



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:34 AM UTC

PDB ID : 8WED / pdb_00008wed
Title : Crystal structure of Arabidopsis thaliana MIK2 ectodomain in complex with BAK1 ectodomain and Fusarium oxysporum SCOOP
Authors : Wan, L.H.; Hu, Y.X.; Wu, H.M.
Deposited on : 2023-09-17
Resolution : 3.30 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

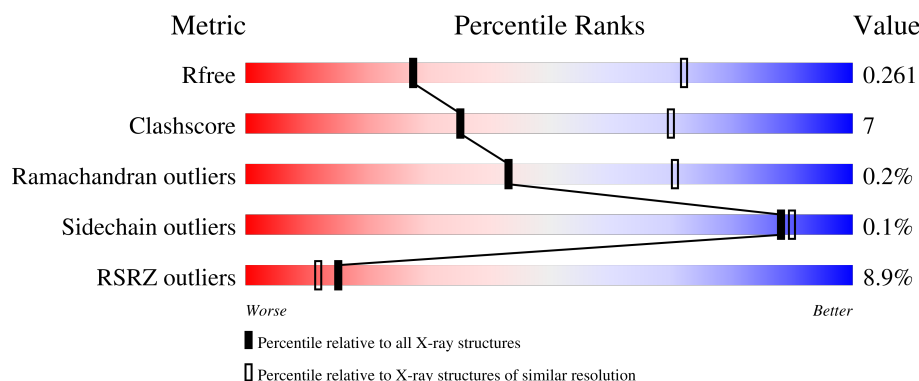
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	683	6% 77% 16% 7%
1	D	683	4% 77% 16% 7%
2	B	230	20% 57% 18% 24%
2	E	230	10% 58% 18% 24%
3	C	13	23% 77% 23%

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Mol	Chain	Length	Quality of chain
3	F	13	
4	G	4	
5	H	2	
5	I	2	
5	J	2	
5	K	2	
5	P	2	
5	Q	2	
5	R	2	
5	U	2	
6	L	3	
7	M	3	
7	N	3	
8	O	4	
9	S	2	
9	T	2	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13354 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 MDIS1-interacting receptor like kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	637	Total	C	N	O	S	0	0	0
			4950	3131	832	972	15			
1	D	637	Total	C	N	O	S	0	0	0
			4950	3131	832	972	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	GLU	LEU	engineered mutation	UNP Q8VZG8
A	164	LYS	ASP	engineered mutation	UNP Q8VZG8
A	564	PHE	SER	engineered mutation	UNP Q8VZG8
D	137	GLU	LEU	engineered mutation	UNP Q8VZG8
D	164	LYS	ASP	engineered mutation	UNP Q8VZG8
D	564	PHE	SER	engineered mutation	UNP Q8VZG8

- Molecule 2 is a protein called BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1332	840	226	263	3			
2	E	174	Total	C	N	O	S	0	0	0
			1325	836	225	261	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	221	HIS	-	expression tag	UNP Q94F62
B	222	HIS	-	expression tag	UNP Q94F62
B	223	HIS	-	expression tag	UNP Q94F62
B	224	HIS	-	expression tag	UNP Q94F62
B	225	HIS	-	expression tag	UNP Q94F62

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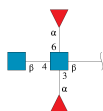
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Chain	Residue	Modelled	Actual	Comment	Reference
B	226	HIS	-	expression tag	UNP Q94F62
B	227	HIS	-	expression tag	UNP Q94F62
B	228	HIS	-	expression tag	UNP Q94F62
B	229	HIS	-	expression tag	UNP Q94F62
B	230	HIS	-	expression tag	UNP Q94F62
E	221	HIS	-	expression tag	UNP Q94F62
E	222	HIS	-	expression tag	UNP Q94F62
E	223	HIS	-	expression tag	UNP Q94F62
E	224	HIS	-	expression tag	UNP Q94F62
E	225	HIS	-	expression tag	UNP Q94F62
E	226	HIS	-	expression tag	UNP Q94F62
E	227	HIS	-	expression tag	UNP Q94F62
E	228	HIS	-	expression tag	UNP Q94F62
E	229	HIS	-	expression tag	UNP Q94F62
E	230	HIS	-	expression tag	UNP Q94F62

- Molecule 3 is a protein called a SCOOP-like peptide from *F. oxysporum* f. sp. *conglutinans* strain Fo5176.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			93	50	21	22			
3	F	13	Total	C	N	O	0	0	0
			93	50	21	22			

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



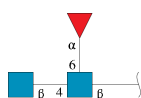
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			48	28	2	18			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



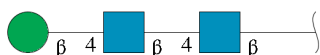
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	U	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- 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.



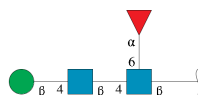
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

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



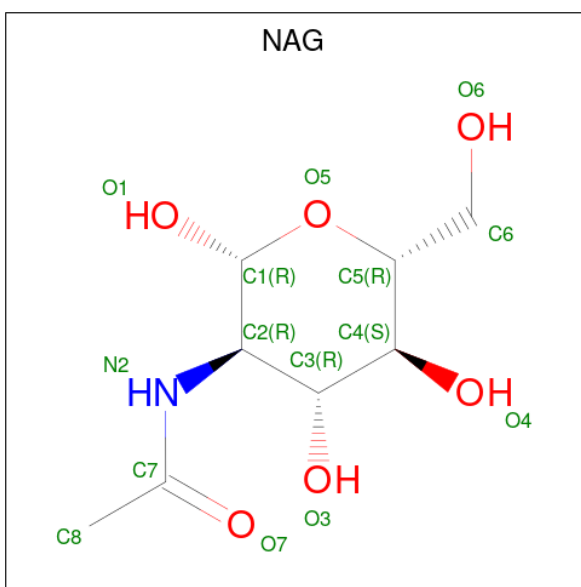
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	O	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



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

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

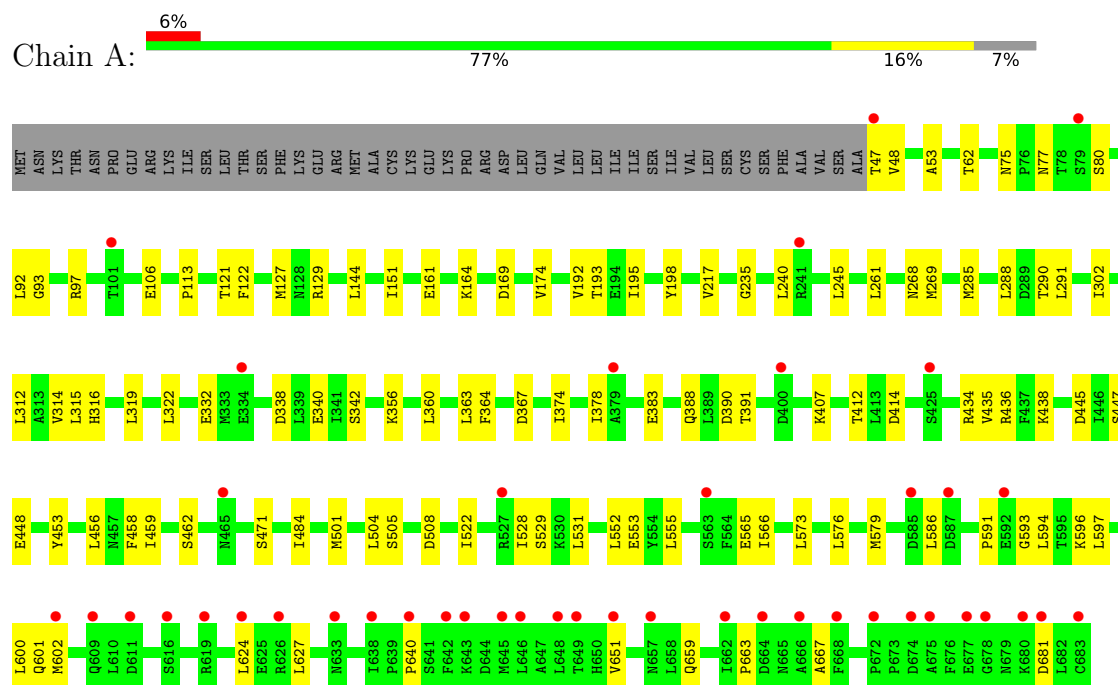


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	D	1	Total	C	N	O	0	0
			14	8	1	5		
10	D	1	Total	C	N	O	0	0
			14	8	1	5		
10	D	1	Total	C	N	O	0	0
			14	8	1	5		
10	D	1	Total	C	N	O	0	0
			14	8	1	5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

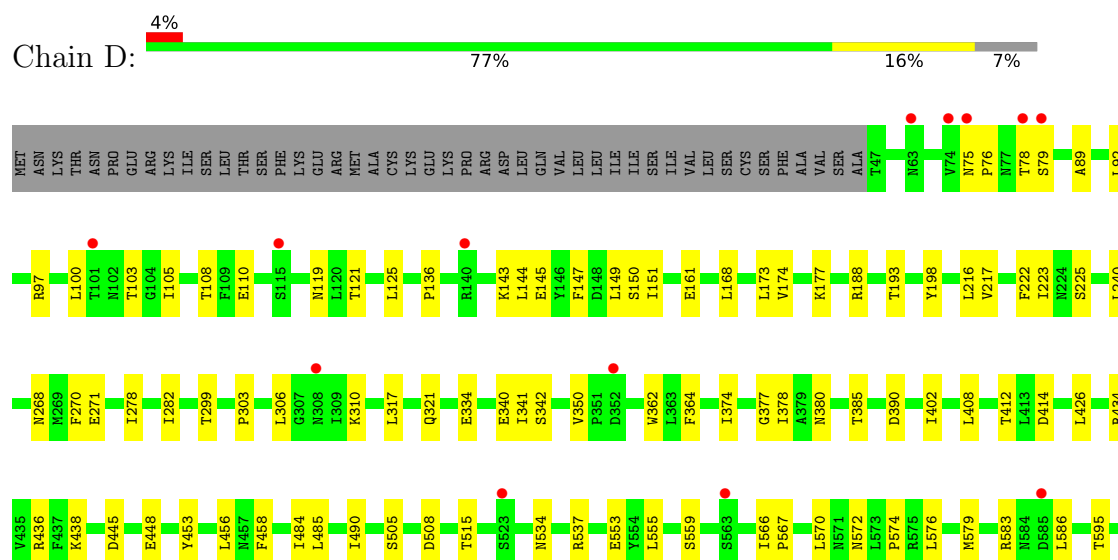
3 Residue-property plots

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: MDIS1-interacting receptor like kinase 2

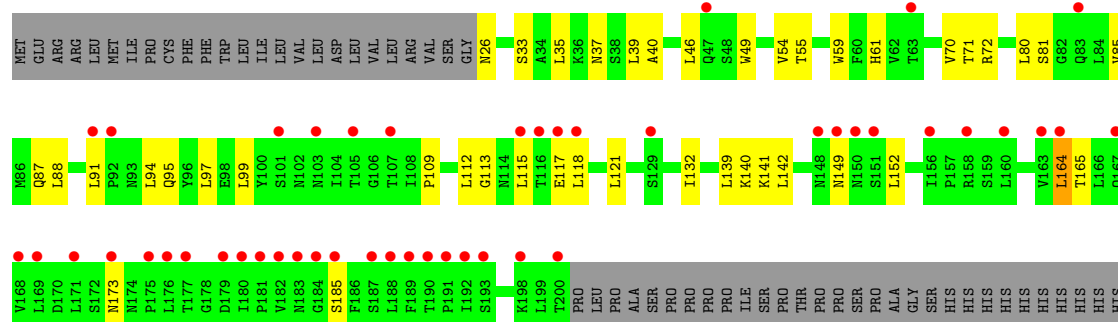


- Molecule 1: MDIS1-interacting receptor like kinase 2

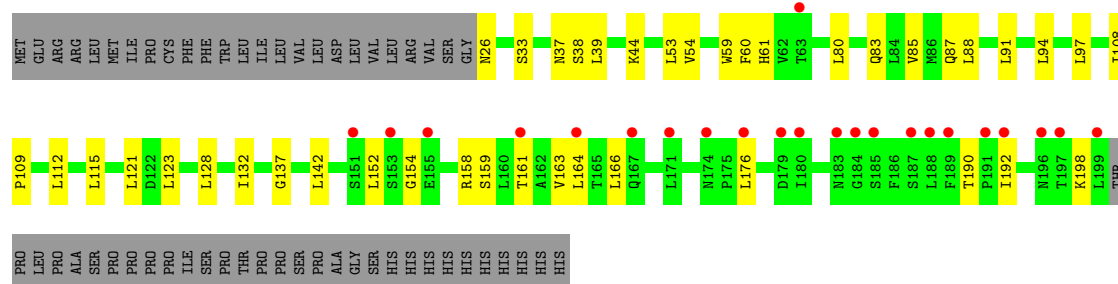




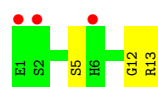
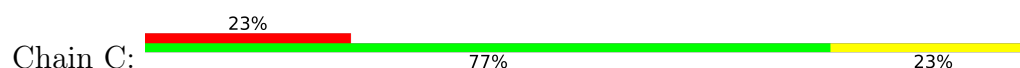
- Molecule 2: BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1



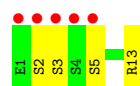
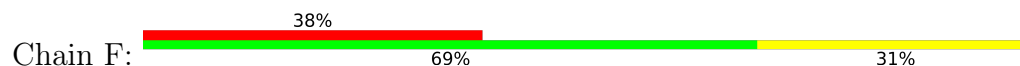
- Molecule 2: BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1



- Molecule 3: a SCOOP-like peptide from *F. oxysporum* f. sp. *conglutinans* strain Fo5176



- Molecule 3: a SCOOP-like peptide from *F. oxysporum* f. sp. *conglutinans* strain Fo5176

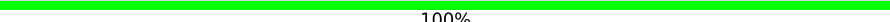


- Molecule 4: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  75% 25%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%

MAG1
MAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%

MAG1
MAG2

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

Chain L:  100%

MAG1
MAG2
FUC3

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

Chain M:  33% 33% 33%

MAG1
MAG2
BMA3

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

Chain N:  33% 33% 33%

MAG1
MAG2
BMA3

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

Chain O:  25% 50% 25%

MAG1
MAG2
BMA3
FUC4

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

Chain S:  100%

MAG1
FUC2

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

Chain T:

100%

MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.67Å 178.12Å 142.26Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	36.34 – 3.30 36.34 – 3.30	Depositor EDS
% Data completeness (in resolution range)	88.9 (36.34-3.30) 89.0 (36.34-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.240 , 0.261 0.240 , 0.261	Depositor DCC
R_{free} test set	2373 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 19.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	13354	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.10	0/5052	0.30	0/6875
1	D	0.10	0/5052	0.30	0/6875
2	B	0.15	0/1354	0.39	0/1852
2	E	0.11	0/1347	0.34	0/1842
3	C	0.16	0/93	0.32	0/121
3	F	0.19	0/93	0.58	0/121
All	All	0.11	0/12991	0.32	0/17686

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4950	0	4909	69	0
1	D	4950	0	4905	74	0
2	B	1332	0	1346	30	0
2	E	1325	0	1339	24	0
3	C	93	0	83	4	0
3	F	93	0	83	5	0
4	G	48	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	28	0	25	0	0
5	I	28	0	25	1	0
5	J	28	0	25	0	0
5	K	28	0	25	1	0
5	P	28	0	25	3	0
5	Q	28	0	25	0	0
5	R	28	0	25	0	0
5	U	28	0	25	1	0
6	L	38	0	34	0	0
7	M	39	0	34	1	0
7	N	39	0	34	1	0
8	O	49	0	43	3	0
9	S	24	0	22	0	0
9	T	24	0	22	0	0
10	A	42	0	39	0	0
10	D	84	0	78	2	0
All	All	13354	0	13214	196	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 7.

All (196) 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:D:583:ARG:HH21	5:P:1:NAG:H4	1.34	0.92
1:A:552:LEU:HD21	1:A:555:LEU:HG	1.57	0.85
2:B:54:VAL:HG23	3:C:12:GLY:H	1.43	0.82
2:B:164:LEU:HD12	2:B:164:LEU:O	1.82	0.80
1:D:643:LYS:HE3	1:D:664:ASP:H	1.49	0.77
2:E:85:VAL:HG12	2:E:87:GLN:H	1.51	0.75
1:A:552:LEU:HD21	1:A:555:LEU:CG	2.16	0.75
1:D:445:ASP:HB3	1:D:448:GLU:HB2	1.70	0.74
1:A:121:THR:HA	1:A:144:LEU:HA	1.70	0.74
2:E:94:LEU:HD21	2:E:97:LEU:HD13	1.71	0.73
1:D:621:LEU:HD23	1:D:624:LEU:HD12	1.71	0.72
2:B:118:LEU:HD11	2:B:121:LEU:HD23	1.72	0.71
8:O:2:NAG:H62	8:O:3:BMA:H2	1.73	0.69
2:B:54:VAL:HG12	2:B:55:THR:HG23	1.75	0.68
1:D:270:PHE:HD1	1:D:271:GLU:HG3	1.58	0.68
1:D:89:ALA:HB3	1:D:97:ARG:HB3	1.75	0.68
2:B:35:LEU:HD12	2:B:88:LEU:HD21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:ILE:HG23	1:D:378:ILE:HD12	1.77	0.67
2:E:39:LEU:HB3	2:E:80:LEU:HD12	1.77	0.67
1:A:268:ASN:ND2	3:C:5:SER:O	2.28	0.65
2:B:33:SER:O	2:B:37:ASN:ND2	2.29	0.65
2:E:142:LEU:HD23	2:E:166:LEU:HD21	1.79	0.65
1:A:445:ASP:HB3	1:A:448:GLU:HB2	1.78	0.64
2:B:94:LEU:HD21	2:B:97:LEU:HD12	1.78	0.64
1:A:383:GLU:OE2	1:A:407:LYS:NZ	2.32	0.63
1:D:225:SER:HB3	5:U:1:NAG:H82	1.80	0.62
1:D:121:THR:HA	1:D:144:LEU:HA	1.81	0.62
1:D:198:TYR:CZ	3:F:3:SER:HB3	2.34	0.62
1:D:92:LEU:HD12	10:D:1401:NAG:H83	1.81	0.62
1:A:62:THR:OG1	1:A:106:GLU:OE1	2.18	0.62
1:D:390:ASP:HB3	1:D:412:THR:HG22	1.83	0.61
1:A:106:GLU:HG3	1:A:129:ARG:HE	1.65	0.61
1:A:434:ARG:HG2	1:A:458:PHE:HB3	1.82	0.61
2:B:142:LEU:O	2:B:165:THR:OG1	2.19	0.60
1:A:434:ARG:NH2	3:C:13:ARG:O	2.33	0.60
1:A:97:ARG:HG3	1:A:122:PHE:HB3	1.83	0.59
1:A:624:LEU:HD21	1:A:627:LEU:HG	1.83	0.59
1:D:317:LEU:HB2	1:D:341:ILE:HG22	1.84	0.59
1:D:143:LYS:NZ	10:D:1401:NAG:O7	2.35	0.59
2:E:33:SER:O	2:E:37:ASN:ND2	2.35	0.59
1:A:552:LEU:HD21	1:A:555:LEU:CD1	2.34	0.58
1:A:531:LEU:HB3	1:A:555:LEU:HD23	1.86	0.57
1:A:601:GLN:OE1	2:B:72:ARG:NH2	2.29	0.57
2:B:109:PRO:O	2:B:112:LEU:HD12	2.03	0.57
2:E:137:GLY:HA3	2:E:159:SER:HB2	1.87	0.57
2:B:70:VAL:HB	2:B:91:LEU:HD12	1.86	0.57
1:A:288:LEU:HD21	1:A:291:LEU:HB2	1.86	0.56
1:A:47:THR:OG1	1:A:48:VAL:N	2.38	0.56
1:A:360:LEU:HD21	1:A:363:LEU:HB2	1.86	0.56
8:O:1:NAG:H61	8:O:2:NAG:C1	2.35	0.56
2:B:97:LEU:HD21	2:B:99:LEU:HD12	1.86	0.56
2:B:140:LYS:HB2	2:B:141:LYS:HE2	1.85	0.56
2:B:71:THR:HA	2:B:94:LEU:HA	1.88	0.56
2:B:85:VAL:HG12	2:B:87:GLN:H	1.71	0.56
1:A:553:GLU:OE2	2:B:61:HIS:ND1	2.31	0.56
1:D:174:VAL:HG11	1:D:198:TYR:CZ	2.41	0.55
1:D:515:THR:HG22	1:D:537:ARG:HB2	1.88	0.55
1:D:390:ASP:HB2	1:D:414:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:576:LEU:HD21	1:D:579:MET:HE3	1.88	0.55
1:A:529:SER:HA	1:A:552:LEU:HA	1.89	0.55
1:A:261:LEU:HB2	1:A:285:MET:HE3	1.87	0.55
2:E:163:VAL:HG11	2:E:166:LEU:HD23	1.88	0.55
1:D:145:GLU:HA	1:D:168:LEU:HA	1.89	0.54
1:A:435:VAL:HB	1:A:459:ILE:HG13	1.89	0.54
1:D:222:PHE:HD2	1:D:223:ILE:HG13	1.72	0.54
2:E:108:ILE:HD11	2:E:128:LEU:HD13	1.88	0.54
1:D:412:THR:HG21	3:F:13:ARG:HB3	1.89	0.54
1:D:377:GLY:HA2	1:D:380:ASN:HB2	1.90	0.53
1:A:591:PRO:HG2	1:A:594:LEU:HD13	1.90	0.53
1:D:567:PRO:HB2	1:D:570:LEU:HD23	1.91	0.53
1:A:92:LEU:HD12	5:I:1:NAG:H83	1.90	0.53
1:A:161:GLU:O	1:A:164:LYS:HG2	2.09	0.53
1:D:78:THR:HG22	1:D:79:SER:H	1.74	0.53
1:D:402:ILE:HG21	1:D:426:LEU:HB2	1.91	0.53
1:A:342:SER:OG	1:A:364:PHE:HB3	2.09	0.53
1:D:485:LEU:HD22	1:D:490:ILE:HG13	1.91	0.53
1:A:390:ASP:HB2	1:A:414:ASP:HB2	1.91	0.52
1:A:505:SER:HA	1:A:528:ILE:HA	1.90	0.52
2:B:39:LEU:HD13	2:B:80:LEU:HB3	1.90	0.52
1:A:388:GLN:HA	1:A:412:THR:HB	1.90	0.52
1:A:245:LEU:HB2	1:A:269:MET:HG2	1.92	0.52
1:A:367:ASP:HA	1:A:391:THR:HB	1.92	0.52
1:D:198:TYR:CE2	3:F:3:SER:HB3	2.46	0.51
1:A:374:ILE:HD12	1:A:378:ILE:HD12	1.92	0.51
1:D:217:VAL:HA	1:D:240:LEU:HA	1.93	0.51
1:D:310:LYS:HD2	1:D:334:GLU:HG3	1.93	0.51
1:D:484:ILE:HG23	1:D:508:ASP:HB3	1.92	0.51
1:A:659:GLN:HB2	1:A:681:ASP:HB3	1.92	0.51
1:D:268:ASN:ND2	3:F:5:SER:O	2.44	0.51
2:E:53:LEU:HD12	2:E:59:TRP:HE1	1.76	0.50
1:D:414:ASP:OD1	1:D:436:ARG:HB3	2.10	0.50
1:D:553:GLU:OE2	2:E:61:HIS:ND1	2.36	0.50
2:E:109:PRO:HD2	2:E:112:LEU:HD22	1.93	0.50
2:B:132:ILE:HD11	2:B:152:LEU:HD23	1.93	0.50
1:A:332:GLU:OE2	1:A:356:LYS:NZ	2.43	0.49
1:D:342:SER:OG	1:D:364:PHE:HB3	2.12	0.49
1:D:566:ILE:HG12	1:D:586:LEU:HD22	1.94	0.49
1:D:103:THR:HB	1:D:105:ILE:HG13	1.95	0.49
1:A:169:ASP:OD1	1:A:193:THR:OG1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:VAL:HG23	3:C:12:GLY:N	2.20	0.49
2:B:164:LEU:HD12	2:B:164:LEU:C	2.36	0.49
1:D:453:TYR:HB2	1:D:456:LEU:HB2	1.95	0.48
2:E:26:ASN:N	2:E:54:VAL:O	2.46	0.48
1:D:278:ILE:HG23	1:D:282:ILE:HD12	1.95	0.48
2:E:163:VAL:O	2:E:164:LEU:HG	2.13	0.48
1:D:583:ARG:NH2	5:P:1:NAG:H4	2.15	0.48
1:A:597:LEU:HB2	1:A:600:LEU:CD1	2.43	0.48
8:O:2:NAG:C6	8:O:3:BMA:H2	2.43	0.48
1:A:566:ILE:HG12	1:A:586:LEU:HD22	1.96	0.47
1:D:350:VAL:HG11	1:D:378:ILE:HD11	1.96	0.47
1:A:217:VAL:HA	1:A:240:LEU:HA	1.96	0.47
1:D:595:THR:HG21	1:D:617:GLN:HB3	1.97	0.47
1:A:414:ASP:OD1	1:A:436:ARG:HB3	2.15	0.47
2:B:95:GLN:HG2	2:B:117:GLU:OE1	2.14	0.47
2:B:87:GLN:OE1	2:B:87:GLN:N	2.47	0.47
1:A:47:THR:HG22	1:A:93:GLY:O	2.15	0.47
1:D:303:PRO:HG2	1:D:306:LEU:HG	1.97	0.46
1:D:559:SER:OG	1:D:583:ARG:HD2	2.14	0.46
1:D:147:PHE:HB2	1:D:168:LEU:HD11	1.96	0.46
1:A:552:LEU:HD21	1:A:555:LEU:HD11	1.97	0.46
2:E:154:GLY:N	2:E:176:LEU:HD12	2.31	0.46
1:A:447:SER:HB2	1:A:471:SER:HB2	1.97	0.46
1:D:108:THR:HG22	1:D:110:GLU:H	1.79	0.46
1:A:340:GLU:HA	1:A:364:PHE:HB2	1.98	0.46
1:D:362:TRP:HE1	7:N:1:NAG:H81	1.79	0.46
2:E:44:LYS:HA	2:E:44:LYS:HD2	1.70	0.46
1:D:674:ASP:HA	1:D:677:GLU:HG3	1.98	0.46
2:E:91:LEU:HD12	2:E:94:LEU:HD22	1.97	0.46
1:A:573:LEU:H	1:A:597:LEU:HD22	1.82	0.45
1:A:302:ILE:HD12	1:A:322:LEU:HD22	1.97	0.45
1:D:651:VAL:HG11	1:D:668:PHE:CE1	2.51	0.45
5:K:1:NAG:H83	5:K:1:NAG:H3	1.98	0.45
1:A:312:LEU:HD21	1:A:315:LEU:HD13	1.98	0.45
2:B:113:GLY:HA2	2:B:139:LEU:HD21	1.99	0.45
1:D:385:THR:HA	1:D:408:LEU:HA	1.99	0.45
2:B:40:ALA:N	2:B:81:SER:O	2.42	0.45
1:A:235:GLY:HA2	1:A:261:LEU:HD11	1.98	0.45
1:A:316:HIS:NE2	1:A:338:ASP:OD2	2.30	0.45
1:D:572:ASN:O	1:D:574:PRO:HD3	2.17	0.45
1:D:434:ARG:HG2	1:D:458:PHE:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:121:LEU:HD23	2:E:123:LEU:HD13	1.99	0.44
2:B:118:LEU:O	2:B:141:LYS:HB2	2.17	0.44
1:D:121:THR:HG22	1:D:143:LYS:HB3	2.00	0.44
1:A:565:GLU:OE2	1:D:188:ARG:NH2	2.45	0.44
7:M:1:NAG:H83	7:M:1:NAG:H2	1.81	0.44
1:D:414:ASP:HA	1:D:438:LYS:O	2.17	0.44
1:D:136:PRO:HB3	1:D:161:GLU:CD	2.43	0.43
1:D:602:MET:HG2	1:D:626:ARG:HB2	2.00	0.43
1:D:75:ASN:HA	1:D:76:PRO:HD3	1.92	0.43
1:A:174:VAL:HG11	1:A:198:TYR:CZ	2.53	0.43
2:B:149:ASN:HA	2:B:173:ASN:HB3	2.00	0.43
1:D:149:LEU:HB2	1:D:173:LEU:HD23	2.00	0.43
1:A:501:MET:HE2	1:A:504:LEU:HD13	2.01	0.43
2:B:88:LEU:O	2:B:115:LEU:HD21	2.18	0.43
1:A:290:THR:HG23	1:A:314:VAL:HB	1.99	0.43
1:A:192:VAL:HG11	1:A:195:ILE:HD11	2.01	0.43
2:E:158:ARG:O	2:E:161:THR:OG1	2.37	0.43
1:A:75:ASN:HD21	1:A:77:ASN:HB2	1.83	0.42
1:A:75:ASN:HB3	1:A:80:SER:OG	2.18	0.42
1:A:127:MET:HE2	1:A:127:MET:HB3	1.88	0.42
1:D:534:ASN:HB2	5:P:1:NAG:H82	2.02	0.42
1:A:484:ILE:HG23	1:A:508:ASP:HB3	2.01	0.42
1:D:119:ASN:HA	1:D:143:LYS:HD2	2.01	0.42
1:D:150:SER:HB3	1:D:174:VAL:HB	2.01	0.42
1:D:177:LYS:HA	1:D:177:LYS:HD3	1.66	0.42
2:E:176:LEU:C	2:E:198:LYS:HG2	2.45	0.42
1:A:601:GLN:HG2	1:A:602:MET:HG3	2.01	0.42
2:E:190:THR:OG1	2:E:192:ILE:HG22	2.20	0.42
1:A:640:PRO:HA	1:A:663:PRO:HB3	2.02	0.42
1:D:299:THR:HG22	1:D:321:GLN:HB2	2.02	0.42
1:D:640:PRO:O	1:D:643:LYS:HD2	2.20	0.41
1:A:53:ALA:HB1	1:A:113:PRO:HB3	2.02	0.41
1:D:555:LEU:HD23	1:D:579:MET:HE2	2.01	0.41
2:E:88:LEU:O	2:E:115:LEU:HD21	2.20	0.41
1:D:193:THR:HA	1:D:216:LEU:HA	2.03	0.41
1:A:453:TYR:HB2	1:A:456:LEU:HB2	2.01	0.41
1:A:438:LYS:HG3	1:A:462:SER:HB2	2.02	0.41
1:A:651:VAL:HG23	1:A:667:ALA:HB1	2.02	0.41
1:A:565:GLU:CD	1:D:188:ARG:HH22	2.29	0.41
1:A:576:LEU:HD21	1:A:579:MET:HB2	2.02	0.41
1:A:593:GLY:HA2	1:A:596:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:ASN:N	2:B:54:VAL:O	2.53	0.41
1:D:340:GLU:HA	1:D:364:PHE:HB2	2.03	0.41
1:D:374:ILE:HD13	1:D:374:ILE:HA	1.92	0.41
2:B:49:TRP:HA	2:B:59:TRP:CD2	2.56	0.41
2:E:38:SER:OG	2:E:83:GLN:O	2.36	0.41
1:A:522:ILE:HD12	1:A:522:ILE:HA	1.91	0.40
1:A:319:LEU:HD23	1:A:319:LEU:HA	1.86	0.40
1:D:100:LEU:HB2	1:D:125:LEU:HD23	2.03	0.40
2:E:132:ILE:HD11	2:E:152:LEU:HD23	2.04	0.40
2:B:46:LEU:HD22	2:B:49:TRP:CE2	2.57	0.40
1:D:222:PHE:HZ	3:F:3:SER:HB2	1.86	0.40
1:D:505:SER:HB3	2:E:60:PHE:CE2	2.57	0.40
1:A:374:ILE:HD13	1:A:374:ILE:HA	1.87	0.40
1:D:78:THR:O	1:D:79:SER:OG	2.29	0.40
1:D:637:GLN:HA	1:D:659:GLN:O	2.22	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	A	635/683 (93%)	631 (99%)	3 (0%)	1 (0%)	43	71
1	D	635/683 (93%)	627 (99%)	7 (1%)	1 (0%)	43	71
2	B	173/230 (75%)	171 (99%)	1 (1%)	1 (1%)	21	52
2	E	172/230 (75%)	169 (98%)	3 (2%)	0	100	100
3	C	11/13 (85%)	9 (82%)	2 (18%)	0	100	100
3	F	11/13 (85%)	10 (91%)	0	1 (9%)	0	3
All	All	1637/1852 (88%)	1617 (99%)	16 (1%)	4 (0%)	43	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	185	SER
3	F	2	SER
1	A	151	ILE
1	D	151	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	576/619 (93%)	576 (100%)	0	100	100
1	D	576/619 (93%)	576 (100%)	0	100	100
2	B	156/207 (75%)	155 (99%)	1 (1%)	78	81
2	E	155/207 (75%)	155 (100%)	0	100	100
3	C	10/10 (100%)	10 (100%)	0	100	100
3	F	10/10 (100%)	10 (100%)	0	100	100
All	All	1483/1672 (89%)	1482 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	164	LEU

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	153	GLN
1	A	249	ASN
1	A	457	ASN
1	A	469	GLN
1	A	503	GLN
1	A	532	GLN
1	A	588	GLN
1	A	657	ASN
2	B	68	ASN

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Mol	Chain	Res	Type
1	D	457	ASN
2	E	111	GLN
2	E	127	ASN
2	E	196	ASN
3	F	6	HIS

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 ⓘ

37 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	G	1	1,4	14,14,15	0.31	0	17,19,21	0.70	0
4	FUC	G	2	4	10,10,11	1.08	1 (10%)	14,14,16	1.24	2 (14%)
4	NAG	G	3	4	14,14,15	0.28	0	17,19,21	0.38	0
4	FUC	G	4	4	10,10,11	0.75	0	14,14,16	0.87	0
5	NAG	H	1	1,5	14,14,15	0.31	0	17,19,21	0.39	0
5	NAG	H	2	5	14,14,15	0.25	0	17,19,21	0.50	0
5	NAG	I	1	1,5	14,14,15	0.29	0	17,19,21	0.49	0
5	NAG	I	2	5	14,14,15	0.22	0	17,19,21	0.41	0
5	NAG	J	1	1,5	14,14,15	0.19	0	17,19,21	0.44	0
5	NAG	J	2	5	14,14,15	0.22	0	17,19,21	0.47	0
5	NAG	K	1	1,5	14,14,15	0.88	1 (7%)	17,19,21	1.90	3 (17%)
5	NAG	K	2	5	14,14,15	0.46	0	17,19,21	0.39	0
6	NAG	L	1	1,6	14,14,15	0.26	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	L	2	6	14,14,15	0.33	0	17,19,21	0.54	0
6	FUC	L	3	6	10,10,11	0.90	0	14,14,16	0.93	0
7	NAG	M	1	1,7	14,14,15	0.71	0	17,19,21	1.61	3 (17%)
7	NAG	M	2	7	14,14,15	0.69	0	17,19,21	1.17	2 (11%)
7	BMA	M	3	7	11,11,12	0.50	0	15,15,17	0.82	0
7	NAG	N	1	1,7	14,14,15	0.69	1 (7%)	17,19,21	1.63	1 (5%)
7	NAG	N	2	7	14,14,15	0.58	0	17,19,21	1.25	2 (11%)
7	BMA	N	3	7	11,11,12	0.43	0	15,15,17	0.66	0
8	NAG	O	1	1,8	14,14,15	0.33	0	17,19,21	1.52	3 (17%)
8	NAG	O	2	8	14,14,15	0.43	0	17,19,21	0.84	0
8	BMA	O	3	8	11,11,12	0.24	0	15,15,17	0.81	0
8	FUC	O	4	8	10,10,11	0.95	0	14,14,16	0.84	0
5	NAG	P	1	1,5	14,14,15	0.37	0	17,19,21	0.55	0
5	NAG	P	2	5	14,14,15	0.31	0	17,19,21	0.62	0
5	NAG	Q	1	1,5	14,14,15	0.19	0	17,19,21	0.46	0
5	NAG	Q	2	5	14,14,15	0.23	0	17,19,21	0.46	0
5	NAG	R	1	1,5	14,14,15	0.28	0	17,19,21	0.62	0
5	NAG	R	2	5	14,14,15	0.25	0	17,19,21	0.56	0
9	NAG	S	1	1,9	14,14,15	0.28	0	17,19,21	0.65	0
9	FUC	S	2	9	10,10,11	0.82	0	14,14,16	0.73	0
9	NAG	T	1	1,9	14,14,15	0.31	0	17,19,21	0.39	0
9	FUC	T	2	9	10,10,11	1.03	0	14,14,16	0.93	0
5	NAG	U	1	1,5	14,14,15	0.29	0	17,19,21	0.66	0
5	NAG	U	2	5	14,14,15	0.32	0	17,19,21	1.00	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
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	FUC	G	2	4	-	-	0/1/1/1
4	NAG	G	3	4	-	0/6/23/26	0/1/1/1
4	FUC	G	4	4	-	-	0/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	NAG	J	1	1,5	-	2/6/23/26	0/1/1/1

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	1	NAG	O5-C1	2.91	1.48	1.43
4	G	2	FUC	C2-C3	2.64	1.56	1.52
7	N	1	NAG	O5-C1	2.45	1.47	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	1	NAG	C1-O5-C5	6.14	120.42	112.19
5	K	1	NAG	C1-O5-C5	5.51	119.57	112.19
7	M	1	NAG	C1-O5-C5	4.72	118.52	112.19
5	K	1	NAG	C2-N2-C7	4.60	129.07	122.90
8	O	1	NAG	C1-O5-C5	3.59	116.99	112.19
7	N	2	NAG	C2-N2-C7	-3.36	118.40	122.90
4	G	2	FUC	C1-C2-C3	3.12	114.18	109.64
8	O	1	NAG	C2-N2-C7	3.08	127.03	122.90
5	U	2	NAG	C1-O5-C5	2.92	116.10	112.19
7	M	1	NAG	O4-C4-C3	-2.42	104.67	110.38
8	O	1	NAG	C4-C3-C2	-2.25	107.71	111.02
7	M	2	NAG	C2-N2-C7	-2.20	119.96	122.90
4	G	2	FUC	C1-O5-C5	2.15	118.04	112.97
7	N	2	NAG	O5-C1-C2	-2.10	108.03	111.29
5	K	1	NAG	C1-C2-N2	2.09	113.72	110.43
7	M	2	NAG	O5-C1-C2	-2.09	108.06	111.29
7	M	1	NAG	C2-N2-C7	-2.03	120.19	122.90

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	2	NAG	C1-C2-N2-C7
5	R	2	NAG	C8-C7-N2-C2
5	R	2	NAG	O7-C7-N2-C2
5	U	2	NAG	C8-C7-N2-C2
5	U	2	NAG	O7-C7-N2-C2
7	M	1	NAG	C8-C7-N2-C2
7	M	1	NAG	O7-C7-N2-C2
8	O	1	NAG	C1-C2-N2-C7
8	O	1	NAG	C8-C7-N2-C2
8	O	1	NAG	O7-C7-N2-C2
5	J	1	NAG	O5-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
7	N	1	NAG	O5-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
8	O	1	NAG	O5-C5-C6-O6
8	O	2	NAG	O7-C7-N2-C2
5	H	2	NAG	C4-C5-C6-O6
6	L	1	NAG	C4-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	P	1	NAG	O5-C5-C6-O6

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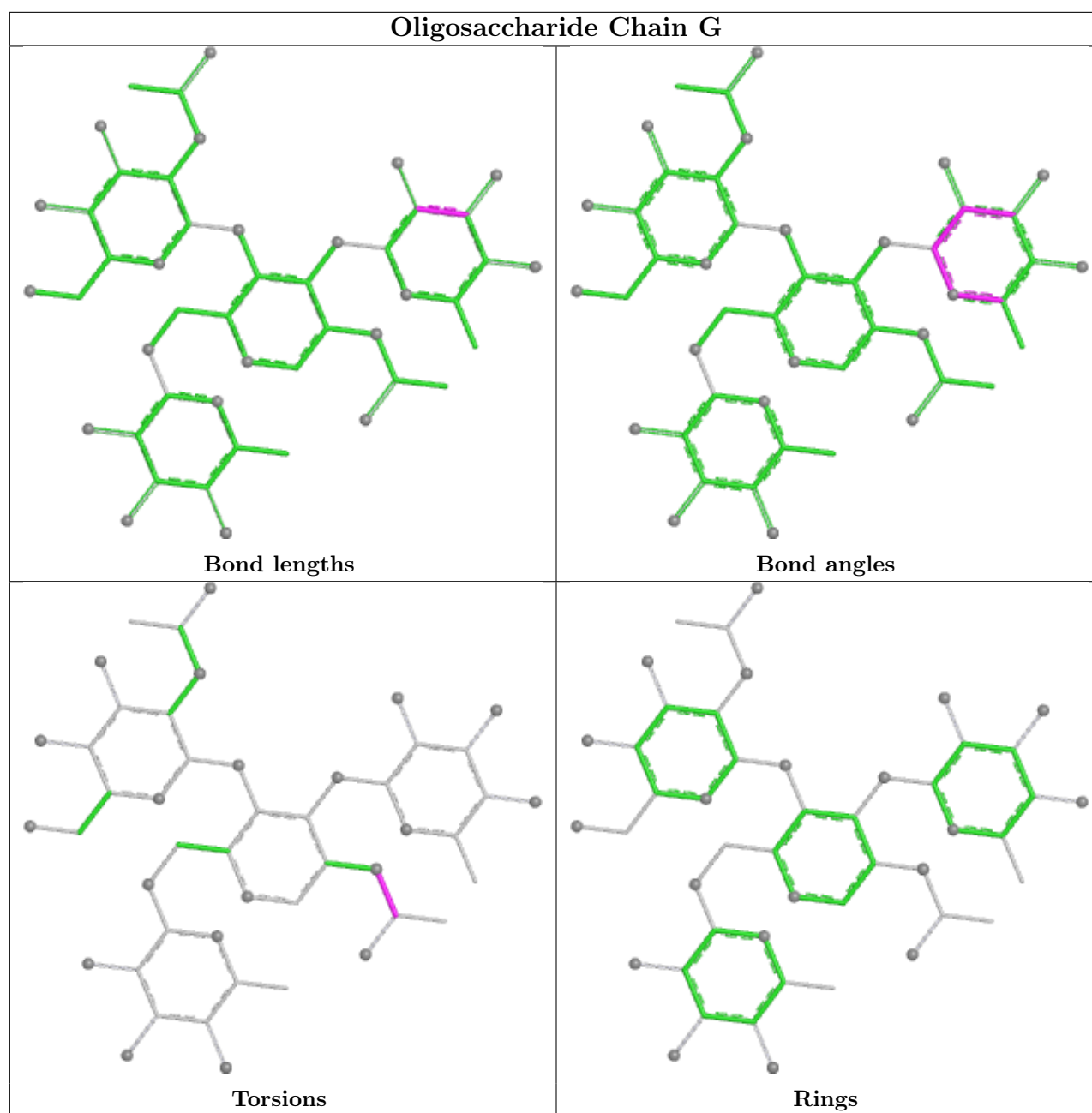
Mol	Chain	Res	Type	Atoms
5	K	1	NAG	C4-C5-C6-O6
6	L	2	NAG	C4-C5-C6-O6
8	O	2	NAG	C8-C7-N2-C2
5	K	1	NAG	O5-C5-C6-O6
7	N	1	NAG	C4-C5-C6-O6
5	Q	1	NAG	C4-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
8	O	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
5	K	1	NAG	C8-C7-N2-C2
5	K	1	NAG	O7-C7-N2-C2
5	Q	1	NAG	C8-C7-N2-C2
5	Q	1	NAG	O7-C7-N2-C2
5	U	1	NAG	C8-C7-N2-C2
7	N	1	NAG	C8-C7-N2-C2
7	N	1	NAG	O7-C7-N2-C2
5	K	2	NAG	O5-C5-C6-O6
5	U	1	NAG	O7-C7-N2-C2
5	P	1	NAG	C4-C5-C6-O6
5	R	1	NAG	C8-C7-N2-C2
5	R	2	NAG	O5-C5-C6-O6
7	M	1	NAG	O5-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
6	L	2	NAG	C1-C2-N2-C7
5	R	1	NAG	O7-C7-N2-C2
5	Q	2	NAG	C4-C5-C6-O6
5	P	2	NAG	C3-C2-N2-C7
6	L	2	NAG	C3-C2-N2-C7
9	S	1	NAG	C3-C2-N2-C7
5	Q	2	NAG	O5-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
5	K	1	NAG	C1-C2-N2-C7
5	P	2	NAG	C1-C2-N2-C7
7	M	2	NAG	C1-C2-N2-C7
9	S	1	NAG	C1-C2-N2-C7
5	K	1	NAG	C3-C2-N2-C7
5	P	1	NAG	C3-C2-N2-C7
9	S	1	NAG	C4-C5-C6-O6

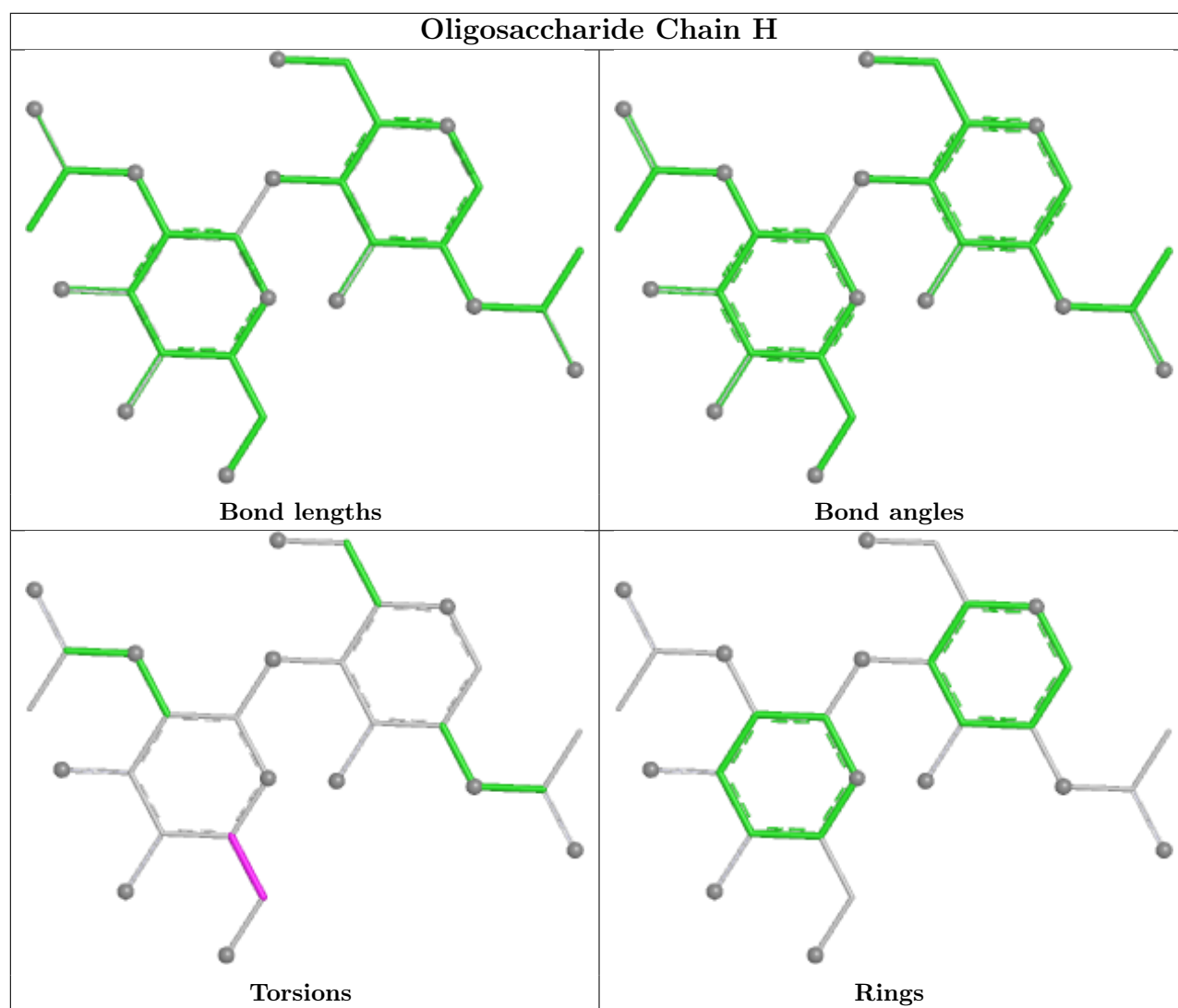
There are no ring outliers.

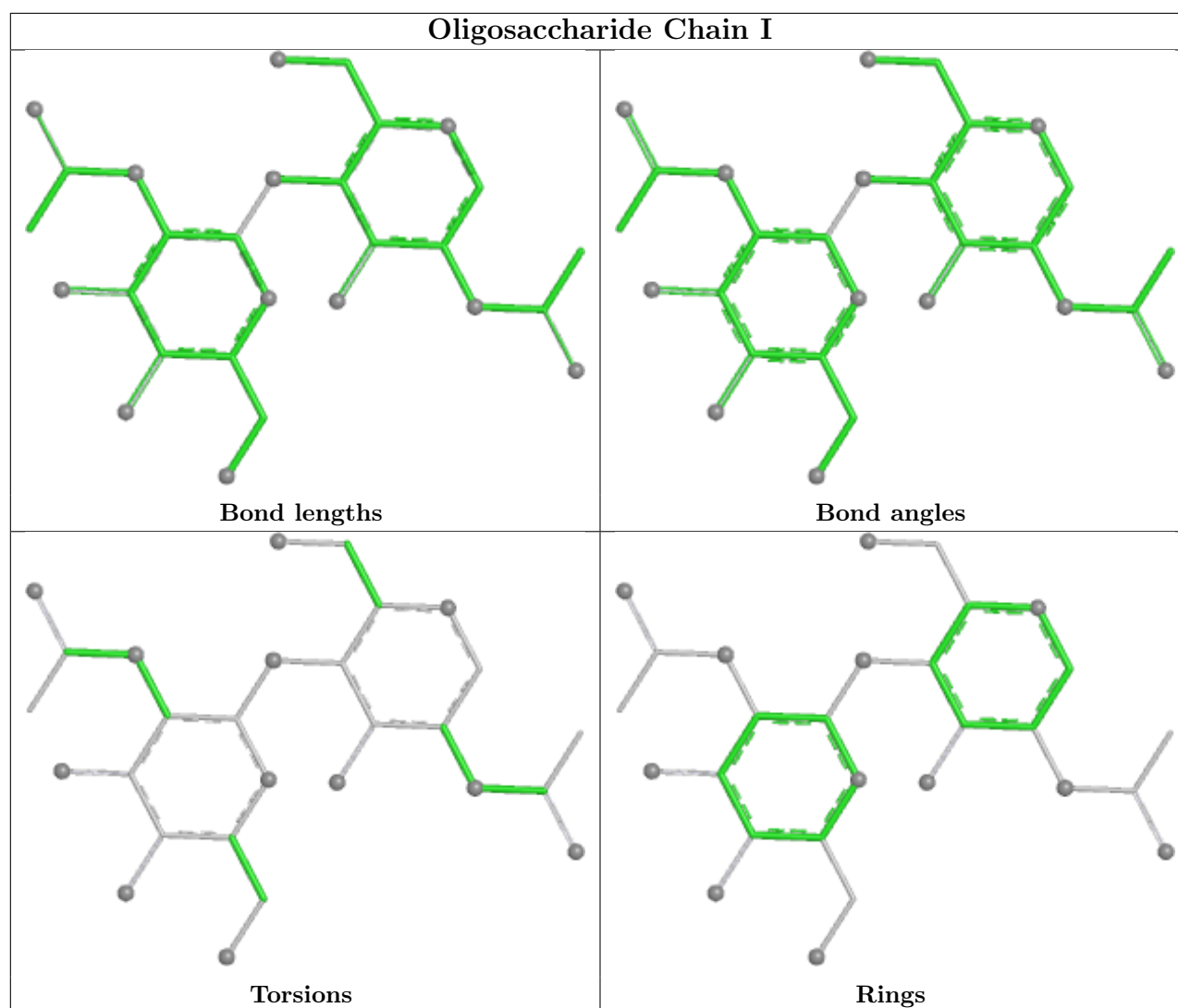
9 monomers are involved in 11 short contacts:

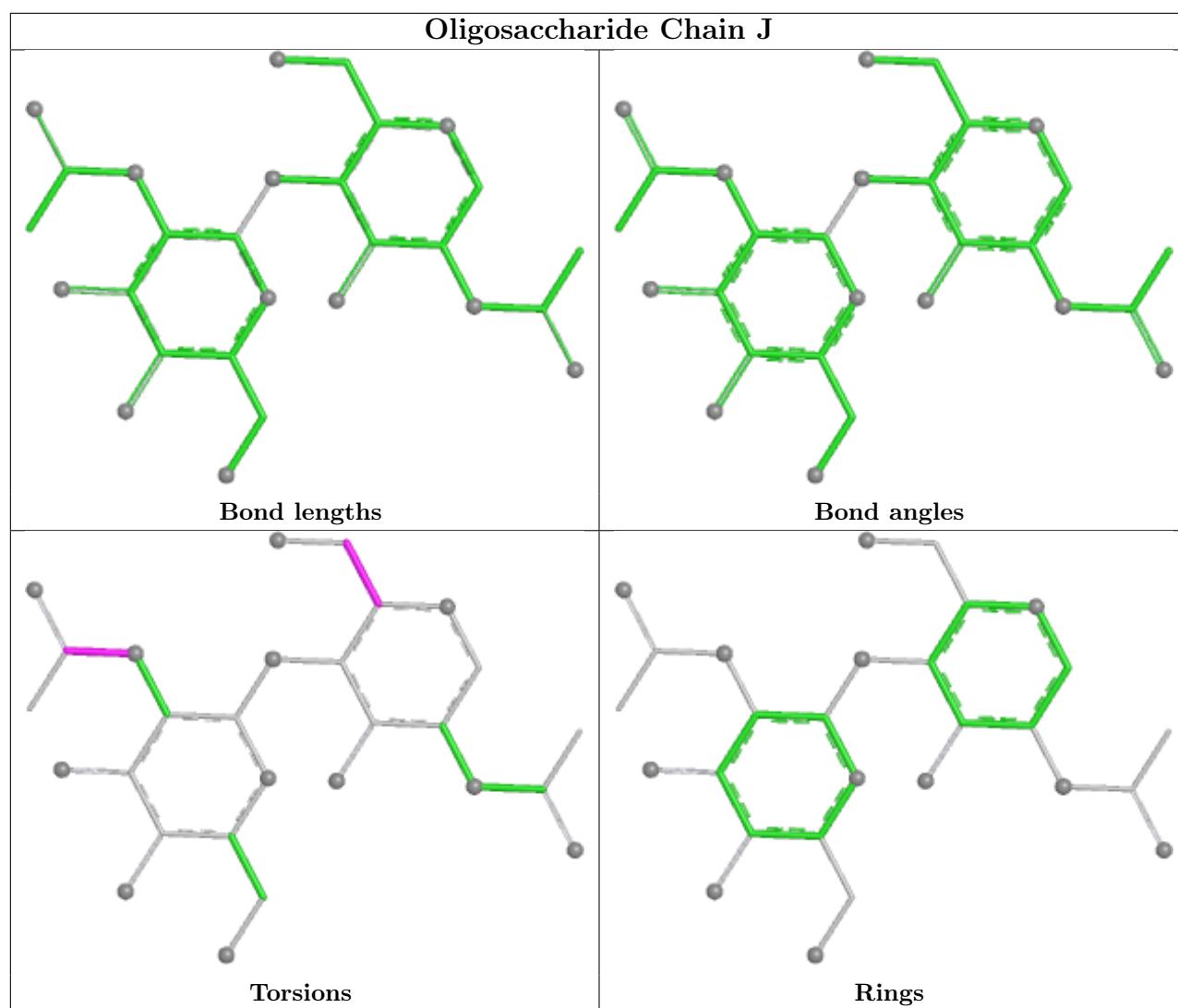
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	O	1	NAG	1	0
8	O	3	BMA	2	0
5	P	1	NAG	3	0
7	N	1	NAG	1	0
5	I	1	NAG	1	0
5	K	1	NAG	1	0
5	U	1	NAG	1	0
7	M	1	NAG	1	0
8	O	2	NAG	3	0

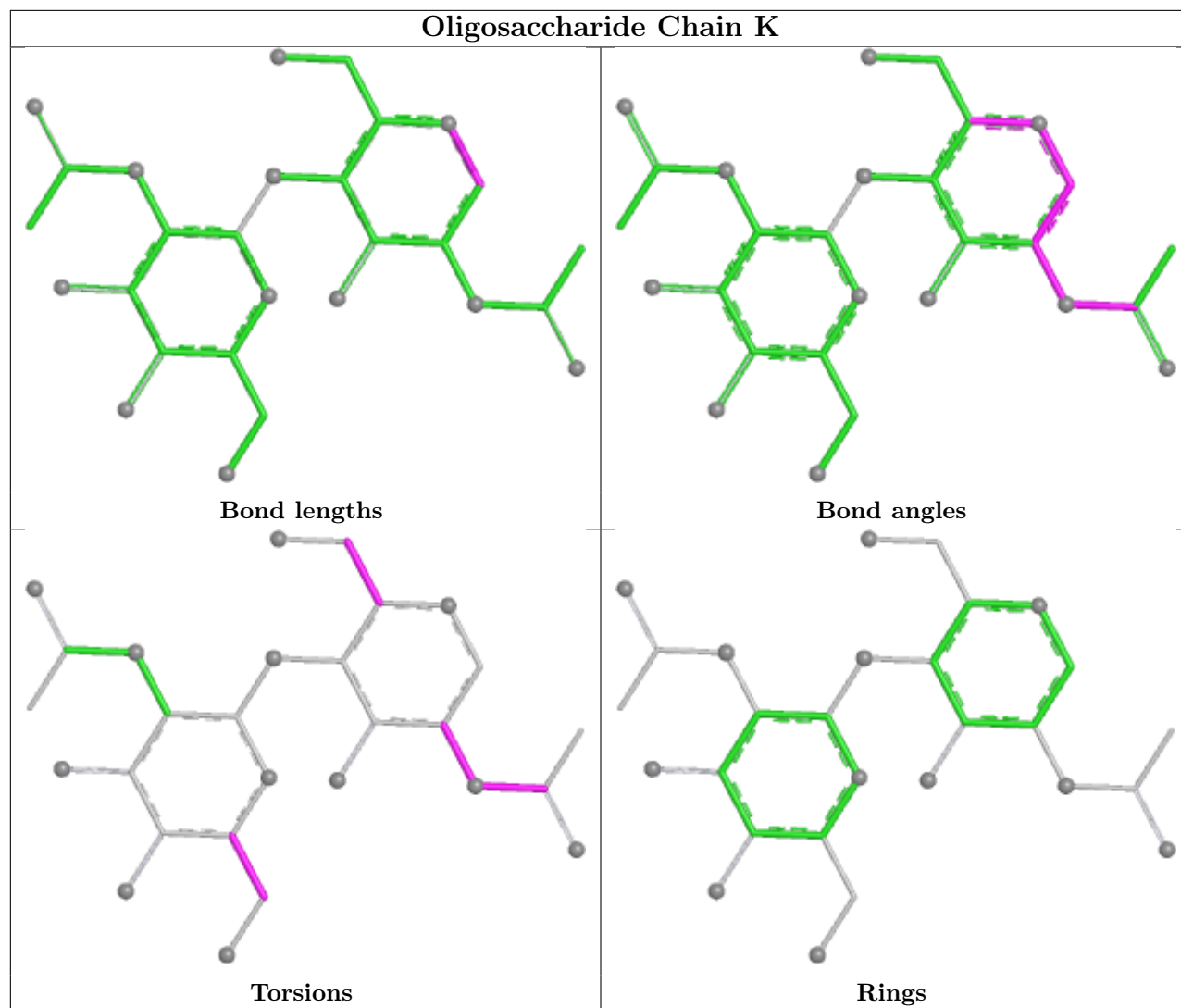
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

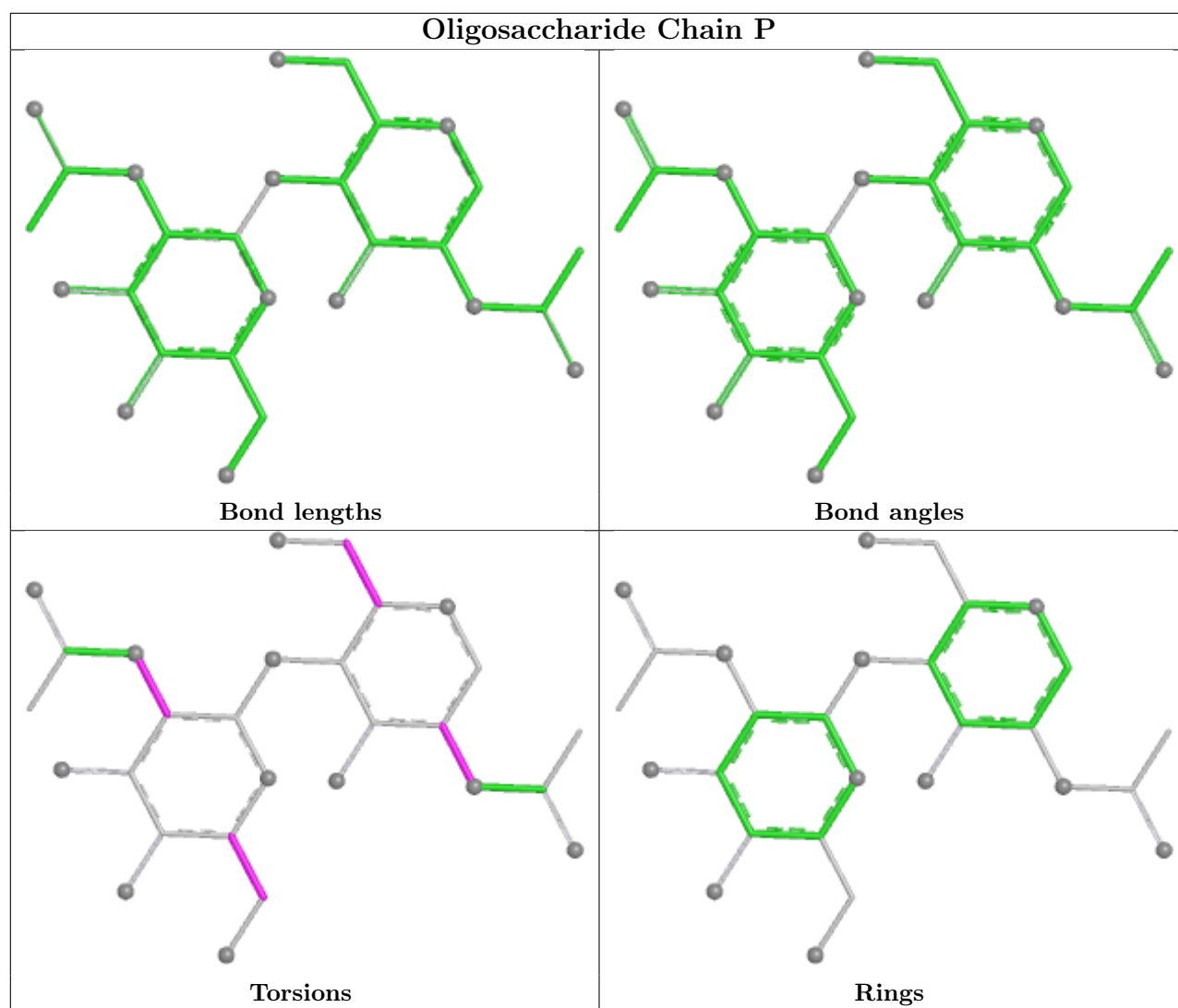


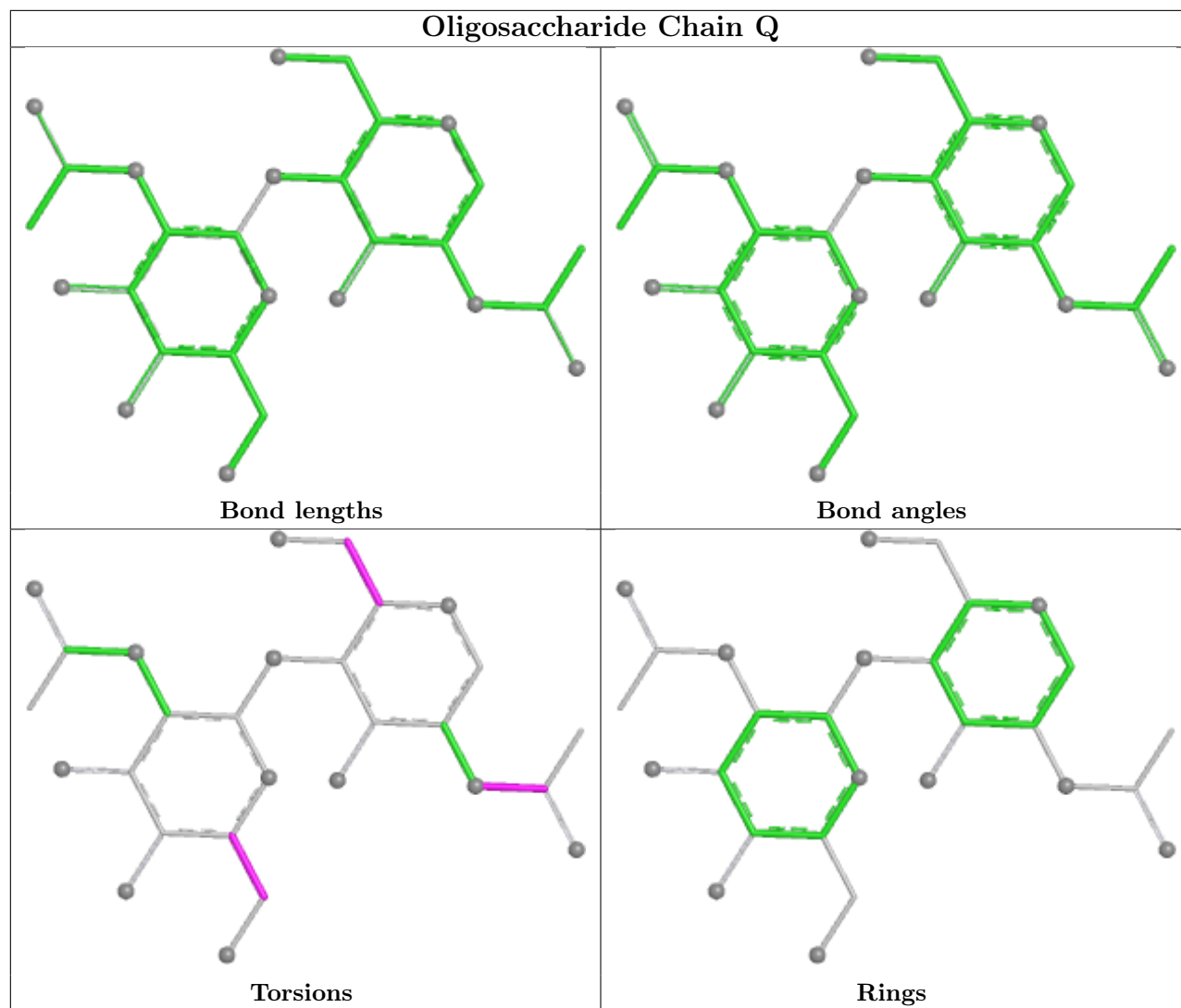


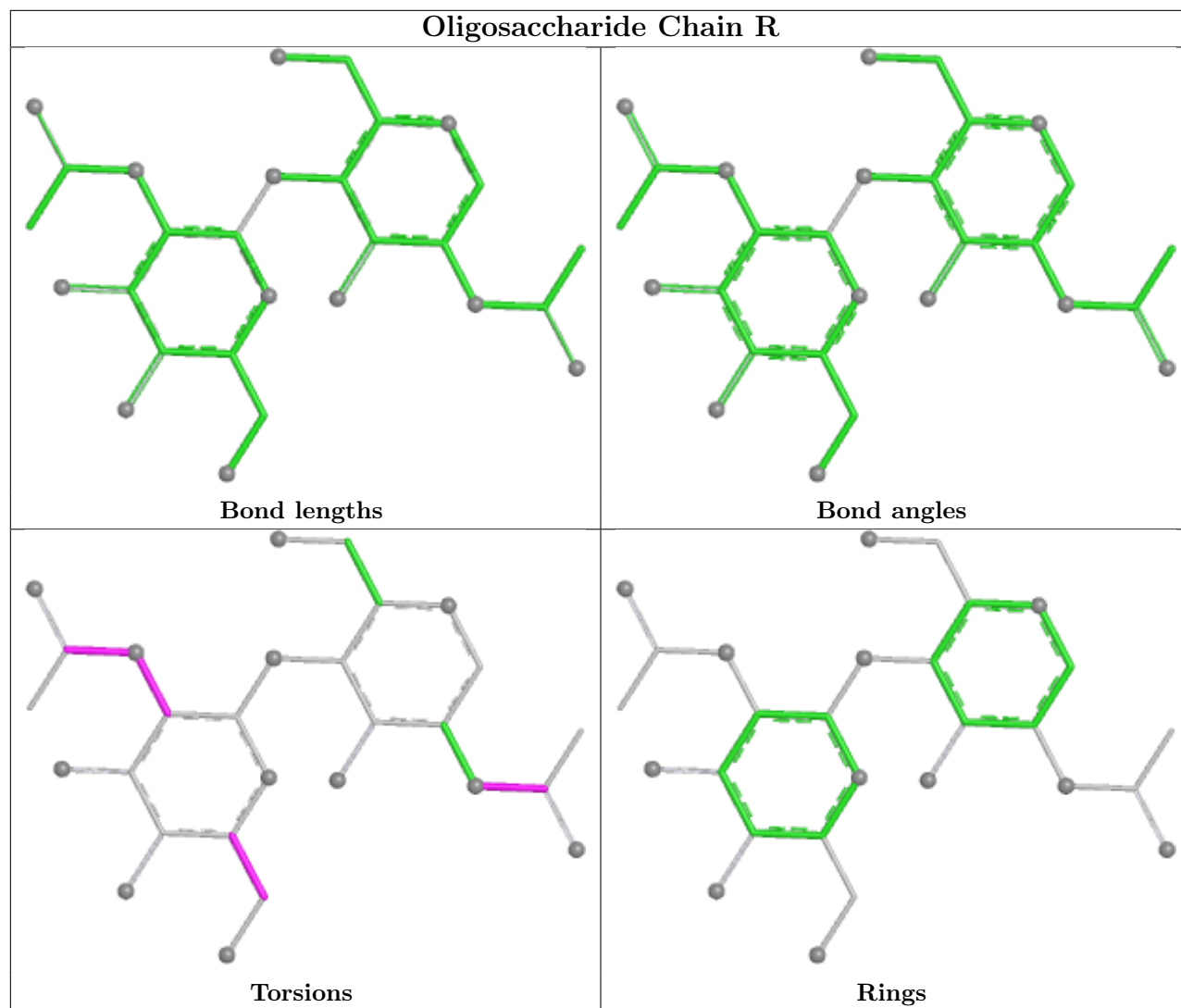


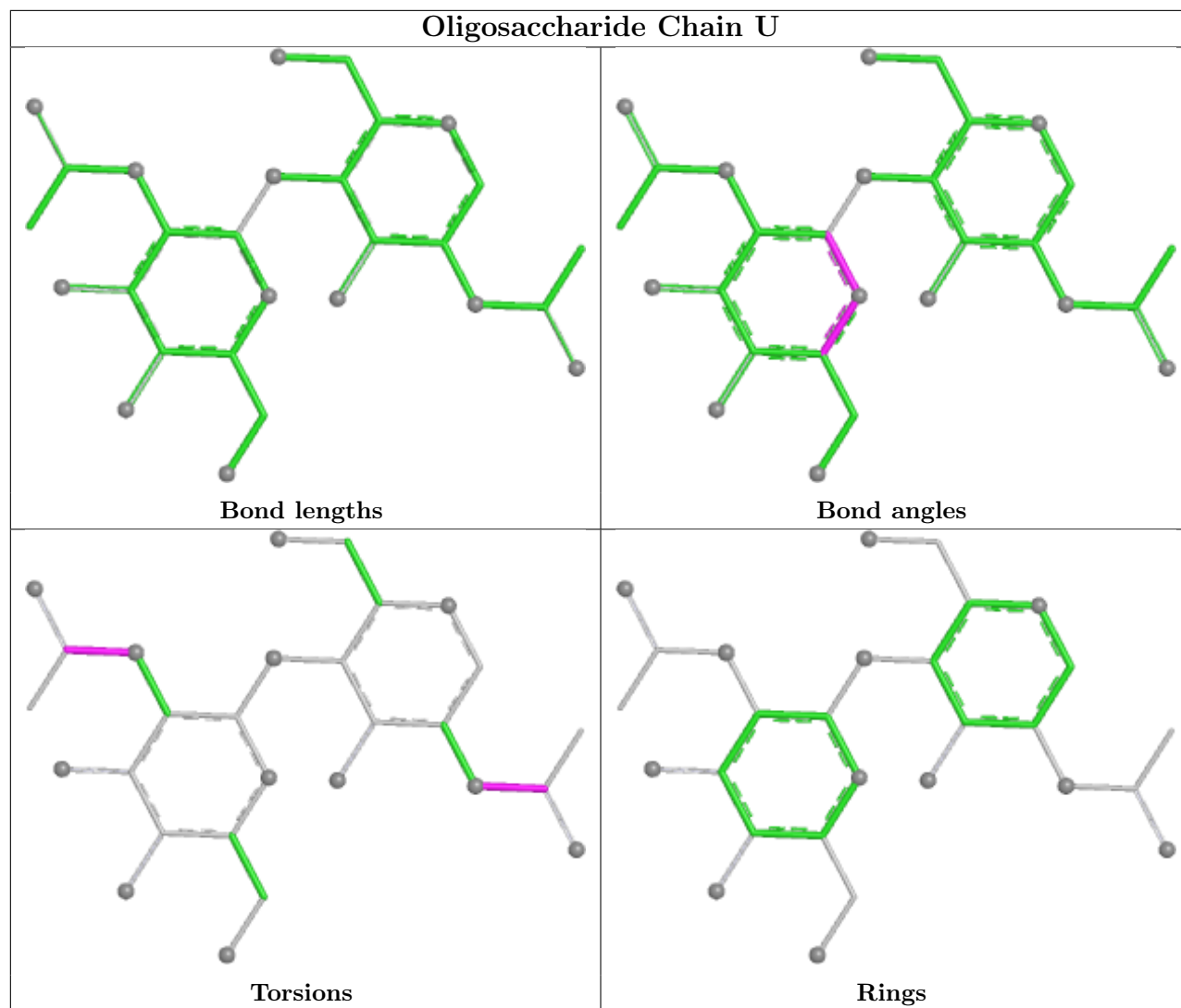


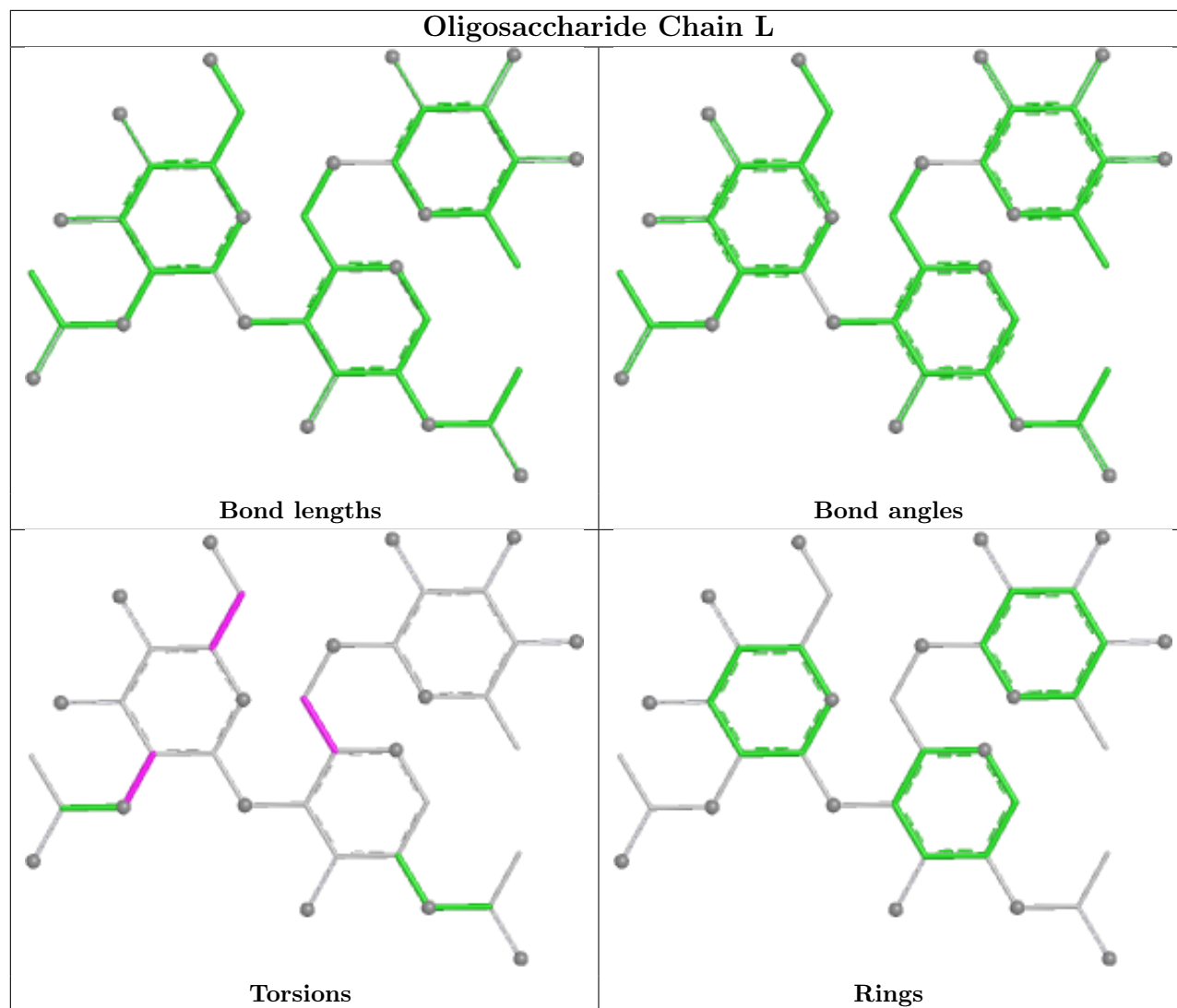


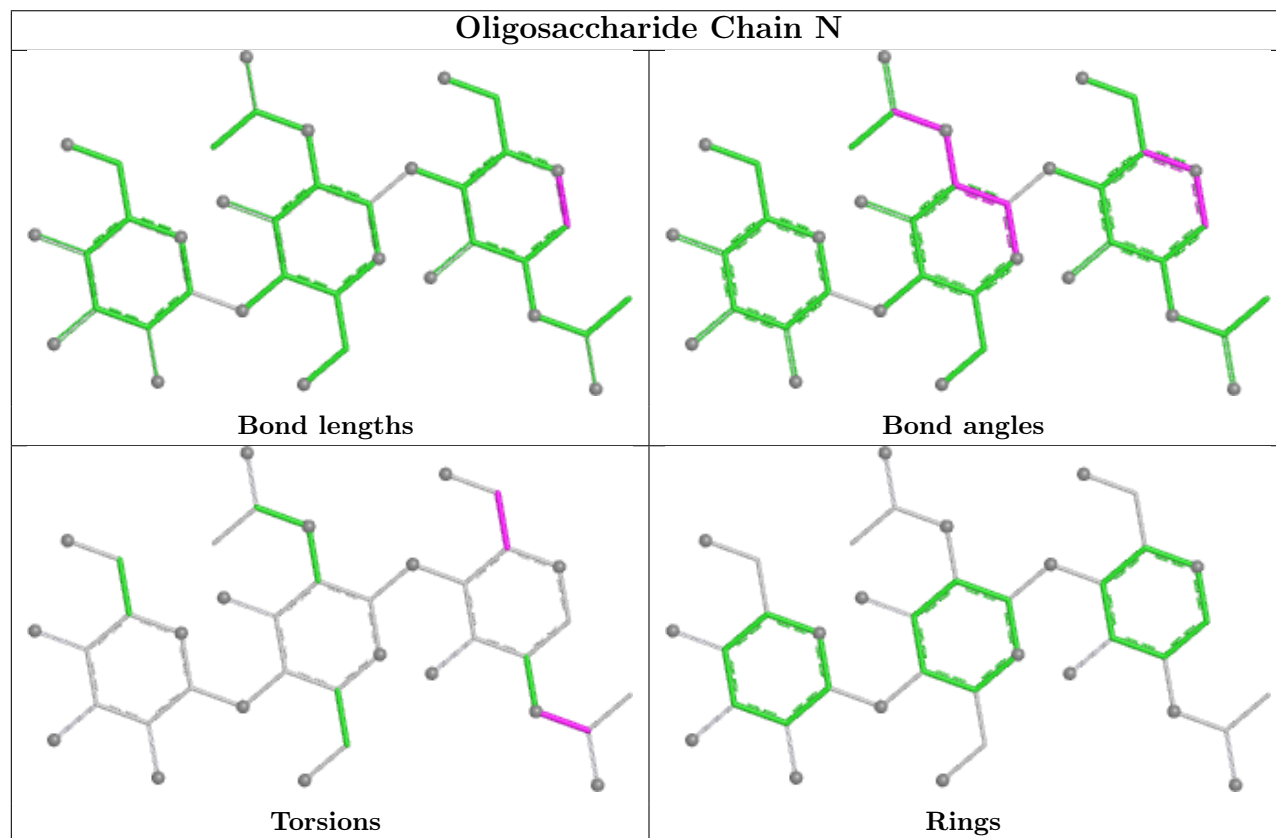
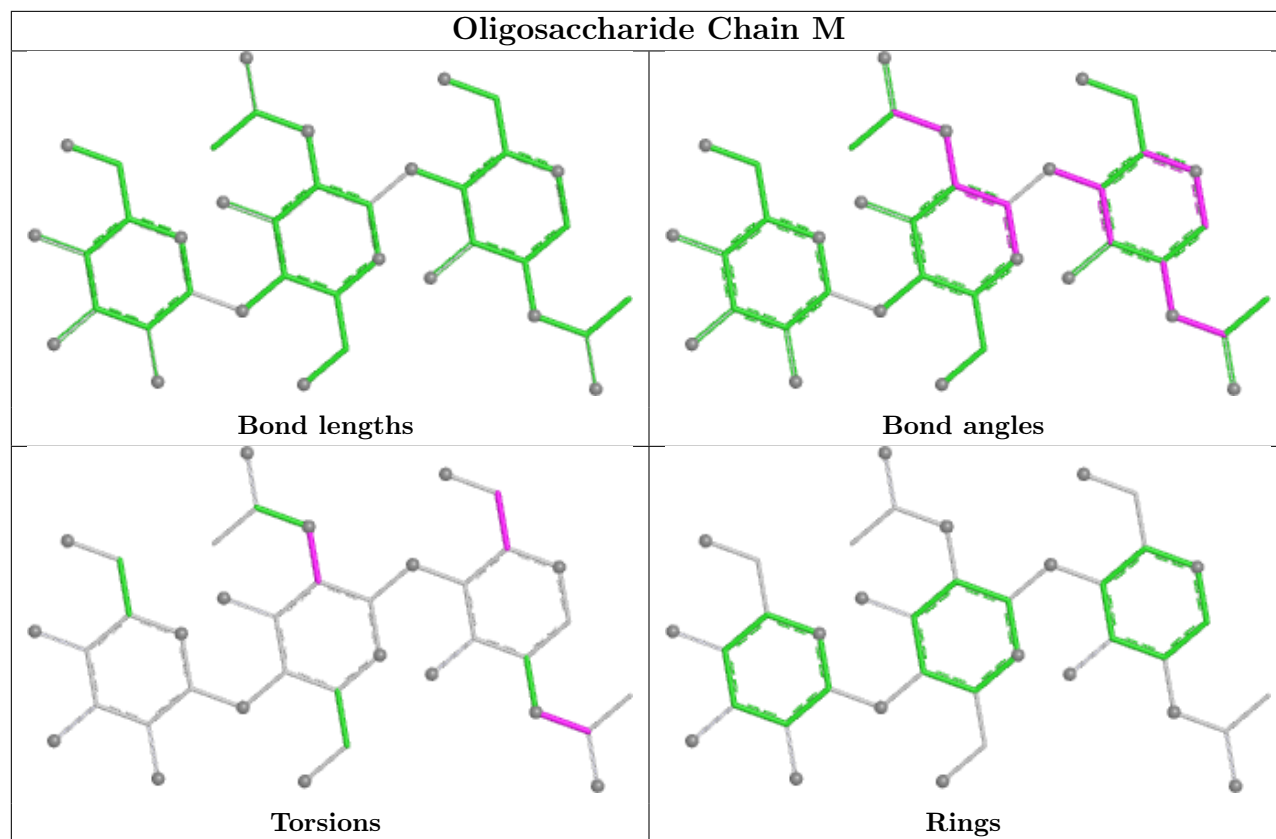


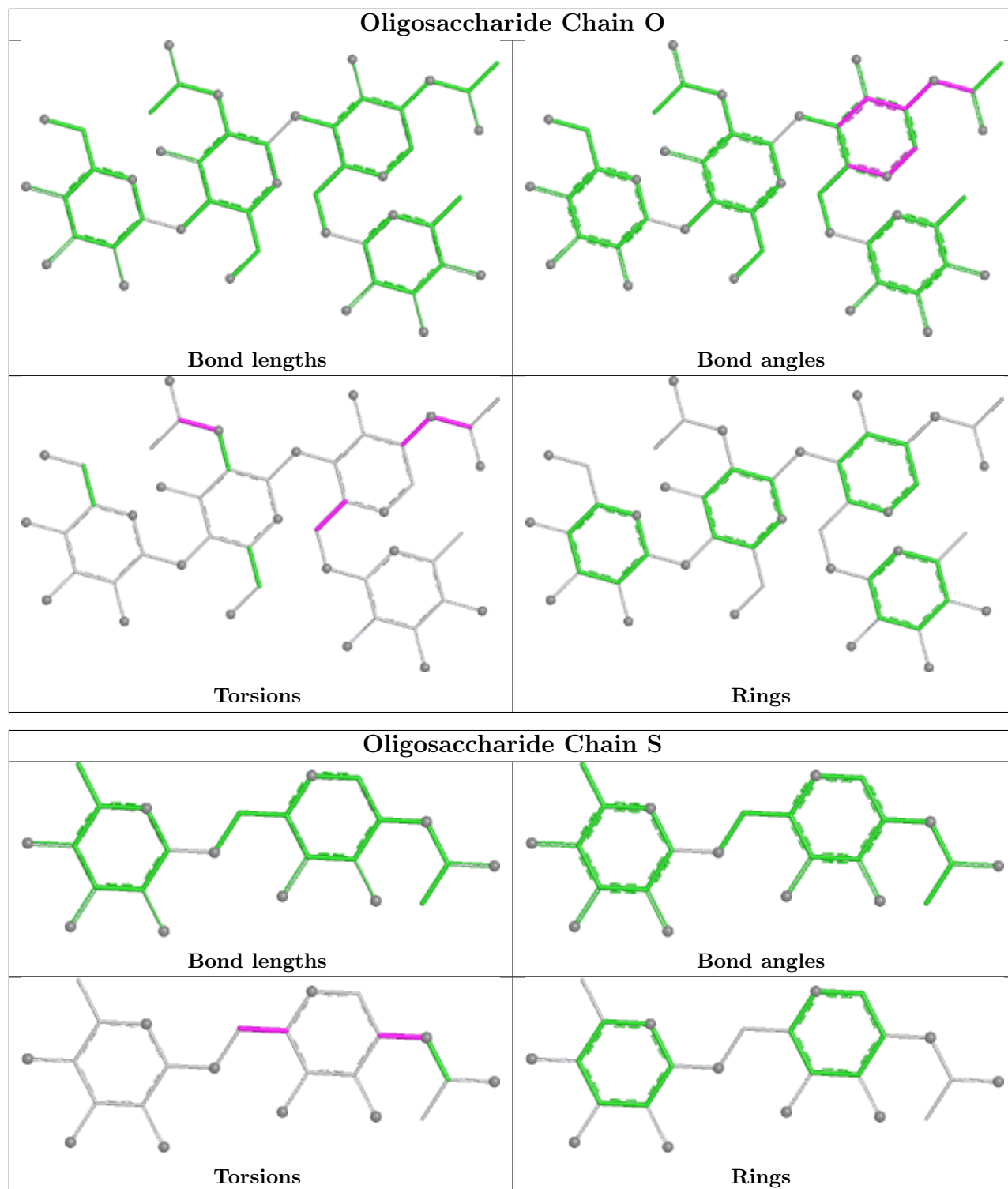


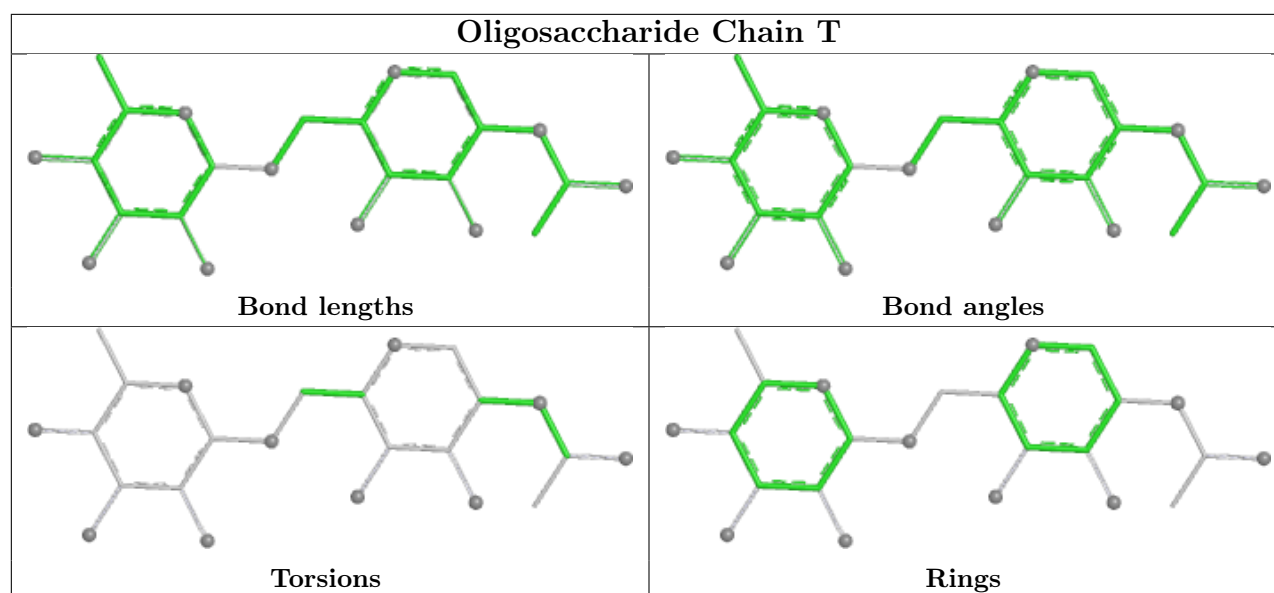












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
10	NAG	A	1601	1	14,14,15	0.48	0	17,19,21	0.38	0
10	NAG	D	1404	1	14,14,15	0.49	0	17,19,21	0.48	0
10	NAG	D	1403	1	14,14,15	0.37	0	17,19,21	0.40	0
10	NAG	D	1405	1	14,14,15	0.28	0	17,19,21	0.50	0
10	NAG	A	1603	1	14,14,15	0.33	0	17,19,21	0.38	0
10	NAG	D	1401	1	14,14,15	0.24	0	17,19,21	0.43	0
10	NAG	D	1402	1	14,14,15	0.42	0	17,19,21	0.37	0
10	NAG	D	1406	1	14,14,15	0.27	0	17,19,21	0.44	0
10	NAG	A	1602	1	14,14,15	0.27	0	17,19,21	0.61	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
10	NAG	A	1601	1	-	2/6/23/26	0/1/1/1
10	NAG	D	1404	1	-	2/6/23/26	0/1/1/1
10	NAG	D	1403	1	-	4/6/23/26	0/1/1/1
10	NAG	D	1405	1	-	2/6/23/26	0/1/1/1
10	NAG	A	1603	1	-	2/6/23/26	0/1/1/1
10	NAG	D	1401	1	-	0/6/23/26	0/1/1/1
10	NAG	D	1402	1	-	2/6/23/26	0/1/1/1
10	NAG	D	1406	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1602	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

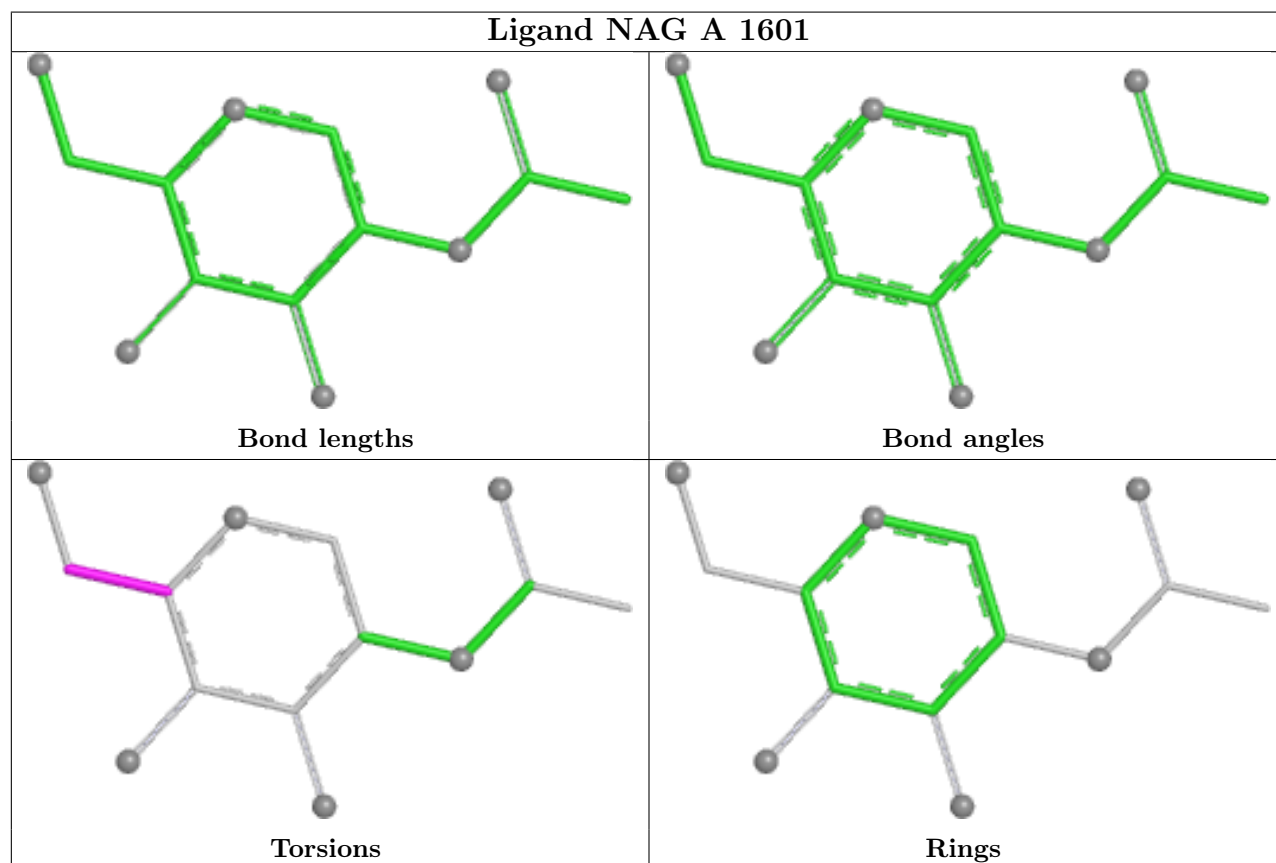
Mol	Chain	Res	Type	Atoms
10	A	1602	NAG	C8-C7-N2-C2
10	A	1602	NAG	O7-C7-N2-C2
10	A	1601	NAG	O5-C5-C6-O6
10	A	1601	NAG	C4-C5-C6-O6
10	D	1405	NAG	O5-C5-C6-O6
10	D	1405	NAG	C4-C5-C6-O6
10	A	1603	NAG	C4-C5-C6-O6
10	A	1603	NAG	O5-C5-C6-O6
10	D	1402	NAG	C8-C7-N2-C2
10	D	1402	NAG	O7-C7-N2-C2
10	D	1403	NAG	C8-C7-N2-C2
10	D	1403	NAG	O7-C7-N2-C2
10	D	1404	NAG	C8-C7-N2-C2
10	D	1404	NAG	O7-C7-N2-C2
10	D	1403	NAG	O5-C5-C6-O6
10	A	1602	NAG	O5-C5-C6-O6
10	D	1403	NAG	C4-C5-C6-O6

There are no ring outliers.

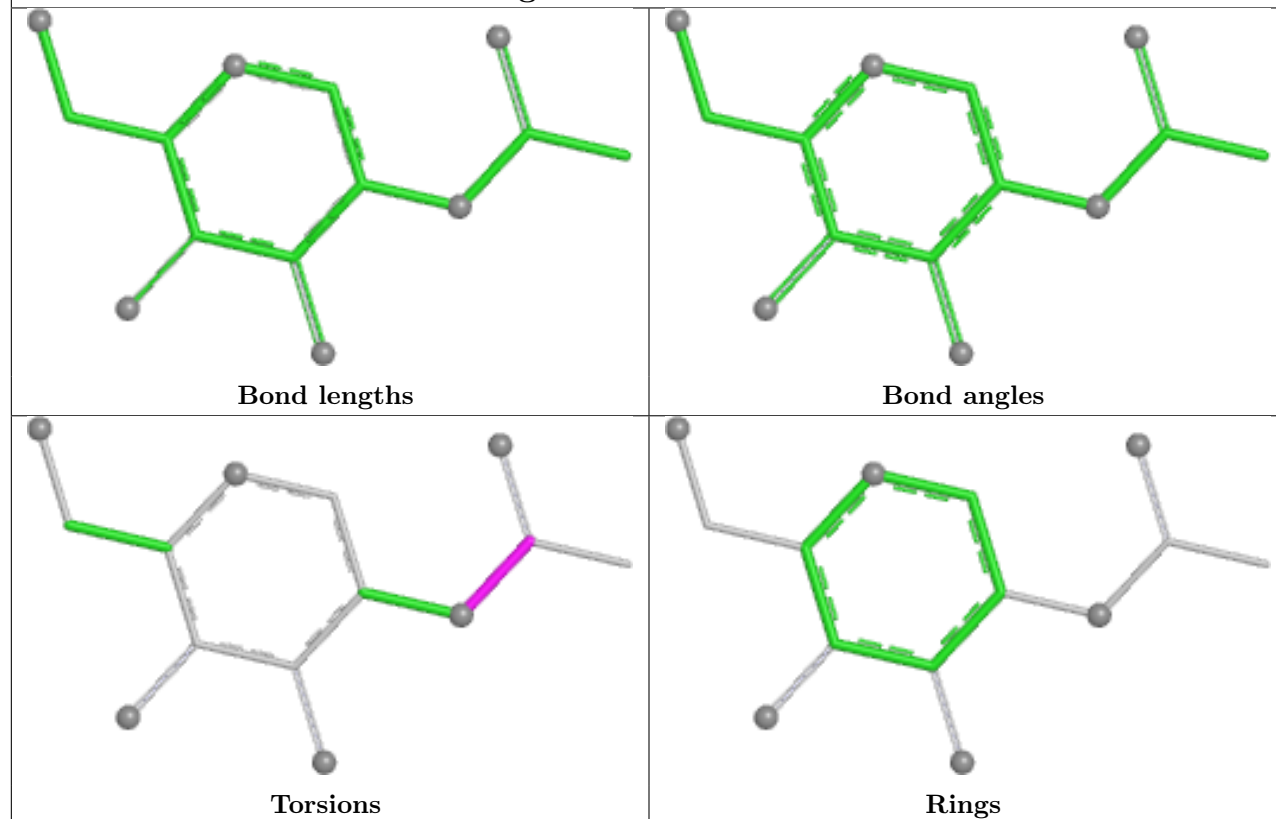
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	1401	NAG	2	0

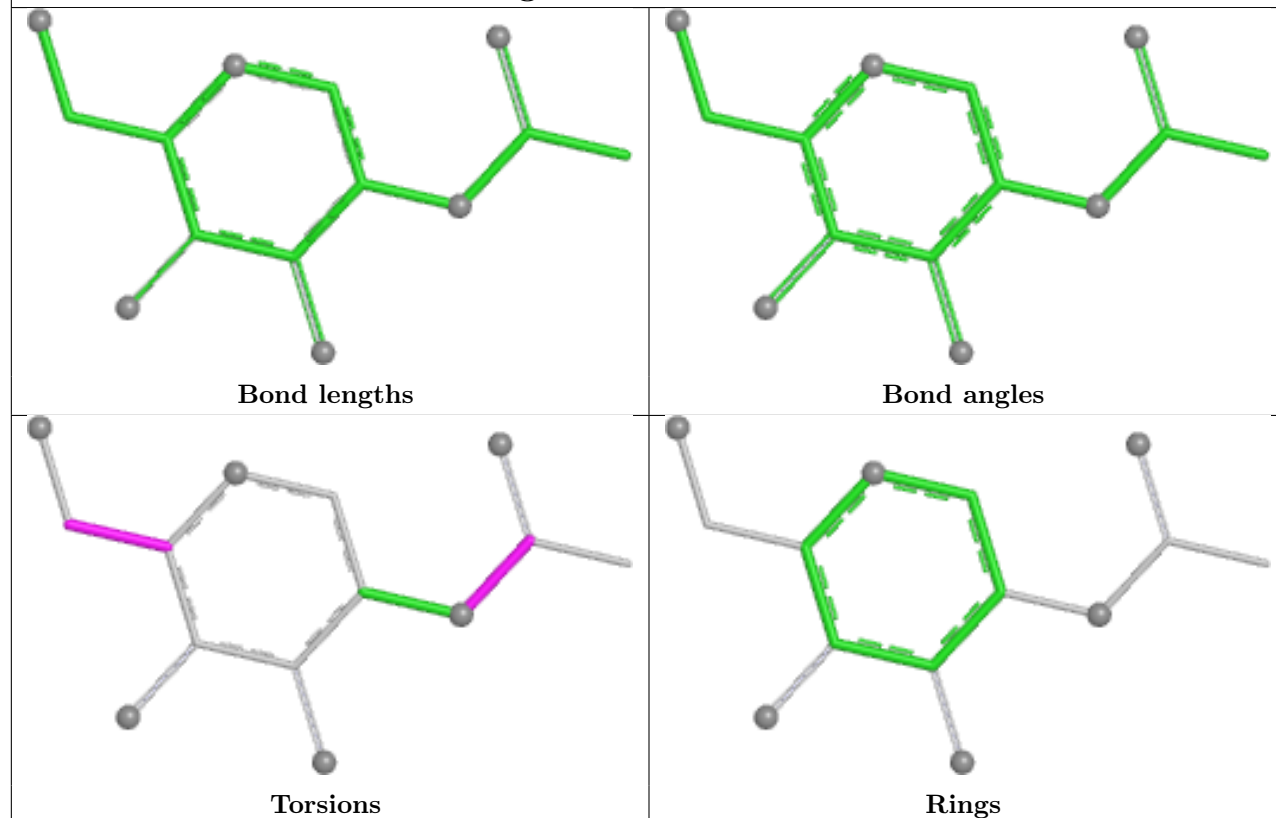
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



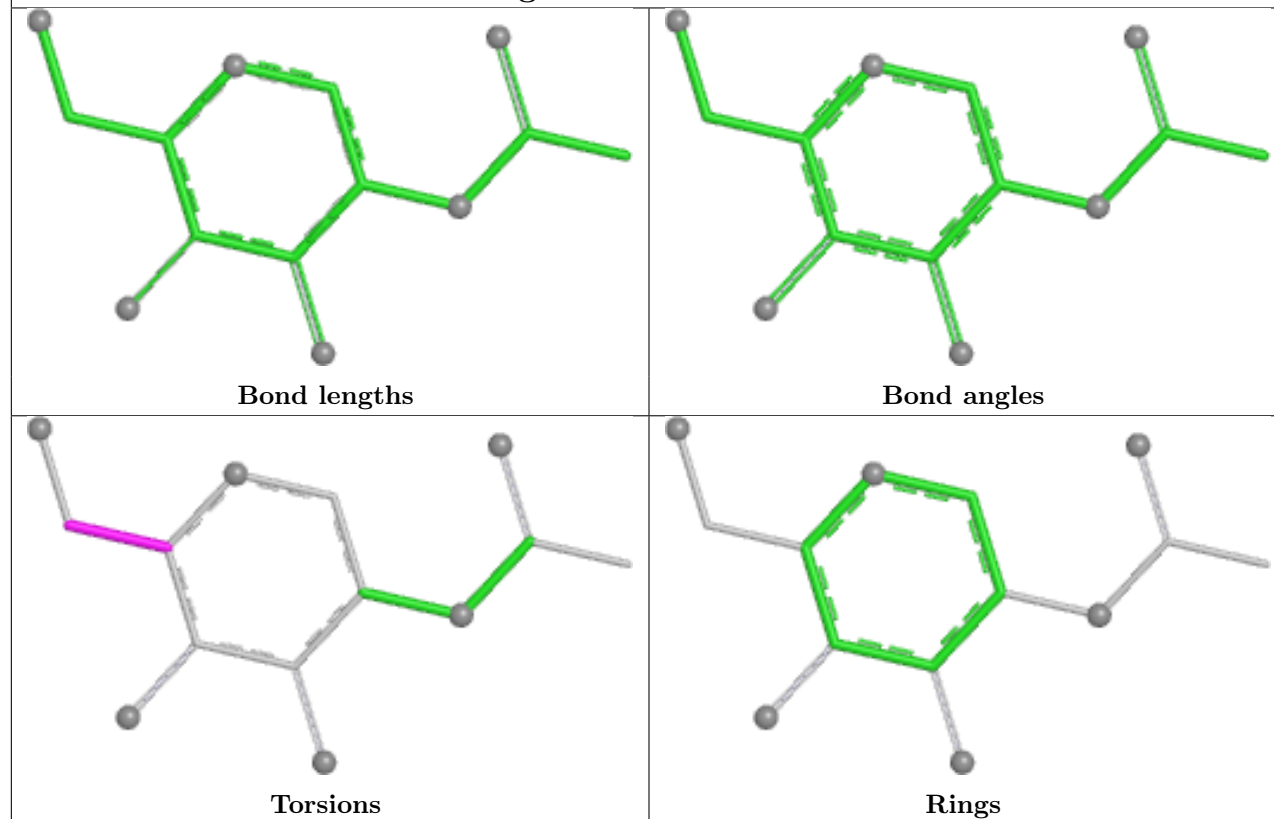
Ligand NAG D 1404



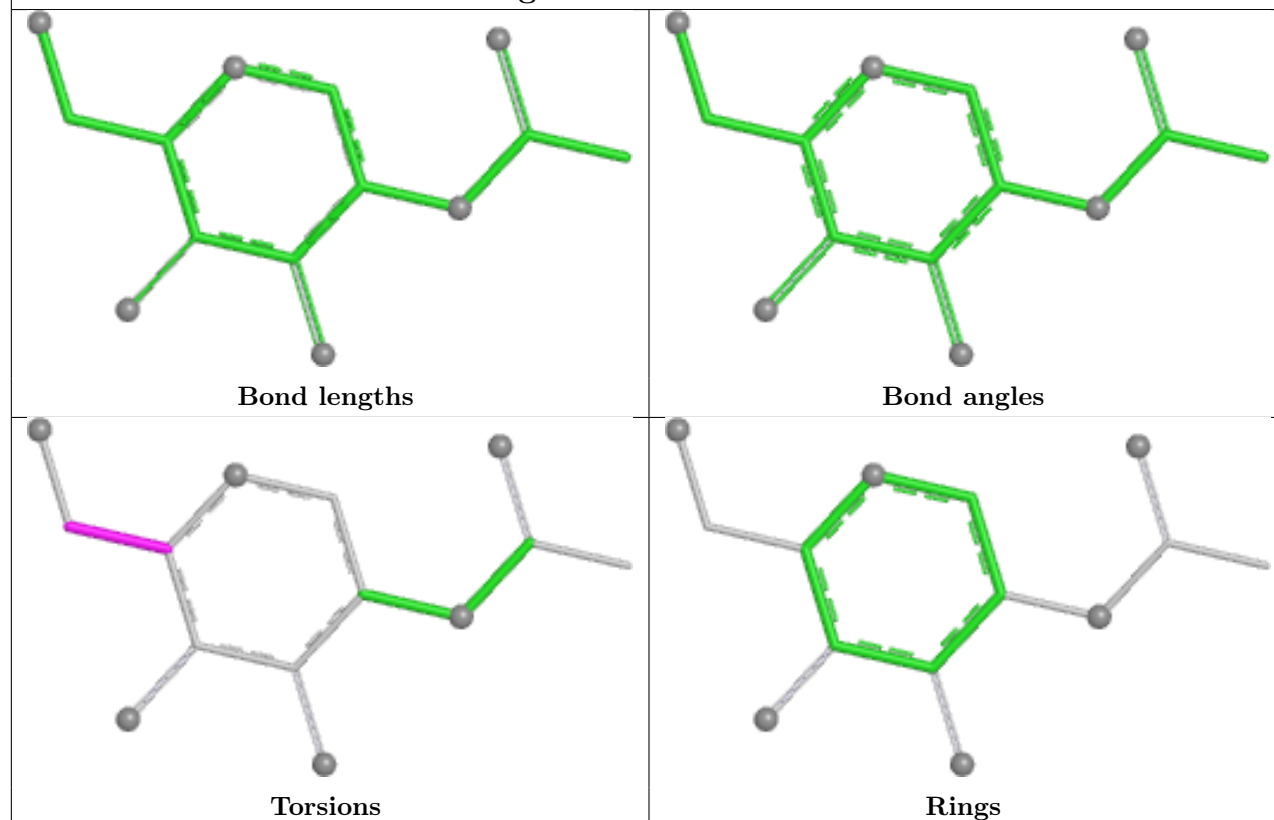
Ligand NAG D 1403



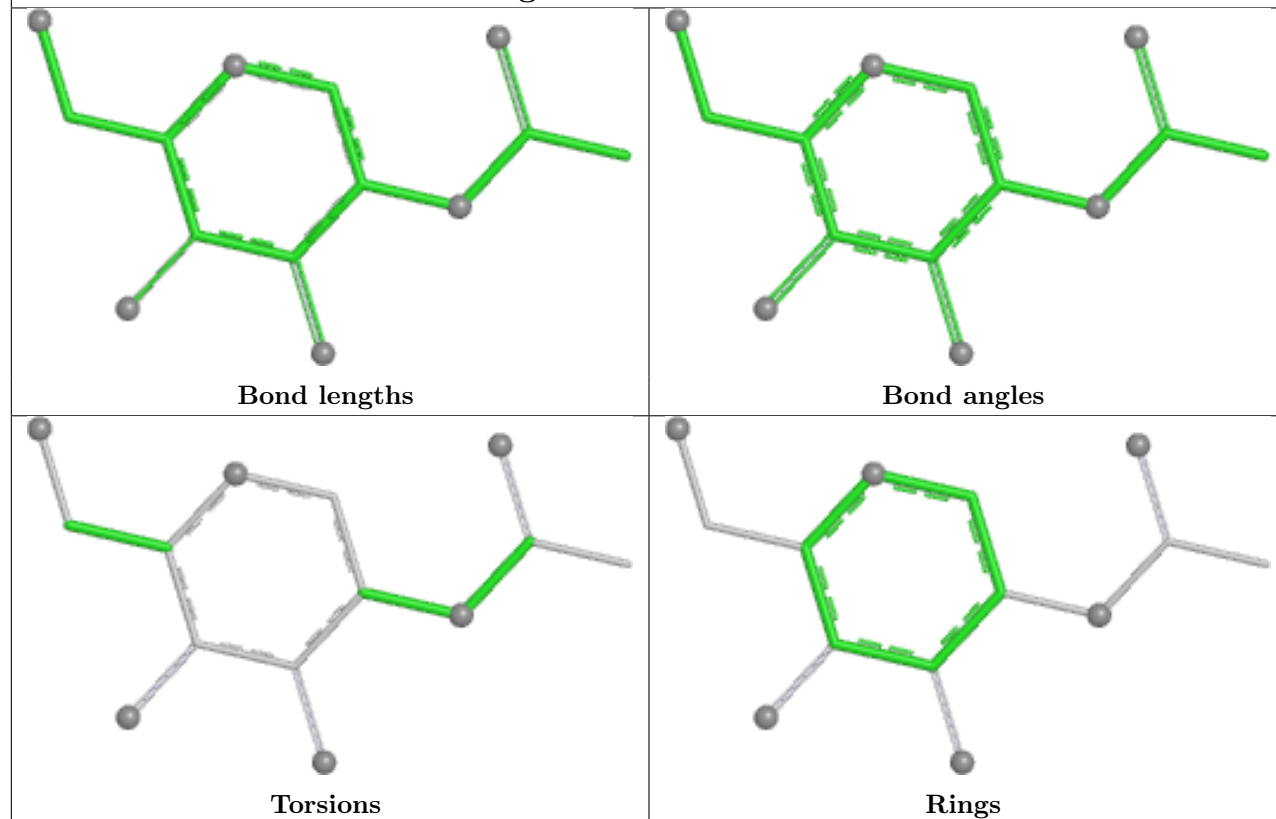
Ligand NAG D 1405



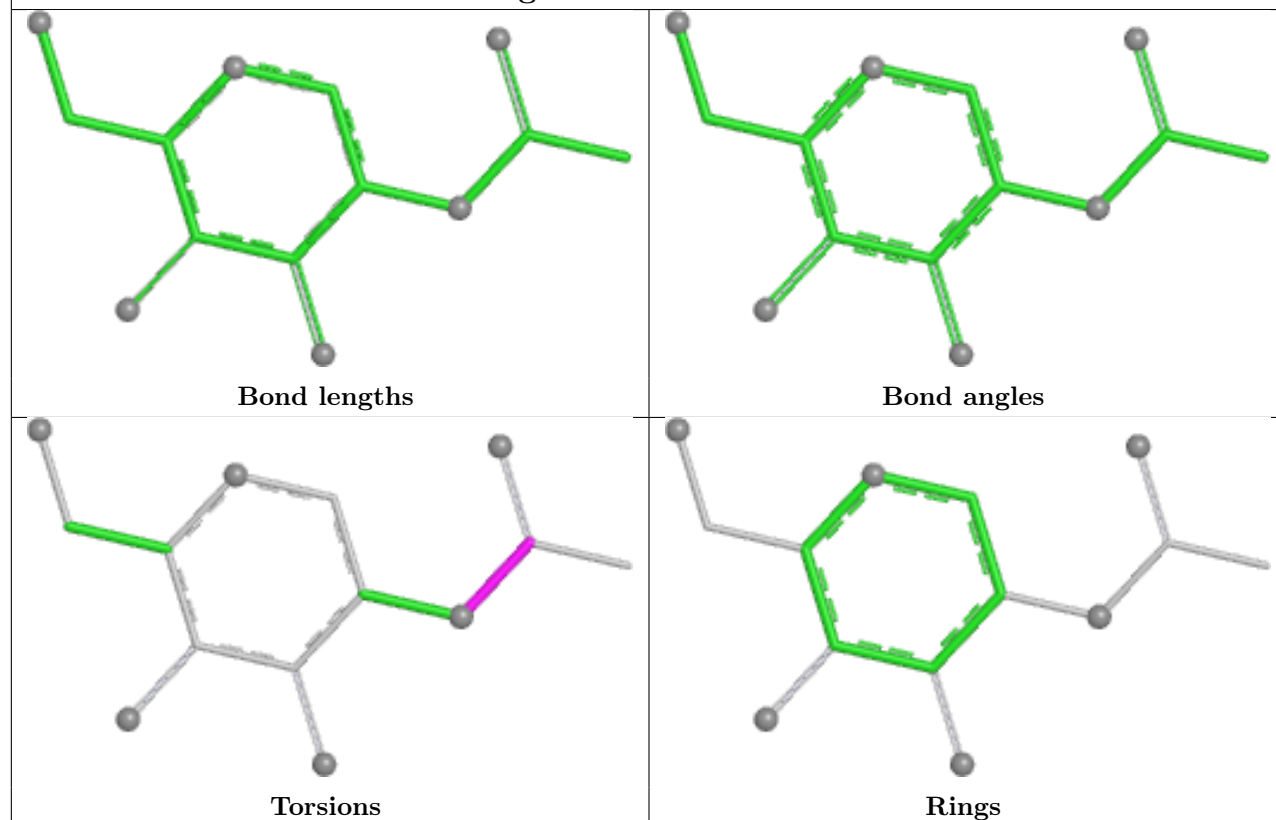
Ligand NAG A 1603



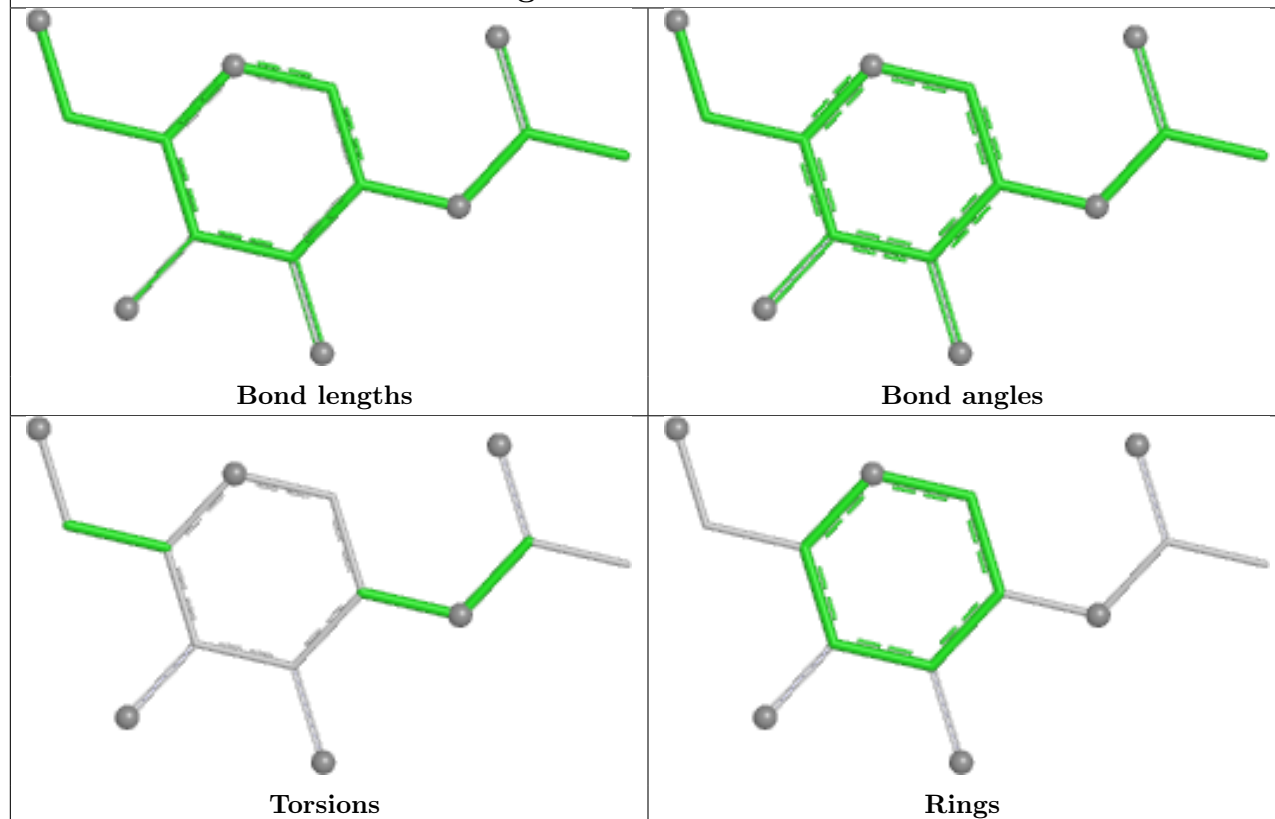
Ligand NAG D 1401



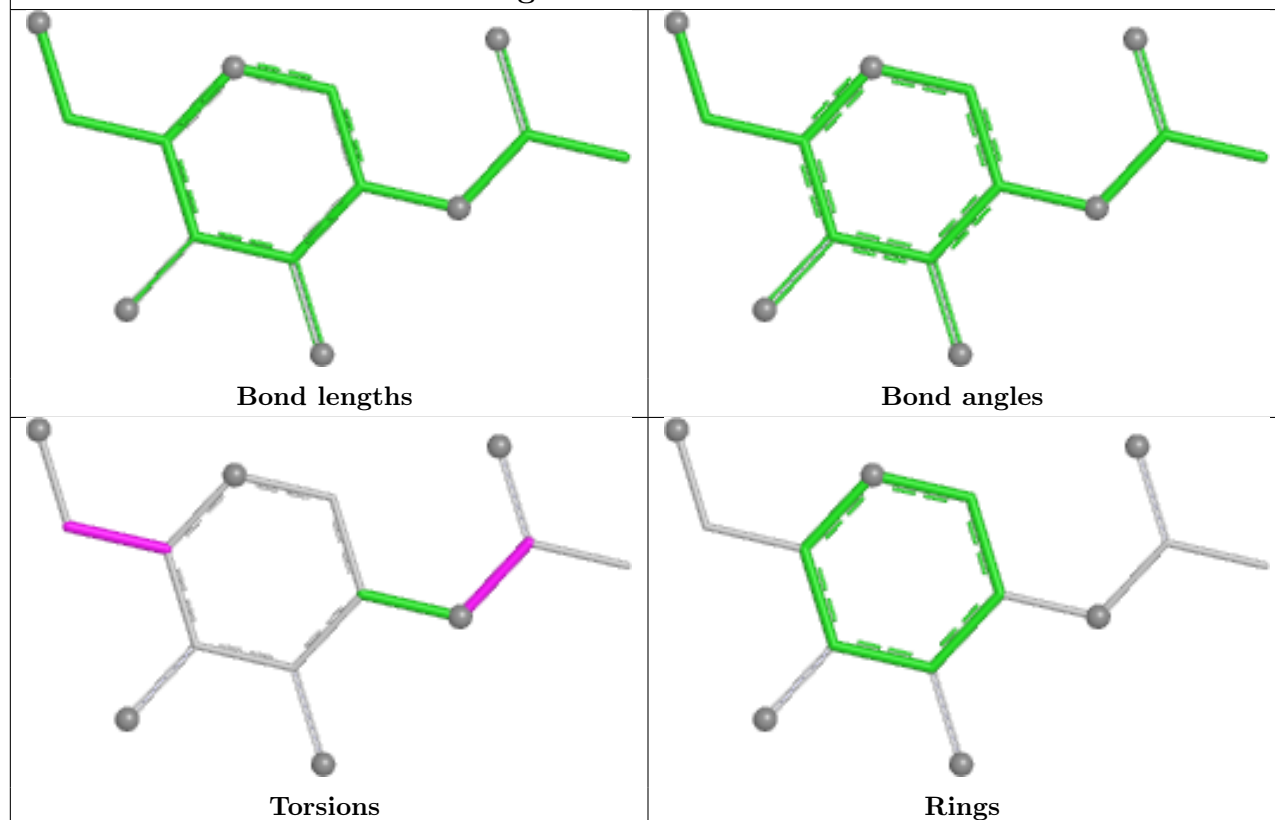
Ligand NAG D 1402



Ligand NAG D 1406



Ligand NAG A 1602



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	637/683 (93%)	0.62	44 (6%)	23 16	25, 44, 90, 107	0
1	D	637/683 (93%)	0.29	25 (3%)	43 29	18, 32, 79, 100	0
2	B	175/230 (76%)	1.57	47 (26%)	1 1	37, 90, 133, 145	0
2	E	174/230 (75%)	0.99	23 (13%)	7 6	24, 65, 107, 113	0
3	C	13/13 (100%)	1.54	3 (23%)	2 2	37, 40, 53, 54	0
3	F	13/13 (100%)	1.55	5 (38%)	1 1	26, 31, 56, 63	0
All	All	1649/1852 (89%)	0.65	147 (8%)	15 12	18, 41, 103, 145	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	199	LEU	6.7
2	B	192	ILE	6.3
2	B	164	LEU	5.6
2	B	190	THR	5.2
2	B	200	THR	5.2
1	A	47	THR	5.0
3	F	1	GLU	4.8
3	C	1	GLU	4.8
2	B	184	GLY	4.2
2	B	191	PRO	4.1
1	D	563	SER	4.1
1	A	563	SER	4.0
1	A	683	CYS	4.0
2	B	189	PHE	3.8
1	D	683	CYS	3.8
2	E	153	SER	3.7
3	C	2	SER	3.7
3	F	3	SER	3.7
2	B	187	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	645	MET	3.6
1	D	682	LEU	3.6
2	B	188	LEU	3.6
2	E	192	ILE	3.6
2	E	164	LEU	3.6
1	A	666	ALA	3.5
1	A	585	ASP	3.4
2	B	177	THR	3.4
2	B	198	LYS	3.4
2	B	103	ASN	3.3
2	B	183	ASN	3.2
1	D	585	ASP	3.1
2	E	151	SER	3.1
1	D	74	VAL	3.0
1	A	465	ASN	3.0
1	D	308	ASN	3.0
2	B	129	SER	3.0
2	B	105	THR	3.0
1	A	662	ILE	3.0
2	B	185	SER	2.9
2	B	180	ILE	2.9
2	E	180	ILE	2.9
2	B	163	VAL	2.9
2	B	193	SER	2.9
1	A	379	ALA	2.9
1	A	640	PRO	2.9
2	B	158	ARG	2.9
1	A	643	LYS	2.8
2	E	185	SER	2.8
1	A	681	ASP	2.8
1	A	642	PHE	2.8
2	E	174	ASN	2.8
1	D	79	SER	2.8
3	F	4	SER	2.8
2	B	176	LEU	2.8
2	B	148	ASN	2.8
2	B	118	LEU	2.8
2	E	188	LEU	2.8
2	B	181	PRO	2.7
1	A	674	ASP	2.7
1	A	602	MET	2.7
2	B	182	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	149	ASN	2.7
2	E	176	LEU	2.7
2	E	63	THR	2.6
2	E	197	THR	2.6
1	A	611	ASP	2.6
1	A	657	ASN	2.6
2	B	160	LEU	2.6
1	A	651	VAL	2.6
2	B	63	THR	2.6
2	B	92	PRO	2.6
2	B	175	PRO	2.6
1	A	616	SER	2.6
1	A	672	PRO	2.6
1	D	681	ASP	2.6
1	A	587	ASP	2.5
2	B	167	GLN	2.5
1	A	649	THR	2.5
1	A	680	LYS	2.5
1	A	527	ARG	2.5
2	B	91	LEU	2.4
2	E	155	GLU	2.4
1	A	664	ASP	2.4
2	E	179	ASP	2.4
1	D	523	SER	2.4
2	B	179	ASP	2.3
2	B	115	LEU	2.3
2	B	107	THR	2.3
2	B	156	ILE	2.3
1	A	626	ARG	2.3
3	C	6	HIS	2.3
2	E	183	ASN	2.3
2	E	167	GLN	2.3
1	A	334	GLU	2.3
1	A	592	GLU	2.3
2	B	151	SER	2.3
2	E	196	ASN	2.3
1	D	646	LEU	2.3
1	D	101	THR	2.2
2	E	161	THR	2.2
1	A	79	SER	2.2
1	D	140	ARG	2.2
2	B	173	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	638	ILE	2.2
2	E	191	PRO	2.2
1	A	648	LEU	2.2
2	B	169	LEU	2.2
2	B	171	LEU	2.2
1	A	425	SER	2.2
2	E	171	LEU	2.2
1	A	638	ILE	2.2
1	D	640	PRO	2.2
1	D	680	LYS	2.2
1	A	400	ASP	2.2
1	A	609	GLN	2.1
1	D	651	VAL	2.1
1	D	78	THR	2.1
2	B	116	THR	2.1
2	B	83	GLN	2.1
1	A	677	GLU	2.1
1	D	660	GLY	2.1
2	B	117	GLU	2.1
2	E	184	GLY	2.1
2	B	150	ASN	2.1
2	E	189	PHE	2.1
1	D	611	ASP	2.1
1	D	643	LYS	2.1
1	A	619	ARG	2.1
3	F	2	SER	2.1
1	A	624	LEU	2.1
1	A	101	THR	2.1
1	A	675	ALA	2.1
3	F	5	SER	2.1
2	B	168	VAL	2.1
1	A	633	ASN	2.1
1	D	63	ASN	2.1
1	D	352	ASP	2.1
2	B	47	GLN	2.1
1	A	668	PHE	2.1
2	B	101	SER	2.0
2	E	187	SER	2.0
1	A	241	ARG	2.0
1	A	646	LEU	2.0
1	D	75	ASN	2.0
1	A	645	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	678	GLY	2.0
1	D	115	SER	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
5	NAG	U	2	14/15	0.04	0.33	73,74,74,75	0
9	FUC	T	2	10/11	0.26	0.28	75,76,78,78	0
4	FUC	G	4	10/11	0.50	0.26	71,71,72,72	0
5	NAG	U	1	14/15	0.50	0.21	57,60,64,65	0
4	NAG	G	3	14/15	0.51	0.29	72,72,73,75	0
5	NAG	J	2	14/15	0.51	0.21	69,69,69,69	0
5	NAG	K	1	14/15	0.51	0.25	73,79,83,86	0
6	FUC	L	3	10/11	0.53	0.21	78,78,78,79	0
6	NAG	L	2	14/15	0.55	0.20	82,82,82,83	0
4	NAG	G	1	14/15	0.55	0.22	63,64,66,66	0
4	FUC	G	2	10/11	0.55	0.22	68,68,69,69	0
8	BMA	O	3	11/12	0.59	0.18	60,60,60,60	0
5	NAG	I	2	14/15	0.59	0.18	54,55,56,56	0
8	FUC	O	4	10/11	0.60	0.20	54,54,54,54	0
5	NAG	P	2	14/15	0.61	0.25	50,51,52,53	0
5	NAG	H	2	14/15	0.62	0.23	59,62,65,65	0
5	NAG	R	2	14/15	0.64	0.20	51,52,54,54	0
5	NAG	K	2	14/15	0.64	0.16	79,80,82,82	0
9	NAG	S	1	14/15	0.66	0.17	56,61,64,65	0
5	NAG	H	1	14/15	0.67	0.23	54,56,58,60	0
5	NAG	Q	2	14/15	0.68	0.17	55,55,55,55	0
5	NAG	P	1	14/15	0.68	0.26	43,45,47,47	0
9	FUC	S	2	10/11	0.70	0.18	62,63,63,63	0
6	NAG	L	1	14/15	0.74	0.16	70,72,74,75	0
9	NAG	T	1	14/15	0.75	0.15	57,62,65,66	0
8	NAG	O	1	14/15	0.76	0.15	31,41,51,67	0

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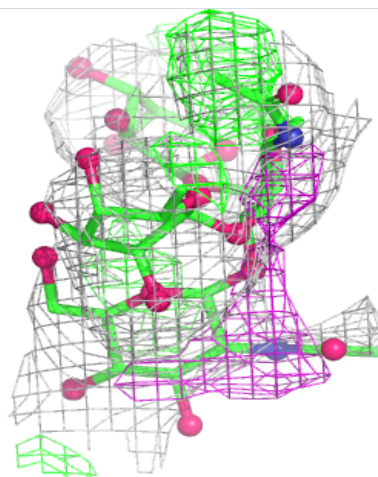
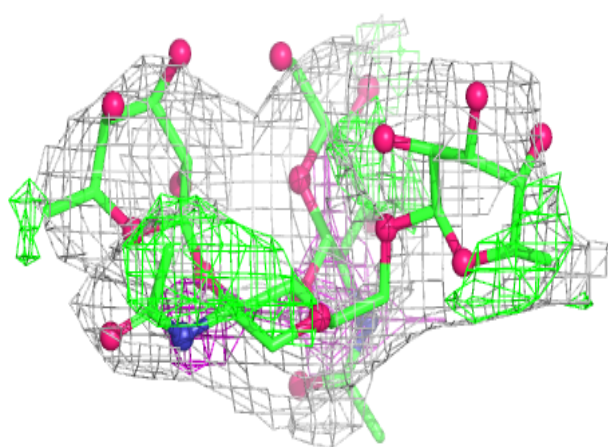
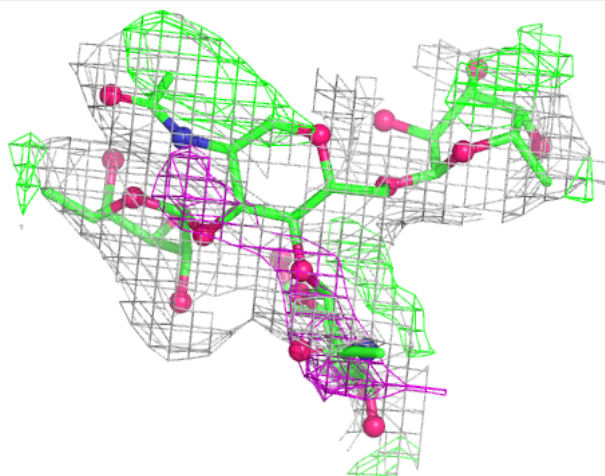
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	N	1	14/15	0.77	0.22	24,26,30,44	0
5	NAG	Q	1	14/15	0.77	0.18	42,43,46,48	0
8	NAG	O	2	14/15	0.78	0.16	58,58,58,58	0
5	NAG	J	1	14/15	0.81	0.15	52,54,57,61	0
7	BMA	M	3	11/12	0.82	0.12	43,43,43,43	0
7	BMA	N	3	11/12	0.83	0.10	40,40,40,40	0
5	NAG	I	1	14/15	0.84	0.17	41,45,50,50	0
5	NAG	R	1	14/15	0.86	0.14	43,50,54,55	0
7	NAG	N	2	14/15	0.89	0.13	22,33,44,46	0
7	NAG	M	1	14/15	0.93	0.13	25,34,63,76	0
7	NAG	M	2	14/15	0.95	0.10	38,38,38,38	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.

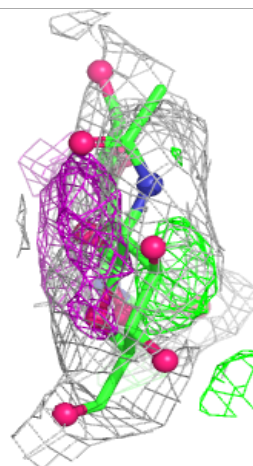
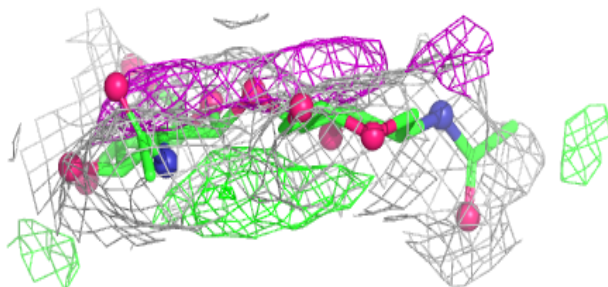
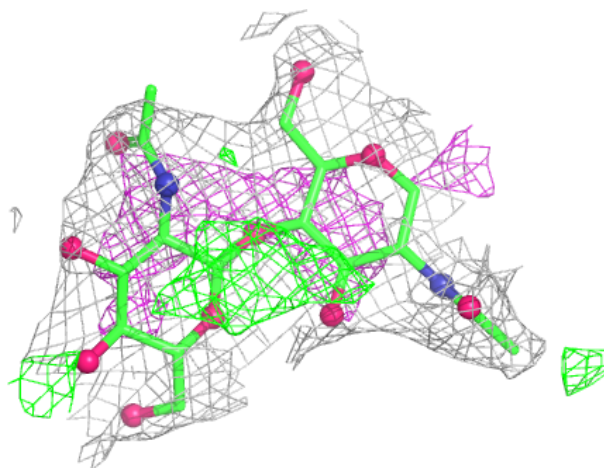
Electron density around Chain G:

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



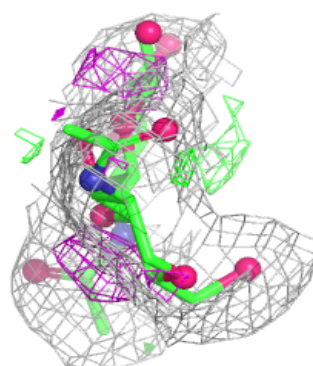
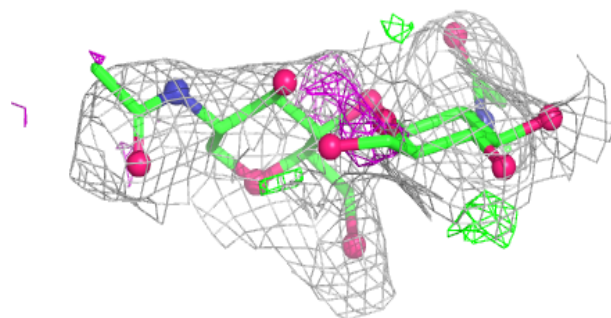
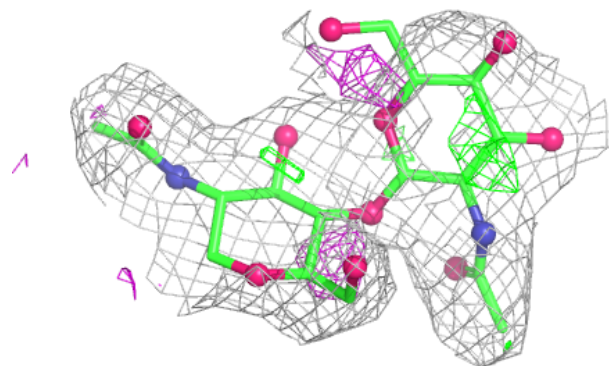
Electron density around Chain H:

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



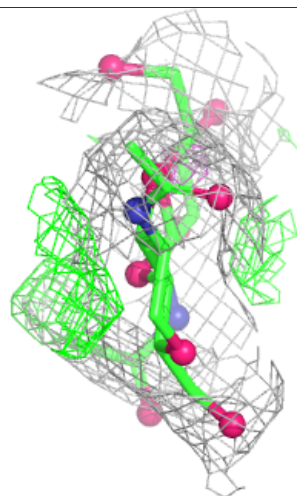
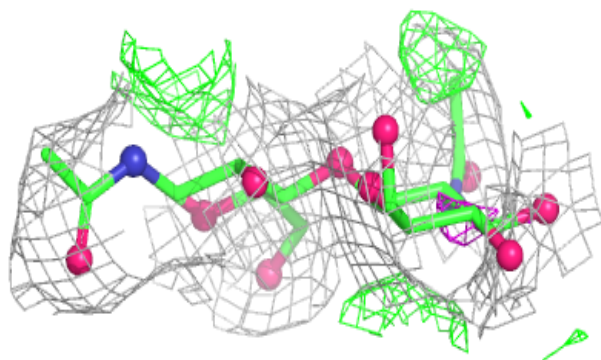
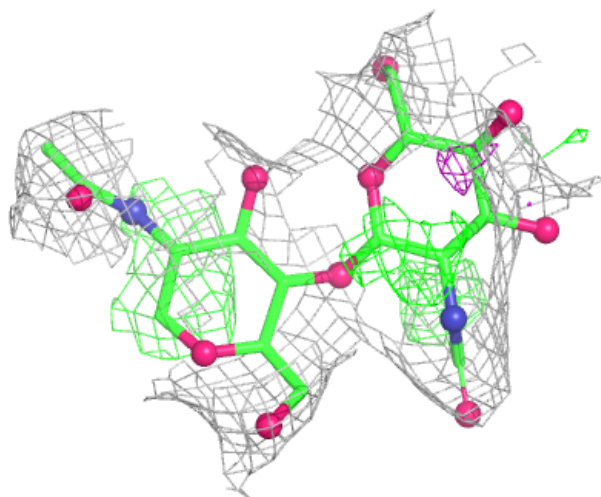
Electron density around Chain I:

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



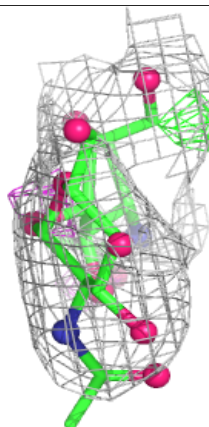
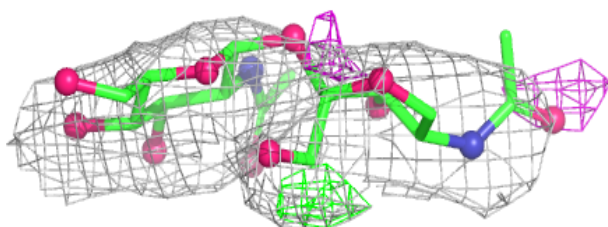
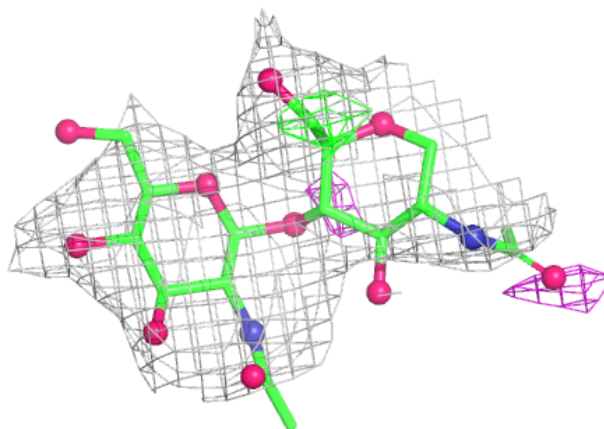
Electron density around Chain J:

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



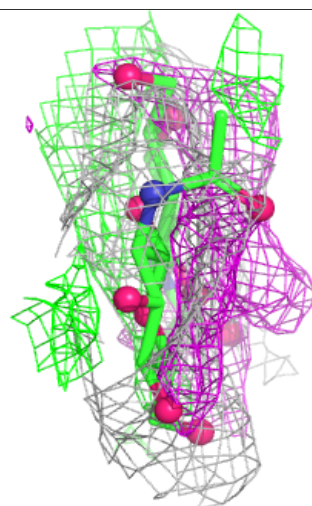
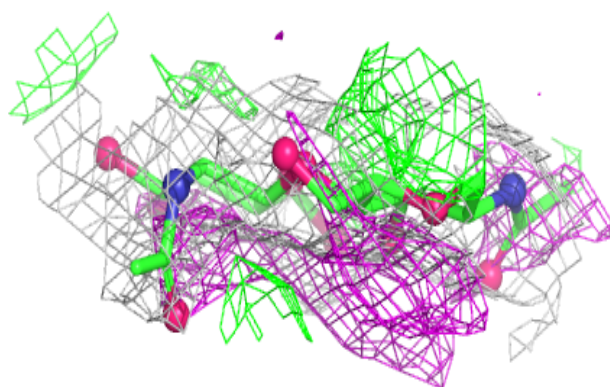
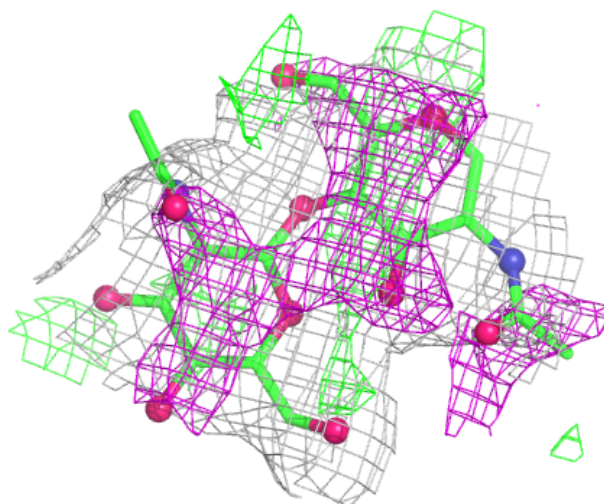
Electron density around Chain K:

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



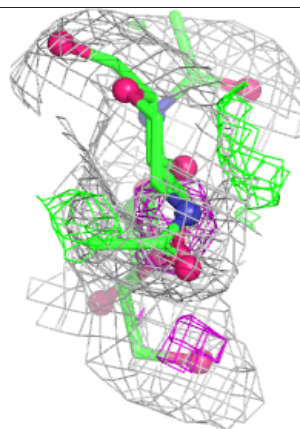
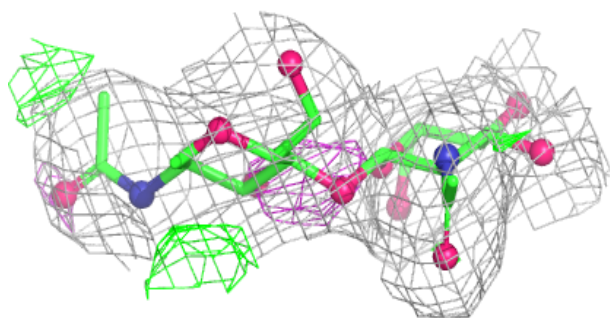
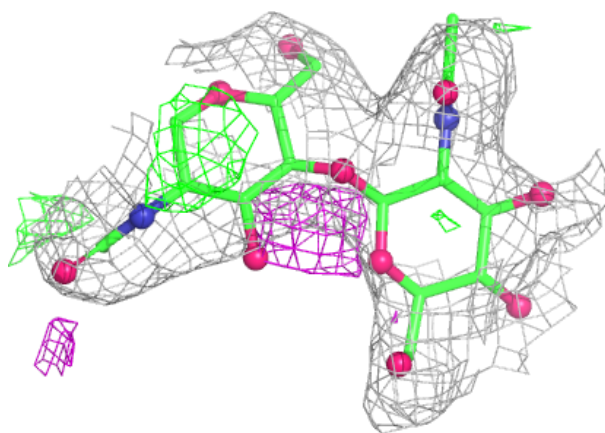
Electron density around Chain P:

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

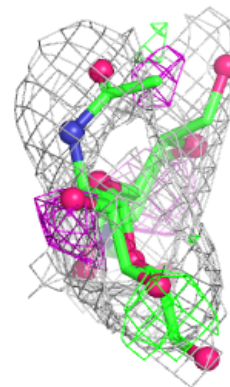
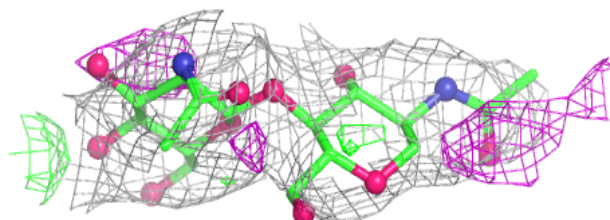
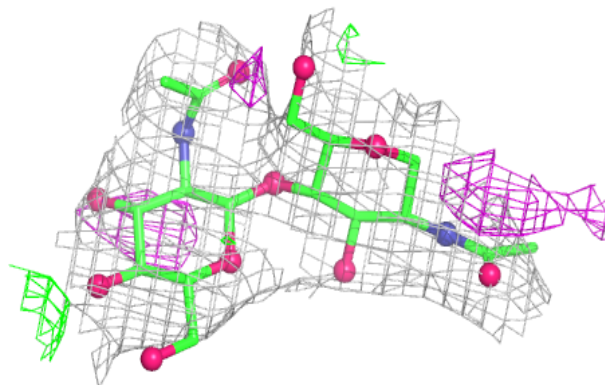


Electron density around Chain Q:

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

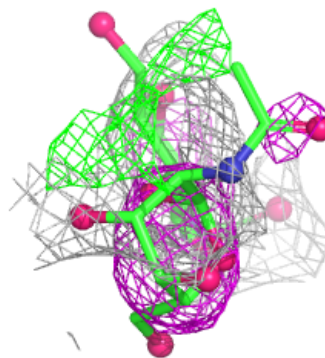
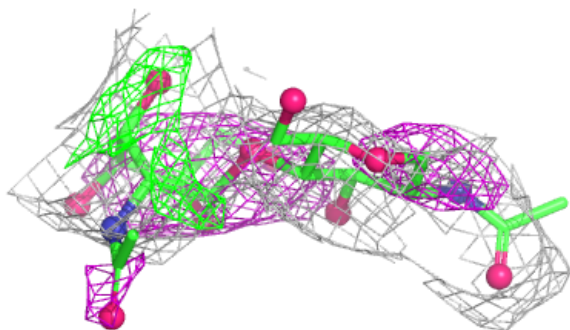
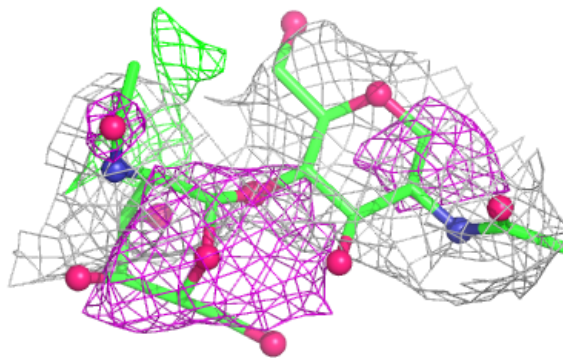
**Electron density around Chain R:**

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



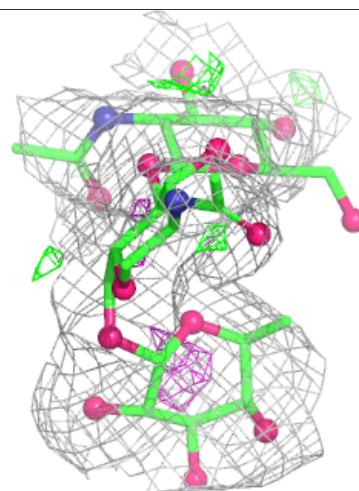
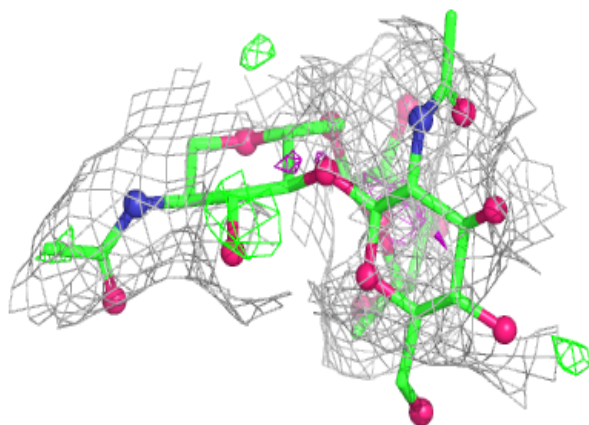
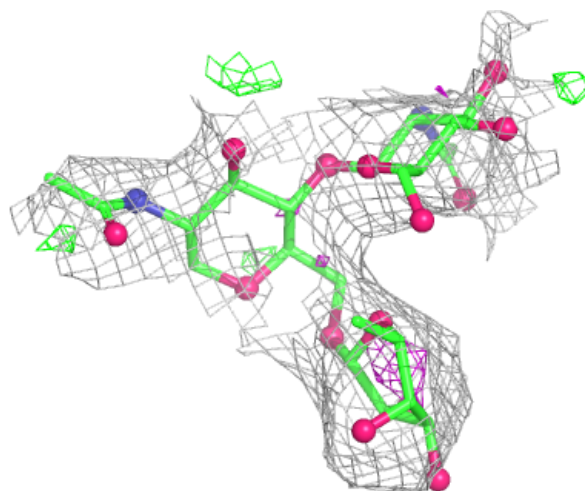
Electron density around Chain U:

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



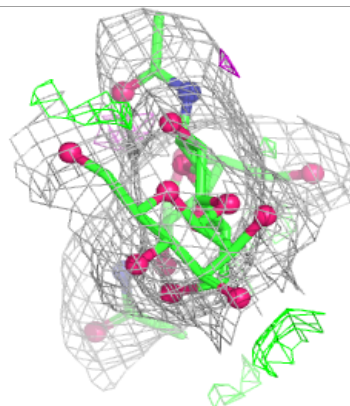
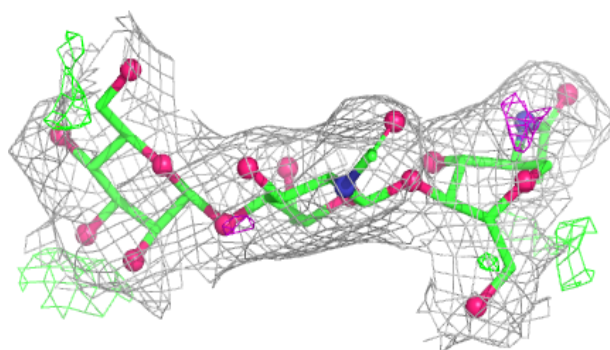
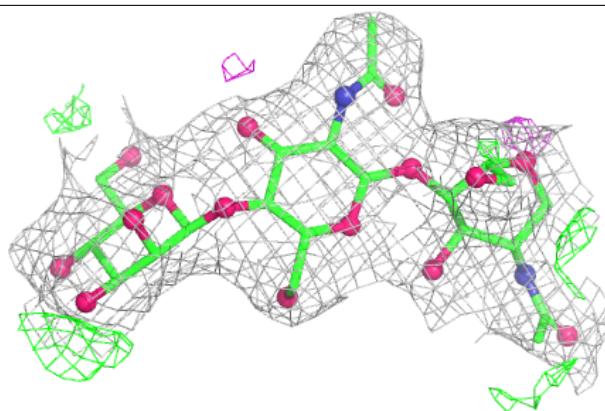
Electron density around Chain L:

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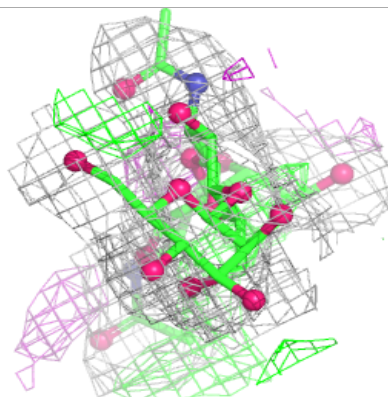
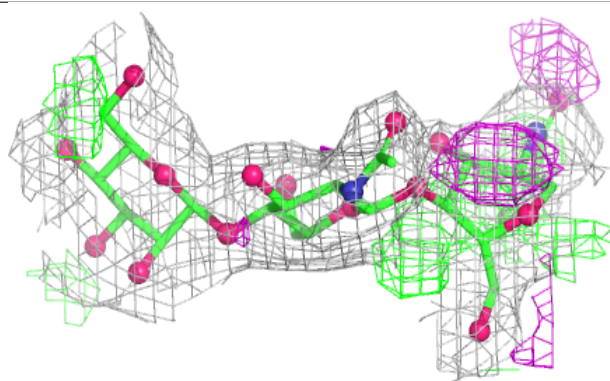
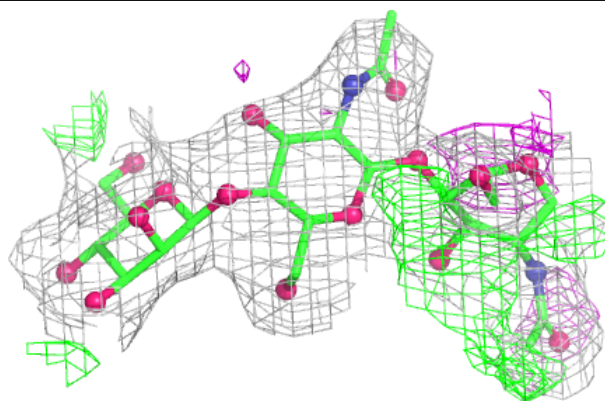


Electron density around Chain M:

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and green (positive)

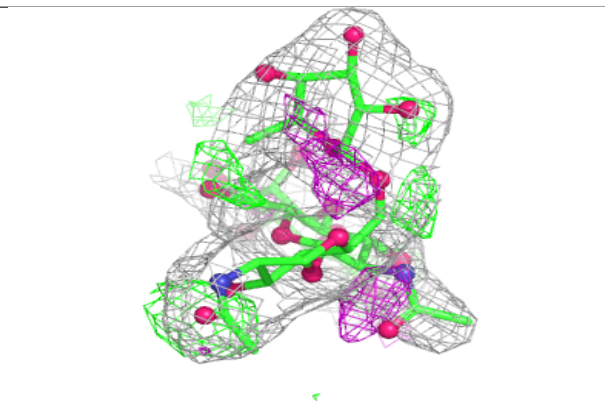
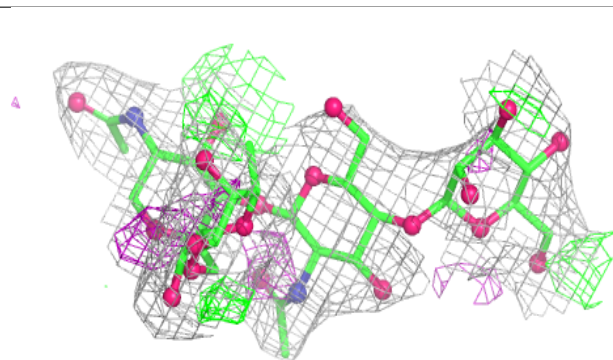
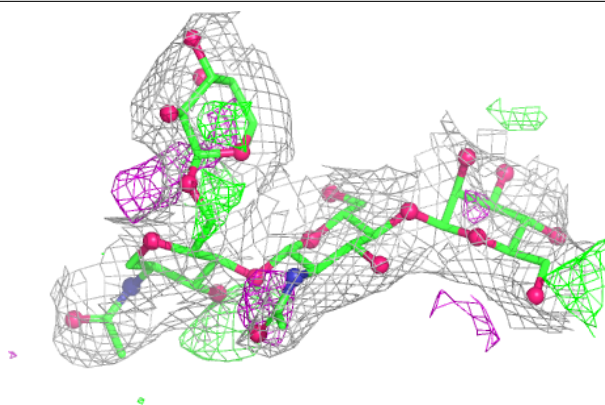
**Electron density around Chain N:**

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and green (positive)

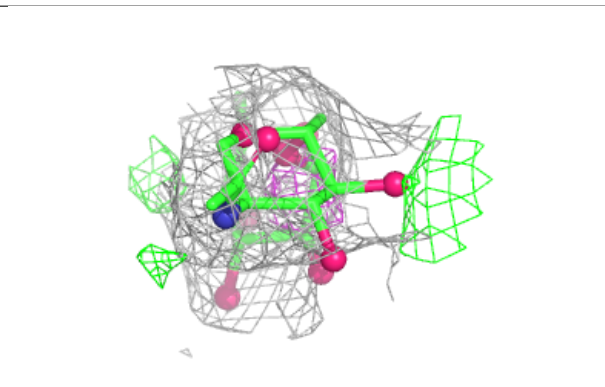
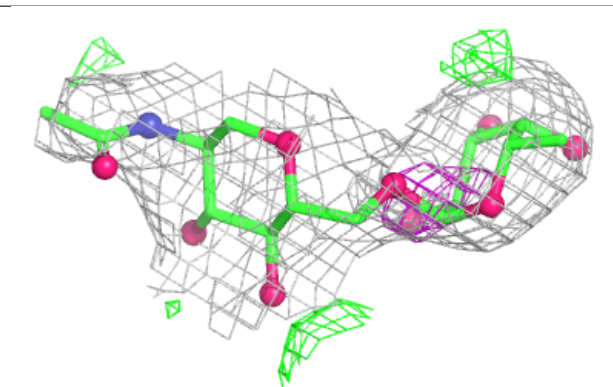
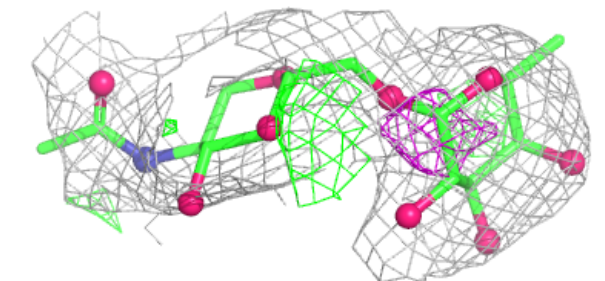


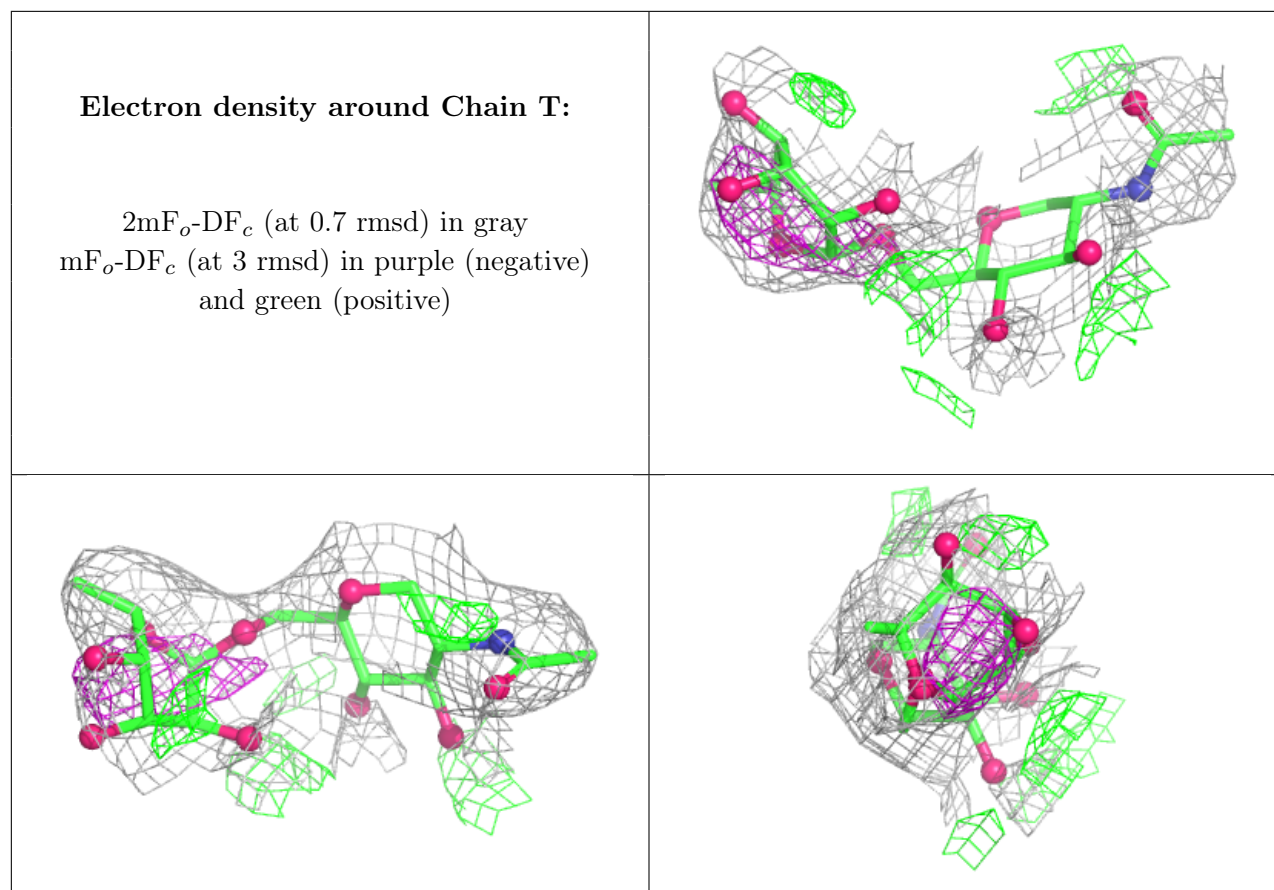
Electron density around Chain O:

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

**Electron density around Chain S:**

$2mF_o-DF_c$ (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.

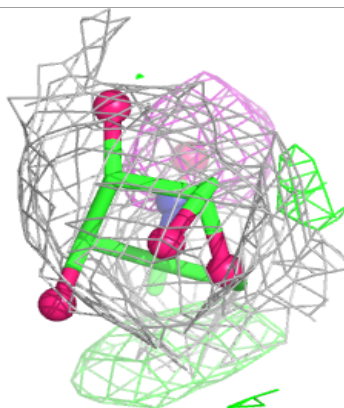
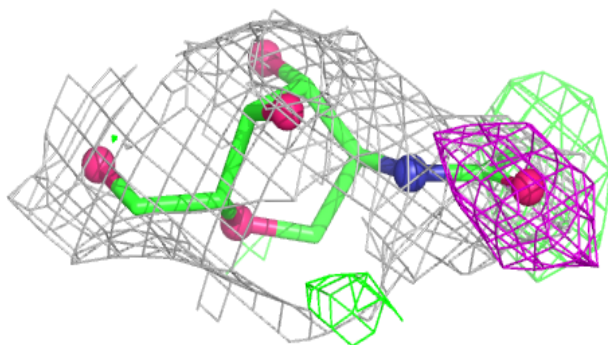
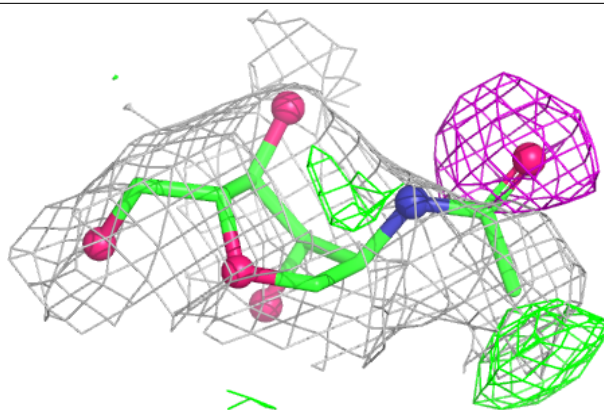
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	NAG	D	1402	14/15	0.50	0.24	55,58,61,64	0
10	NAG	D	1403	14/15	0.52	0.22	54,57,60,61	0
10	NAG	D	1404	14/15	0.52	0.26	82,85,88,89	0
10	NAG	A	1603	14/15	0.54	0.23	68,71,74,76	0
10	NAG	A	1602	14/15	0.59	0.21	60,63,67,68	0
10	NAG	D	1405	14/15	0.67	0.17	56,58,59,61	0
10	NAG	D	1401	14/15	0.69	0.21	35,37,40,42	0
10	NAG	D	1406	14/15	0.76	0.17	53,55,57,59	0
10	NAG	A	1601	14/15	0.77	0.17	61,63,66,66	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

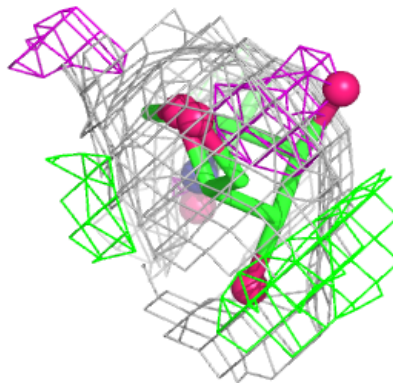
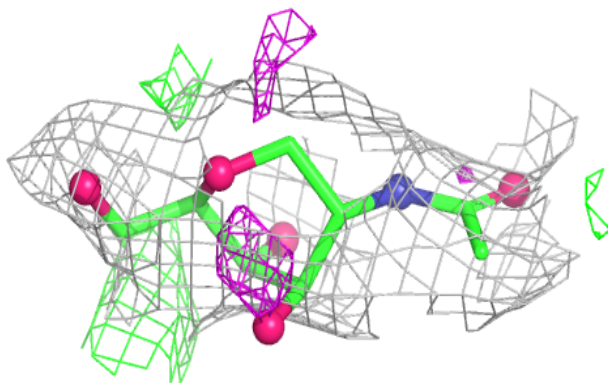
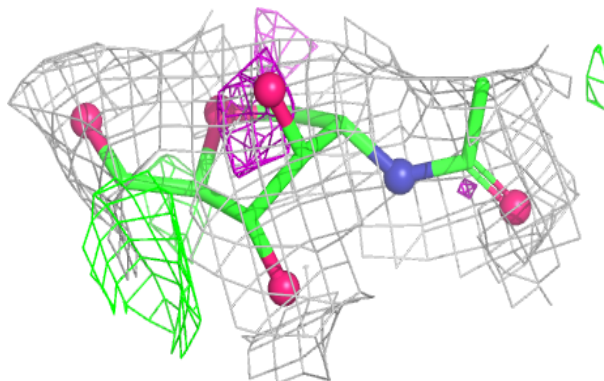
Electron density around NAG D 1402:

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



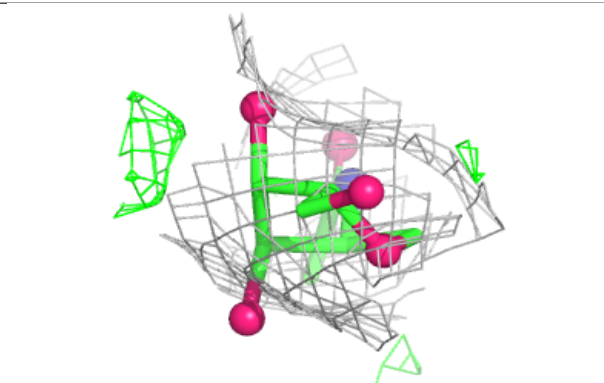
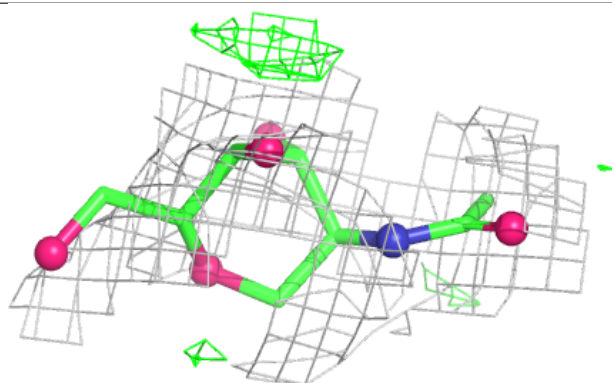
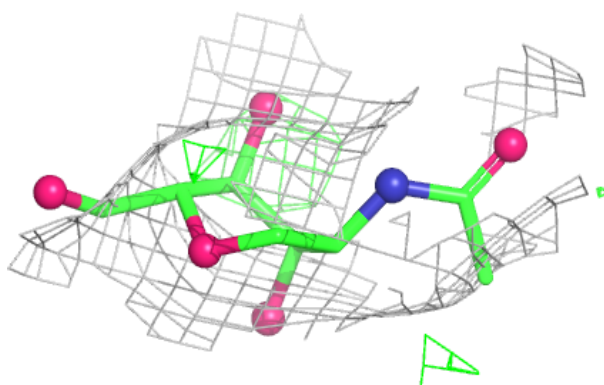
Electron density around NAG D 1403:

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

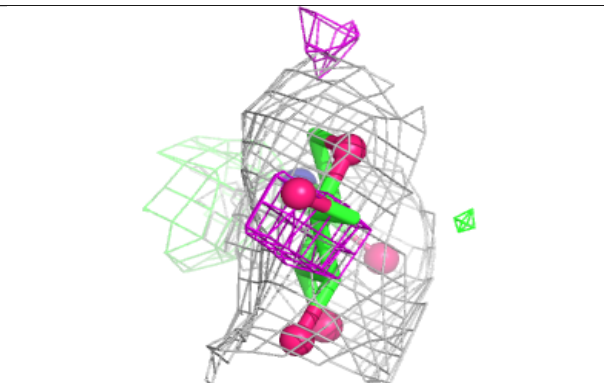
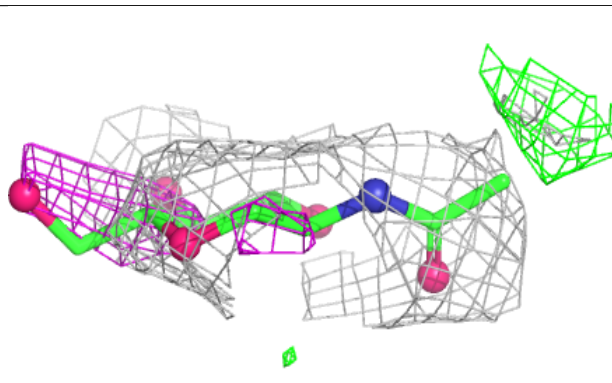
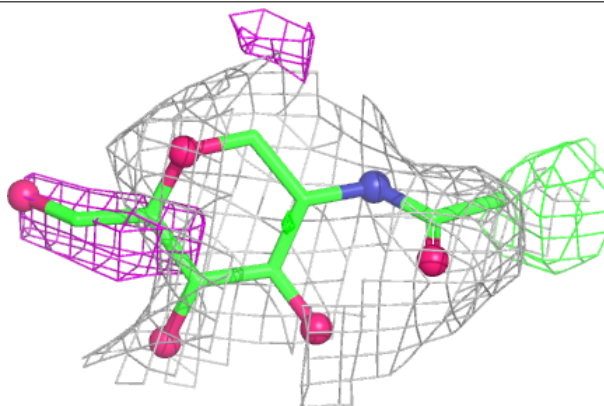


Electron density around NAG D 1404:

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

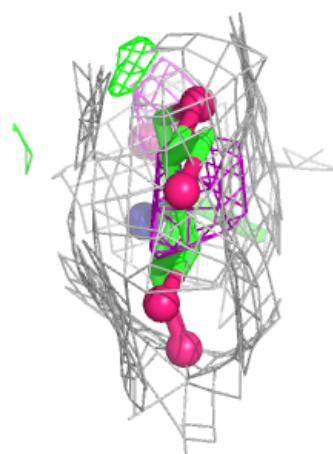
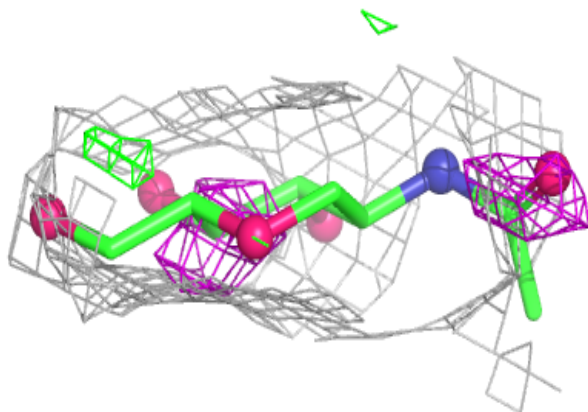
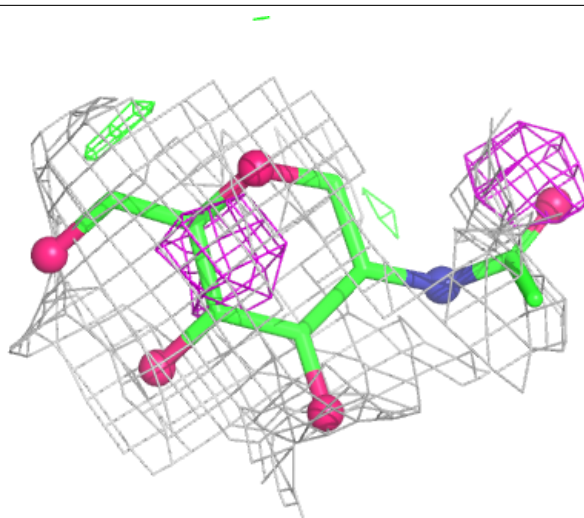
**Electron density around NAG A 1603:**

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



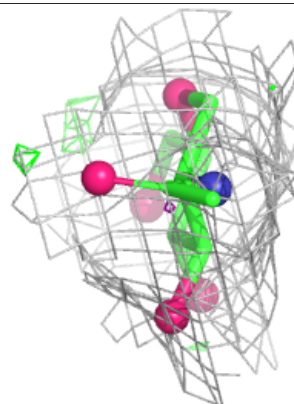
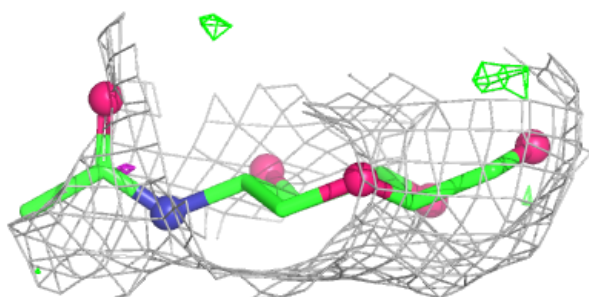
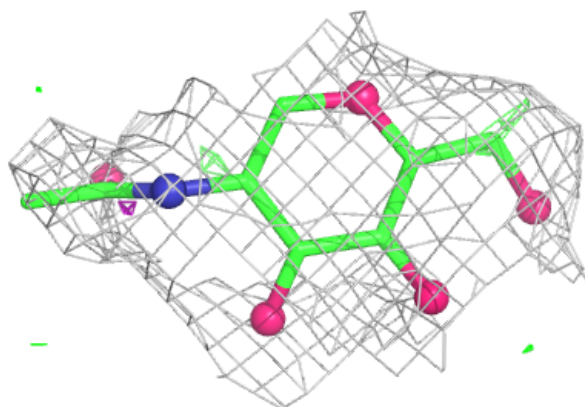
Electron density around NAG A 1602:

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

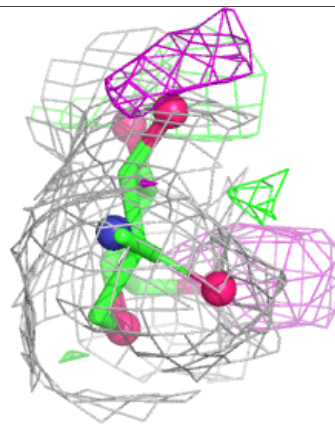
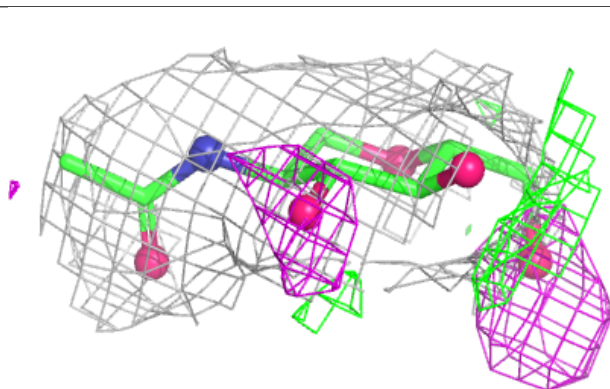
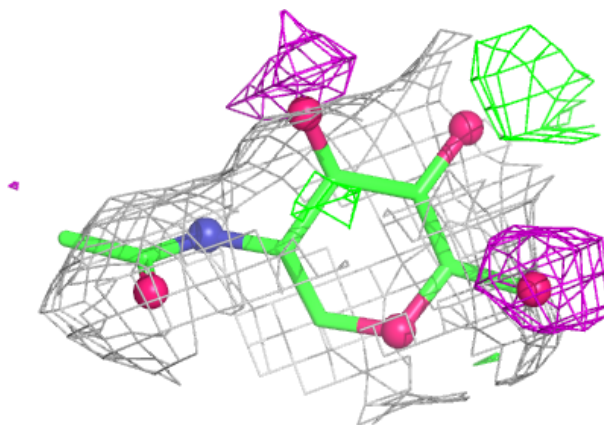


Electron density around NAG D 1405:

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

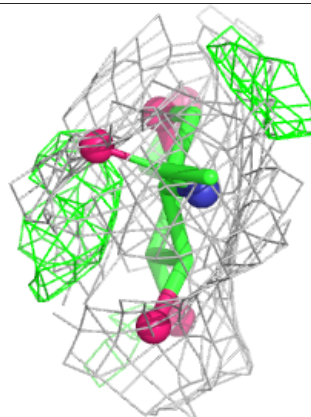
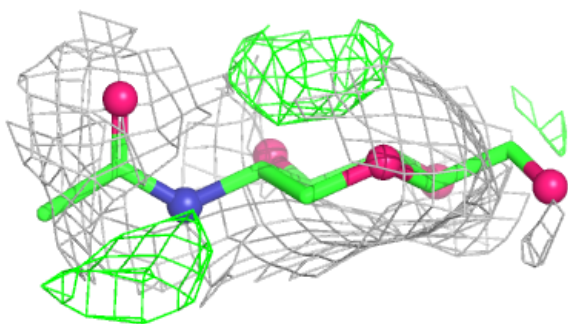
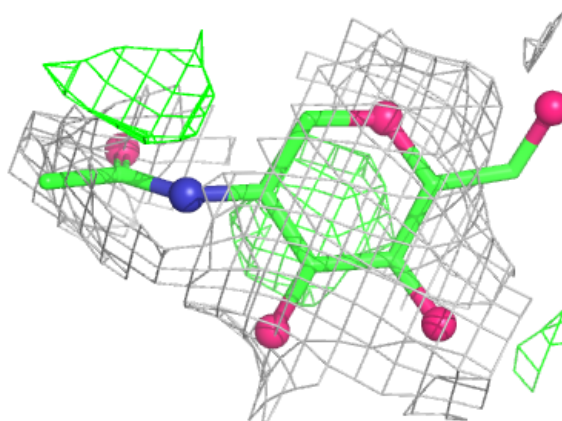
**Electron density around NAG D 1401:**

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



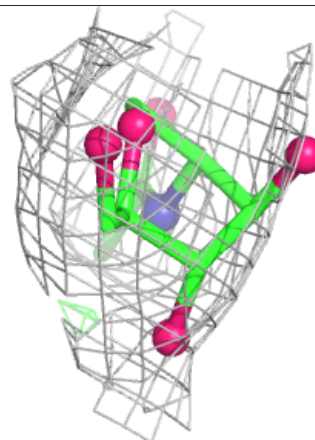
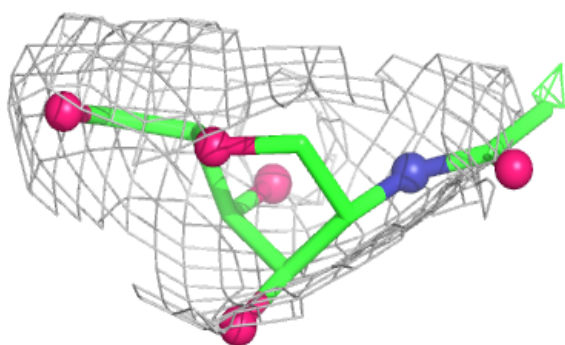
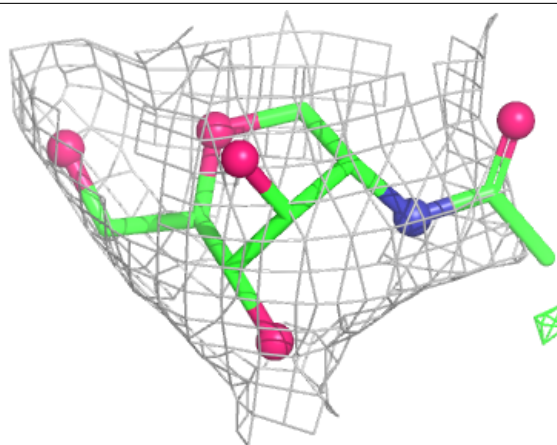
Electron density around NAG D 1406:

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



Electron density around NAG A 1601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.