	MAN	1	0
4	O	6	MAN	1	0
6	R	2	NAG	2	0
4	I	3	BMA	1	0

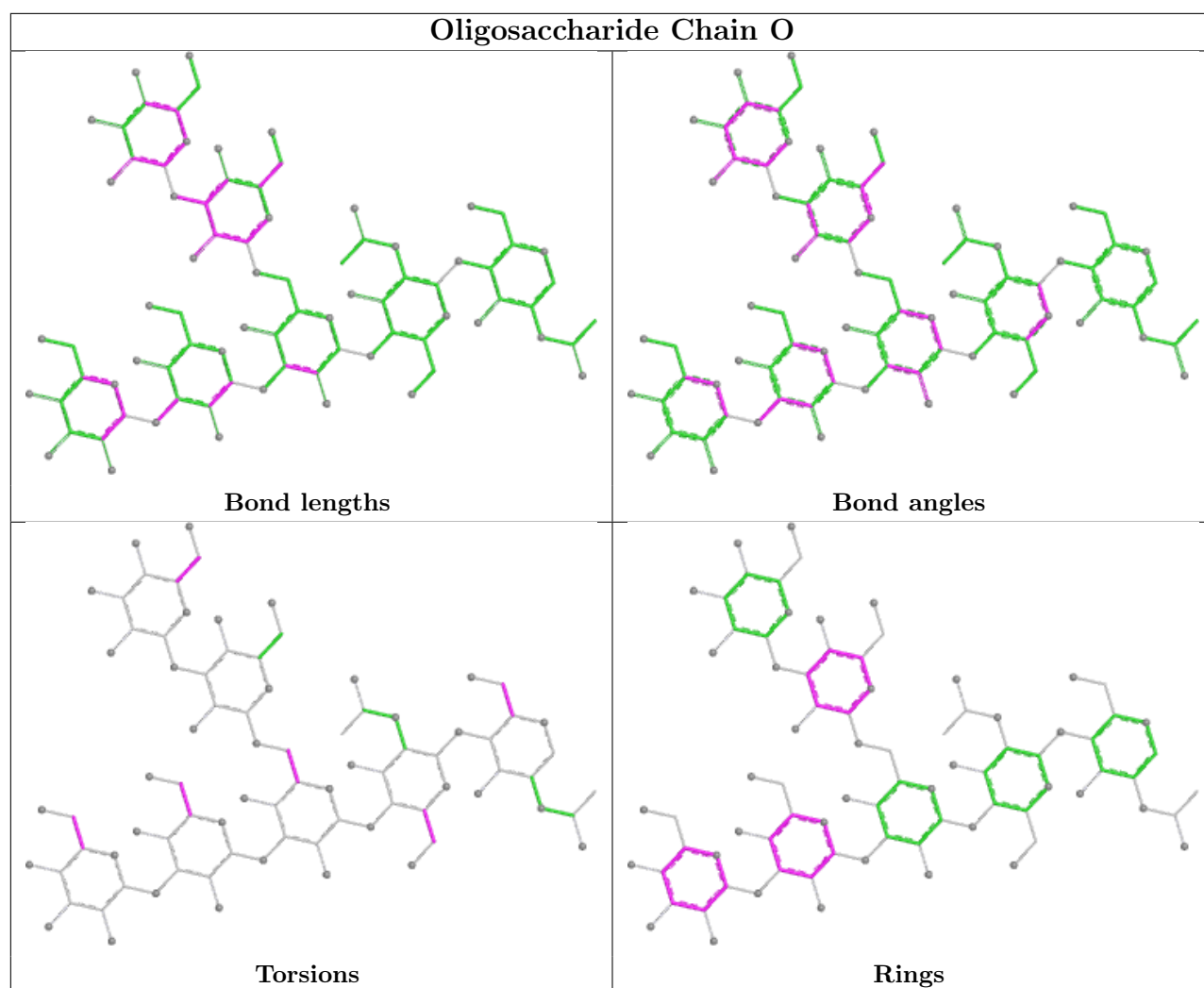
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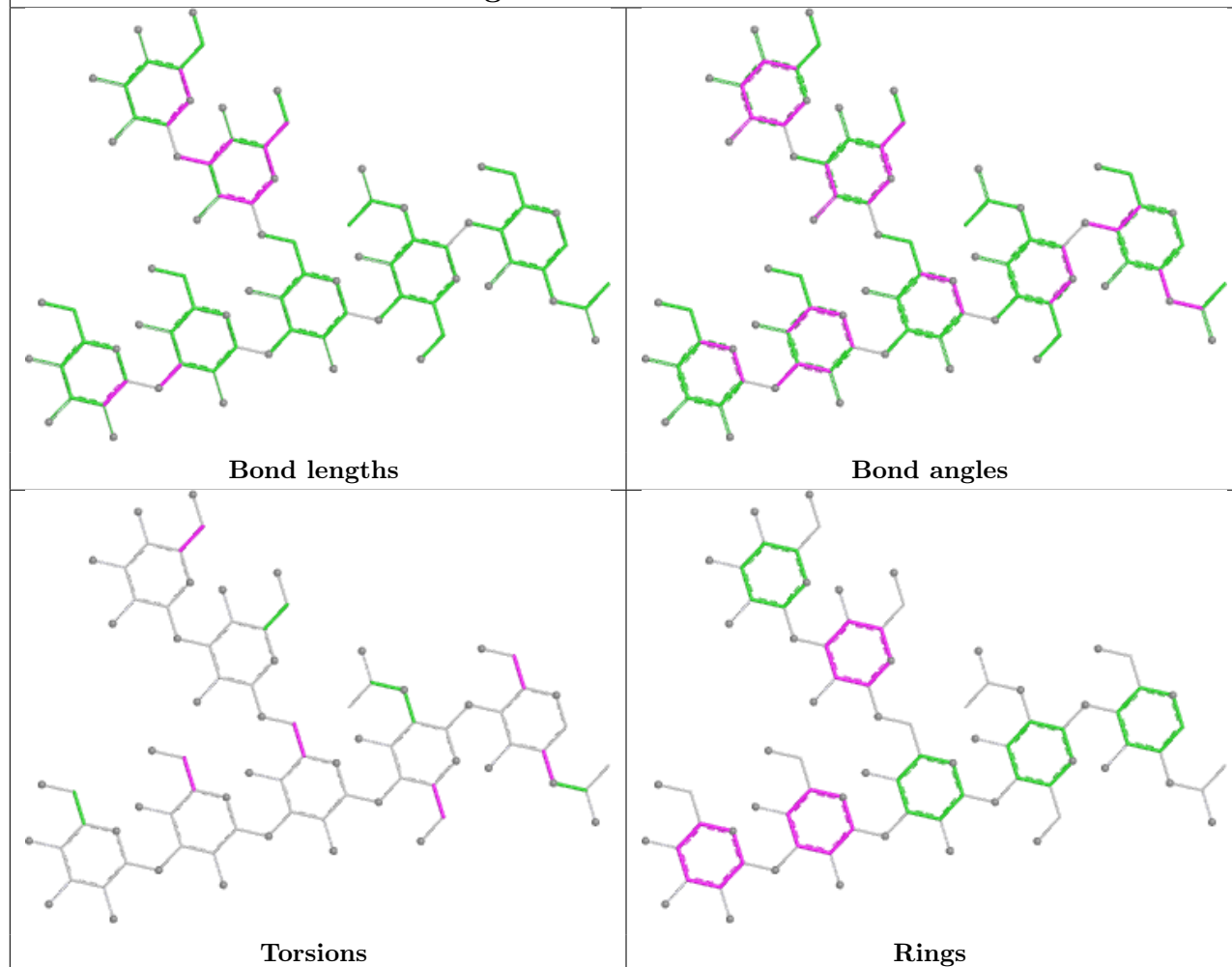
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	5	MAN	2	0

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





Oligosaccharide Chain X



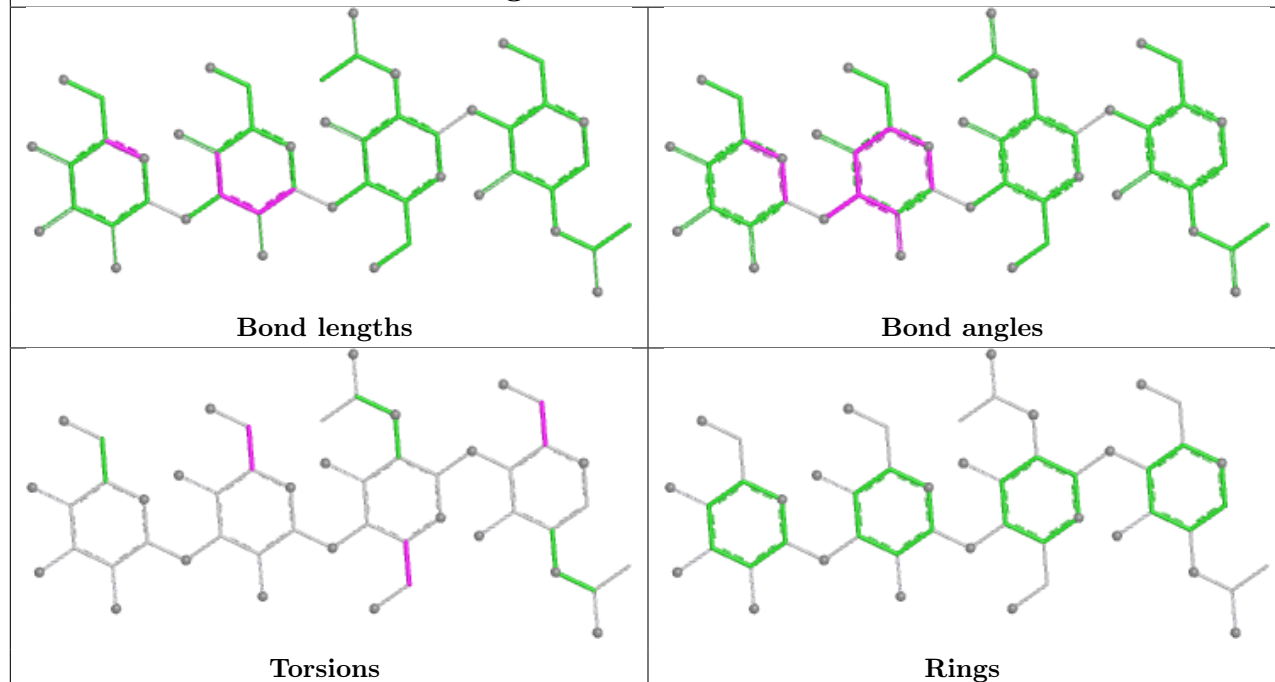
Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

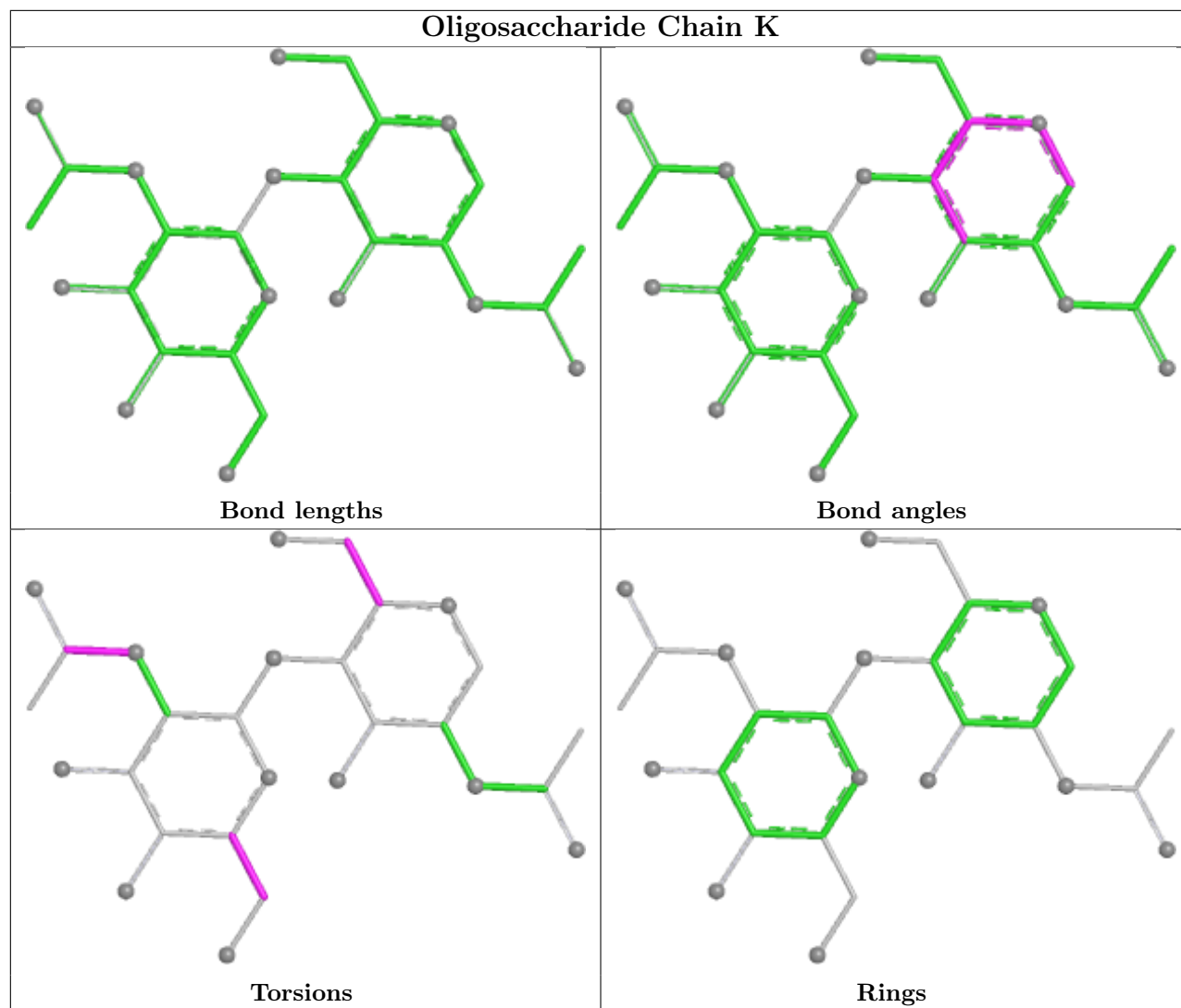


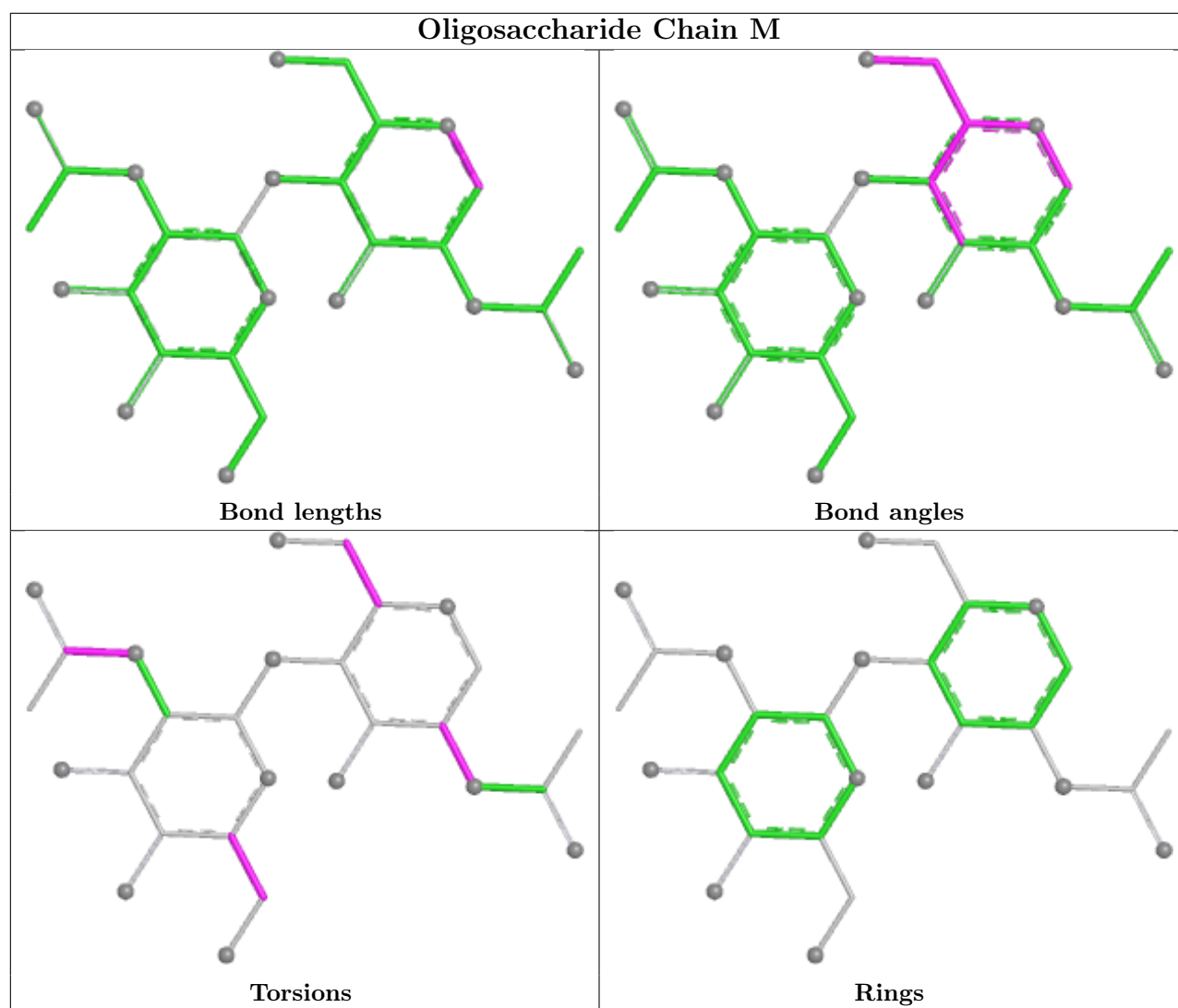
Bond lengths

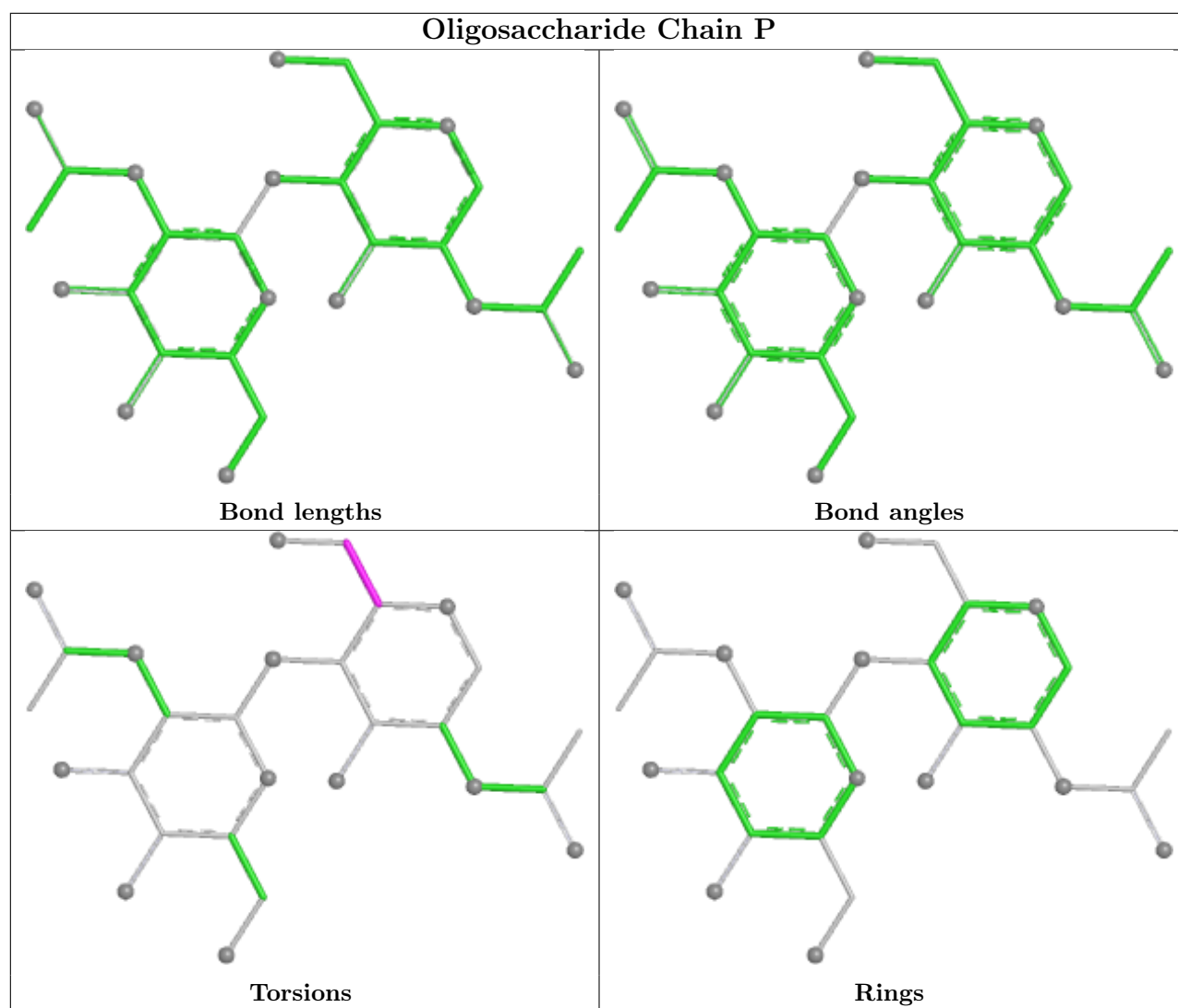
Bond angles

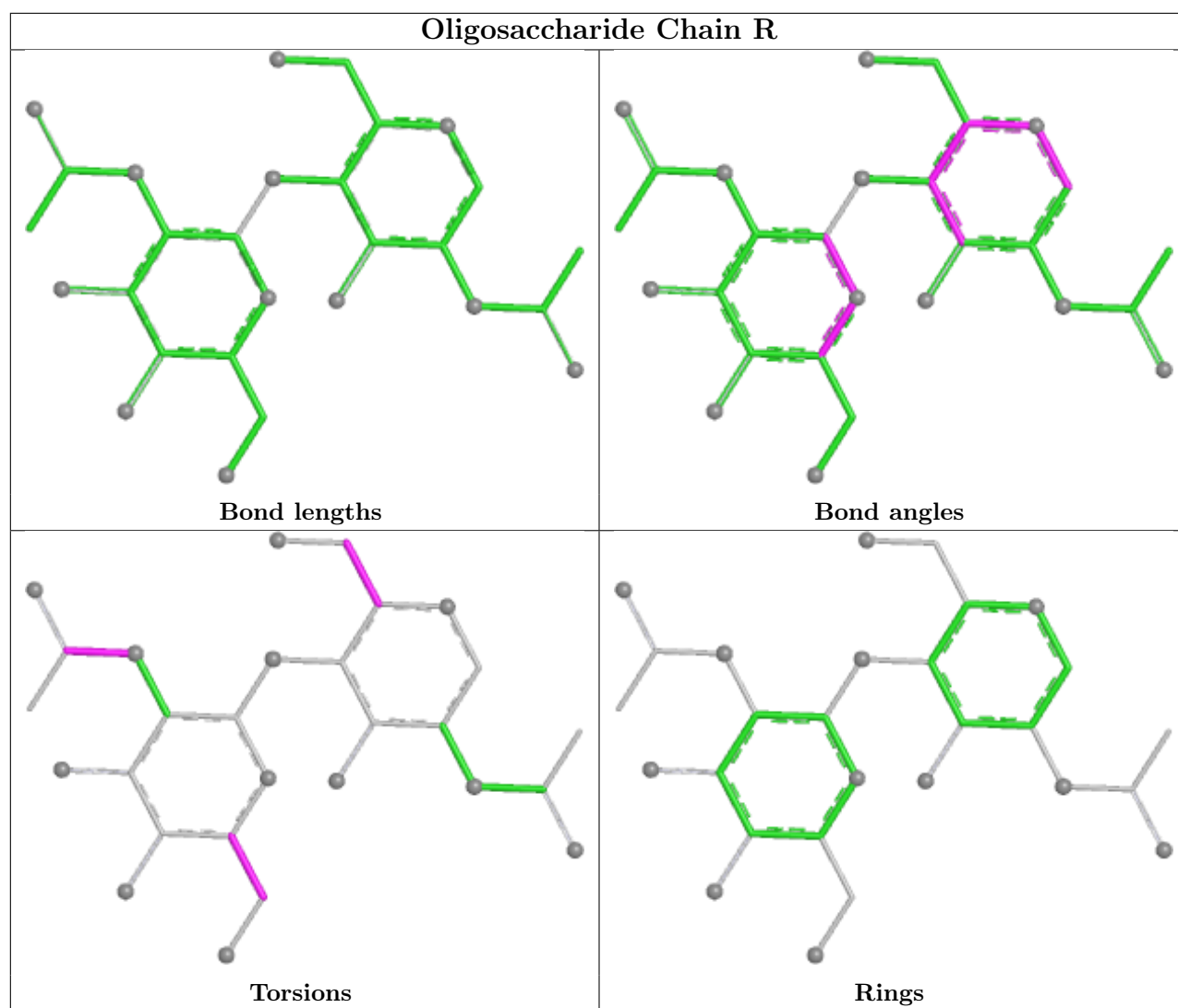
Torsions

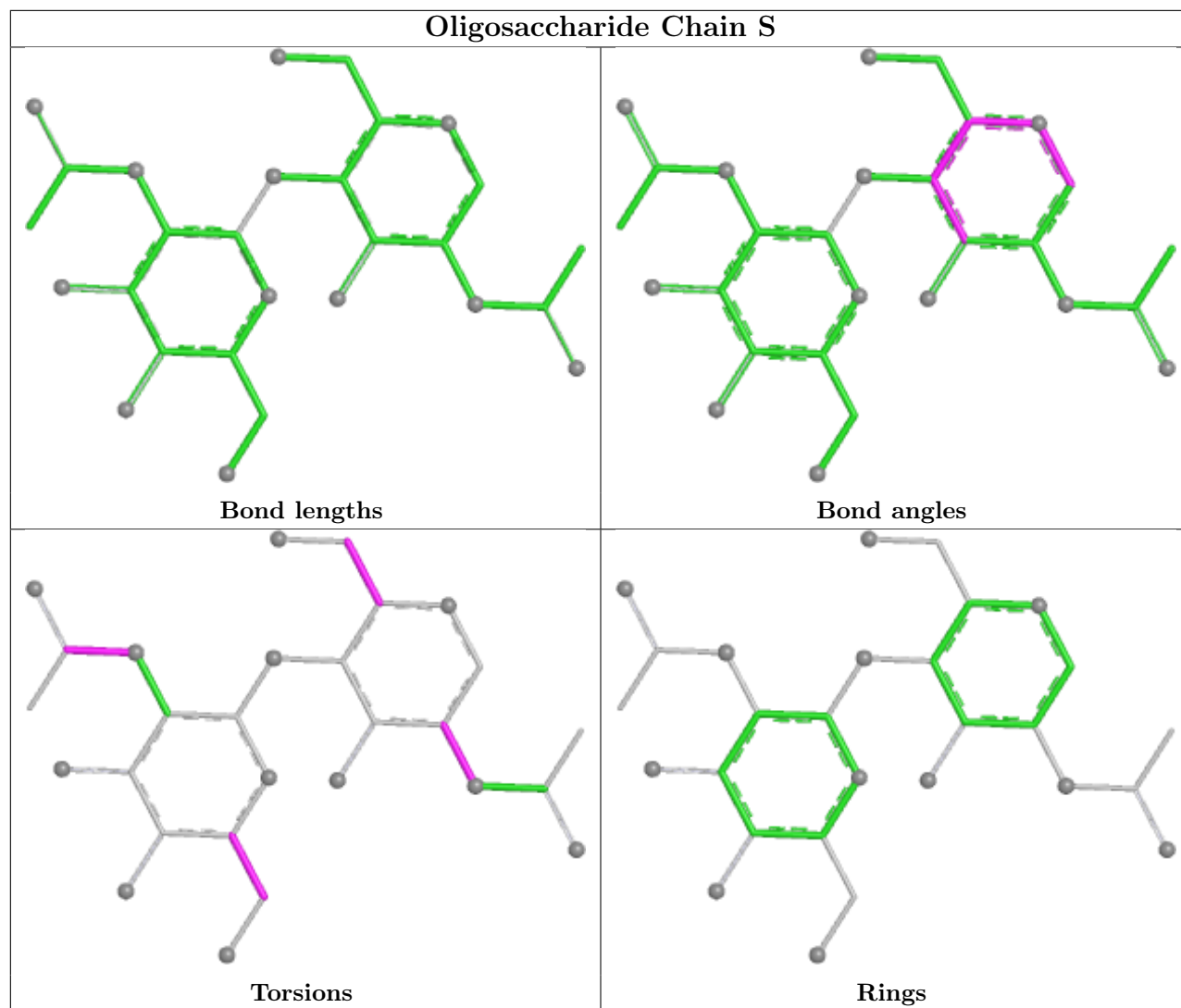
Rings

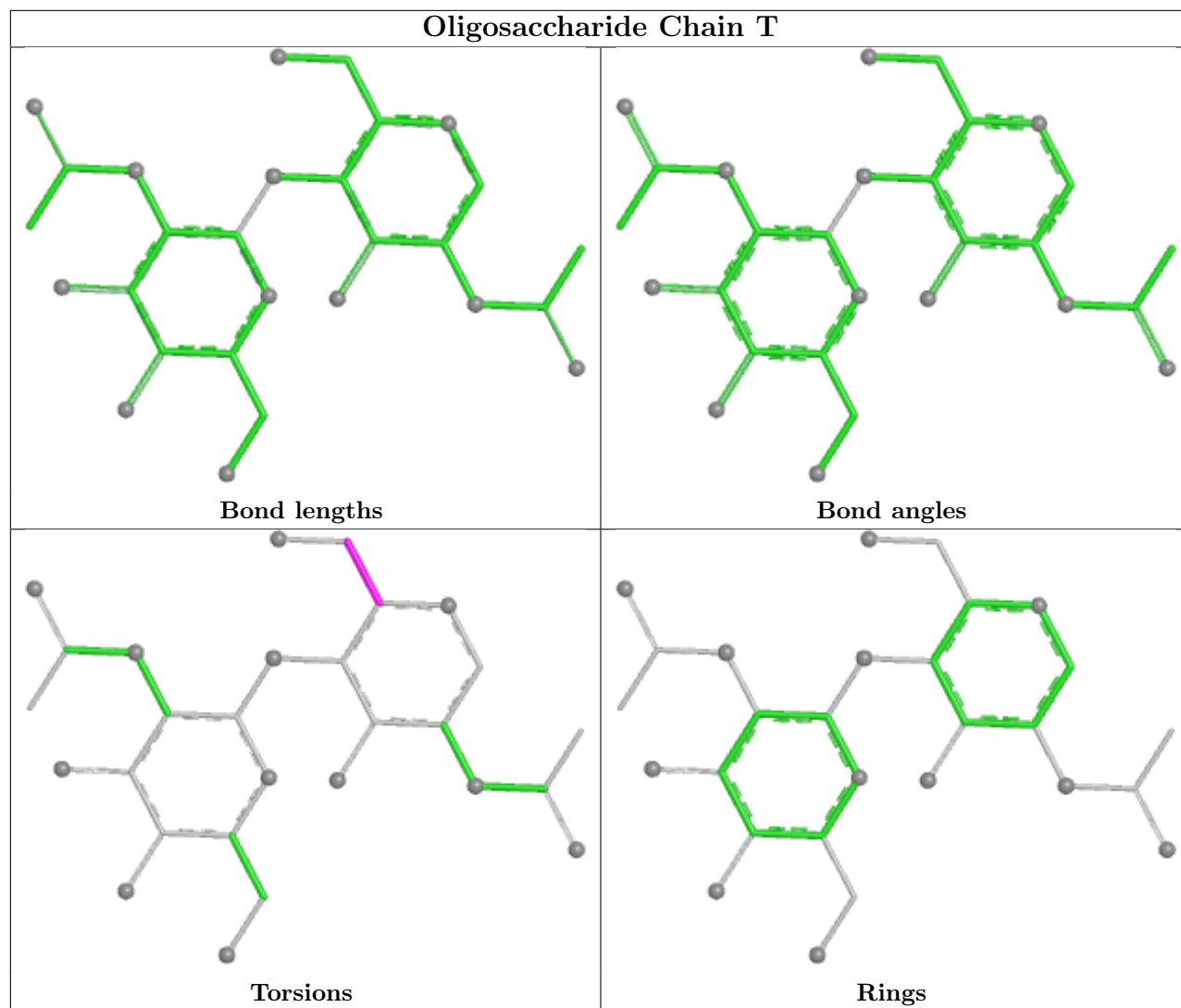


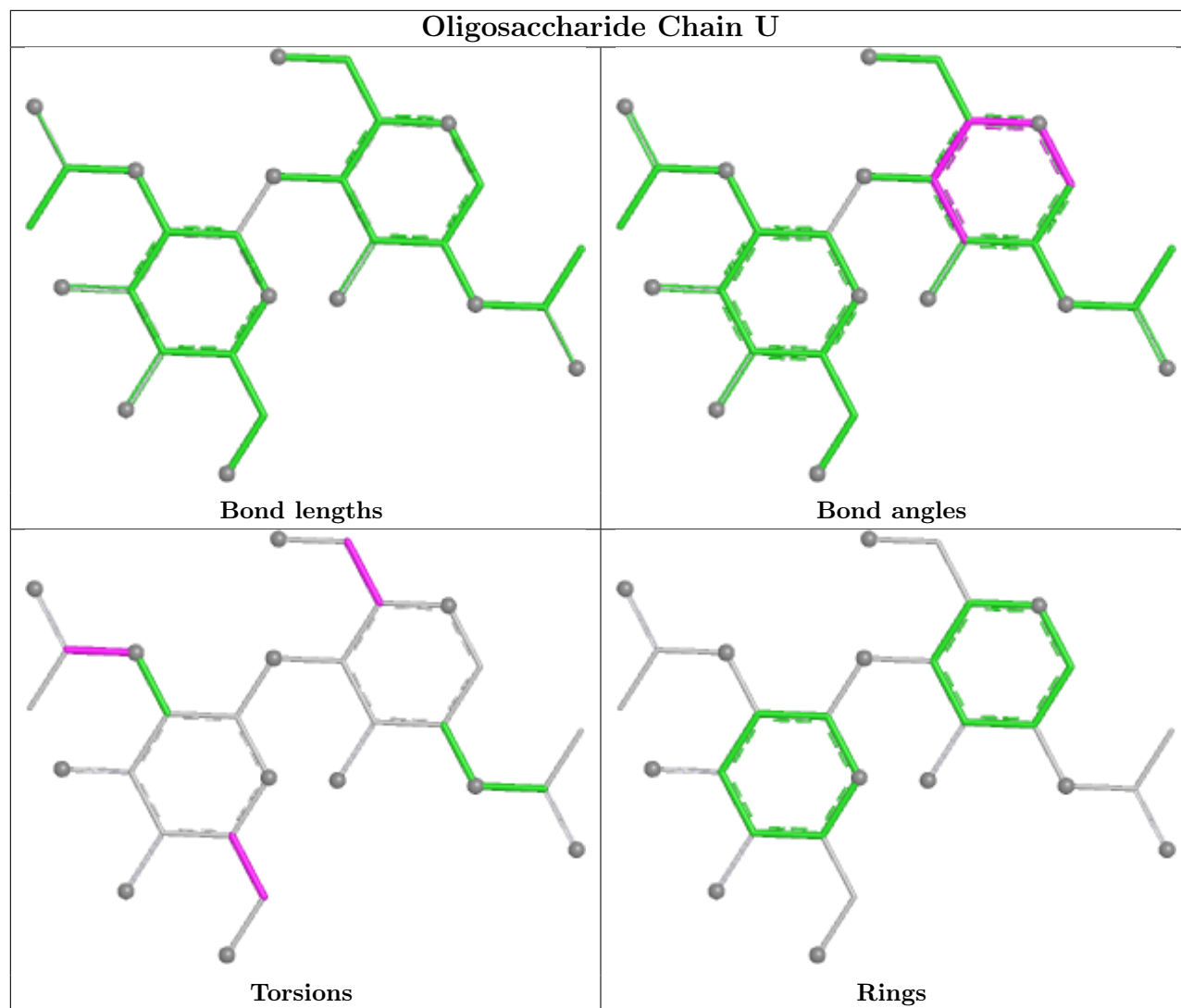


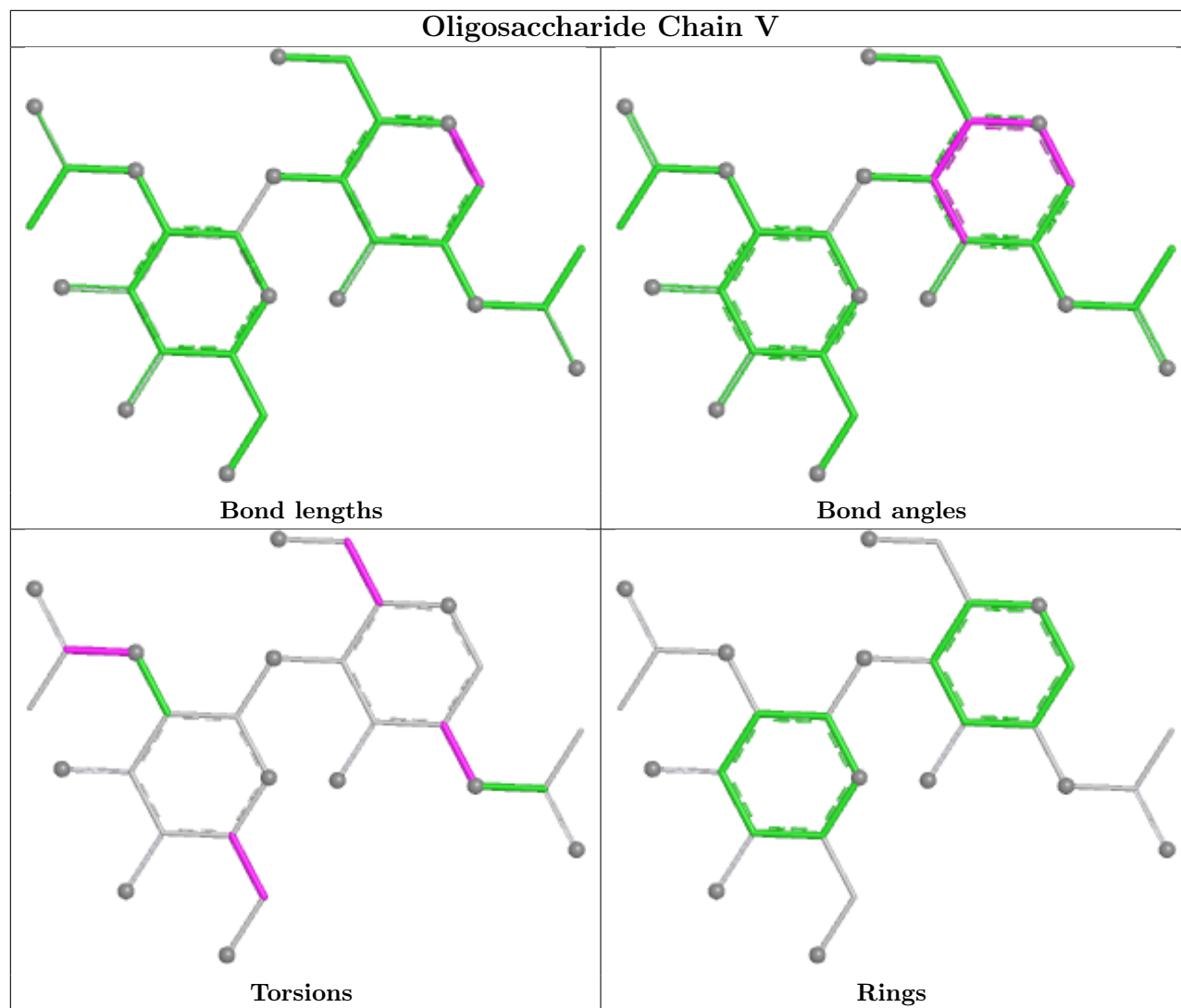


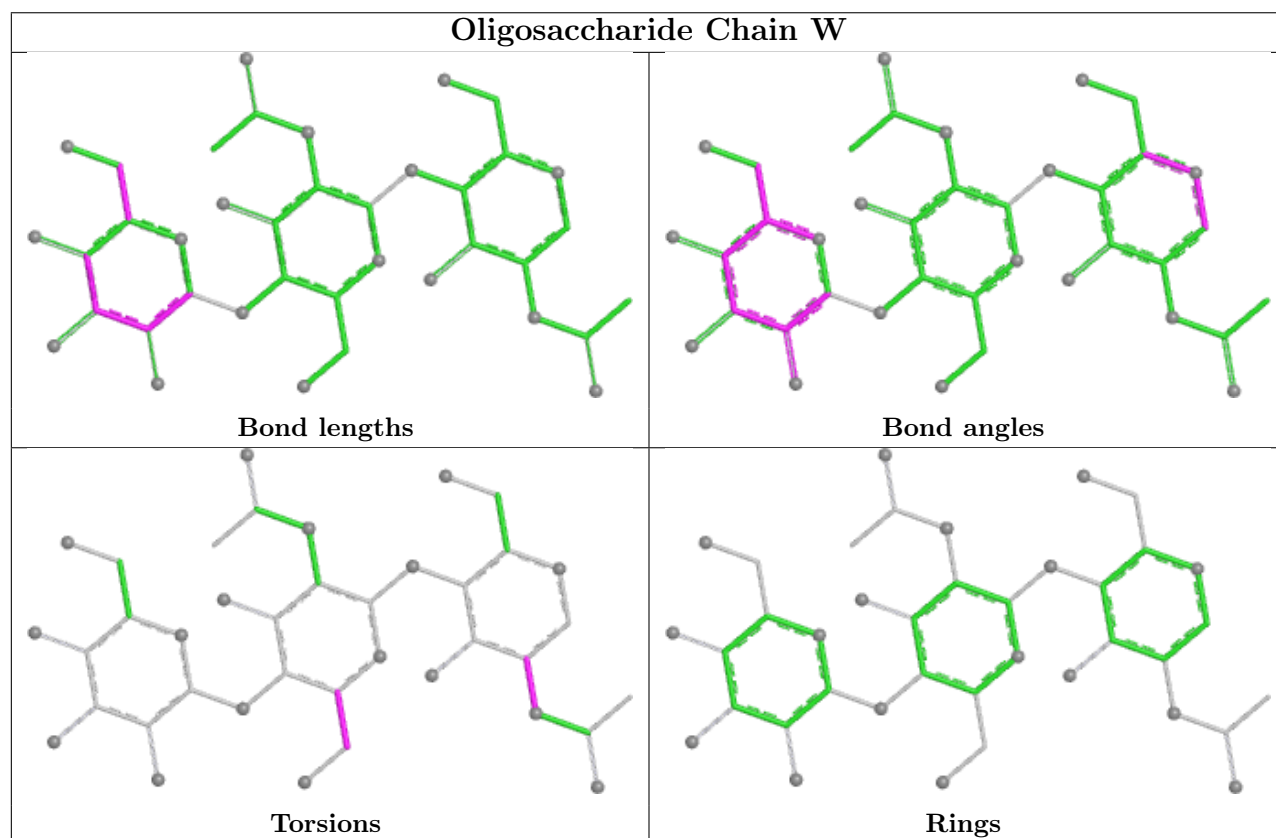
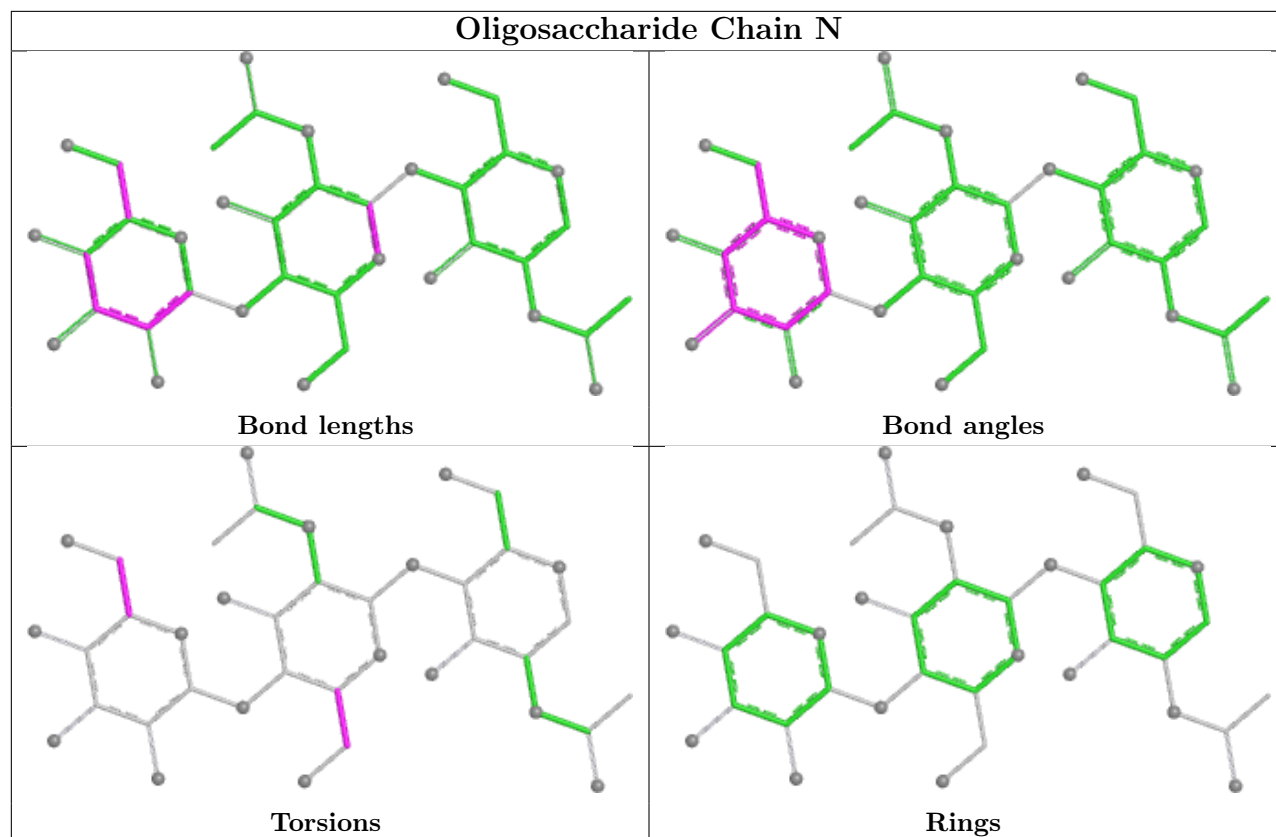


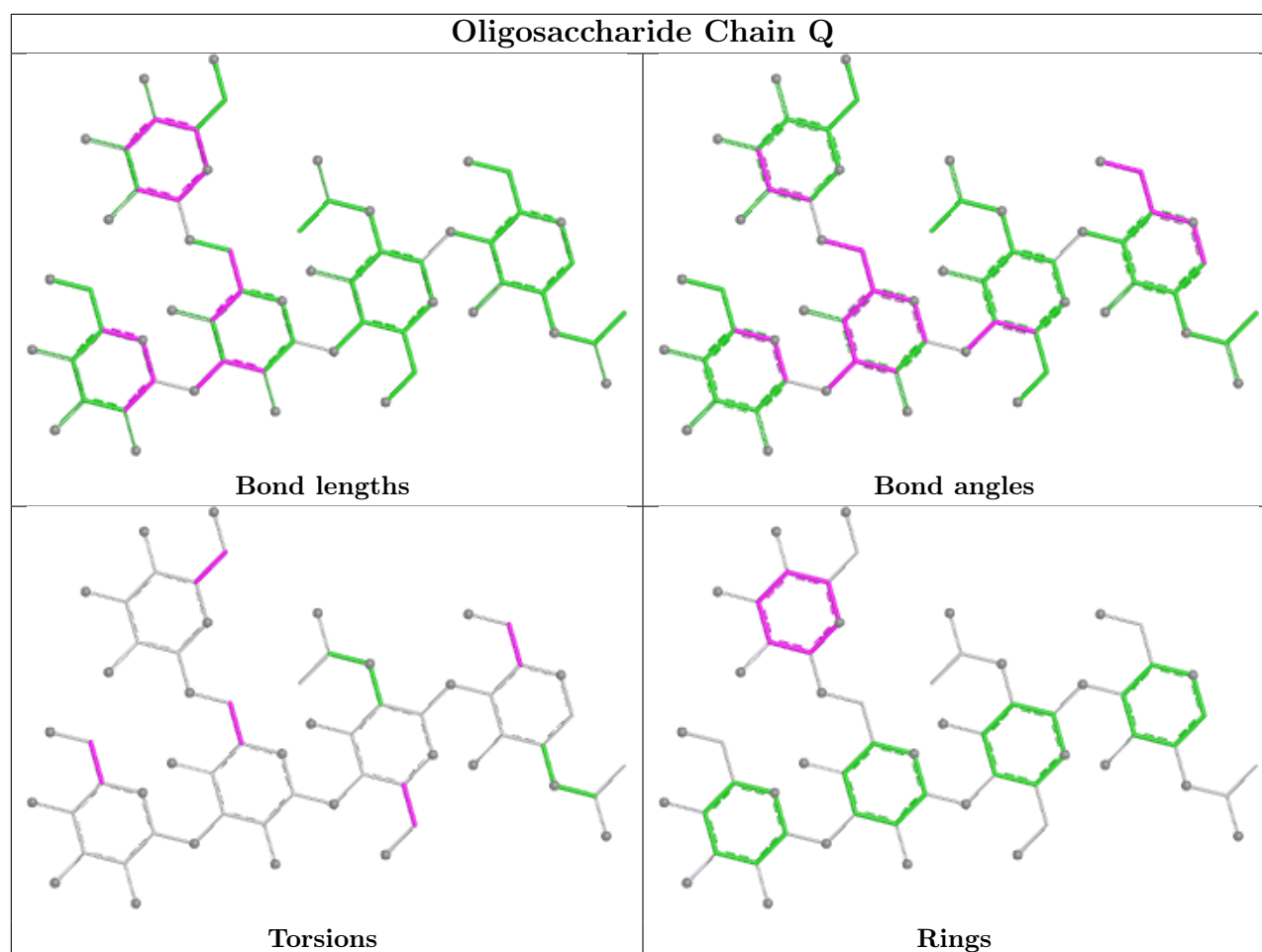












5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
9	NAG	C	501	1	14,14,15	0.31	0	17,19,21	0.47	0
9	NAG	B	409	1	14,14,15	0.31	0	17,19,21	0.60	0
9	NAG	C	502	1	14,14,15	0.94	2 (14%)	17,19,21	0.75	1 (5%)
9	NAG	B	408	1	14,14,15	0.47	0	17,19,21	0.74	0
9	NAG	A	410	1	14,14,15	1.36	1 (7%)	17,19,21	1.07	2 (11%)
9	NAG	B	410	1	14,14,15	1.19	1 (7%)	17,19,21	1.17	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	C	503	1	14,14,15	1.22	1 (7%)	17,19,21	1.12	2 (11%)
9	NAG	A	408	1	14,14,15	0.29	0	17,19,21	0.46	0
9	NAG	A	409	1	14,14,15	1.34	2 (14%)	17,19,21	0.91	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
9	NAG	C	501	1	-	0/6/23/26	0/1/1/1
9	NAG	B	409	1	-	0/6/23/26	0/1/1/1
9	NAG	C	502	1	-	2/6/23/26	0/1/1/1
9	NAG	B	408	1	-	0/6/23/26	0/1/1/1
9	NAG	A	410	1	-	4/6/23/26	0/1/1/1
9	NAG	B	410	1	-	3/6/23/26	0/1/1/1
9	NAG	C	503	1	-	4/6/23/26	0/1/1/1
9	NAG	A	408	1	-	2/6/23/26	0/1/1/1
9	NAG	A	409	1	-	3/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	410	NAG	O5-C1	-4.92	1.35	1.43
9	B	410	NAG	O5-C1	-4.24	1.36	1.43
9	A	409	NAG	O5-C1	4.11	1.50	1.43
9	C	503	NAG	O5-C1	-4.09	1.36	1.43
9	C	502	NAG	O5-C1	2.77	1.48	1.43
9	A	409	NAG	C1-C2	2.55	1.55	1.52
9	C	502	NAG	C1-C2	2.05	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	410	NAG	C1-O5-C5	-2.98	108.20	112.19
9	C	503	NAG	C1-O5-C5	-2.79	108.45	112.19
9	B	410	NAG	C3-C4-C5	2.71	115.14	110.23
9	C	503	NAG	C3-C4-C5	2.68	115.09	110.23
9	A	410	NAG	C3-C4-C5	2.56	114.88	110.23
9	C	502	NAG	C1-O5-C5	2.53	115.57	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	410	NAG	C1-O5-C5	-2.45	108.90	112.19
9	A	409	NAG	C1-O5-C5	2.35	115.34	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	409	NAG	C4-C5-C6-O6
9	B	410	NAG	O5-C5-C6-O6
9	C	502	NAG	C4-C5-C6-O6
9	A	408	NAG	O5-C5-C6-O6
9	C	502	NAG	O5-C5-C6-O6
9	A	409	NAG	O5-C5-C6-O6
9	A	410	NAG	O5-C5-C6-O6
9	C	503	NAG	O5-C5-C6-O6
9	B	410	NAG	C4-C5-C6-O6
9	A	408	NAG	C4-C5-C6-O6
9	C	503	NAG	C4-C5-C6-O6
9	A	410	NAG	C4-C5-C6-O6
9	A	410	NAG	C1-C2-N2-C7
9	A	410	NAG	C3-C2-N2-C7
9	C	503	NAG	C3-C2-N2-C7
9	C	503	NAG	C1-C2-N2-C7
9	A	409	NAG	C3-C2-N2-C7
9	B	410	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	A	336/336 (100%)	-0.52	0 100 100	30, 47, 76, 97	0
1	B	336/336 (100%)	-0.26	7 (2%) 63 40	38, 62, 96, 133	0
1	C	336/336 (100%)	0.11	11 (3%) 49 28	43, 74, 117, 143	0
2	D	120/132 (90%)	0.57	11 (9%) 14 8	49, 92, 129, 157	0
2	F	120/132 (90%)	0.22	7 (5%) 29 15	43, 71, 107, 153	0
2	H	128/132 (96%)	-0.35	5 (3%) 43 24	32, 44, 90, 147	0
3	E	111/111 (100%)	-0.15	4 (3%) 46 26	45, 64, 95, 126	0
3	G	111/111 (100%)	-0.33	1 (0%) 81 61	43, 57, 85, 103	0
3	L	111/111 (100%)	-0.52	1 (0%) 81 61	33, 47, 72, 86	0
All	All	1709/1737 (98%)	-0.17	47 (2%) 55 32	30, 61, 106, 157	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	-7	GLY	6.8
2	H	-4	SER	6.3
1	C	302	SER	5.5
1	C	353	SER	5.2
2	H	120	SER	4.8
2	F	120	SER	4.3
1	C	44	TRP	4.0
2	F	119	SER	3.9
1	B	353	SER	3.3
2	D	119	SER	3.3
2	D	108	ASP	3.2
1	C	95	THR	3.2
1	B	62	ARG	3.1
1	C	219	TYR	3.1
2	F	65	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	77	TYR	3.0
2	D	74	LYS	2.9
2	D	13	LYS	2.9
1	C	139	THR	2.9
1	C	303	ILE	2.8
3	E	136	LYS	2.8
2	F	1	GLU	2.8
1	C	176	CYS	2.7
1	B	44	TRP	2.7
2	D	63	LYS	2.6
2	D	66	VAL	2.6
2	D	43	GLN	2.5
3	E	96	SER	2.5
2	D	120	SER	2.5
2	F	74	LYS	2.5
3	E	26	ASP	2.5
2	H	-6	GLY	2.4
3	G	136	LYS	2.4
2	F	43	GLN	2.4
2	D	1	GLU	2.4
1	B	302	SER	2.4
1	B	139	THR	2.3
3	L	136	LYS	2.3
2	H	-3	GLY	2.3
1	B	350	SER	2.2
2	D	41	PRO	2.2
2	D	57	ASP	2.1
1	C	214	CYS	2.1
1	C	96	THR	2.1
1	B	107	GLN	2.1
3	E	105	HIS	2.1
2	F	117	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	I	1	14/15	-	-	27,33,43,52	0
4	NAG	I	2	14/15	-	-	27,34,52,64	0
4	BMA	I	3	11/12	-	-	27,39,47,51	0
4	MAN	I	4	11/12	-	-	64,81,93,112	0
4	MAN	I	5	11/12	-	-	82,113,122,123	0
4	MAN	I	6	11/12	-	-	46,64,87,93	0
4	MAN	I	7	11/12	-	-	52,69,75,78	0
6	NAG	P	1	14/15	0.35	0.21	122,143,148,149	0
4	MAN	O	5	11/12	0.55	0.23	114,126,140,140	0
8	MAN	Q	4	11/12	0.56	0.23	137,146,156,159	0
6	NAG	T	2	14/15	0.60	0.19	128,143,157,162	0
6	NAG	P	2	14/15	0.60	0.16	126,147,152,152	0
6	NAG	V	2	14/15	0.61	0.21	131,160,174,179	0
4	MAN	X	5	11/12	0.66	0.21	131,145,152,154	0
6	NAG	M	2	14/15	0.68	0.23	107,117,129,143	0
4	MAN	X	4	11/12	0.71	0.24	107,115,126,135	0
6	NAG	S	2	14/15	0.72	0.25	131,163,173,176	0
6	NAG	V	1	14/15	0.75	0.14	56,91,109,130	0
5	MAN	J	4	11/12	0.75	0.24	118,128,135,137	0
7	BMA	N	3	11/12	0.75	0.18	71,91,105,109	0
6	NAG	R	2	14/15	0.75	0.21	63,95,121,124	0
4	MAN	X	6	11/12	0.76	0.17	60,86,96,103	0
8	MAN	Q	5	11/12	0.76	0.12	103,121,125,127	0
6	NAG	U	2	14/15	0.77	0.18	71,89,103,115	0
4	MAN	O	6	11/12	0.77	0.19	62,88,104,113	0
6	NAG	S	1	14/15	0.79	0.19	76,87,107,138	0
6	NAG	M	1	14/15	0.81	0.12	43,66,84,104	0
8	BMA	Q	3	11/12	0.81	0.15	89,96,115,123	0
4	MAN	O	4	11/12	0.82	0.17	71,89,110,119	0
6	NAG	U	1	14/15	0.82	0.12	53,74,87,90	0
7	BMA	W	3	11/12	0.82	0.14	78,104,116,117	0
6	NAG	R	1	14/15	0.86	0.13	58,66,81,86	0
4	MAN	O	7	11/12	0.86	0.15	69,86,96,96	0
4	MAN	X	7	11/12	0.87	0.15	70,97,106,107	0
4	BMA	X	3	11/12	0.88	0.10	81,89,95,105	0
7	NAG	W	1	14/15	0.88	0.13	76,84,110,117	0
6	NAG	T	1	14/15	0.90	0.13	78,96,115,116	0
7	NAG	W	2	14/15	0.91	0.12	97,104,120,123	0
8	NAG	Q	2	14/15	0.93	0.11	44,69,79,81	0
4	BMA	O	3	11/12	0.93	0.08	56,66,75,78	0
6	NAG	K	2	14/15	0.94	0.10	64,86,91,92	0

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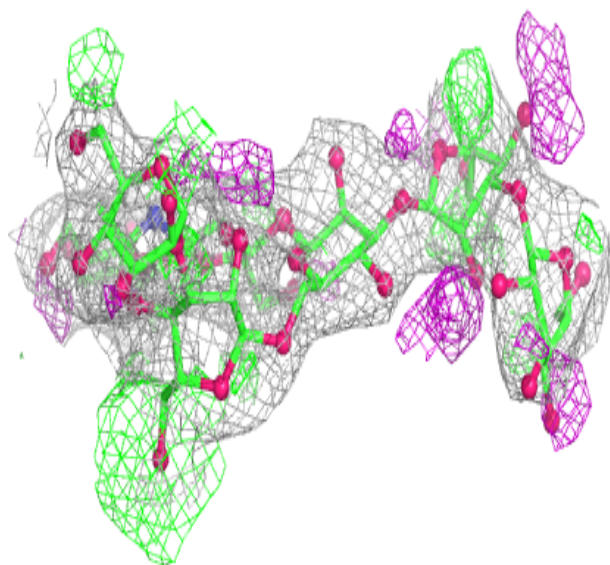
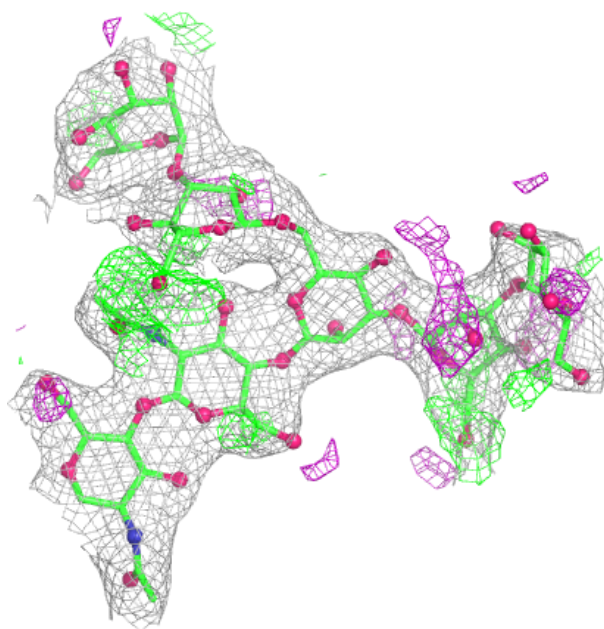
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	Q	1	14/15	0.95	0.09	40,51,77,87	0
4	NAG	X	1	14/15	0.95	0.12	57,63,89,96	0
5	BMA	J	3	11/12	0.95	0.07	88,108,124,130	0
4	NAG	X	2	14/15	0.95	0.12	55,65,100,106	0
7	NAG	N	1	14/15	0.95	0.07	50,56,66,70	0
7	NAG	N	2	14/15	0.96	0.09	54,70,82,87	0
4	NAG	O	2	14/15	0.96	0.09	36,50,63,85	0
5	NAG	J	1	14/15	0.97	0.07	35,37,50,55	0
5	NAG	J	2	14/15	0.97	0.07	40,55,69,71	0
4	NAG	O	1	14/15	0.98	0.06	36,41,54,62	0
6	NAG	K	1	14/15	0.98	0.06	36,51,68,69	0

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

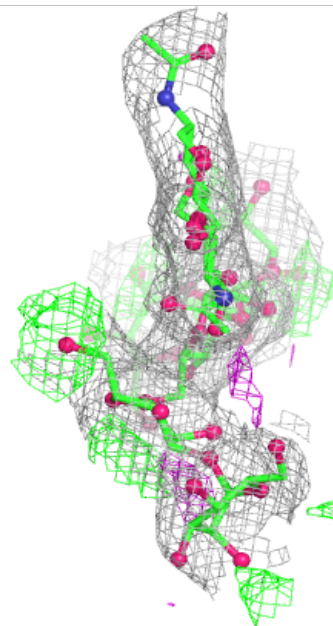
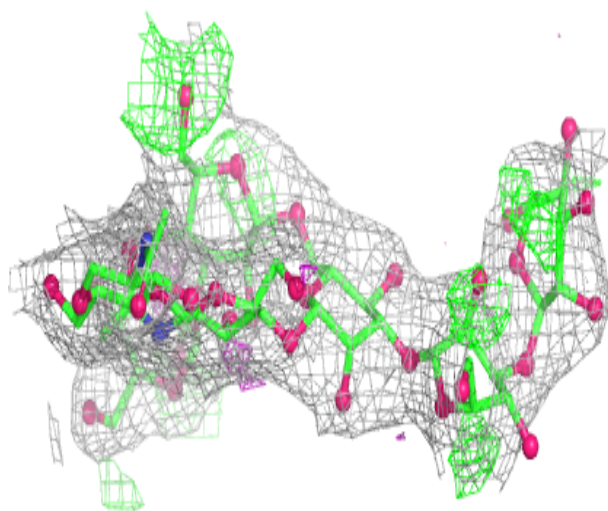
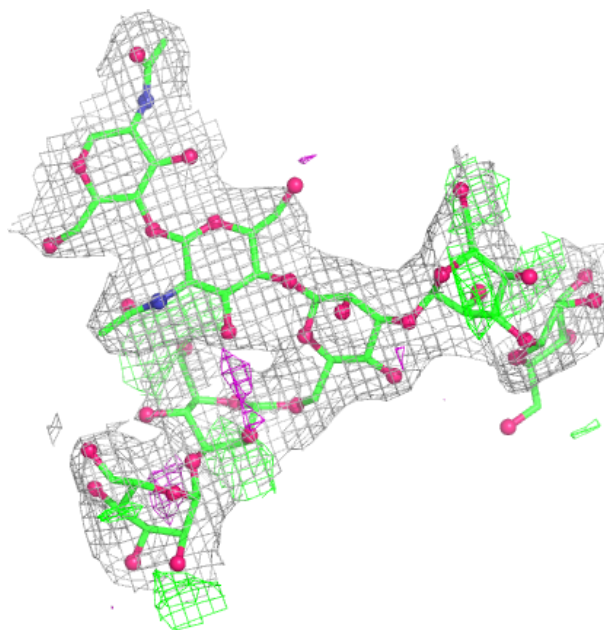
Electron density around Chain I:

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



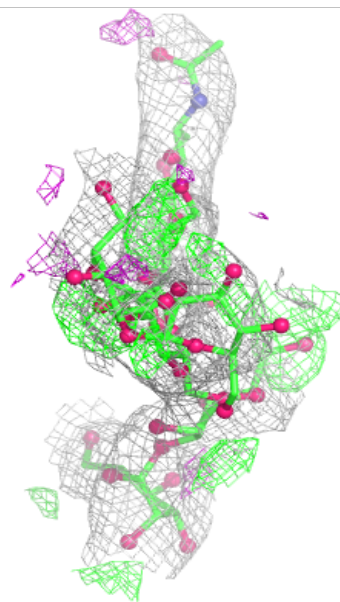
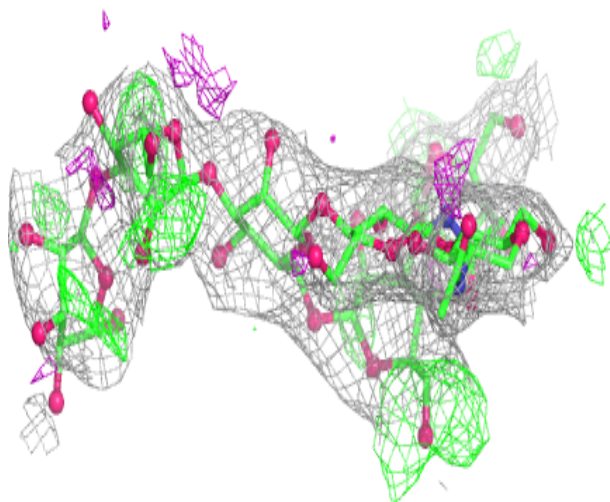
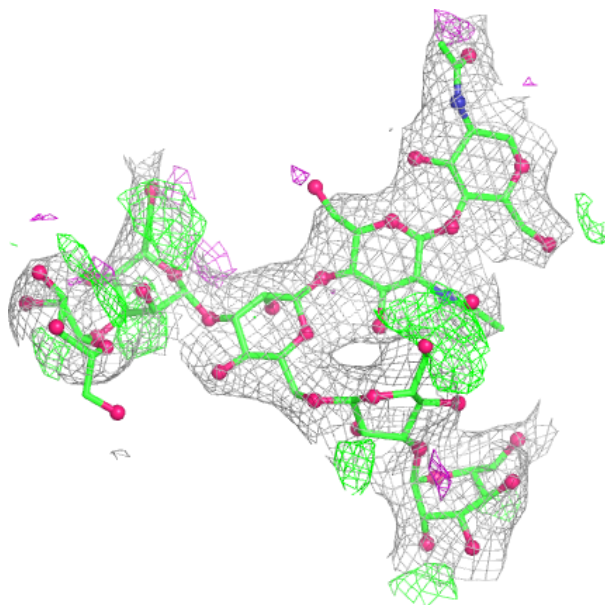
Electron density around Chain O:

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



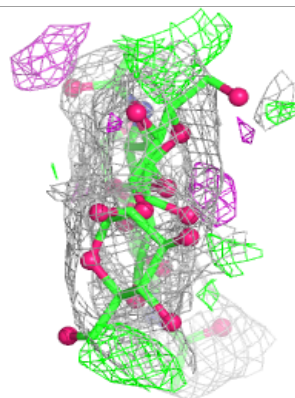
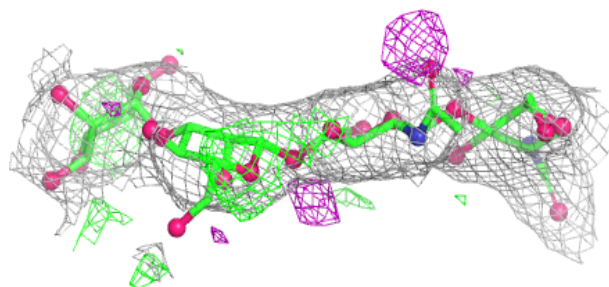
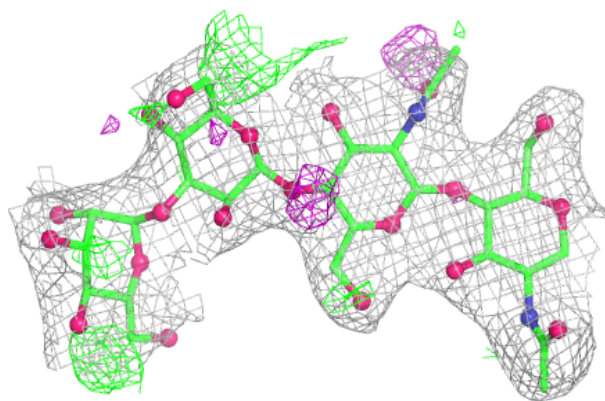
Electron density around Chain X:

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



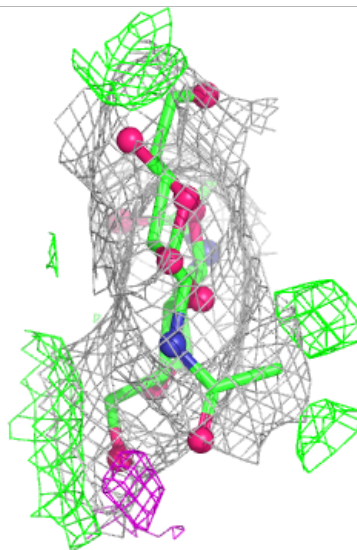
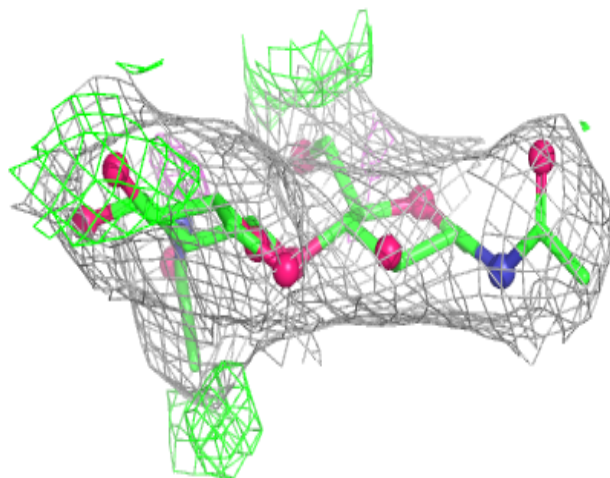
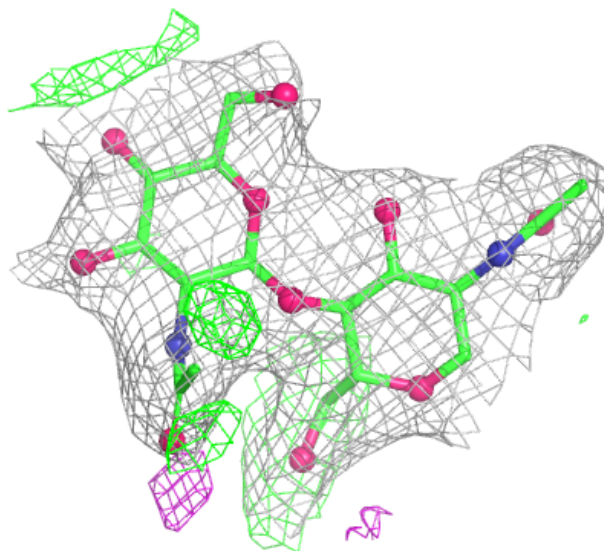
Electron density around Chain J:

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



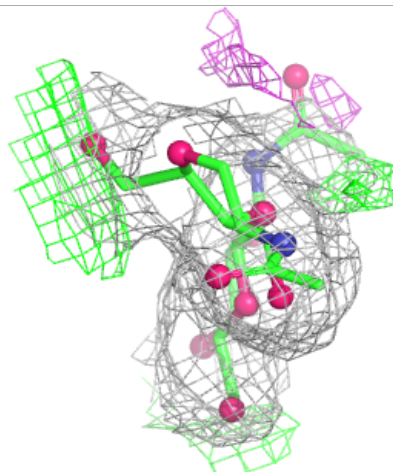
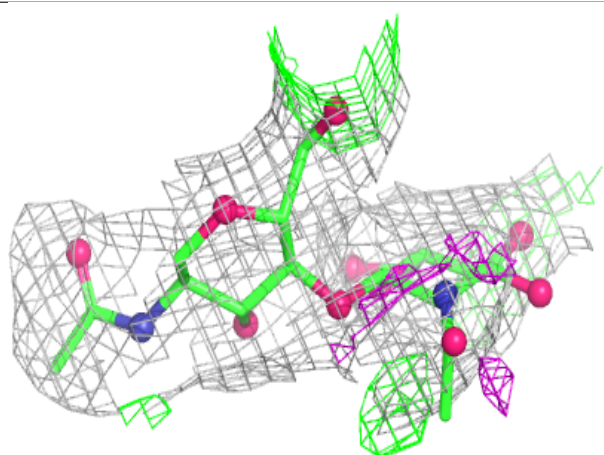
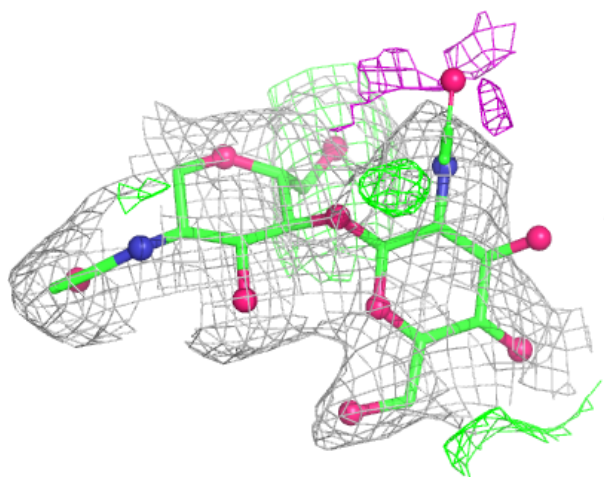
Electron density around Chain K:

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



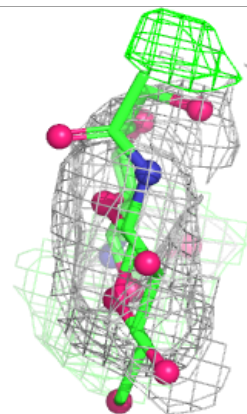
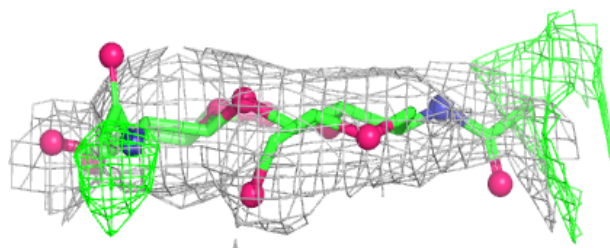
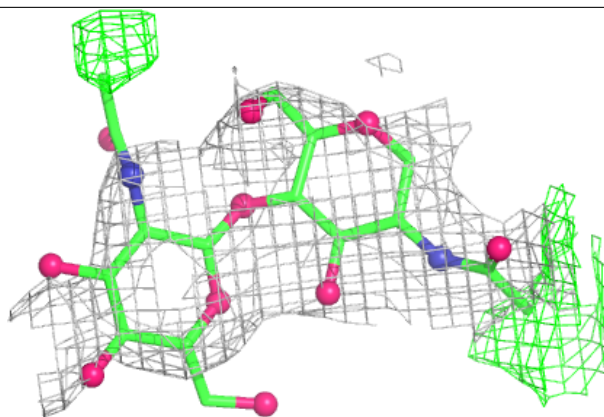
Electron density around Chain M:

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



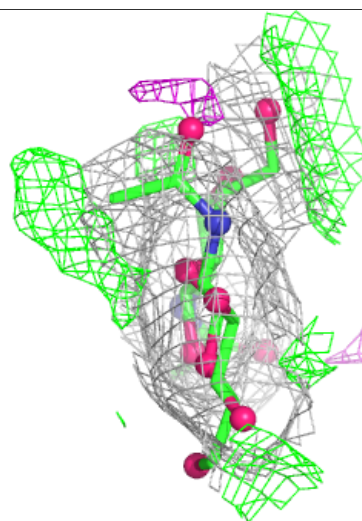
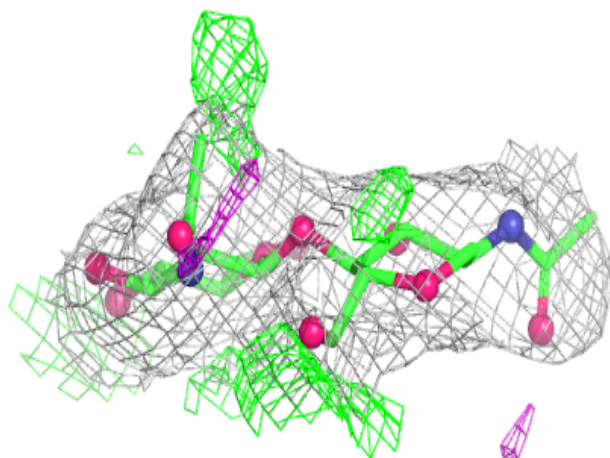
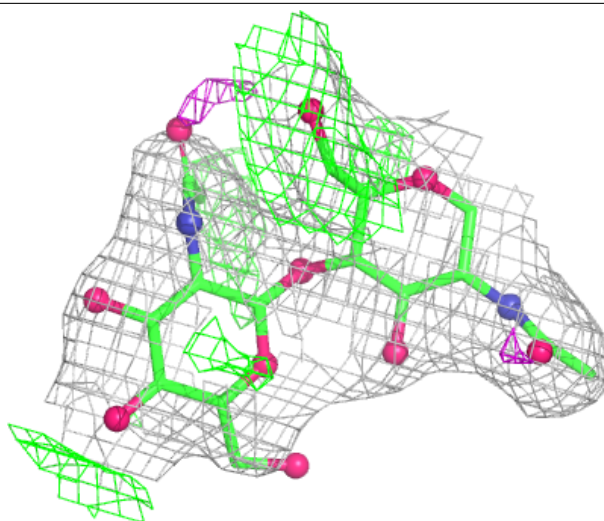
Electron density around Chain P:

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



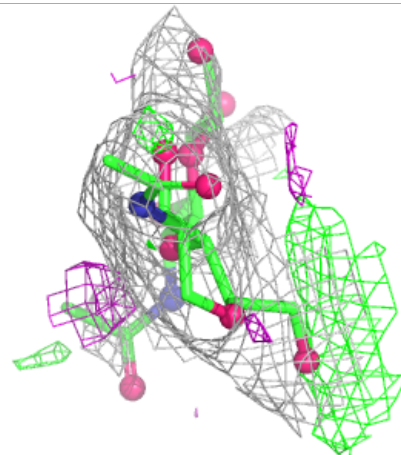
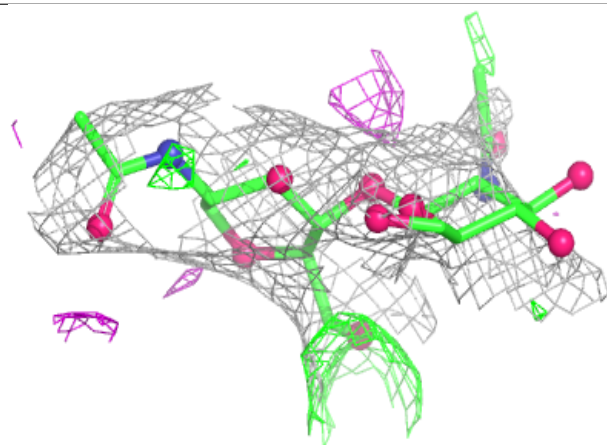
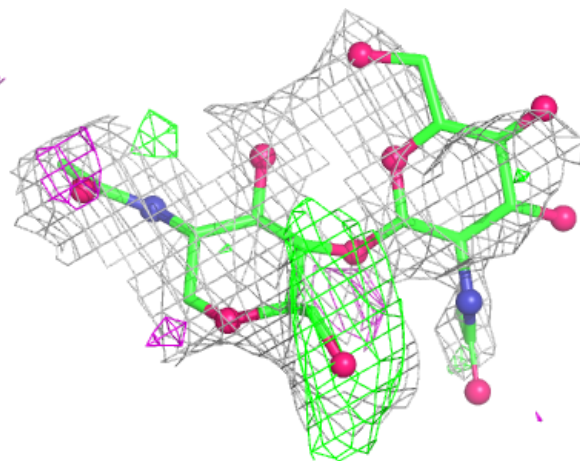
Electron density around Chain R:

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



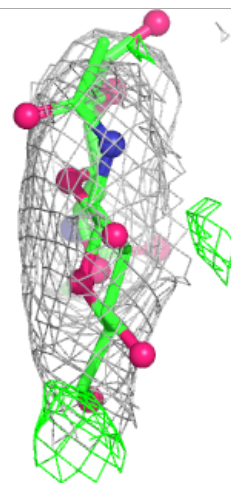
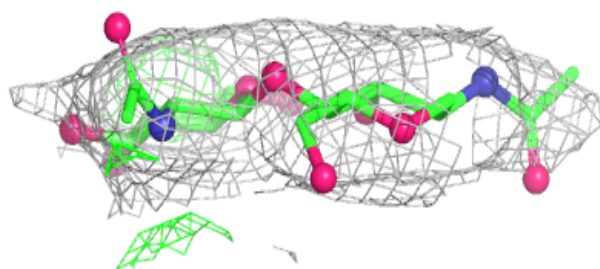
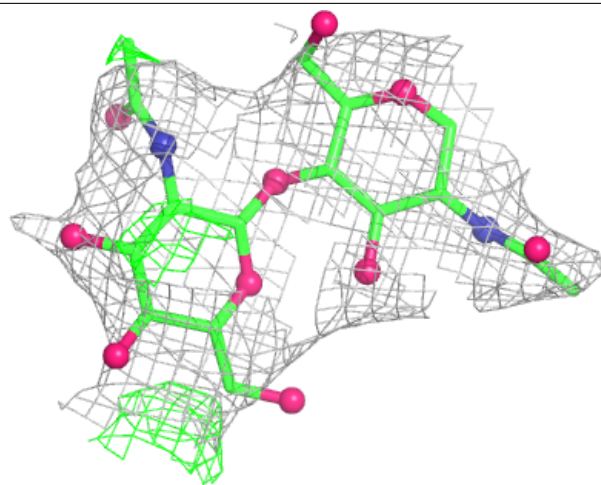
Electron density around Chain S:

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



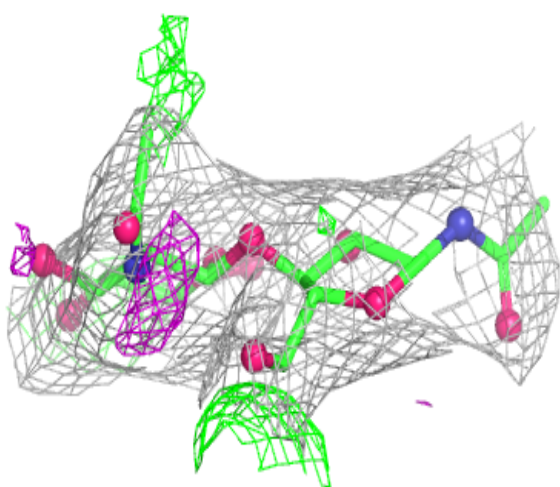
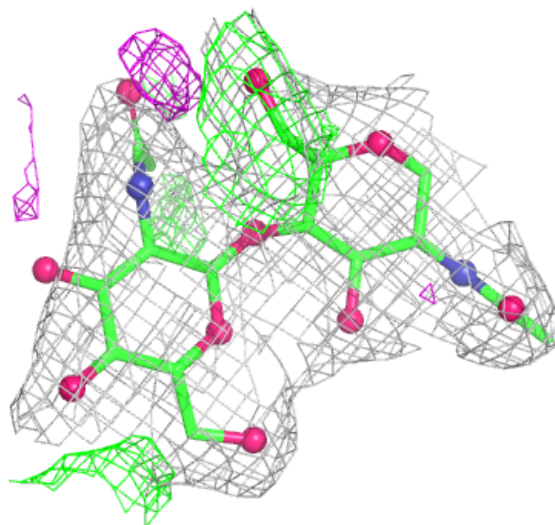
Electron density around Chain T:

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



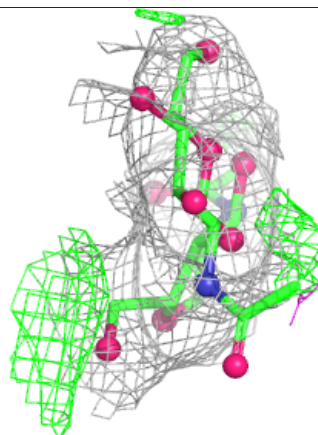
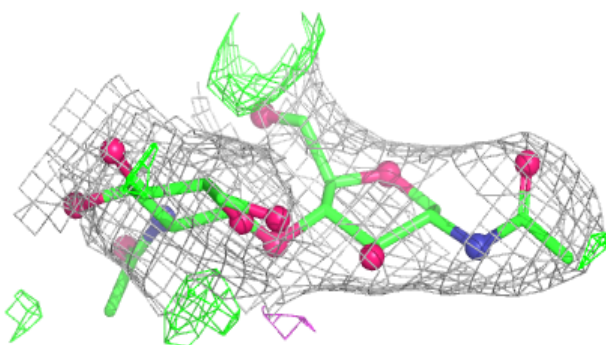
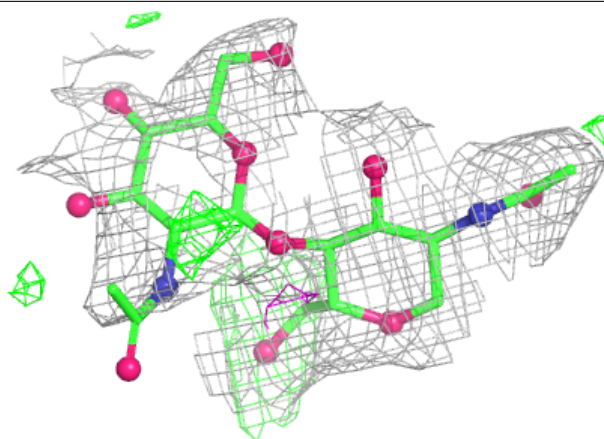
Electron density around Chain U:

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

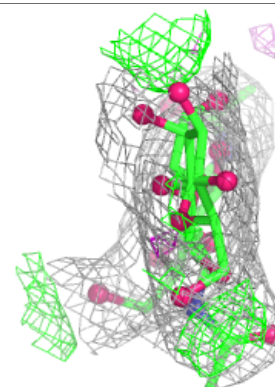
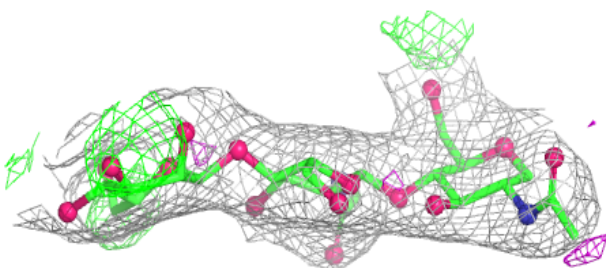
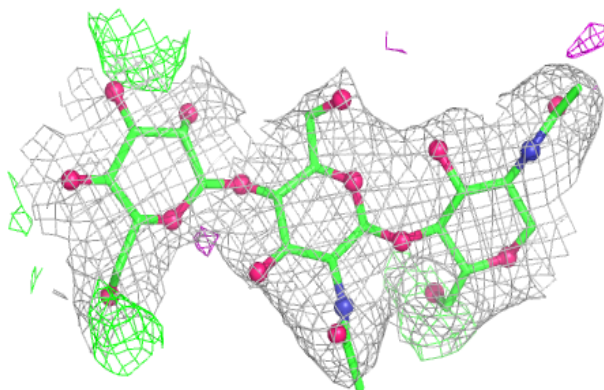


Electron density around Chain V:

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

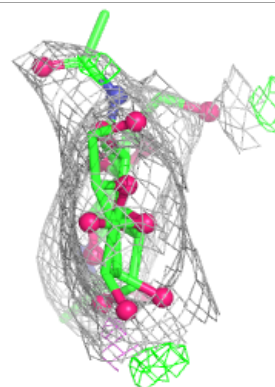
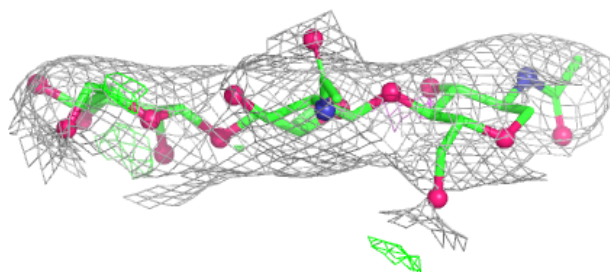
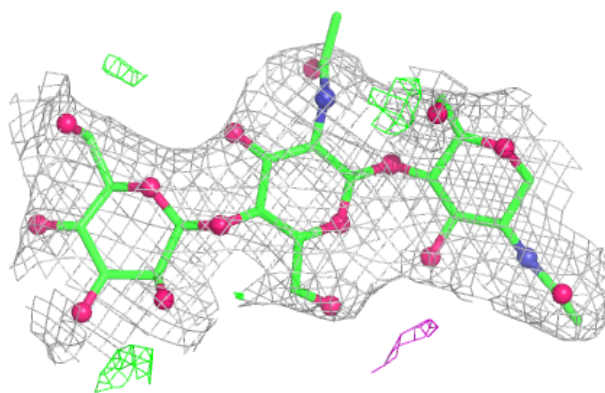
**Electron density around Chain N:**

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

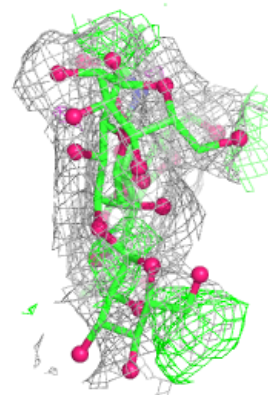
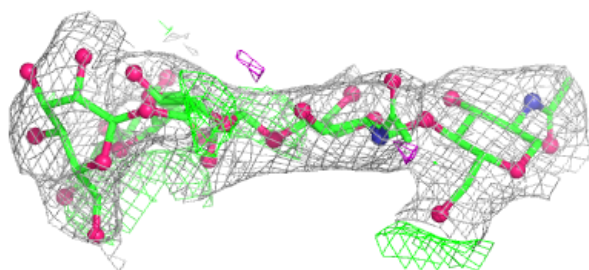
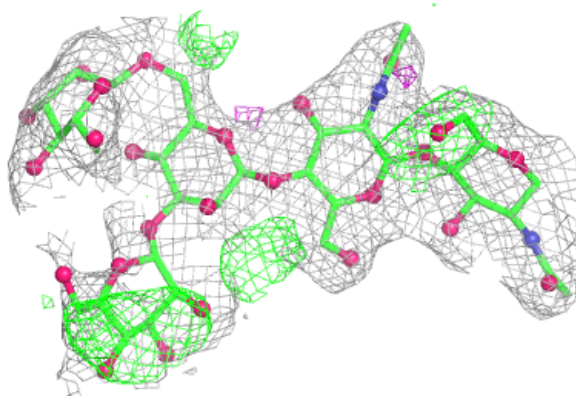


Electron density around Chain W:

$2mF_o-DF_c$ (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)



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(Å ²)	Q<0.9
9	NAG	C	503	14/15	0.49	0.25	112,128,139,140	0
9	NAG	C	502	14/15	0.62	0.22	115,151,154,156	0
9	NAG	B	409	14/15	0.66	0.19	126,140,146,152	0
9	NAG	A	410	14/15	0.71	0.21	106,122,129,135	0
9	NAG	C	501	14/15	0.73	0.17	106,132,142,144	0
9	NAG	A	408	14/15	0.76	0.15	95,119,132,136	0
9	NAG	B	408	14/15	0.76	0.20	75,97,109,120	0
9	NAG	B	410	14/15	0.77	0.17	112,124,135,135	0
9	NAG	A	409	14/15	0.80	0.18	81,108,114,118	0

6.5 Other polymers

There are no such residues in this entry.