



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2024 – 04:22 PM JST

PDB ID : 8WEC  
Title : Crystal structure of Arabidopsis thaliana MIK2 ectodomain in complex with BAK1 ectodomain and SCOOP12  
Authors : Wan, L.H.; Hu, Y.X.; Wu, H.M.  
Deposited on : 2023-09-17  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

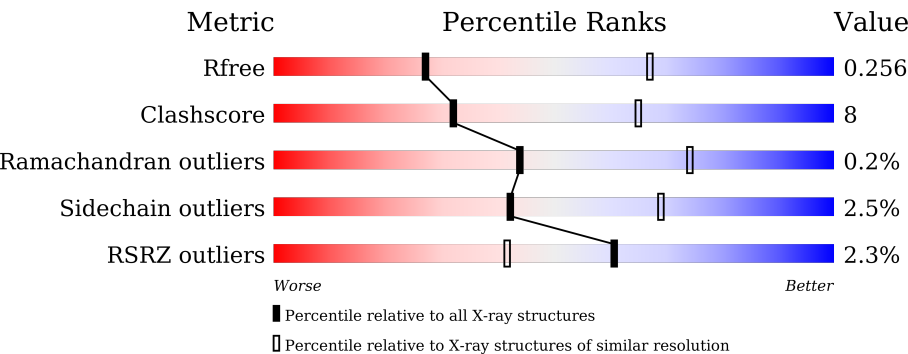
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

# 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 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div><div>%</div><div><div></div><div>78%</div><div>14%</div><div>•</div><div>7%</div></div></div>
1	D	683	<div><div></div><div>80%</div><div>13%</div><div>7%</div></div>
2	B	230	<div><div>7%</div><div><div></div><div>53%</div><div>22%</div><div>24%</div></div></div>
2	E	230	<div><div>4%</div><div><div></div><div>47%</div><div>27%</div><div>•</div><div>24%</div></div></div>
3	C	13	<div><div></div><div>92%</div><div>8%</div></div>
3	F	13	<div><div></div><div>77%</div><div>15%</div><div>8%</div></div>

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Mol	Chain	Length	Quality of chain
4	G	2	100%
4	I	2	50% 50%
4	J	2	100%
4	K	2	100%
4	L	2	50% 50%
4	Q	2	100%
4	R	2	50% 50%
4	S	2	50% 50%
4	W	2	50% 50%
5	H	4	50% 50%
6	M	3	33% 67%
6	O	3	67% 33%
7	N	3	67% 33%
7	T	3	100%
8	P	2	50% 50%
9	U	2	100%
9	V	2	50% 50%

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13386 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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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 SERINE-RICH ENDOGENOUS PEPTIDE (SCOOP).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			91	51	21	19			
3	F	13	Total	C	N	O	0	0	0
			91	51	21	19			

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



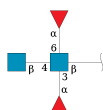
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			27	16	2	9			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

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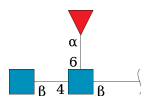
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	W	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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.



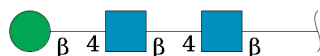
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	4	Total	C	N	O	0	0	0
			48	28	2	18			

- 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	M	3	Total	C	N	O	0	0	0
			38	22	2	14			
6	O	3	Total	C	N	O	0	0	0
			37	22	2	13			

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

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranoside.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	P	2	Total	C	O		0	0	0
			23	12	11				

- 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	U	2	Total	C	N	O	0	0	0
			24	14	1	9			
9	V	2	Total	C	N	O	0	0	0
			24	14	1	9			

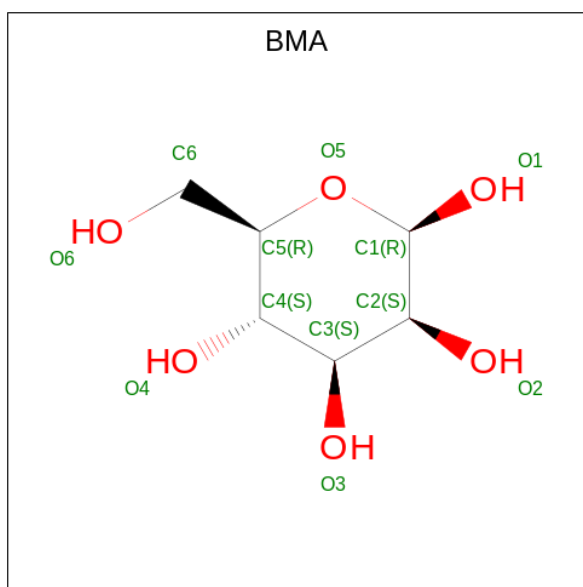
- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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		

- Molecule 11 is beta-D-mannopyranose (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ) (labeled as "Ligand of Interest" by depositor).



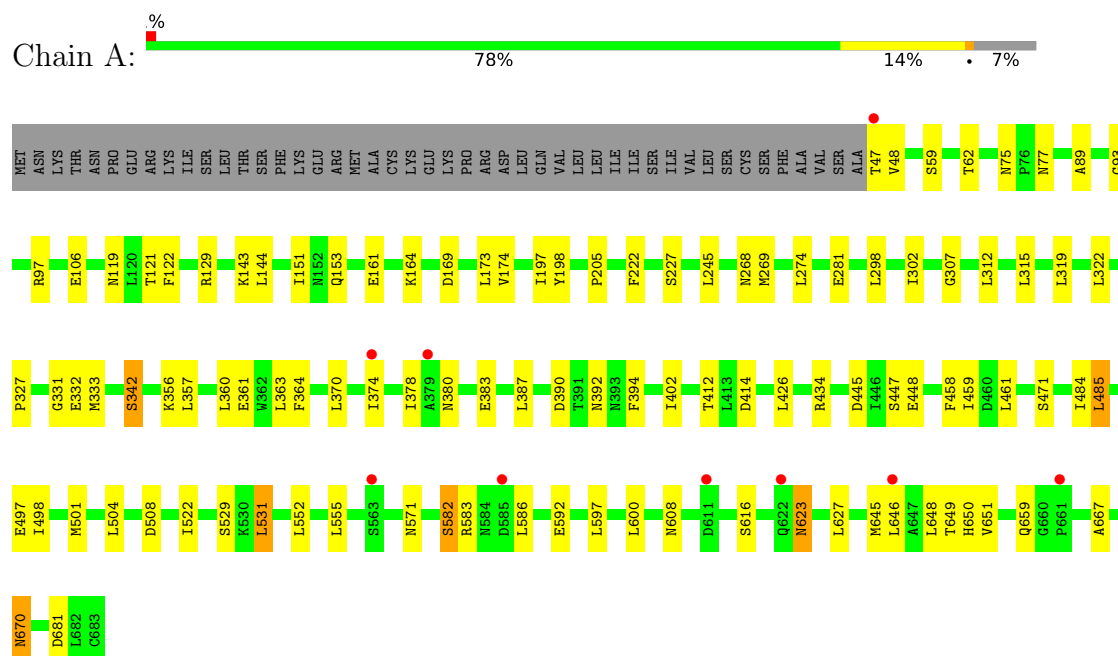


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			12	6	6		

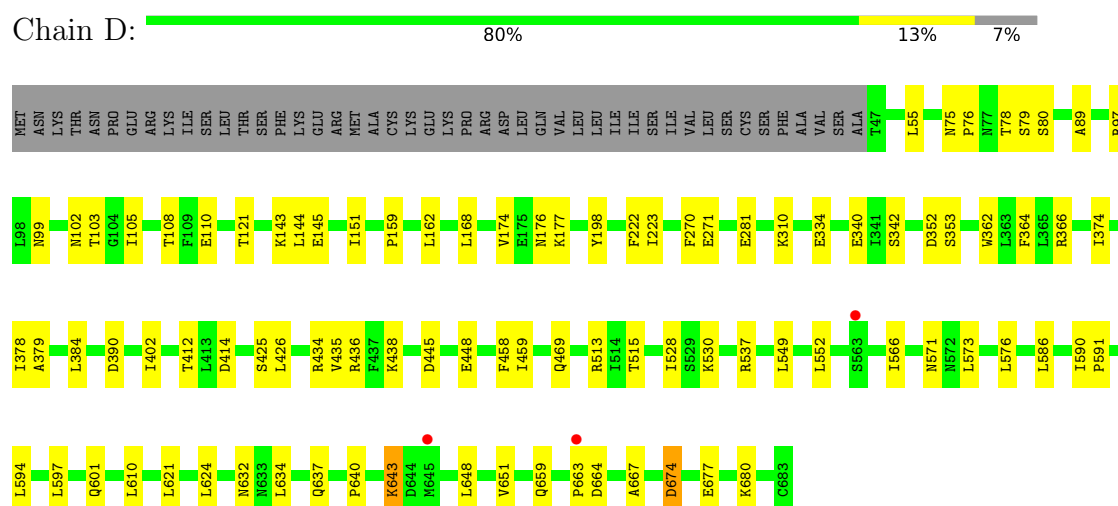
### 3 Residue-property plots [i](#)

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

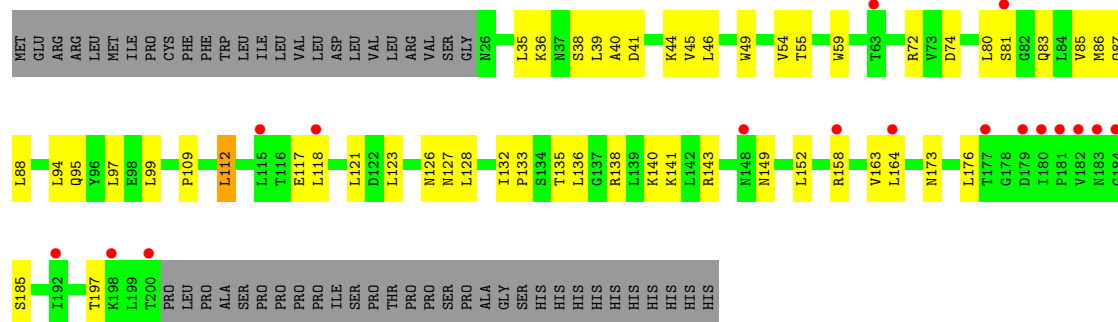
- Molecule 1: MDIS1-interacting receptor like kinase 2



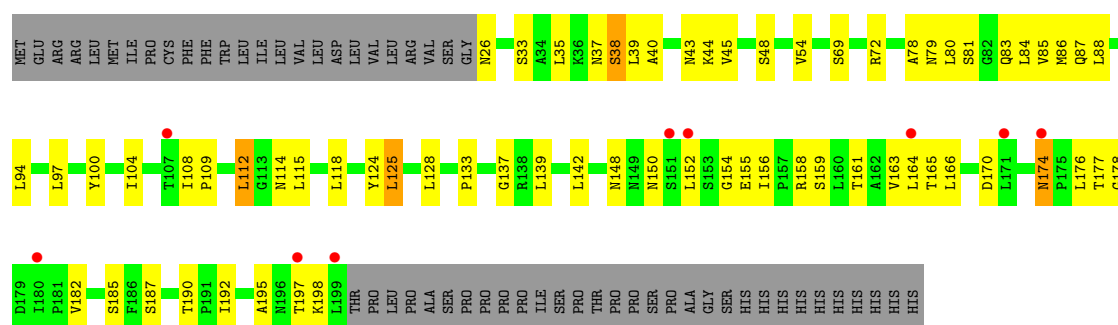
- Molecule 1: MDIS1-interacting receptor like kinase 2



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



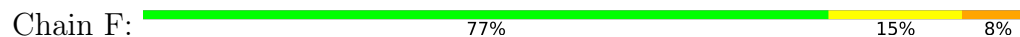
- Molecule 2: BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1



- Molecule 3: SERINE-RICH ENDOGENOUS PEPTIDE (SCOOP)



- Molecule 3: SERINE-RICH ENDOGENOUS PEPTIDE (SCOOP)



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



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

Chain I:  50% 50%

MAG1  
MAG2

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

Chain J:  100%

MAG1  
MAG2

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

Chain K:  100%

MAG1  
MAG2

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

Chain L:  50% 50%

MAG1  
MAG2

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

Chain Q:  100%

MAG1  
MAG2

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

Chain R:  50% 50%

MAG1  
MAG2

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

Chain S:  50% 50%



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

Chain W:



- Molecule 5: 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 H:



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

Chain M:



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

Chain O:



- 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:



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

Chain T:



- Molecule 8: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose

Chain P:  50% 50%

BM1  
MAN2

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

Chain U:  100%

MAG1  
FUC2

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

Chain V:  50% 50%

MAG1  
FUC2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.00Å 178.69Å 144.16Å 90.00° 90.79° 90.00°	Depositor
Resolution (Å)	46.15 – 3.10 46.15 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.15-3.10) 99.7 (46.15-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.245 , 0.256 0.244 , 0.256	Depositor DCC
$R_{free}$ test set	3314 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.6	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13386	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, FUC, 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	0.28	0/5052	0.53	0/6875
1	D	0.29	0/5052	0.51	0/6875
2	B	0.30	0/1354	0.66	0/1852
2	E	0.35	0/1347	0.60	0/1842
3	C	0.26	0/91	0.57	0/119
3	F	0.27	0/91	0.58	0/119
All	All	0.29	0/12987	0.55	0/17682

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	71	0
1	D	4950	0	4905	57	0
2	B	1332	0	1346	33	0
2	E	1325	0	1339	47	0
3	C	91	0	91	1	0
3	F	91	0	91	3	0
4	G	27	0	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	2	0
4	L	28	0	25	1	0
4	Q	28	0	25	0	0
4	R	28	0	25	1	0
4	S	28	0	25	0	0
4	W	28	0	25	0	0
5	H	48	0	43	0	0
6	M	38	0	34	1	0
6	O	37	0	32	3	0
7	N	39	0	34	1	0
7	T	39	0	34	0	0
8	P	23	0	20	2	0
9	U	24	0	22	0	0
9	V	24	0	22	0	0
10	A	42	0	39	0	0
10	D	70	0	65	0	0
11	B	12	0	11	0	0
All	All	13386	0	13260	210	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 8.

All (210) 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)
6:O:2:NAG:C4	8:P:1:BMA:O1	1.66	1.42
2:E:35:LEU:HD12	2:E:88:LEU:HD21	1.49	0.94
1:A:62:THR:OG1	1:A:106:GLU:OE1	1.87	0.91
2:B:118:LEU:HD11	2:B:121:LEU:HD23	1.57	0.86
2:B:94:LEU:HD21	2:B:97:LEU:HD12	1.58	0.85
2:E:85:VAL:HG12	2:E:87:GLN:H	1.42	0.83
1:D:621:LEU:HD23	1:D:624:LEU:HD12	1.59	0.83
1:A:597:LEU:HB2	1:A:600:LEU:HD11	1.62	0.79
2:E:94:LEU:HD21	2:E:97:LEU:HD13	1.65	0.77
1:A:121:THR:HA	1:A:144:LEU:HA	1.69	0.74
2:B:54:VAL:HG12	2:B:55:THR:HG23	1.69	0.73
2:E:124:TYR:CD1	2:E:125:LEU:HD12	2.24	0.72
1:A:97:ARG:HG3	1:A:122:PHE:HB3	1.72	0.71
2:E:39:LEU:HB3	2:E:80:LEU:HD12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:GLU:OE1	1:D:281:GLU:N	2.16	0.71
2:E:142:LEU:HD23	2:E:166:LEU:HD21	1.72	0.71
1:D:643:LYS:HE3	1:D:664:ASP:H	1.57	0.68
1:A:597:LEU:HB2	1:A:600:LEU:CD1	2.23	0.68
1:A:312:LEU:HD21	1:A:315:LEU:HD13	1.78	0.64
1:A:586:LEU:HD13	1:A:608:ASN:HD21	1.63	0.64
2:E:38:SER:OG	2:E:83:GLN:O	2.15	0.64
1:D:340:GLU:OE2	3:F:9:GLN:HG2	1.98	0.63
1:D:390:ASP:HB3	1:D:412:THR:HG22	1.80	0.63
2:B:87:GLN:OE1	2:B:87:GLN:N	2.33	0.62
1:D:270:PHE:HD1	1:D:271:GLU:HG3	1.65	0.61
2:B:95:GLN:HG2	2:B:117:GLU:OE1	2.00	0.61
2:E:163:VAL:HG11	2:E:166:LEU:HD23	1.82	0.61
1:A:552:LEU:HD21	1:A:555:LEU:HG	1.82	0.61
2:B:35:LEU:HD12	2:B:88:LEU:HD21	1.83	0.59
2:B:97:LEU:HD21	2:B:99:LEU:HD12	1.84	0.59
6:O:2:NAG:C4	8:P:1:BMA:C1	2.76	0.59
2:B:40:ALA:N	2:B:81:SER:O	2.34	0.58
1:A:586:LEU:HD12	1:A:586:LEU:H	1.68	0.57
2:B:140:LYS:HB2	2:B:141:LYS:HE2	1.86	0.57
2:E:33:SER:O	2:E:37:ASN:ND2	2.35	0.57
1:D:99:ASN:HD22	4:R:1:NAG:H83	1.70	0.57
2:E:108:ILE:HD11	2:E:128:LEU:HD13	1.87	0.56
2:B:132:ILE:HD11	2:B:152:LEU:HD23	1.88	0.56
1:A:281:GLU:OE1	1:A:281:GLU:N	2.26	0.56
1:A:307:GLY:HA2	1:A:333:MET:HG2	1.88	0.55
2:B:109:PRO:O	2:B:112:LEU:HD12	2.06	0.55
1:D:586:LEU:HD12	1:D:586:LEU:H	1.71	0.55
1:A:582:SER:OG	1:A:583:ARG:NH1	2.38	0.55
1:D:362:TRP:HE1	7:N:1:NAG:H81	1.72	0.55
1:A:342:SER:OG	1:A:364:PHE:HB3	2.07	0.54
2:E:137:GLY:HA3	2:E:159:SER:HB2	1.89	0.54
2:B:140:LYS:HA	2:B:163:VAL:HG23	1.90	0.54
1:A:501:MET:HE2	1:A:504:LEU:HD13	1.90	0.54
2:B:121:LEU:HD12	2:B:123:LEU:HD21	1.90	0.53
1:A:586:LEU:HD13	1:A:608:ASN:ND2	2.24	0.53
2:E:118:LEU:HD23	2:E:139:LEU:HD13	1.89	0.53
2:E:45:VAL:HG21	2:E:78:ALA:HB1	1.90	0.53
1:D:571:ASN:HA	1:D:597:LEU:HD21	1.90	0.52
6:O:1:NAG:H3	6:O:1:NAG:H83	1.91	0.52
1:A:651:VAL:HG23	1:A:667:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:MET:HE2	1:A:648:LEU:HD22	1.91	0.51
2:B:141:LYS:HE2	2:B:141:LYS:N	2.25	0.51
1:D:108:THR:HG22	1:D:110:GLU:H	1.76	0.51
1:D:121:THR:HA	1:D:144:LEU:HA	1.93	0.51
2:E:124:TYR:HD1	2:E:125:LEU:HD12	1.75	0.51
1:D:103:THR:HB	1:D:105:ILE:HG13	1.93	0.51
1:A:370:LEU:HB2	1:A:394:PHE:CE1	2.46	0.51
1:A:649:THR:HG21	2:B:143:ARG:HH12	1.75	0.50
2:B:126:ASN:HB3	2:B:128:LEU:HD13	1.93	0.50
2:E:152:LEU:HB2	2:E:174:ASN:HD22	1.76	0.50
1:A:582:SER:HG	1:A:583:ARG:HH11	1.58	0.50
2:E:154:GLY:O	2:E:177:THR:N	2.43	0.50
1:D:174:VAL:HG11	1:D:198:TYR:CZ	2.47	0.50
1:D:390:ASP:OD2	3:F:13:ARG:HD2	2.12	0.50
2:E:148:ASN:ND2	2:E:170:ASP:OD2	2.45	0.50
1:A:274:LEU:HB3	1:A:298:LEU:HD21	1.93	0.49
1:A:374:ILE:HD12	1:A:378:ILE:HD12	1.94	0.49
2:E:177:THR:C	2:E:198:LYS:HD2	2.34	0.49
2:B:127:ASN:OD1	2:B:127:ASN:O	2.31	0.48
1:D:222:PHE:HD2	1:D:223:ILE:HG13	1.78	0.48
1:D:342:SER:OG	1:D:364:PHE:HB3	2.12	0.48
1:D:515:THR:HG22	1:D:537:ARG:HB2	1.95	0.48
1:D:674:ASP:HA	1:D:677:GLU:HG3	1.95	0.48
1:A:529:SER:HA	1:A:552:LEU:HA	1.95	0.48
1:A:659:GLN:HB2	1:A:681:ASP:HB3	1.95	0.48
1:A:47:THR:OG1	1:A:48:VAL:N	2.43	0.48
2:B:118:LEU:HD11	2:B:121:LEU:CD2	2.35	0.48
1:D:648:LEU:HD21	1:D:651:VAL:HG22	1.95	0.48
2:B:41:ASP:OD1	2:B:44:LYS:N	2.47	0.48
2:B:45:VAL:HG12	2:B:46:LEU:HD23	1.95	0.48
1:A:434:ARG:HG2	1:A:458:PHE:HB3	1.95	0.48
1:A:571:ASN:HA	1:A:597:LEU:HD21	1.95	0.48
1:A:649:THR:HG1	1:A:650:HIS:CE1	2.26	0.48
2:B:38:SER:OG	2:B:83:GLN:O	2.27	0.48
2:E:100:TYR:HB2	2:E:124:TYR:CE1	2.49	0.48
1:D:78:THR:HG22	1:D:79:SER:H	1.79	0.47
1:A:445:ASP:HB3	1:A:448:GLU:HB2	1.95	0.47
2:E:158:ARG:O	2:E:161:THR:OG1	2.29	0.47
1:A:75:ASN:HD21	1:A:77:ASN:HB2	1.78	0.47
1:D:374:ILE:HD12	1:D:378:ILE:HD12	1.96	0.47
1:D:159:PRO:HG2	1:D:162:LEU:HG	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:43:ASN:OD1	2:E:79:ASN:ND2	2.47	0.47
2:B:36:LYS:NZ	2:B:46:LEU:O	2.48	0.47
1:D:121:THR:HG22	1:D:143:LYS:HB3	1.96	0.47
1:D:414:ASP:OD1	1:D:436:ARG:HB3	2.14	0.47
2:B:140:LYS:HB2	2:B:141:LYS:CE	2.44	0.47
1:D:89:ALA:HB3	1:D:97:ARG:HB3	1.97	0.47
1:D:640:PRO:O	1:D:643:LYS:HD2	2.15	0.47
1:A:302:ILE:HG22	1:A:327:PRO:HG2	1.98	0.46
1:D:643:LYS:HE3	1:D:663:PRO:HA	1.96	0.46
2:E:40:ALA:N	2:E:81:SER:O	2.41	0.46
2:B:176:LEU:HD23	2:B:197:THR:CG2	2.46	0.46
1:A:322:LEU:HD12	1:A:322:LEU:H	1.81	0.46
2:B:163:VAL:O	2:B:164:LEU:HG	2.15	0.46
2:E:35:LEU:CD2	2:E:39:LEU:HD22	2.45	0.46
2:E:108:ILE:HG22	2:E:133:PRO:HG2	1.98	0.46
1:A:374:ILE:HD13	1:A:374:ILE:HA	1.82	0.46
1:A:531:LEU:HB3	1:A:555:LEU:HD23	1.97	0.46
1:A:161:GLU:O	1:A:164:LYS:HG2	2.15	0.46
1:D:145:GLU:HA	1:D:168:LEU:HA	1.98	0.46
1:A:174:VAL:HG11	1:A:198:TYR:CZ	2.51	0.46
2:E:190:THR:OG1	2:E:192:ILE:HG22	2.15	0.46
1:D:637:GLN:HA	1:D:659:GLN:O	2.16	0.45
4:L:1:NAG:H3	4:L:1:NAG:H83	1.99	0.45
2:E:182:VAL:HG13	2:E:187:SER:HA	1.98	0.45
1:A:447:SER:HB2	1:A:471:SER:HB2	1.98	0.45
1:A:498:ILE:O	1:A:501:MET:HG3	2.16	0.45
1:D:379:ALA:HA	1:D:384:LEU:HD22	1.98	0.45
1:D:640:PRO:HA	1:D:643:LYS:NZ	2.31	0.45
1:A:89:ALA:HB3	1:A:97:ARG:HB3	1.99	0.45
2:B:176:LEU:HD23	2:B:197:THR:HG23	1.97	0.45
1:D:648:LEU:HD22	1:D:667:ALA:CB	2.47	0.45
1:A:623:ASN:OD1	1:A:623:ASN:N	2.50	0.45
1:D:374:ILE:HG23	1:D:378:ILE:HD12	1.99	0.45
1:A:484:ILE:HG23	1:A:508:ASP:HB3	1.99	0.44
1:A:173:LEU:HB2	1:A:197:ILE:HG23	1.99	0.44
1:A:360:LEU:HD21	1:A:363:LEU:HB2	1.99	0.44
1:A:370:LEU:HB2	1:A:394:PHE:CZ	2.52	0.44
1:D:643:LYS:HE3	1:D:664:ASP:N	2.29	0.44
2:E:100:TYR:HB2	2:E:124:TYR:CD1	2.53	0.44
1:D:435:VAL:HB	1:D:459:ILE:HD12	1.99	0.44
2:B:49:TRP:HA	2:B:59:TRP:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ASN:OD1	1:D:80:SER:HB3	2.18	0.44
1:A:361:GLU:HG2	1:A:383:GLU:HB3	2.00	0.44
2:E:88:LEU:O	2:E:115:LEU:HD21	2.17	0.44
1:D:310:LYS:HD2	1:D:334:GLU:HG3	2.00	0.43
1:D:566:ILE:HG12	1:D:586:LEU:HD23	2.00	0.43
2:B:39:LEU:HD13	2:B:80:LEU:HB3	2.00	0.43
2:B:72:ARG:HD3	2:B:74:ASP:OD2	2.17	0.43
1:A:459:ILE:HD11	1:A:461:LEU:HD21	2.00	0.43
2:E:154:GLY:N	2:E:176:LEU:HD12	2.33	0.43
1:A:319:LEU:HD23	1:A:319:LEU:HA	1.78	0.43
1:D:445:ASP:HB3	1:D:448:GLU:HB2	2.00	0.43
2:E:163:VAL:O	2:E:164:LEU:HG	2.19	0.43
2:E:174:ASN:OD1	2:E:174:ASN:N	2.50	0.43
2:E:78:ALA:HB3	2:E:80:LEU:HD23	2.01	0.43
2:E:114:ASN:HD22	2:E:114:ASN:N	2.17	0.43
2:E:109:PRO:HG2	2:E:112:LEU:HD13	1.99	0.43
2:E:182:VAL:HG12	2:E:182:VAL:O	2.19	0.43
1:A:122:PHE:CZ	4:K:1:NAG:H82	2.53	0.43
1:A:649:THR:OG1	1:A:650:HIS:ND1	2.34	0.43
2:E:44:LYS:HA	2:E:44:LYS:HD2	1.75	0.43
1:D:390:ASP:HB2	1:D:414:ASP:HB2	1.99	0.43
1:A:392:ASN:HB3	1:A:394:PHE:CD1	2.53	0.42
1:A:119:ASN:OD1	1:A:143:LYS:NZ	2.42	0.42
1:A:390:ASP:HB2	1:A:414:ASP:HB2	2.00	0.42
1:A:645:MET:CE	1:A:648:LEU:HD22	2.49	0.42
1:D:640:PRO:HA	1:D:643:LYS:HZ2	1.84	0.42
2:E:84:LEU:HD12	2:E:104:ILE:HG21	2.02	0.42
1:A:402:ILE:HG21	1:A:426:LEU:HB2	2.01	0.42
1:A:646:LEU:H	1:A:646:LEU:HD12	1.85	0.42
2:B:135:THR:O	2:B:138:ARG:HG3	2.19	0.42
2:E:176:LEU:C	2:E:198:LYS:HG2	2.39	0.42
1:A:245:LEU:HB2	1:A:269:MET:HG2	2.02	0.42
1:A:315:LEU:HD22	1:A:333:MET:HE1	2.01	0.42
2:E:198:LYS:HB2	2:E:198:LYS:NZ	2.34	0.42
1:D:591:PRO:HG2	1:D:594:LEU:HD13	2.02	0.42
2:E:26:ASN:N	2:E:54:VAL:O	2.53	0.42
2:E:35:LEU:HD21	2:E:39:LEU:HD22	2.02	0.42
1:A:331:GLY:HA2	1:A:357:LEU:HD21	2.02	0.41
1:A:332:GLU:OE2	1:A:356:LYS:NZ	2.53	0.41
2:B:149:ASN:HA	2:B:173:ASN:HB3	2.01	0.41
1:D:573:LEU:HD12	1:D:576:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:155:GLU:OE2	2:E:178:GLY:HA3	2.20	0.41
2:E:195:ALA:O	2:E:197:THR:HG23	2.20	0.41
1:D:176:ASN:O	1:D:177:LYS:HD3	2.20	0.41
1:A:205:PRO:HA	1:A:227:SER:O	2.20	0.41
1:A:497:GLU:HG3	6:M:1:NAG:H81	2.03	0.41
2:B:133:PRO:O	2:B:136:LEU:HG	2.21	0.41
1:D:75:ASN:HA	1:D:76:PRO:HD3	1.89	0.41
2:E:142:LEU:O	2:E:165:THR:HB	2.21	0.41
2:E:150:ASN:HB3	2:E:152:LEU:HD13	2.03	0.41
1:A:47:THR:HG22	1:A:93:GLY:O	2.20	0.41
2:E:156:ILE:CD1	2:E:198:LYS:HE3	2.51	0.41
1:A:122:PHE:CE2	4:K:1:NAG:H82	2.56	0.41
1:A:129:ARG:CZ	1:A:153:GLN:HE22	2.34	0.41
1:A:461:LEU:HD12	1:A:485:LEU:HG	2.02	0.41
2:B:85:VAL:HG13	2:B:87:GLN:OE1	2.20	0.41
1:D:412:THR:HG21	3:F:13:ARG:HB3	2.02	0.41
1:A:268:ASN:ND2	3:C:5:SER:O	2.54	0.41
1:A:390:ASP:HB3	1:A:412:THR:HG22	2.03	0.41
1:A:522:ILE:HD12	1:A:522:ILE:HA	1.88	0.41
1:D:549:LEU:O	1:D:552:LEU:HB2	2.21	0.41
1:D:610:LEU:HD12	1:D:632:ASN:OD1	2.20	0.41
1:A:390:ASP:HB3	1:A:412:THR:CG2	2.51	0.40
1:D:402:ILE:HG21	1:D:426:LEU:HB2	2.03	0.40
1:D:601:GLN:OE1	2:E:72:ARG:NH1	2.45	0.40
1:D:55:LEU:HD12	1:D:55:LEU:HA	1.92	0.40
1:D:414:ASP:HA	1:D:438:LYS:O	2.21	0.40
1:D:528:ILE:HD11	1:D:530:LYS:O	2.21	0.40
1:A:333:MET:HB3	1:A:333:MET:HE3	2.00	0.40
1:A:670:ASN:OD1	1:A:670:ASN:N	2.54	0.40
1:D:177:LYS:HD3	1:D:177:LYS:HA	1.78	0.40
1:D:434:ARG:HG2	1:D:458:PHE:HB3	2.04	0.40
1:D:590:ILE:HD11	1:D:634:LEU:HD21	2.02	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	635/683 (93%)	628 (99%)	6 (1%)	1 (0%)	44	74
1	D	635/683 (93%)	629 (99%)	5 (1%)	1 (0%)	44	74
2	B	173/230 (75%)	169 (98%)	3 (2%)	1 (1%)	22	53
2	E	172/230 (75%)	168 (98%)	4 (2%)	0	100	100
3	C	11/13 (85%)	11 (100%)	0	0	100	100
3	F	11/13 (85%)	11 (100%)	0	0	100	100
All	All	1637/1852 (88%)	1616 (99%)	18 (1%)	3 (0%)	44	74

All (3) Ramachandran outliers are listed below:

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

### 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	576/619 (93%)	562 (98%)	14 (2%)	44	70
1	D	576/619 (93%)	566 (98%)	10 (2%)	56	78
2	B	156/207 (75%)	153 (98%)	3 (2%)	52	75
2	E	155/207 (75%)	147 (95%)	8 (5%)	19	48
3	C	10/10 (100%)	10 (100%)	0	100	100
3	F	10/10 (100%)	8 (80%)	2 (20%)	1	4
All	All	1483/1672 (89%)	1446 (98%)	37 (2%)	42	69

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	SER
1	A	169	ASP
1	A	222	PHE
1	A	342	SER
1	A	380	ASN
1	A	387	LEU
1	A	485	LEU
1	A	531	LEU
1	A	582	SER
1	A	592	GLU
1	A	616	SER
1	A	623	ASN
1	A	627	LEU
1	A	670	ASN
2	B	86	MET
2	B	112	LEU
2	B	158	ARG
1	D	102	ASN
1	D	352	ASP
1	D	353	SER
1	D	366	ARG
1	D	425	SER
1	D	469	GLN
1	D	513	ARG
1	D	643	LYS
1	D	674	ASP
1	D	680	LYS
2	E	38	SER
2	E	48	SER
2	E	69	SER
2	E	86	MET
2	E	112	LEU
2	E	125	LEU
2	E	174	ASN
2	E	185	SER
3	F	8	SER
3	F	9	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
2	B	37	ASN

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Mol	Chain	Res	Type
3	C	6	GLN
1	D	102	ASN
1	D	236	ASN
1	D	321	GLN
2	E	114	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

40 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	4,1	14,14,15	0.87	1 (7%)	17,19,21	1.52	1 (5%)
4	NAG	G	2	4	13,13,15	0.72	0	14,17,21	1.50	2 (14%)
5	NAG	H	1	5,1	14,14,15	0.20	0	17,19,21	1.00	1 (5%)
5	FUC	H	2	5	10,10,11	1.18	1 (10%)	14,14,16	1.35	3 (21%)
5	NAG	H	3	5	14,14,15	0.41	0	17,19,21	0.42	0
5	FUC	H	4	5	10,10,11	0.72	0	14,14,16	0.92	0
4	NAG	I	1	4,1	14,14,15	0.53	0	17,19,21	0.38	0
4	NAG	I	2	4	14,14,15	0.21	0	17,19,21	0.62	1 (5%)
4	NAG	J	1	4,1	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	J	2	4	14,14,15	0.26	0	17,19,21	0.40	0
4	NAG	K	1	4,1	14,14,15	0.20	0	17,19,21	0.65	0
4	NAG	K	2	4	14,14,15	0.34	0	17,19,21	0.85	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	L	1	4,1	14,14,15	0.79	1 (7%)	17,19,21	1.86	2 (11%)
4	NAG	L	2	4	14,14,15	0.44	0	17,19,21	0.36	0
6	NAG	M	1	6,1	14,14,15	0.34	0	17,19,21	0.52	0
6	NAG	M	2	6	14,14,15	0.35	0	17,19,21	0.59	0
6	FUC	M	3	6	10,10,11	1.14	1 (10%)	14,14,16	1.03	1 (7%)
7	NAG	N	1	7,1	14,14,15	0.56	0	17,19,21	1.48	1 (5%)
7	NAG	N	2	7	14,14,15	0.52	0	17,19,21	1.99	3 (17%)
7	BMA	N	3	7	11,11,12	0.72	0	15,15,17	1.18	1 (6%)
6	NAG	O	1	6,1	14,14,15	0.30	0	17,19,21	1.42	2 (11%)
6	NAG	O	2	6	13,13,15	0.27	0	14,17,21	0.40	0
6	FUC	O	3	6	10,10,11	0.96	1 (10%)	14,14,16	0.90	1 (7%)
8	BMA	P	1	8	12,12,12	0.49	0	17,17,17	1.01	1 (5%)
8	MAN	P	2	8	11,11,12	0.24	0	15,15,17	1.02	1 (6%)
4	NAG	Q	1	4,1	14,14,15	0.54	0	17,19,21	0.62	0
4	NAG	Q	2	4	14,14,15	0.42	0	17,19,21	0.61	0
4	NAG	R	1	4,1	14,14,15	0.30	0	17,19,21	0.47	0
4	NAG	R	2	4	14,14,15	0.24	0	17,19,21	0.57	0
4	NAG	S	1	4,1	14,14,15	0.51	0	17,19,21	0.50	0
4	NAG	S	2	4	14,14,15	0.26	0	17,19,21	1.17	2 (11%)
7	NAG	T	1	7,1	14,14,15	0.34	0	17,19,21	0.97	1 (5%)
7	NAG	T	2	7	14,14,15	0.58	0	17,19,21	1.08	1 (5%)
7	BMA	T	3	7	11,11,12	0.49	0	15,15,17	0.72	1 (6%)
9	NAG	U	1	9,1	14,14,15	0.23	0	17,19,21	0.97	1 (5%)
9	FUC	U	2	9	10,10,11	0.96	0	14,14,16	0.90	1 (7%)
9	NAG	V	1	9,1	14,14,15	0.42	0	17,19,21	0.51	0
9	FUC	V	2	9	10,10,11	1.21	1 (10%)	14,14,16	1.28	3 (21%)
4	NAG	W	1	4,1	14,14,15	0.35	0	17,19,21	0.54	0
4	NAG	W	2	4	14,14,15	0.45	0	17,19,21	1.23	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	4,1	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/19/26	0/1/1/1
5	NAG	H	1	5,1	-	2/6/23/26	0/1/1/1

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	NAG	O5-C1	3.12	1.48	1.43
5	H	2	FUC	C2-C3	2.79	1.56	1.52
4	L	1	NAG	O5-C1	2.63	1.47	1.43
9	V	2	FUC	C1-C2	2.36	1.57	1.52
6	O	3	FUC	C1-C2	2.12	1.57	1.52
6	M	3	FUC	C2-C3	2.03	1.55	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	C1-O5-C5	5.87	120.15	112.19
4	L	1	NAG	C1-O5-C5	5.59	119.76	112.19
7	N	2	NAG	C4-C3-C2	-5.24	103.34	111.02
7	N	1	NAG	C1-O5-C5	4.94	118.89	112.19
4	W	2	NAG	C1-O5-C5	4.48	118.26	112.19
6	O	1	NAG	C2-N2-C7	4.35	129.10	122.90
7	N	2	NAG	O5-C1-C2	-4.34	104.44	111.29
4	L	1	NAG	C2-N2-C7	4.32	129.05	122.90
4	S	2	NAG	C1-O5-C5	3.80	117.34	112.19
8	P	2	MAN	O5-C1-C2	-3.48	105.39	110.77
8	P	1	BMA	C1-O5-C5	-3.20	107.62	113.66
5	H	2	FUC	C1-C2-C3	3.10	113.47	109.67
5	H	1	NAG	O3-C3-C2	3.04	115.76	109.47
9	U	1	NAG	C1-O5-C5	2.79	115.97	112.19
4	G	2	NAG	O5-C5-C4	-2.71	106.27	110.65
9	V	2	FUC	C1-C2-C3	2.69	112.97	109.67
7	N	3	BMA	C1-C2-C3	-2.60	106.46	109.67
7	T	1	NAG	O5-C1-C2	-2.54	107.28	111.29
4	K	2	NAG	C1-O5-C5	2.48	115.56	112.19
7	N	2	NAG	C2-N2-C7	2.43	126.37	122.90
6	O	1	NAG	C1-O5-C5	2.40	115.44	112.19
5	H	2	FUC	O5-C1-C2	2.33	114.37	110.77
5	H	2	FUC	C1-O5-C5	2.29	117.97	112.78
7	T	2	NAG	O5-C1-C2	-2.27	107.71	111.29
9	U	2	FUC	O2-C2-C1	2.24	113.73	109.15
4	S	2	NAG	C3-C4-C5	2.23	114.22	110.24
4	G	2	NAG	C2-N2-C7	-2.19	119.79	122.90
9	V	2	FUC	O5-C5-C4	2.14	113.36	109.52
7	T	3	BMA	O5-C1-C2	-2.12	107.50	110.77
4	I	2	NAG	C1-O5-C5	2.07	115.00	112.19
9	V	2	FUC	O2-C2-C1	2.03	113.31	109.15
6	M	3	FUC	C1-C2-C3	2.02	112.15	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	3	FUC	O2-C2-C1	2.01	113.27	109.15

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	O	2	NAG	C4-C5-C6-O6
6	O	2	NAG	O5-C5-C6-O6
7	T	1	NAG	C1-C2-N2-C7
7	T	1	NAG	C8-C7-N2-C2
7	T	1	NAG	O7-C7-N2-C2
4	I	2	NAG	C4-C5-C6-O6
6	M	1	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
8	P	2	MAN	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
8	P	2	MAN	C4-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
6	O	1	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
6	M	1	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
6	M	2	NAG	C4-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
6	M	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	K	2	NAG	C8-C7-N2-C2
4	K	2	NAG	O7-C7-N2-C2
4	L	1	NAG	C8-C7-N2-C2
4	L	1	NAG	O7-C7-N2-C2
4	R	1	NAG	C8-C7-N2-C2
4	R	1	NAG	O7-C7-N2-C2
4	S	1	NAG	C8-C7-N2-C2
4	S	1	NAG	O7-C7-N2-C2
4	S	2	NAG	C8-C7-N2-C2
4	S	2	NAG	O7-C7-N2-C2
4	W	2	NAG	C8-C7-N2-C2
4	W	2	NAG	O7-C7-N2-C2
5	H	1	NAG	C8-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
6	O	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	O	1	NAG	O7-C7-N2-C2
6	O	2	NAG	C8-C7-N2-C2
6	O	2	NAG	O7-C7-N2-C2
7	N	1	NAG	C8-C7-N2-C2
7	N	1	NAG	O7-C7-N2-C2
4	R	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
6	O	1	NAG	C4-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
5	H	3	NAG	O5-C5-C6-O6
7	N	2	NAG	C1-C2-N2-C7
4	W	1	NAG	C4-C5-C6-O6
7	N	1	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	C1-C2-N2-C7
7	T	3	BMA	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	Q	2	NAG	C3-C2-N2-C7
6	M	2	NAG	C3-C2-N2-C7
9	V	1	NAG	C4-C5-C6-O6
5	H	3	NAG	C4-C5-C6-O6
9	V	1	NAG	O5-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
7	N	2	NAG	O7-C7-N2-C2
7	N	2	NAG	C8-C7-N2-C2
4	L	1	NAG	C3-C2-N2-C7
6	O	1	NAG	C3-C2-N2-C7
9	U	1	NAG	C3-C2-N2-C7
4	G	2	NAG	C4-C5-C6-O6
9	U	1	NAG	C1-C2-N2-C7

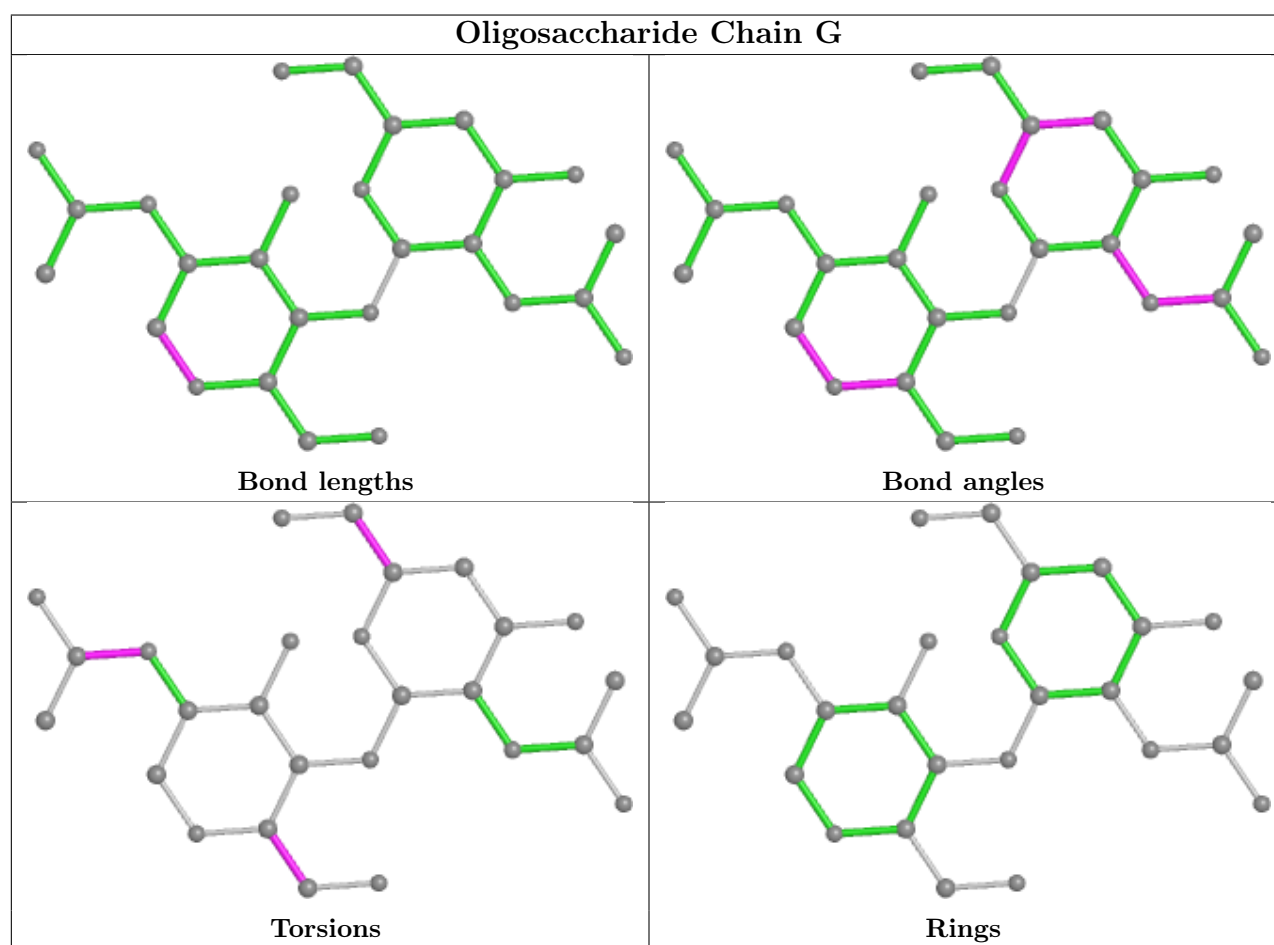
All (1) ring outliers are listed below:

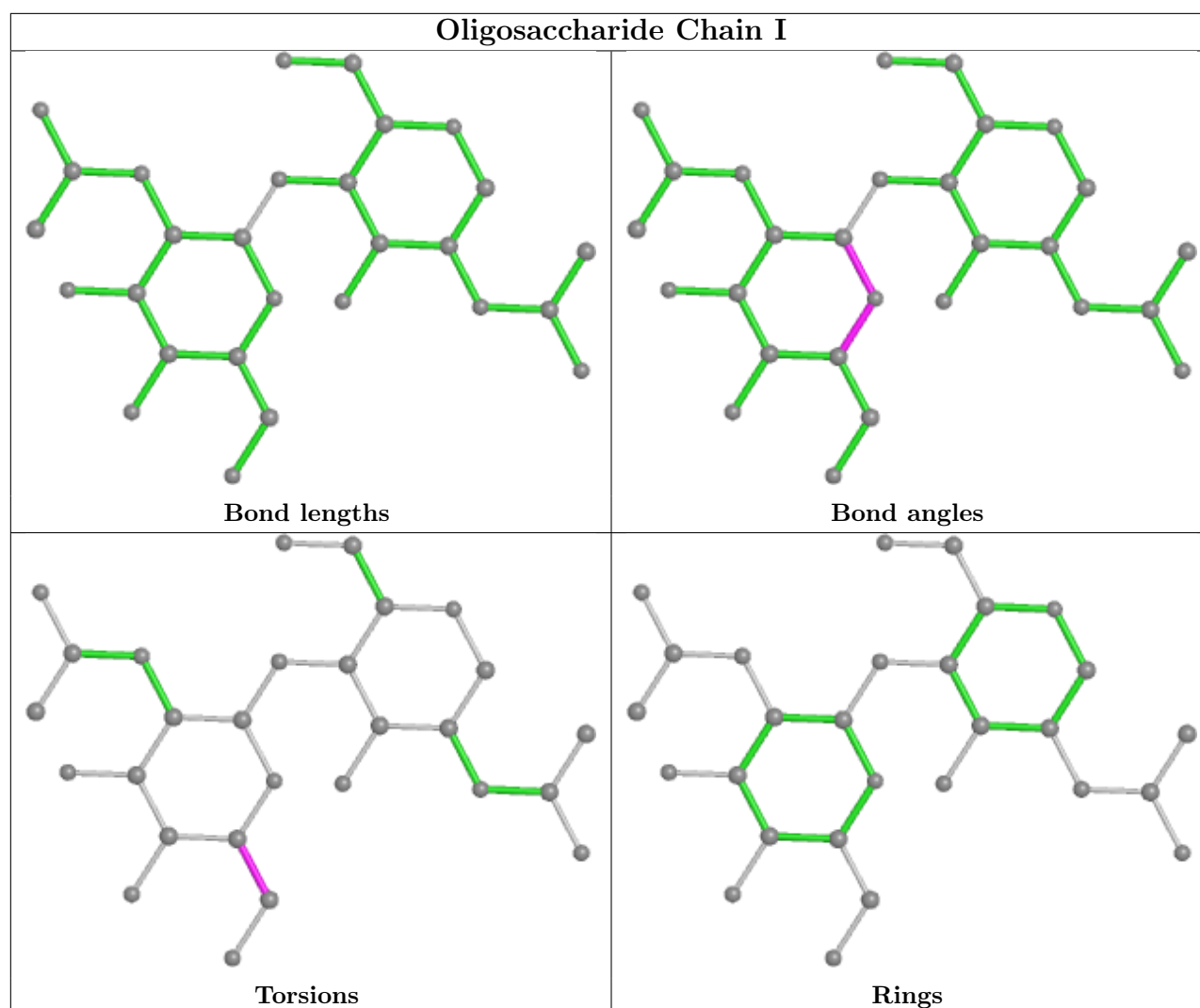
Mol	Chain	Res	Type	Atoms
7	N	3	BMA	C1-C2-C3-C4-C5-O5

8 monomers are involved in 9 short contacts:

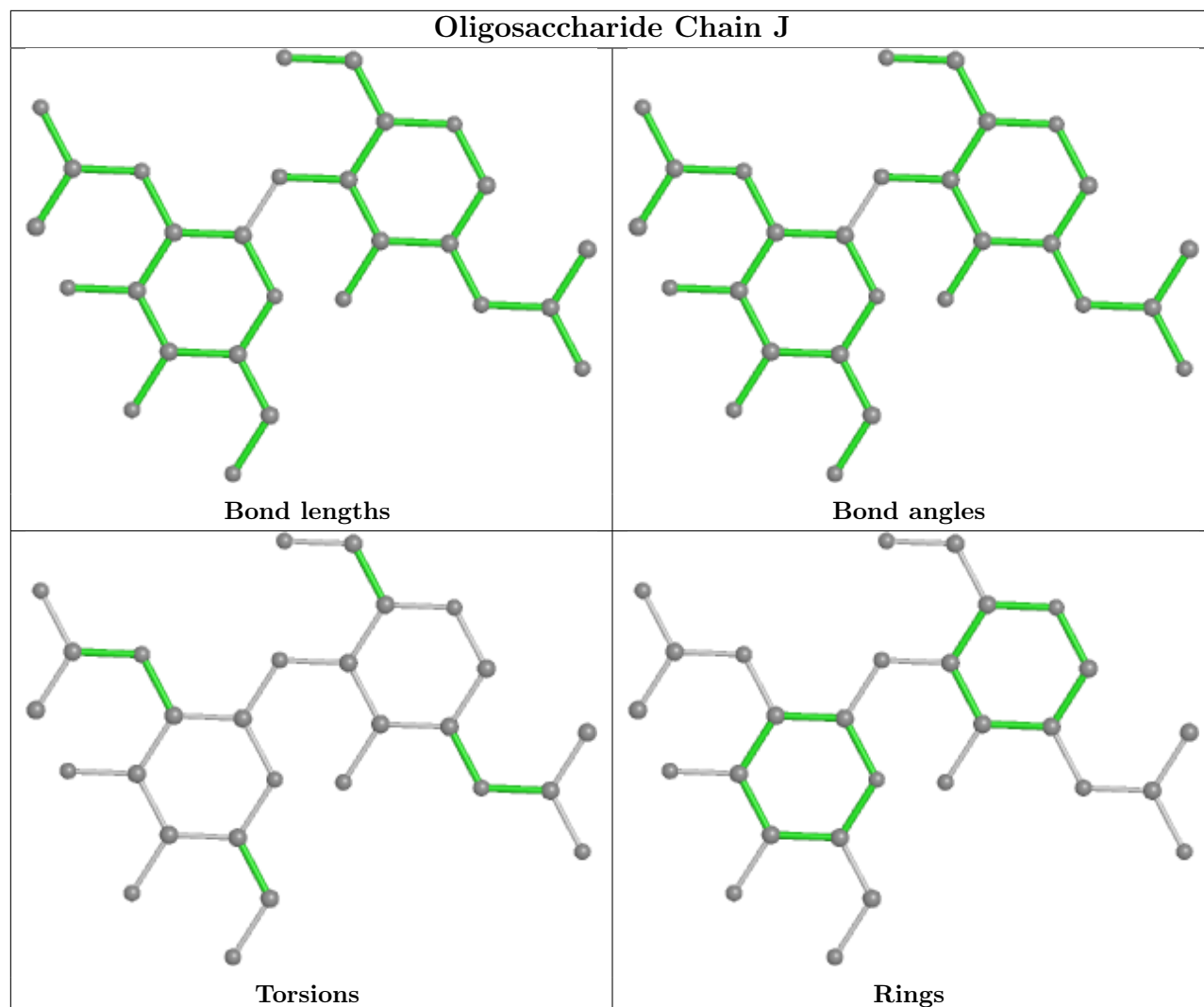
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	NAG	2	0
6	O	1	NAG	1	0
6	M	1	NAG	1	0
6	O	2	NAG	2	0
8	P	1	BMA	2	0
7	N	1	NAG	1	0
4	R	1	NAG	1	0
4	L	1	NAG	1	0

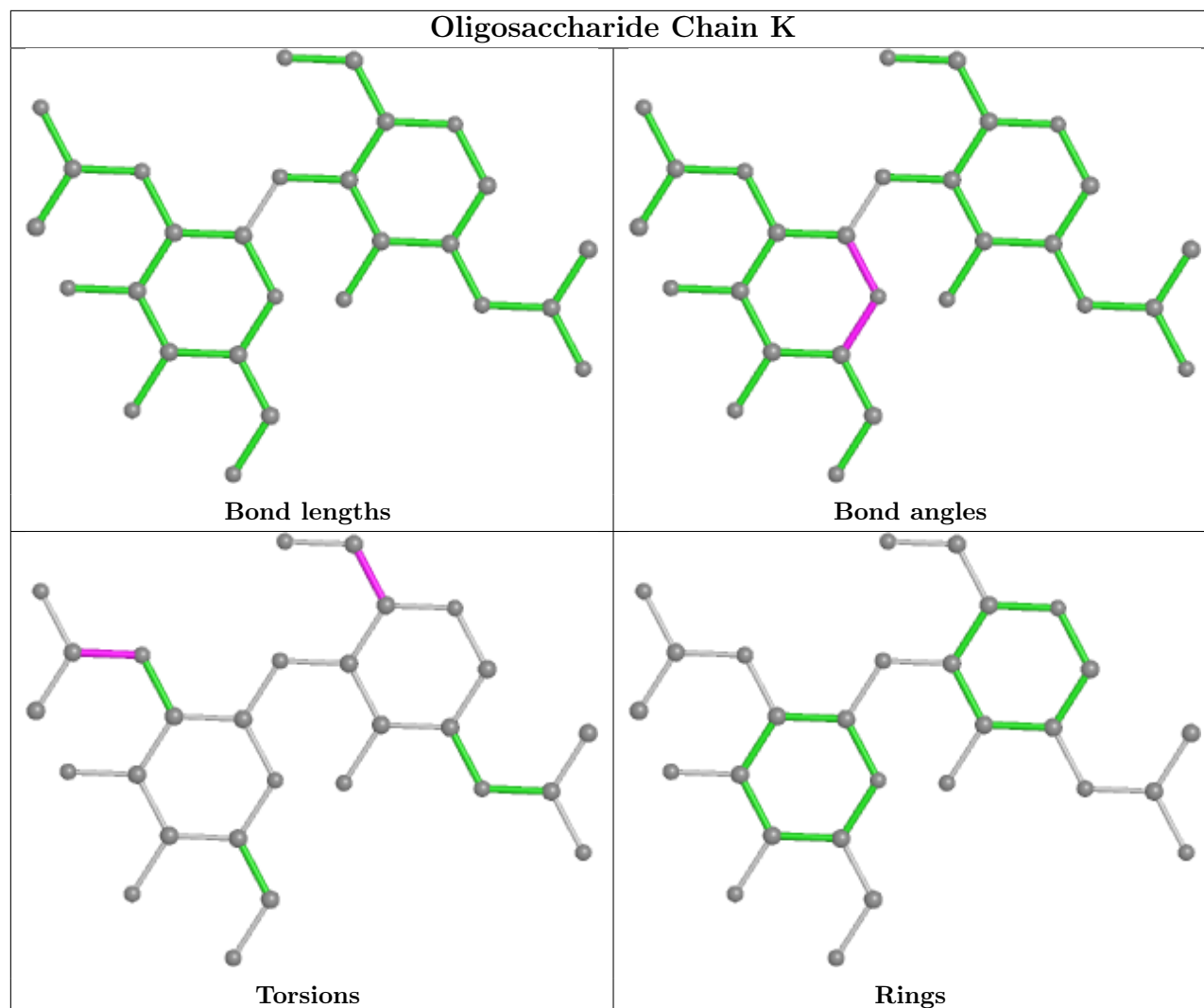
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

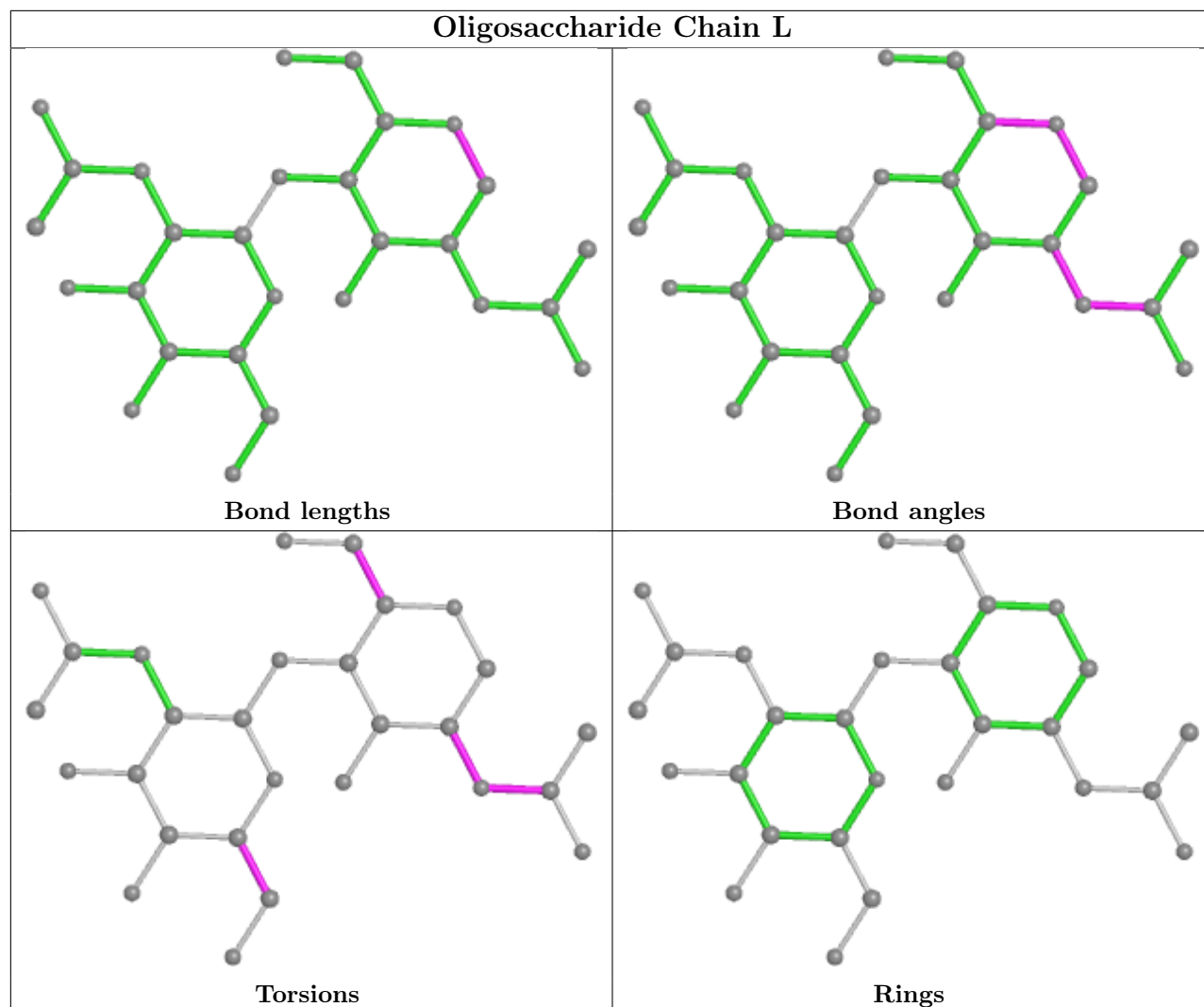


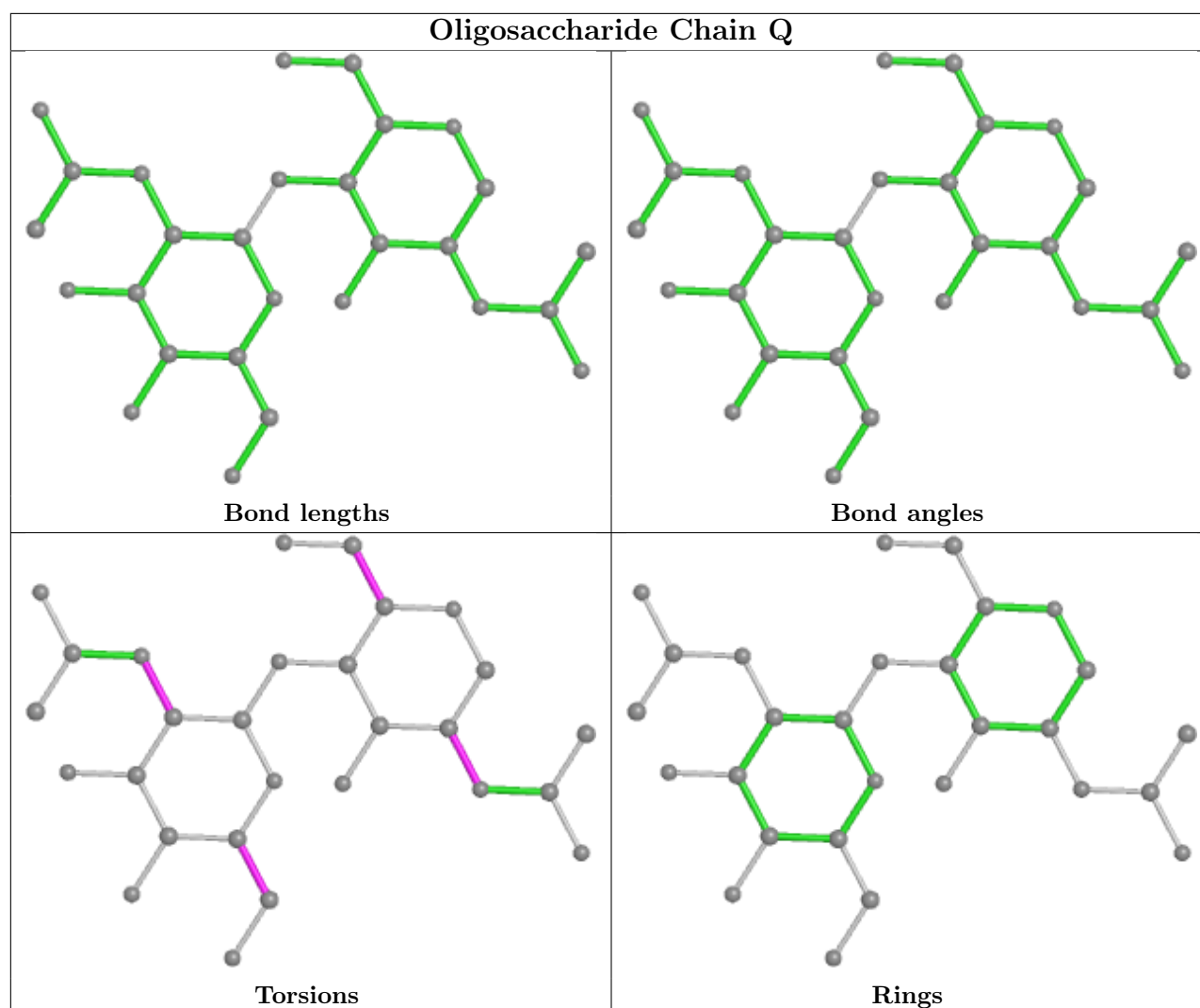


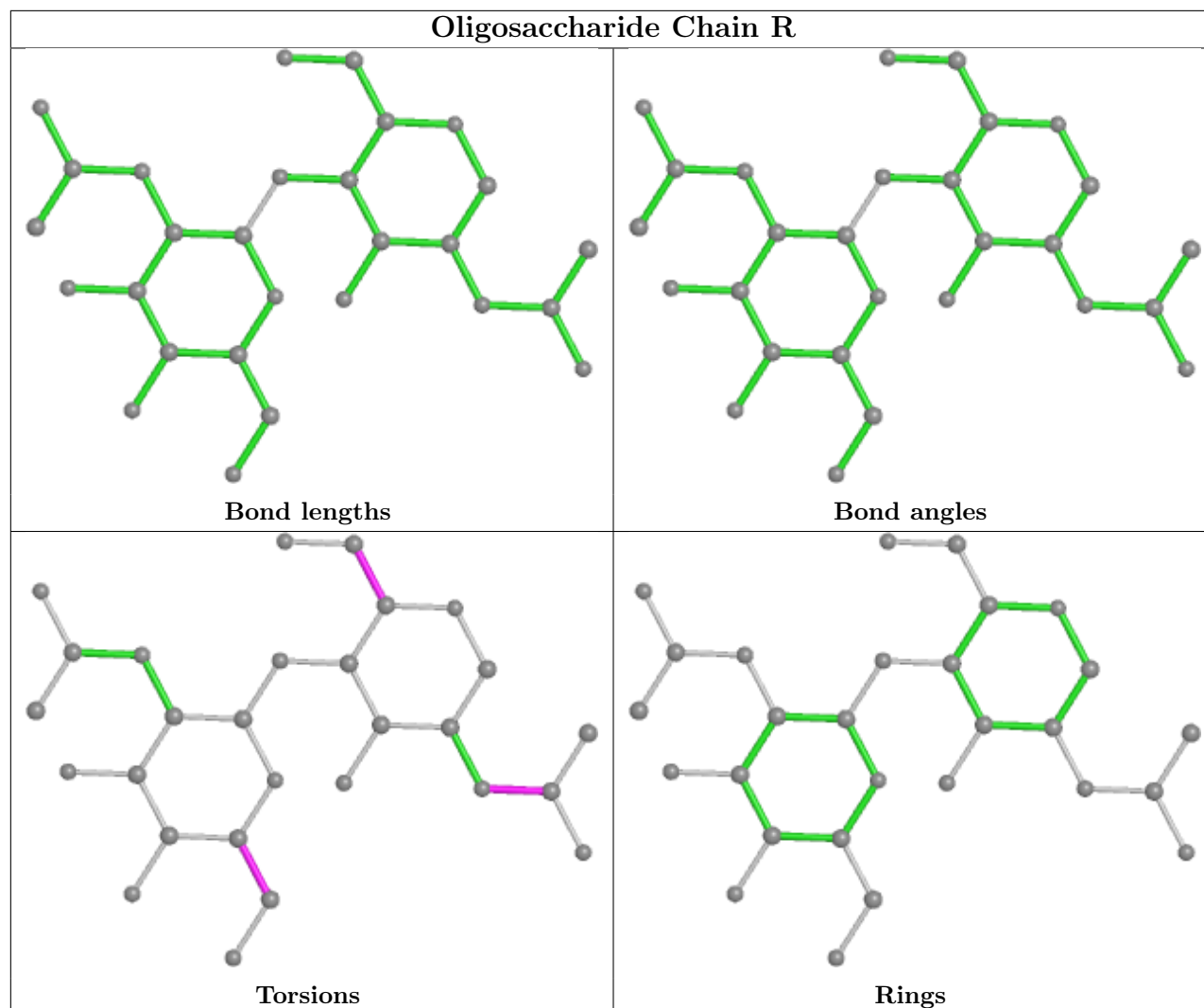


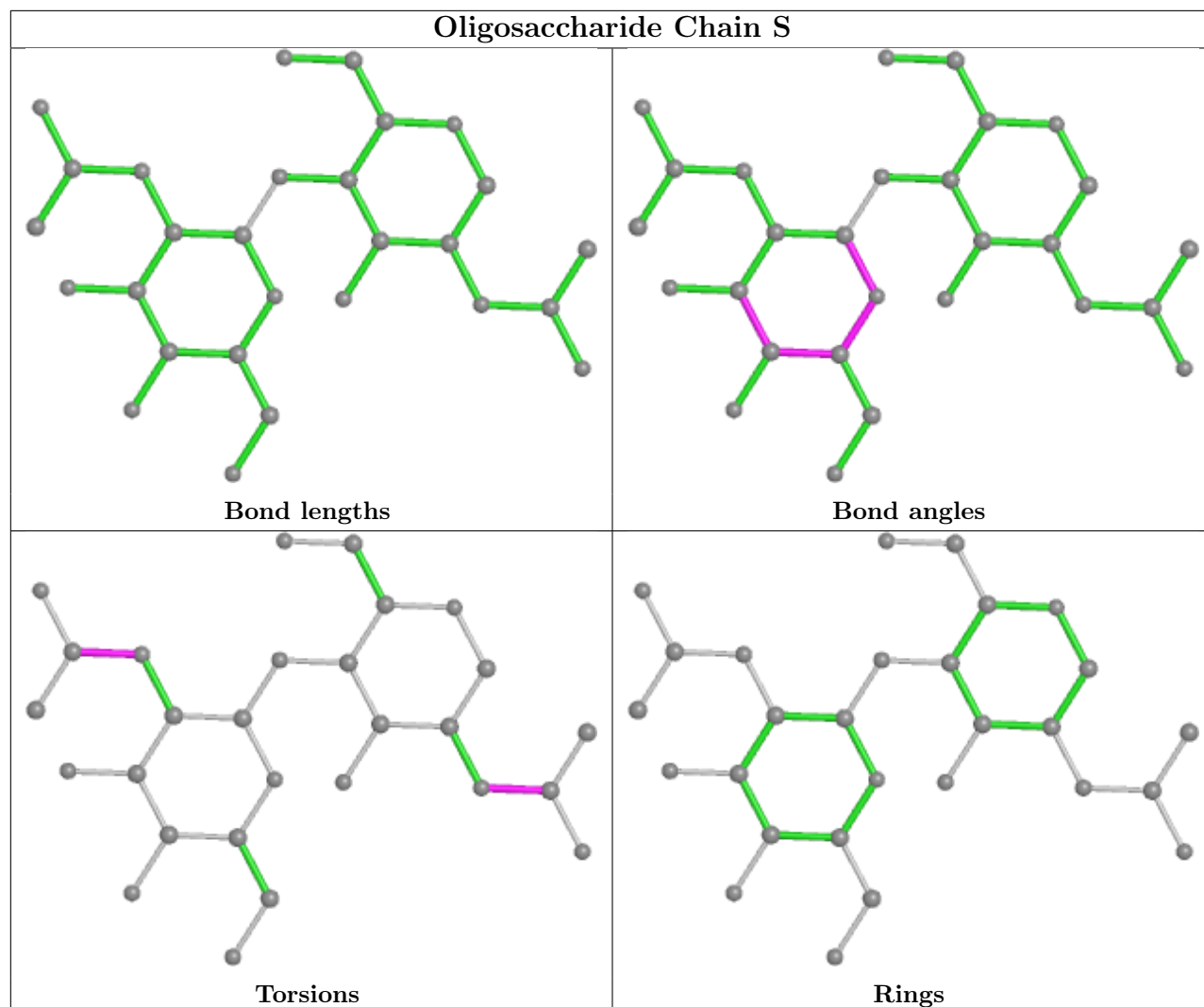


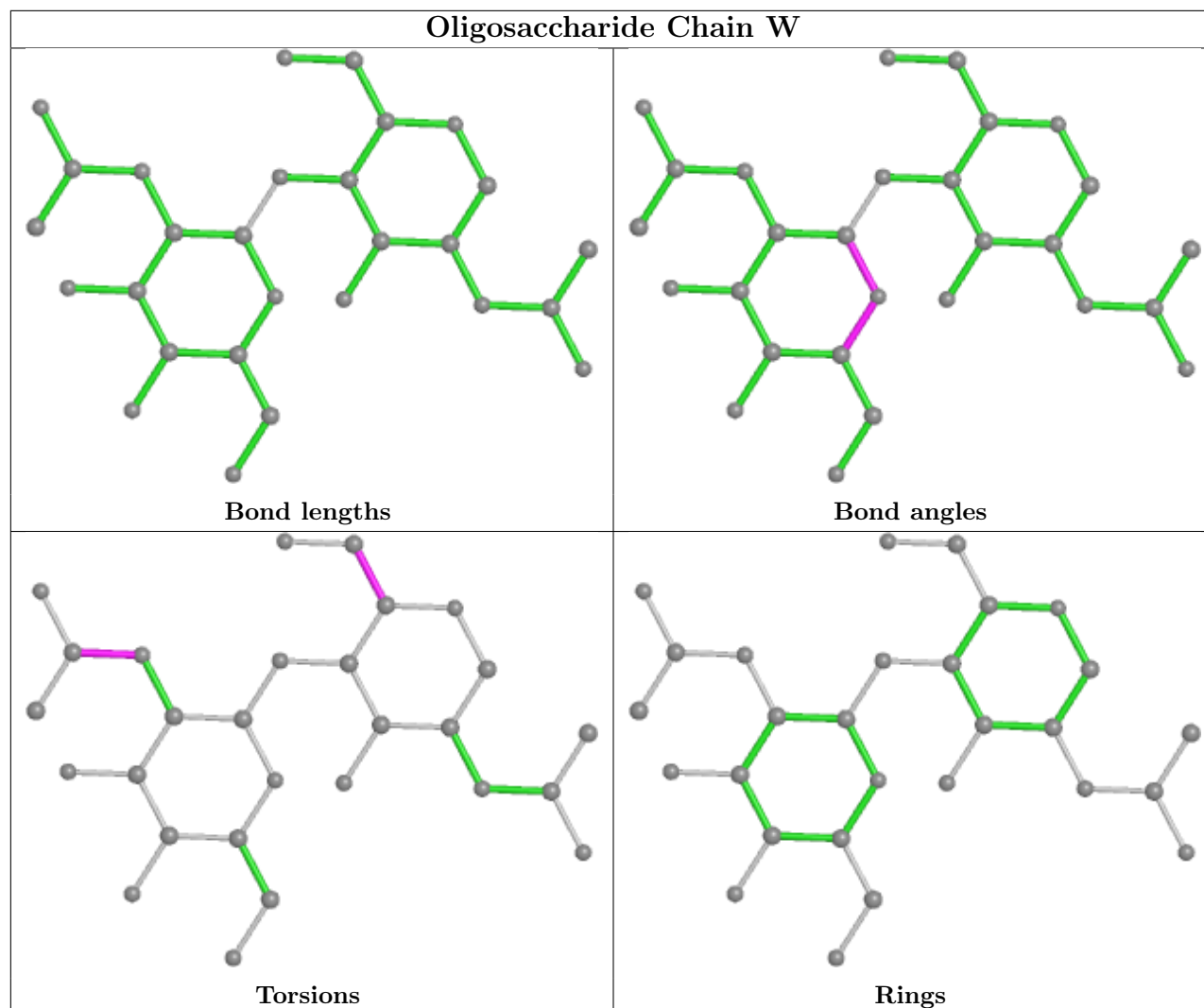




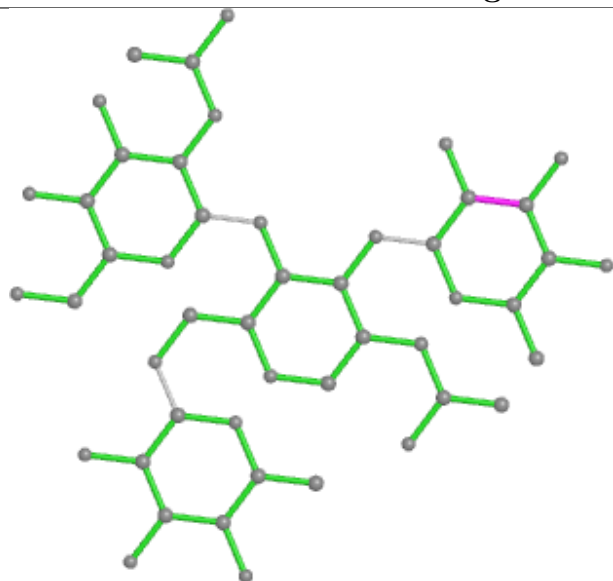




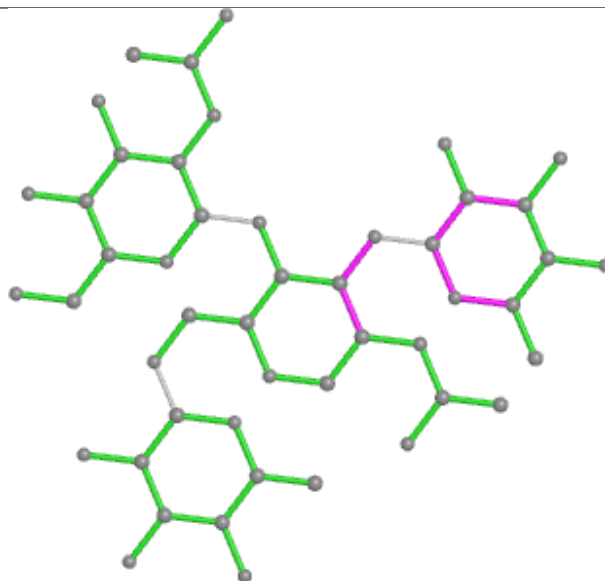




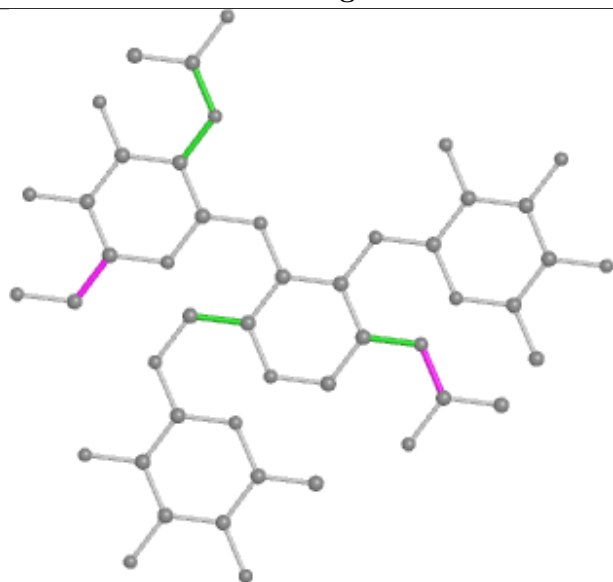
## Oligosaccharide Chain H



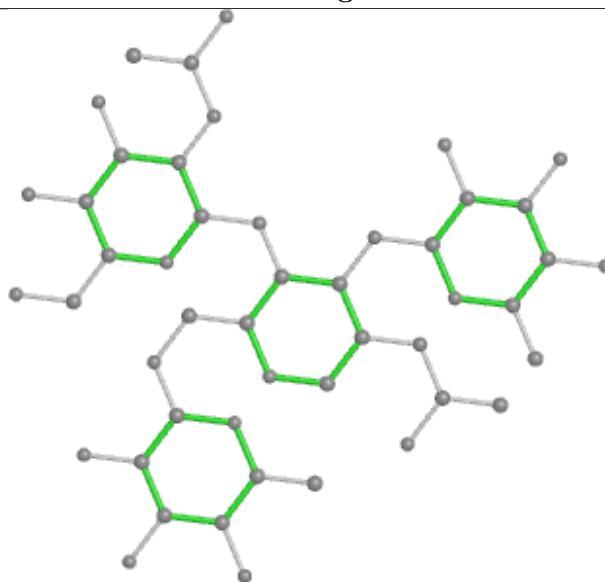
Bond lengths



Bond angles

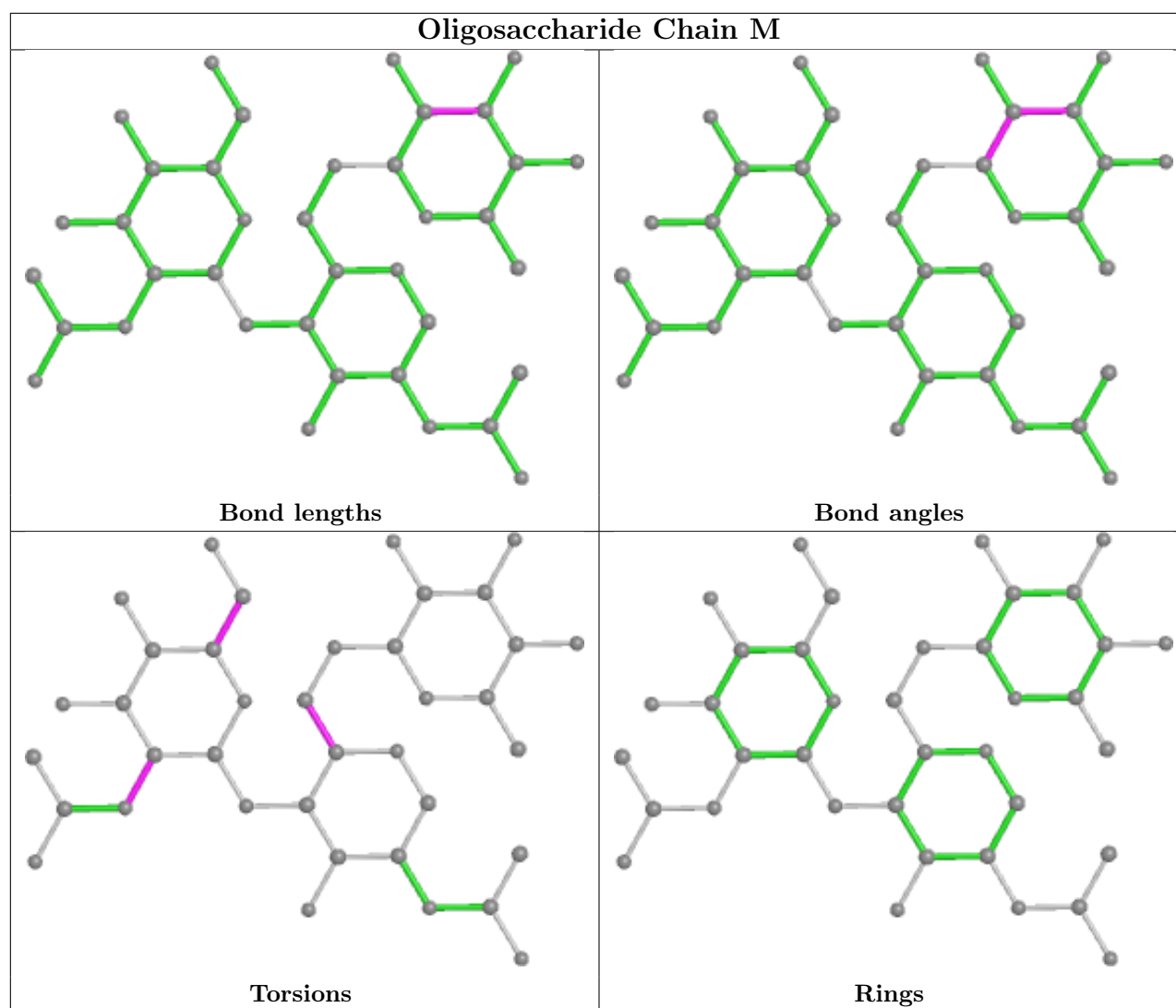


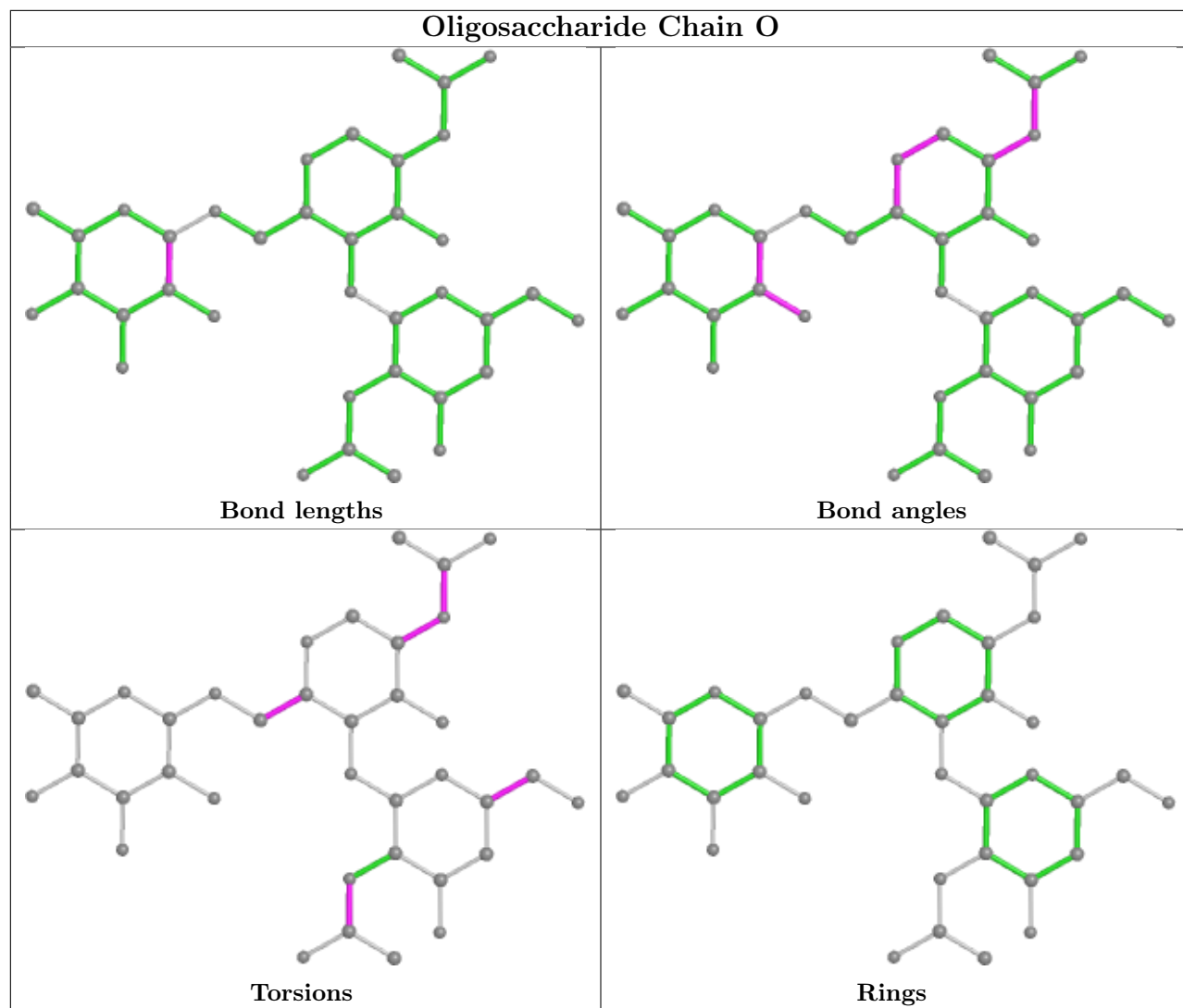
Torsions

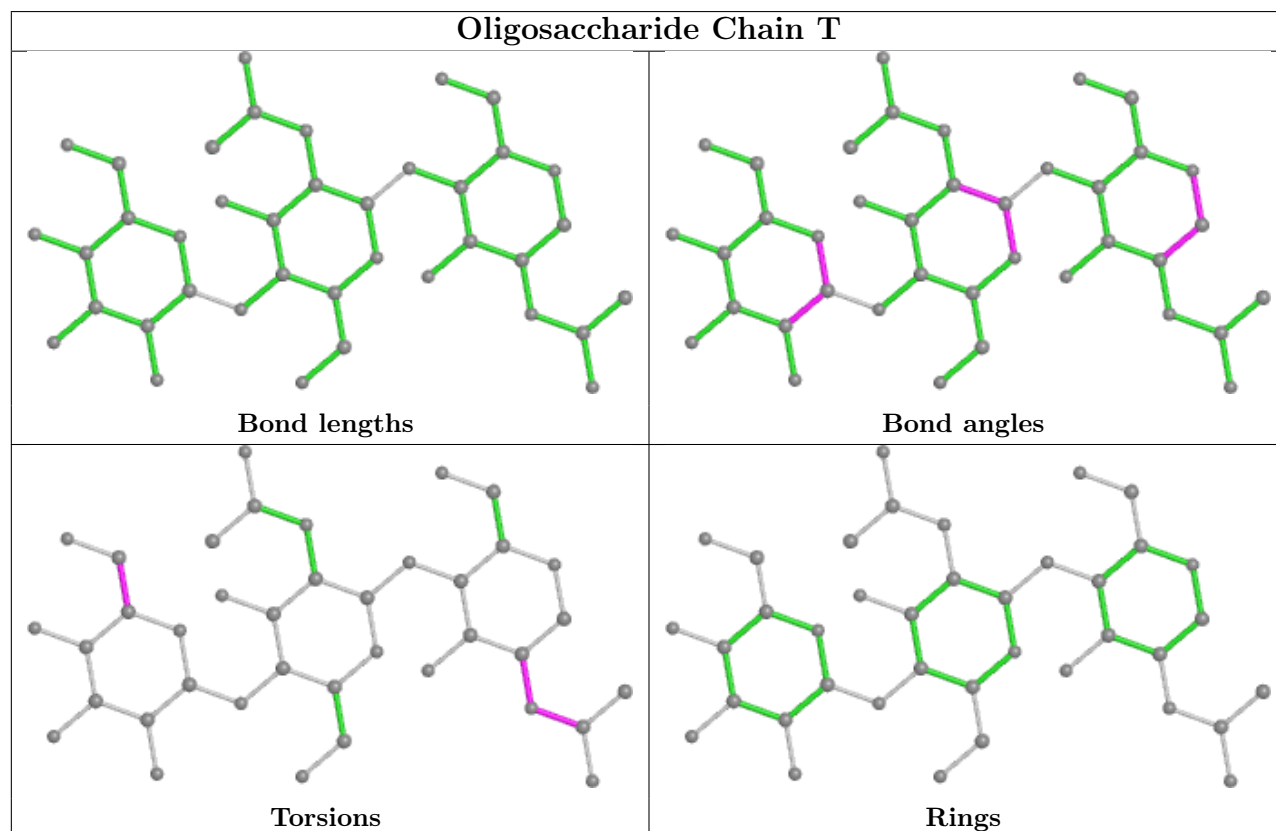
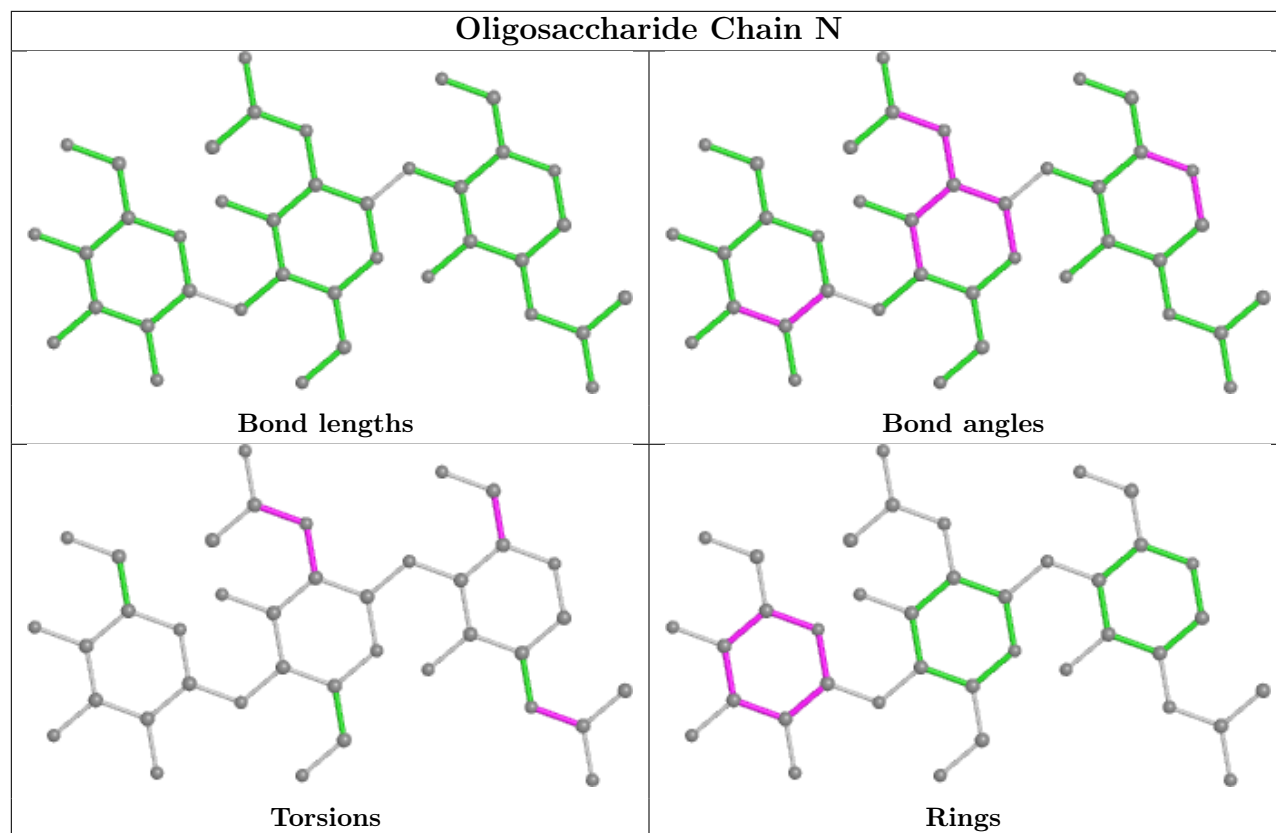


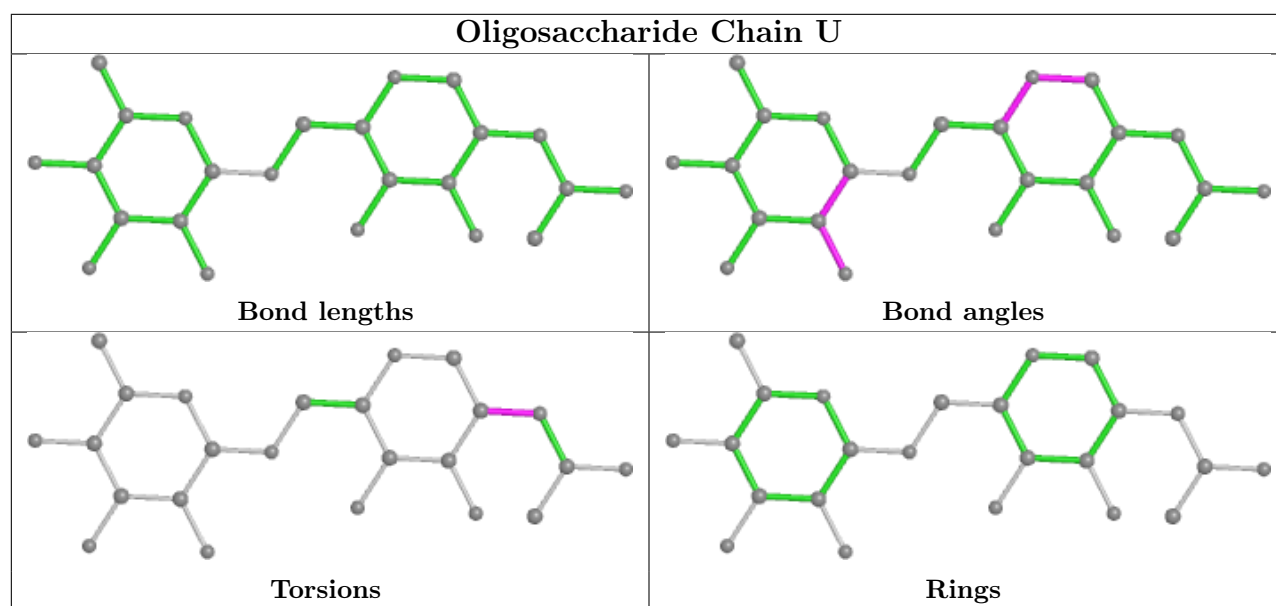
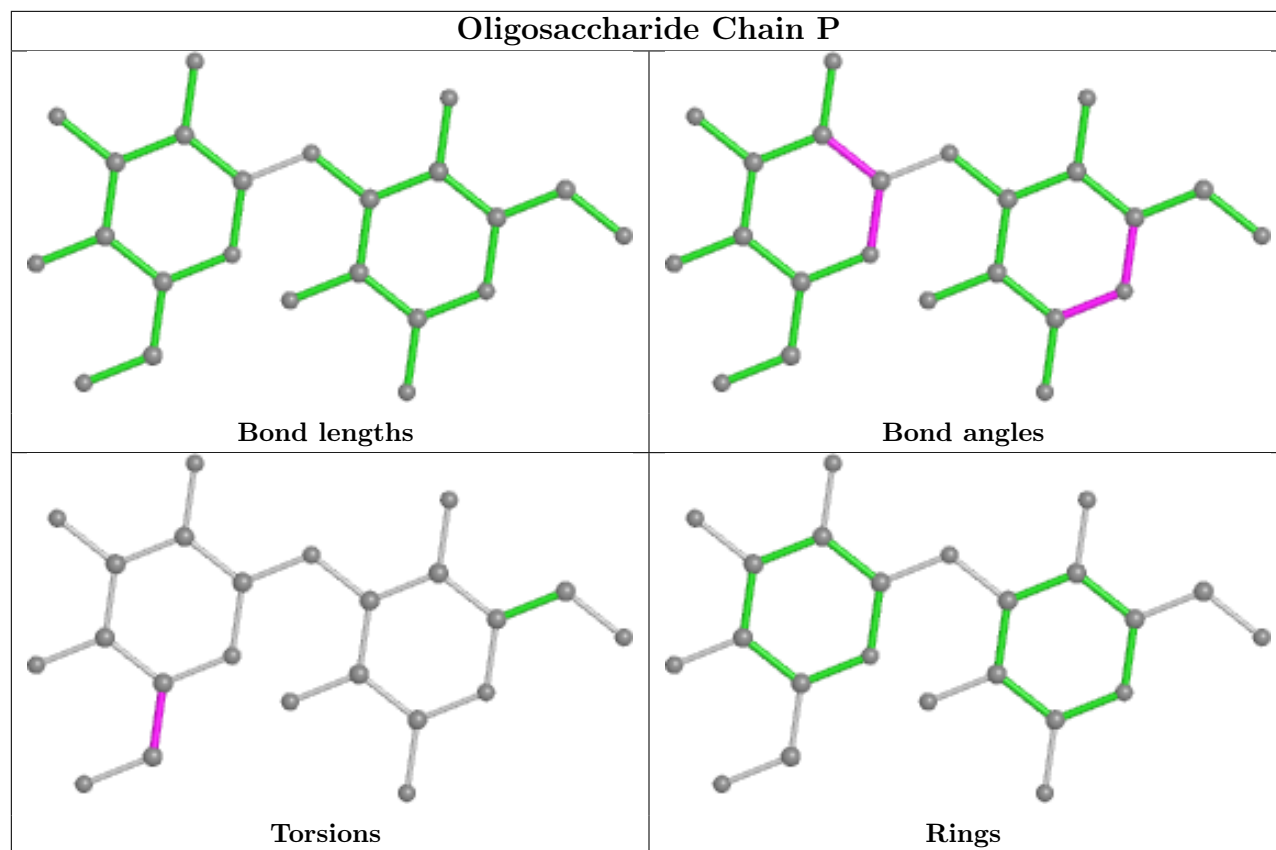
Rings

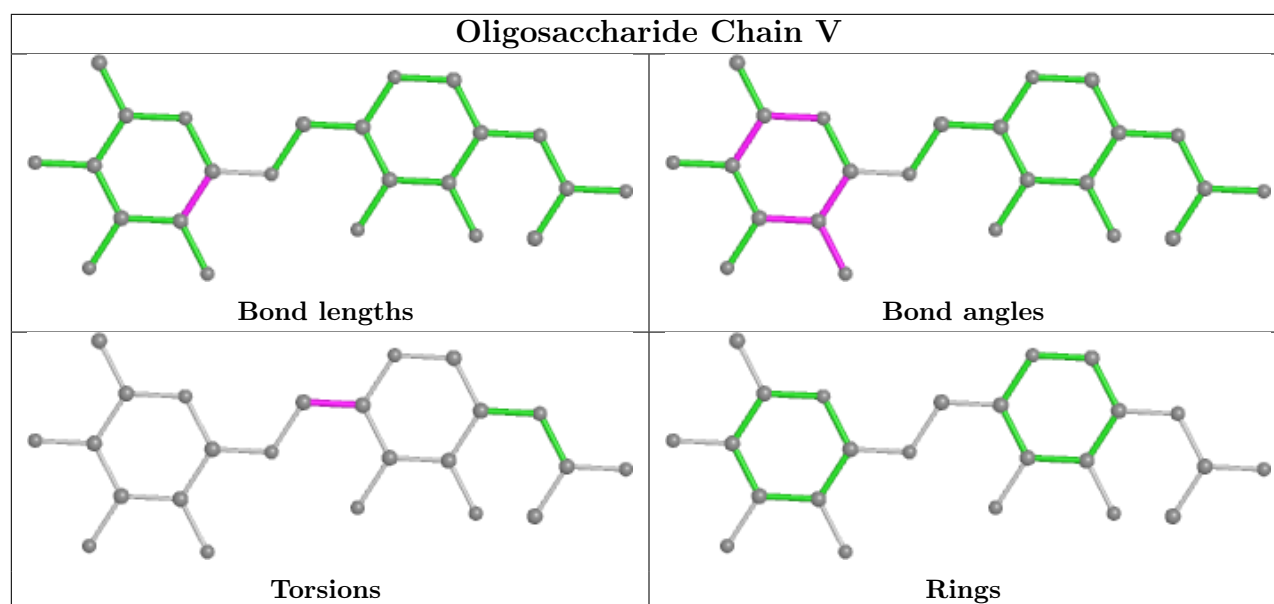












## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
10	NAG	D	1401	1	14,14,15	0.18	0	17,19,21	0.48	0
10	NAG	A	1602	1	14,14,15	0.41	0	17,19,21	0.58	0
10	NAG	D	1403	1	14,14,15	0.42	0	17,19,21	0.41	0
10	NAG	D	1402	1	14,14,15	0.38	0	17,19,21	0.45	0
10	NAG	D	1404	1	14,14,15	0.28	0	17,19,21	0.56	0
10	NAG	A	1601	1	14,14,15	0.35	0	17,19,21	0.43	0
11	BMA	B	301	-	12,12,12	0.54	0	17,17,17	0.75	0
10	NAG	D	1405	1	14,14,15	0.28	0	17,19,21	0.40	0
10	NAG	A	1603	1	14,14,15	0.35	0	17,19,21	0.34	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	D	1401	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1602	1	-	3/6/23/26	0/1/1/1
10	NAG	D	1403	1	-	4/6/23/26	0/1/1/1
10	NAG	D	1402	1	-	2/6/23/26	0/1/1/1
10	NAG	D	1404	1	-	2/6/23/26	0/1/1/1
10	NAG	A	1601	1	-	2/6/23/26	0/1/1/1
11	BMA	B	301	-	-	0/2/22/22	0/1/1/1
10	NAG	D	1405	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1603	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

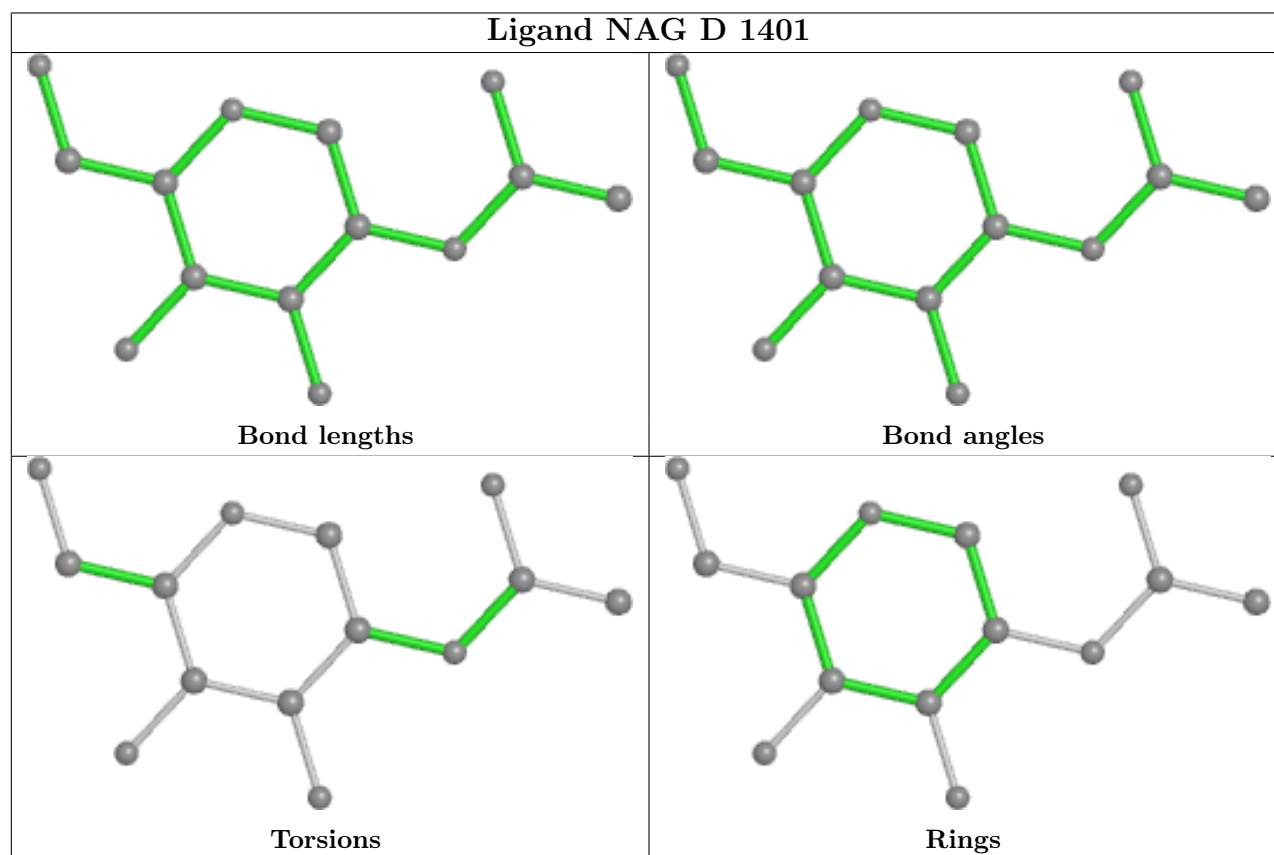
Mol	Chain	Res	Type	Atoms
10	A	1601	NAG	O5-C5-C6-O6
10	D	1404	NAG	O5-C5-C6-O6
10	D	1403	NAG	O5-C5-C6-O6
10	A	1603	NAG	C4-C5-C6-O6
10	D	1403	NAG	C4-C5-C6-O6
10	A	1601	NAG	C4-C5-C6-O6
10	A	1602	NAG	C8-C7-N2-C2
10	A	1602	NAG	O7-C7-N2-C2
10	D	1402	NAG	C8-C7-N2-C2
10	D	1402	NAG	O7-C7-N2-C2
10	D	1403	NAG	C8-C7-N2-C2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

There are no ring outliers.

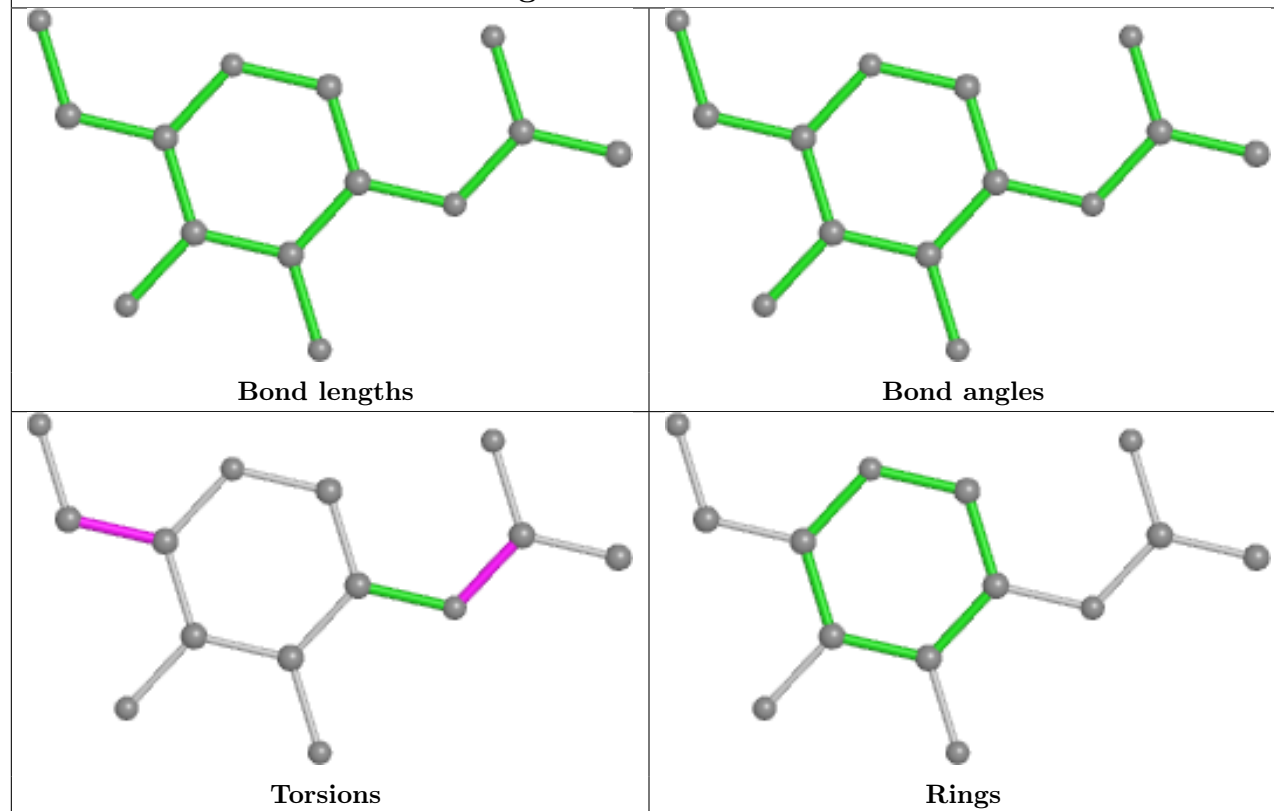
No monomer is involved in short contacts.

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

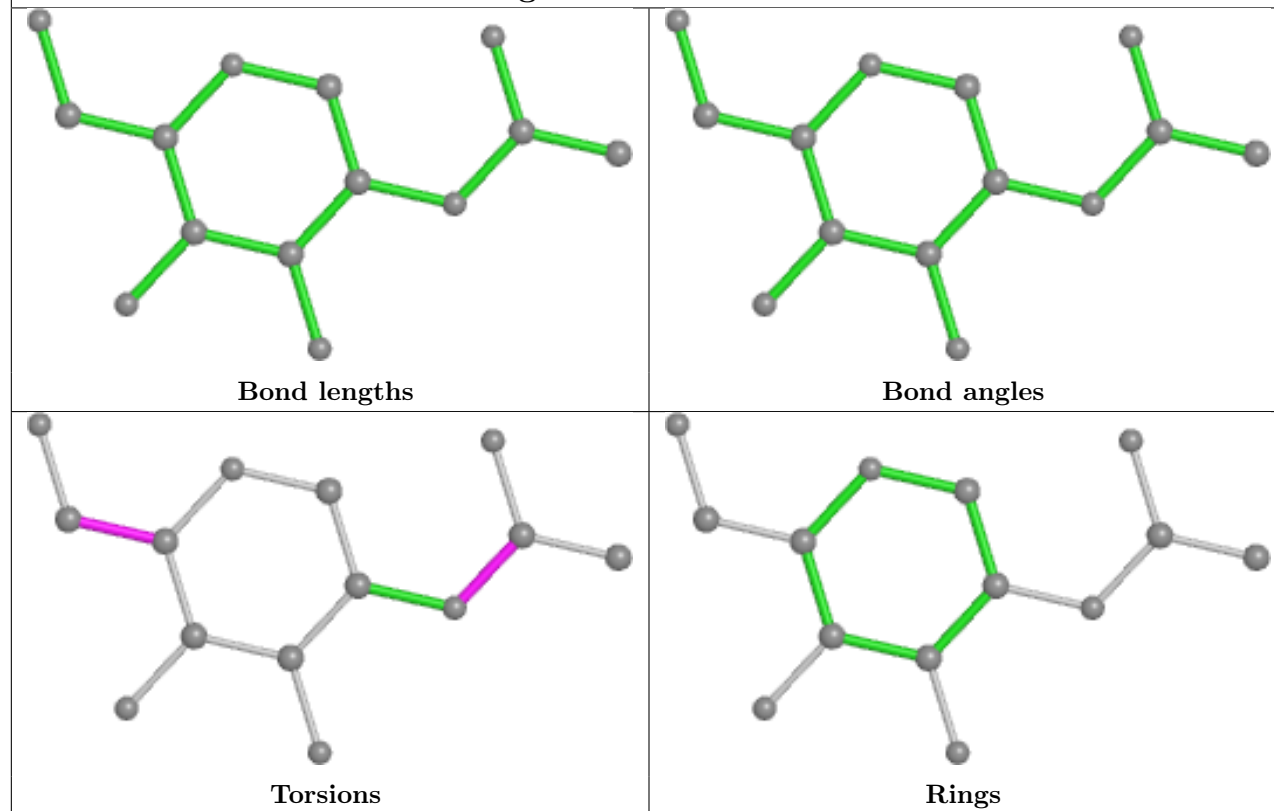
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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 A 1602

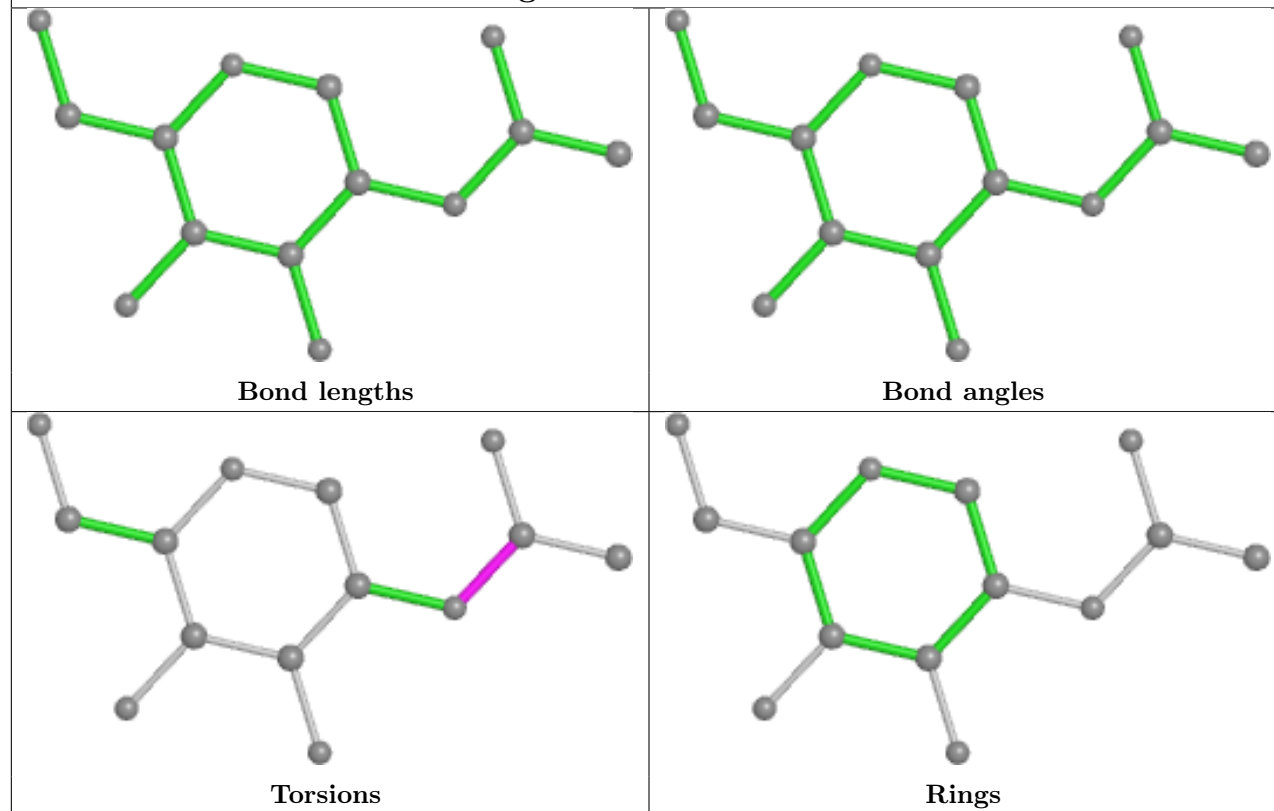


## Ligand NAG D 1403

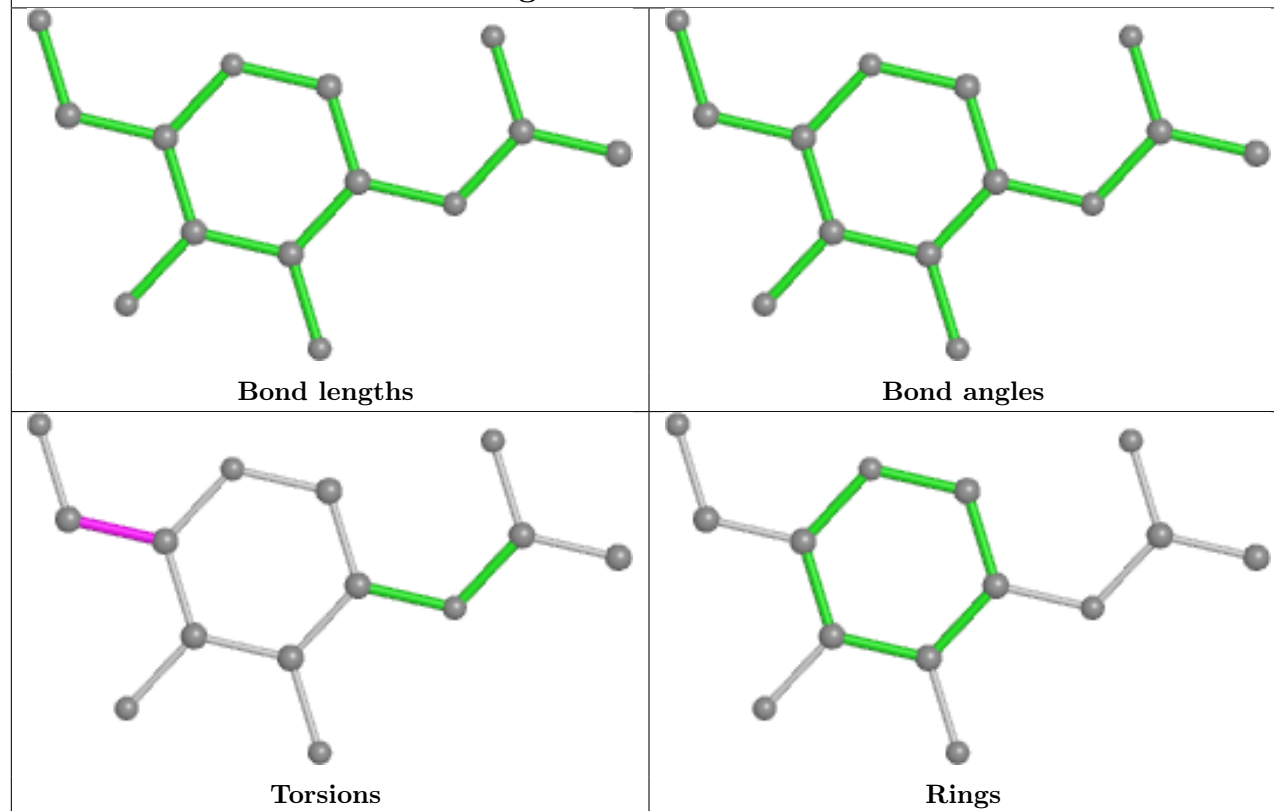


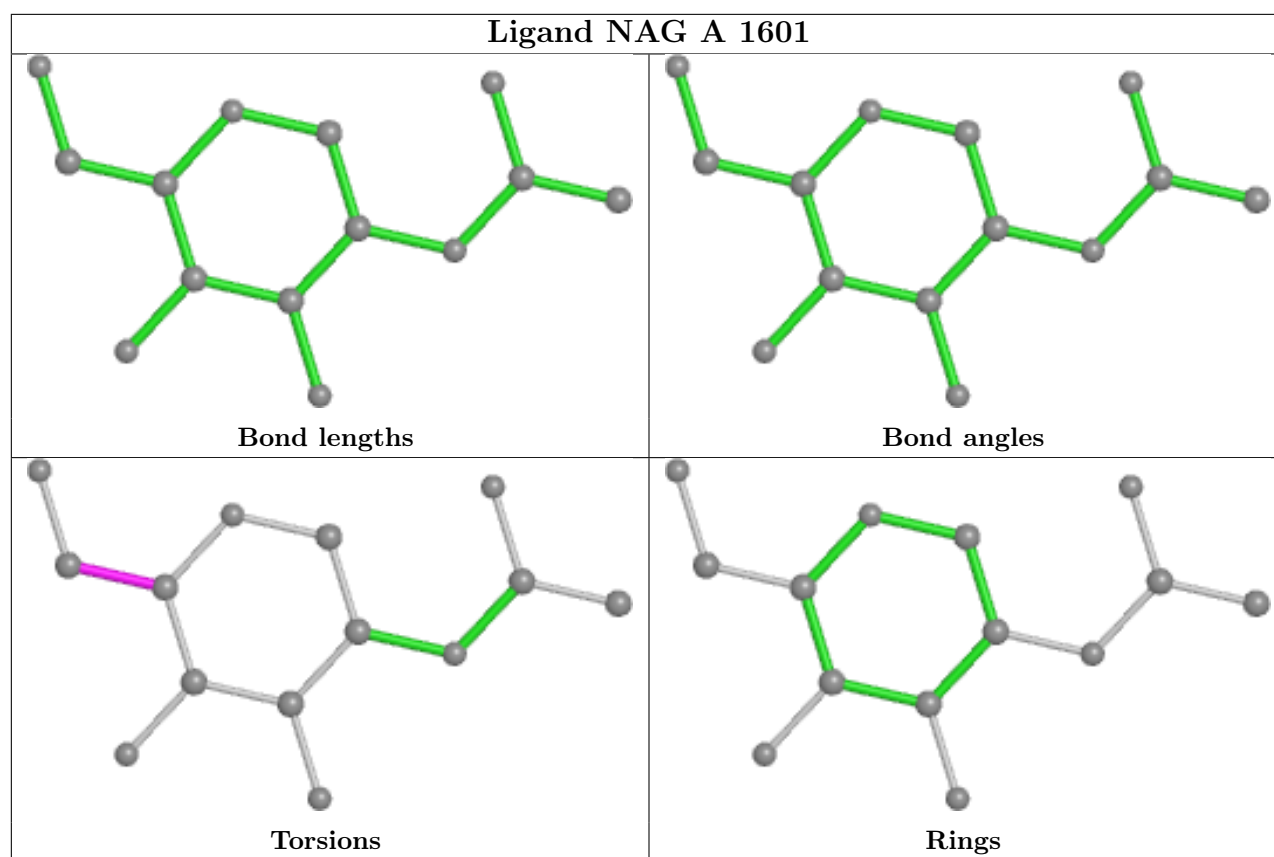


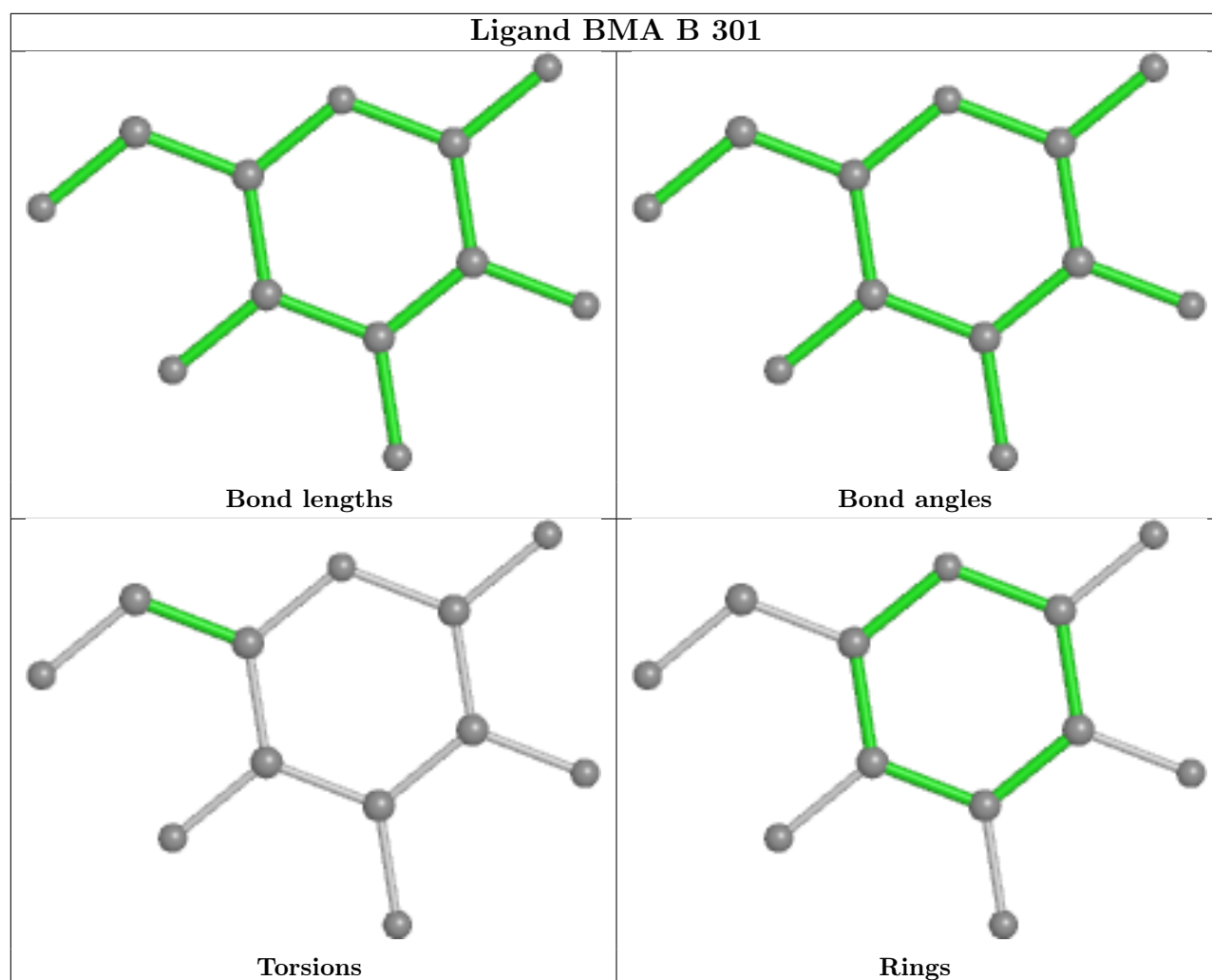
## Ligand NAG D 1402

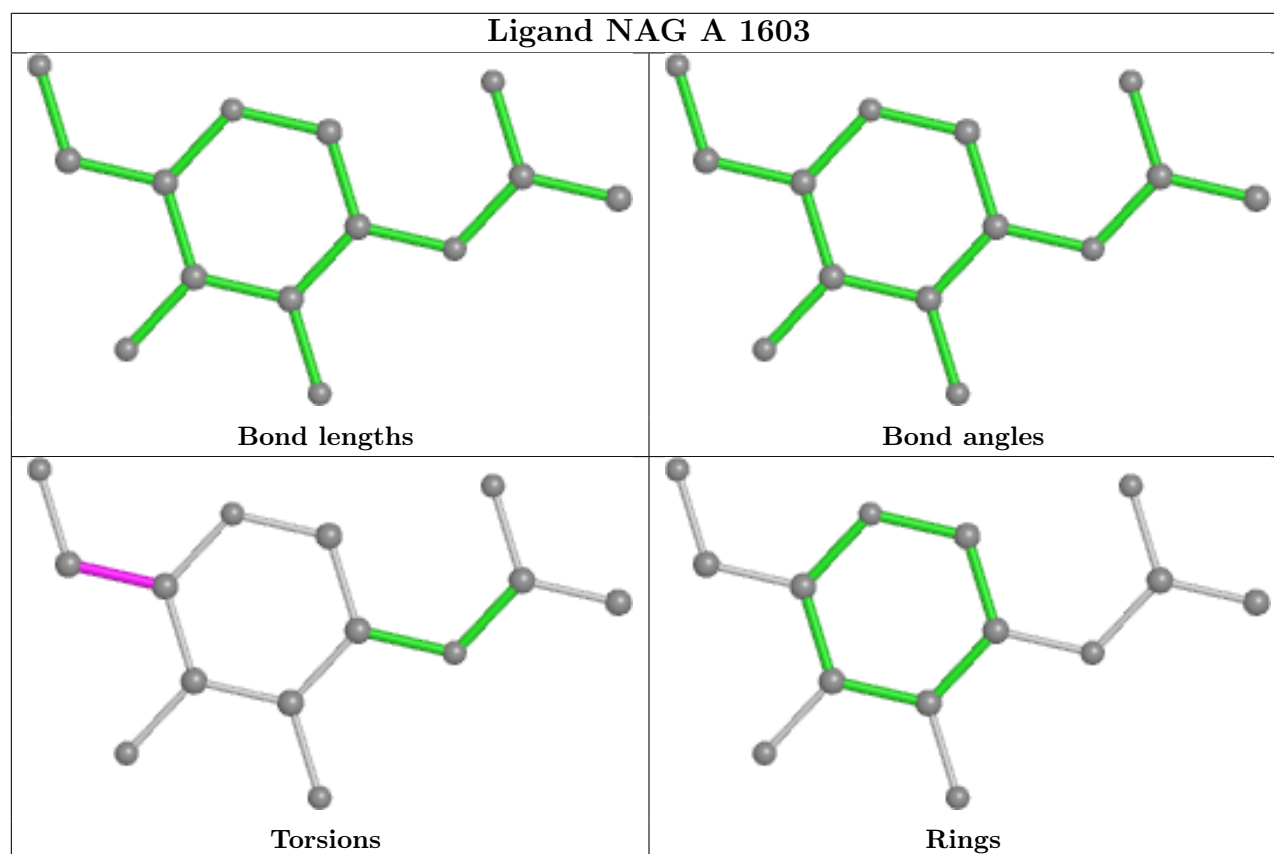
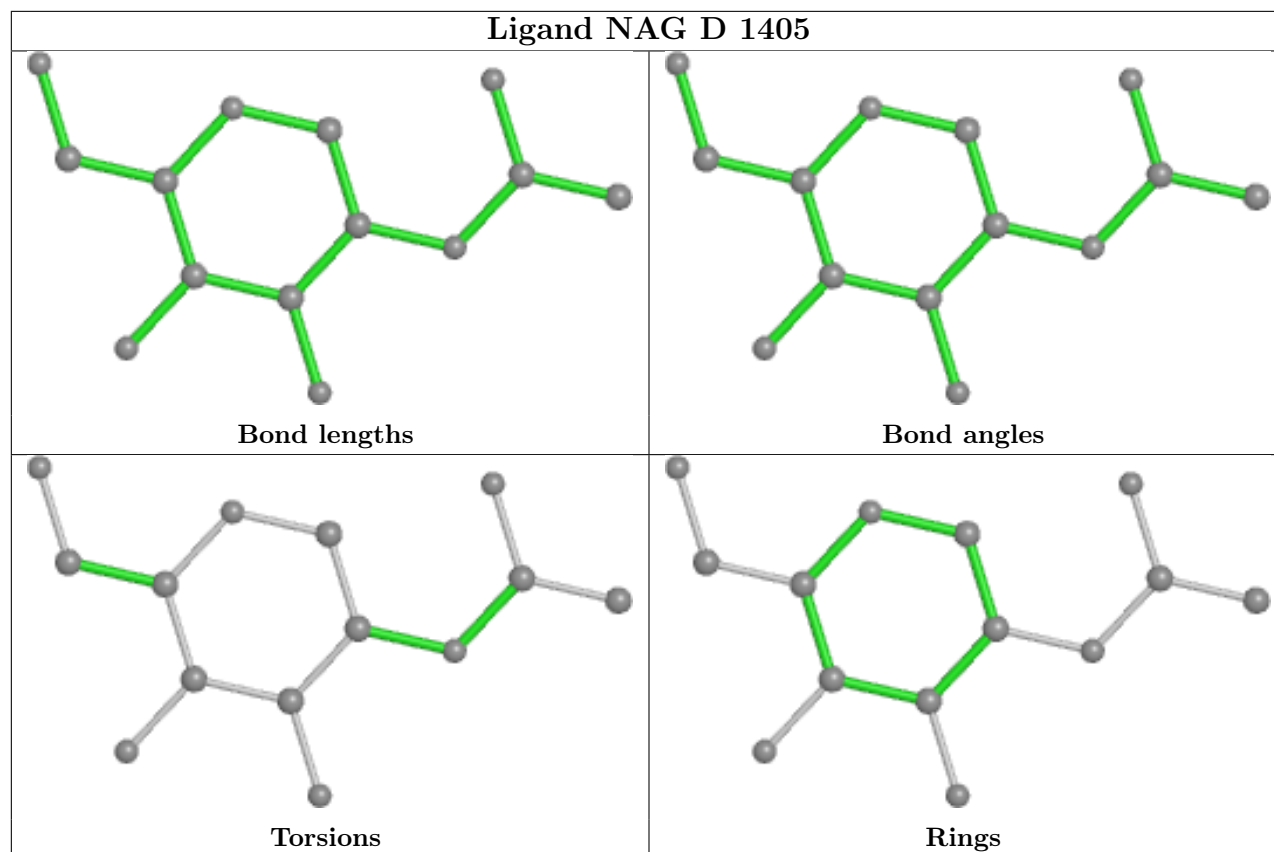


## Ligand NAG D 1404









## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	637/683 (93%)	0.05	9 (1%) 73 56	49, 72, 124, 148	0
1	D	637/683 (93%)	-0.11	3 (0%) 87 75	40, 61, 106, 129	0
2	B	175/230 (76%)	0.78	17 (9%) 15 8	64, 121, 172, 189	0
2	E	174/230 (75%)	0.59	9 (5%) 34 20	52, 96, 135, 154	0
3	C	13/13 (100%)	0.14	0 100 100	65, 69, 75, 77	0
3	F	13/13 (100%)	0.40	0 100 100	63, 66, 71, 74	0
All	All	1649/1852 (89%)	0.13	38 (2%) 61 42	40, 70, 134, 189	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	199	LEU	5.5
2	B	200	THR	5.0
1	A	611	ASP	4.1
2	B	192	ILE	4.1
2	B	184	GLY	3.3
1	A	47	THR	3.0
2	E	164	LEU	3.0
2	B	148	ASN	3.0
2	E	174	ASN	3.0
2	B	183	ASN	2.8
2	B	182	VAL	2.8
1	D	563	SER	2.8
2	B	181	PRO	2.7
2	E	151	SER	2.7
1	A	563	SER	2.7
2	E	180	ILE	2.6
1	A	661	PRO	2.6
1	D	645	MET	2.5
2	B	177	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	379	ALA	2.4
2	B	158	ARG	2.4
1	A	646	LEU	2.3
2	B	63	THR	2.3
2	B	198	LYS	2.3
2	E	171	LEU	2.3
2	E	197	THR	2.2
1	A	374	ILE	2.2
1	A	585	ASP	2.2
2	E	107	THR	2.2
1	D	663	PRO	2.2
2	B	164	LEU	2.2
2	B	115	LEU	2.2
2	B	118	LEU	2.2
2	E	152	LEU	2.2
2	B	180	ILE	2.0
2	B	179	ASP	2.0
1	A	622	GLN	2.0
2	B	81	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
8	MAN	P	2	11/12	0.13	0.21	128,128,128,128	0
4	NAG	S	2	14/15	0.34	0.19	125,137,142,143	0
8	BMA	P	1	12/12	0.38	0.19	120,120,120,120	0
7	BMA	T	3	11/12	0.49	0.15	103,103,103,103	0
4	NAG	K	2	14/15	0.53	0.17	94,109,115,116	0
4	NAG	W	2	14/15	0.55	0.18	103,103,103,103	0
6	NAG	M	2	14/15	0.57	0.17	116,116,116,116	0
7	BMA	N	3	11/12	0.58	0.17	79,79,79,79	0
9	FUC	V	2	10/11	0.58	0.15	100,100,100,100	0

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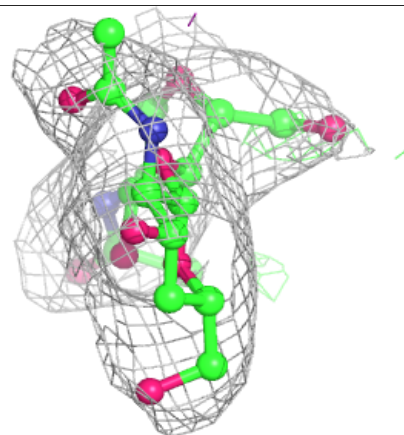
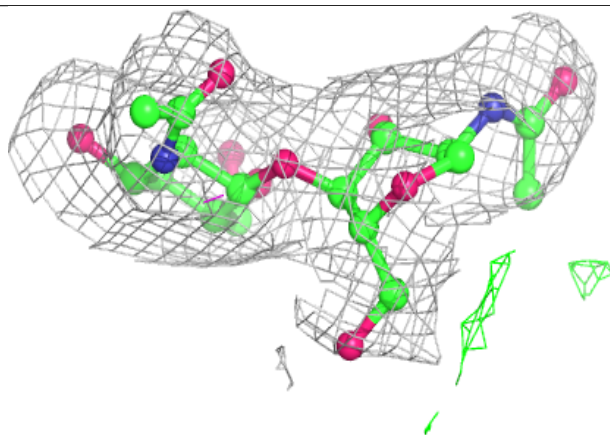
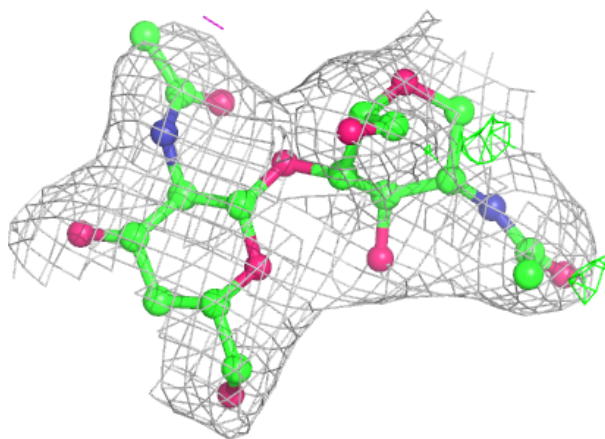
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	W	1	14/15	0.61	0.17	92,92,92,92	0
4	NAG	L	2	14/15	0.61	0.13	94,109,117,120	0
4	NAG	S	1	14/15	0.63	0.16	101,123,130,136	0
5	FUC	H	4	10/11	0.64	0.18	101,101,101,101	0
6	FUC	M	3	10/11	0.65	0.14	100,100,100,100	0
4	NAG	R	2	14/15	0.68	0.14	84,103,106,107	0
6	NAG	M	1	14/15	0.69	0.15	77,102,114,129	0
7	NAG	T	1	14/15	0.69	0.18	61,79,83,88	0
4	NAG	J	2	14/15	0.71	0.14	67,86,100,103	0
5	NAG	H	3	14/15	0.72	0.16	80,106,112,112	0
5	FUC	H	2	10/11	0.73	0.13	97,97,97,97	0
9	NAG	U	1	14/15	0.73	0.17	77,95,106,110	0
9	NAG	V	1	14/15	0.73	0.15	89,89,89,89	0
4	NAG	L	1	14/15	0.73	0.14	82,99,105,110	0
6	FUC	O	3	10/11	0.78	0.12	88,88,88,88	0
6	NAG	O	2	13/15	0.79	0.14	86,100,109,111	0
5	NAG	H	1	14/15	0.81	0.13	71,84,103,109	0
6	NAG	O	1	14/15	0.81	0.12	64,74,85,100	0
9	FUC	U	2	10/11	0.82	0.13	94,94,94,94	0
4	NAG	I	2	14/15	0.83	0.12	78,85,101,102	0
4	NAG	K	1	14/15	0.84	0.12	70,83,97,105	0
4	NAG	Q	1	14/15	0.84	0.15	59,69,83,84	0
7	NAG	N	2	14/15	0.86	0.13	51,62,73,76	0
7	NAG	T	2	14/15	0.86	0.10	69,85,99,100	0
4	NAG	R	1	14/15	0.86	0.11	63,78,89,95	0
7	NAG	N	1	14/15	0.87	0.11	52,54,58,73	0
4	NAG	Q	2	14/15	0.88	0.12	62,76,88,105	0
4	NAG	J	1	14/15	0.89	0.12	51,70,77,82	0
4	NAG	G	1	14/15	0.91	0.13	52,61,90,103	0
4	NAG	I	1	14/15	0.92	0.10	64,77,83,90	0
4	NAG	G	2	13/15	0.96	0.09	53,68,75,85	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.



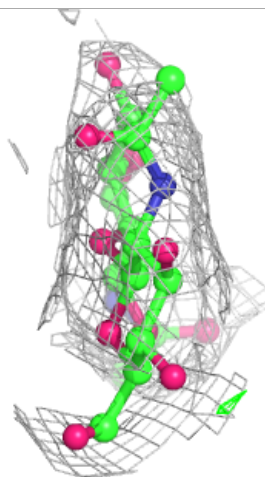
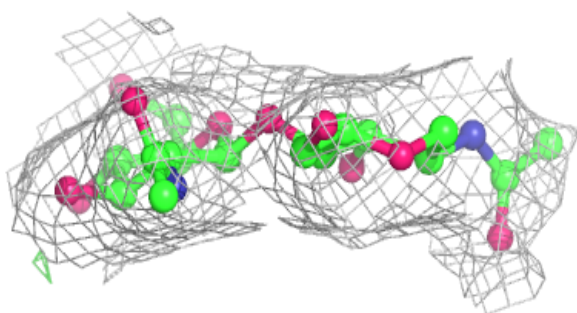
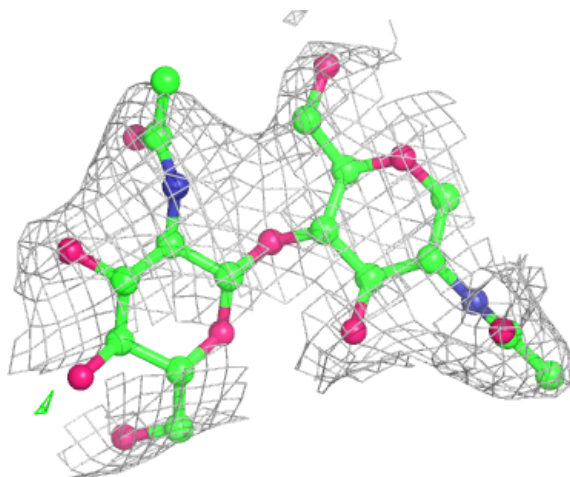
**Electron density around Chain G:**

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



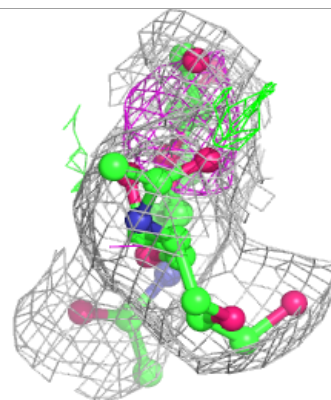
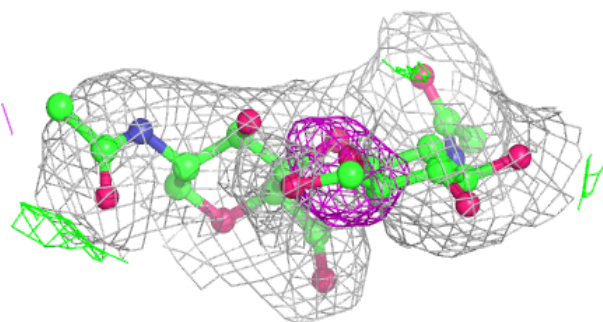
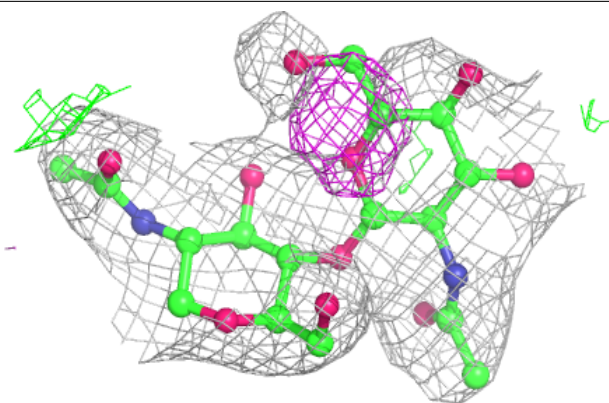
**Electron density around Chain I:**

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

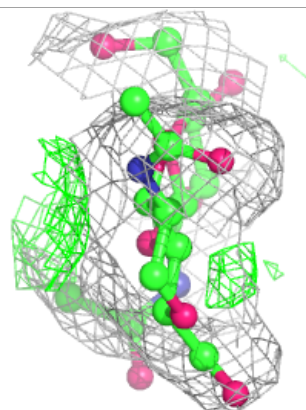
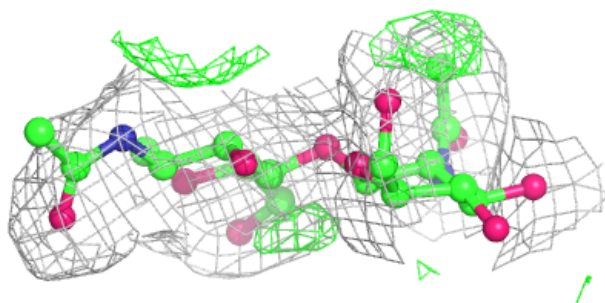
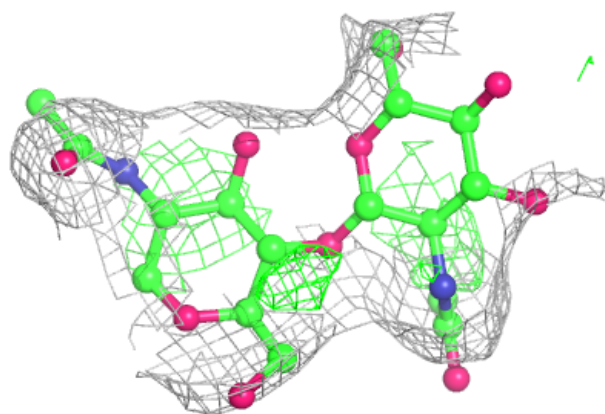


**Electron density around Chain J:**

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

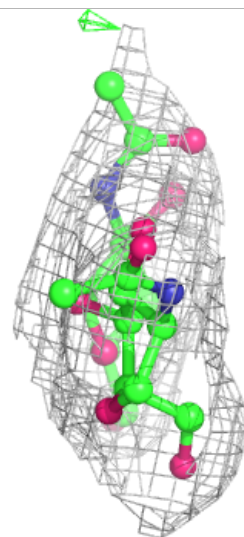
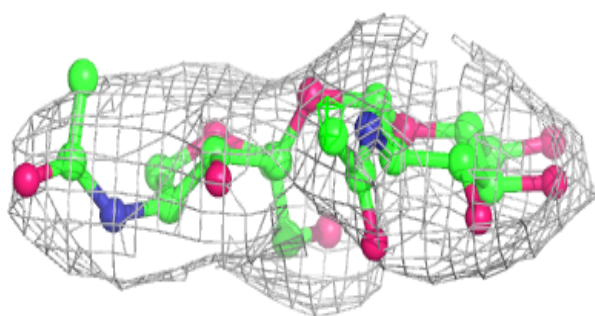
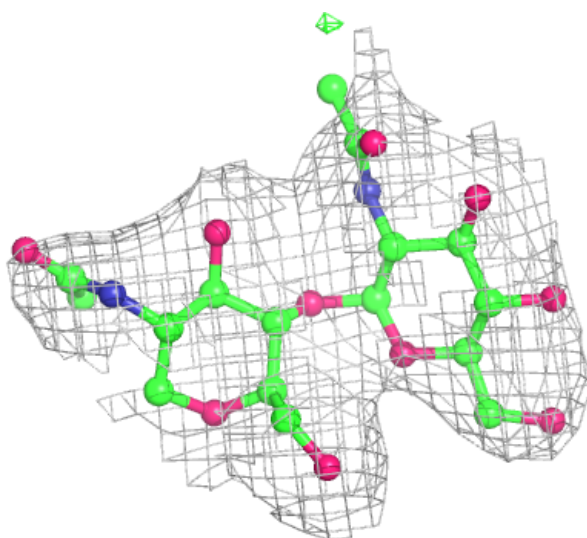
**Electron density around Chain K:**

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



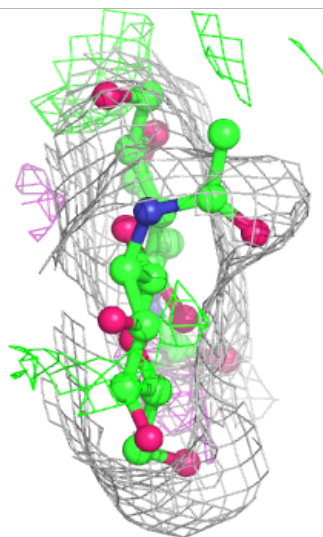
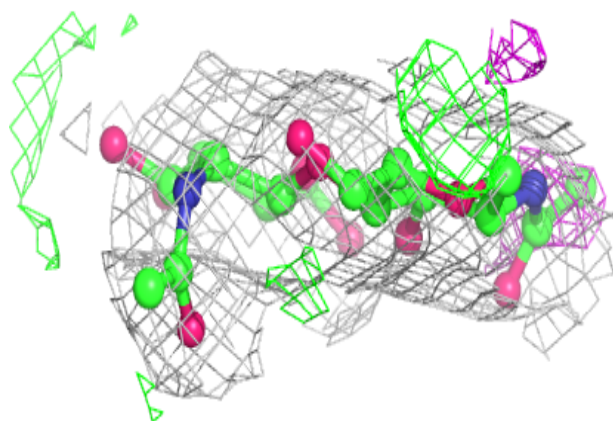
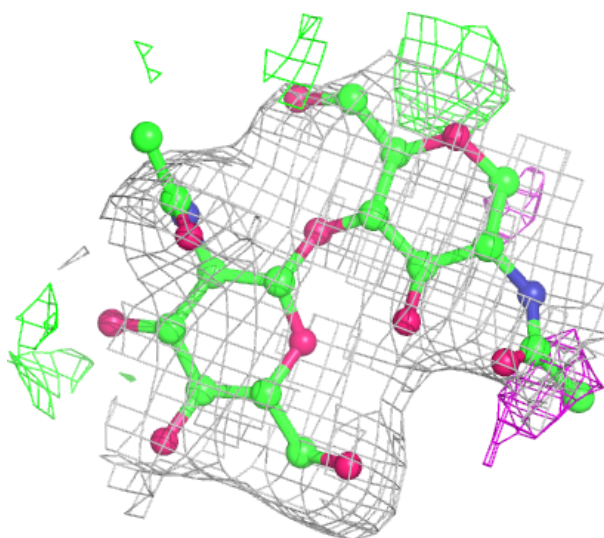
**Electron density around Chain L:**

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and green (positive)



**Electron density around Chain Q:**

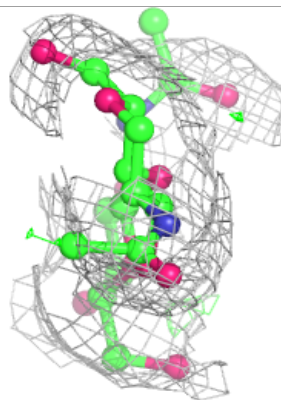
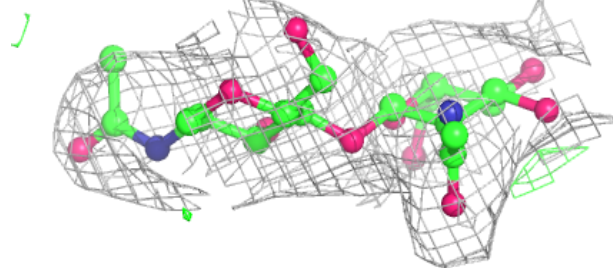
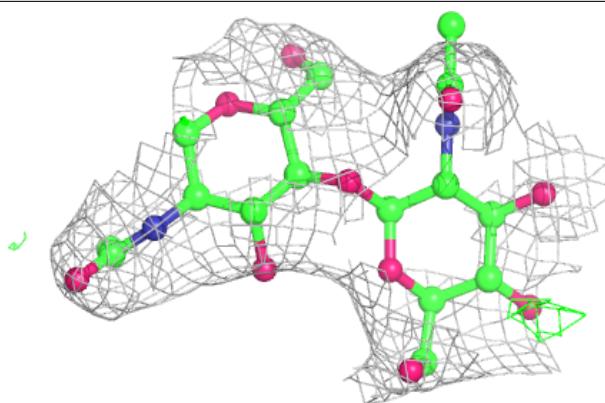
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





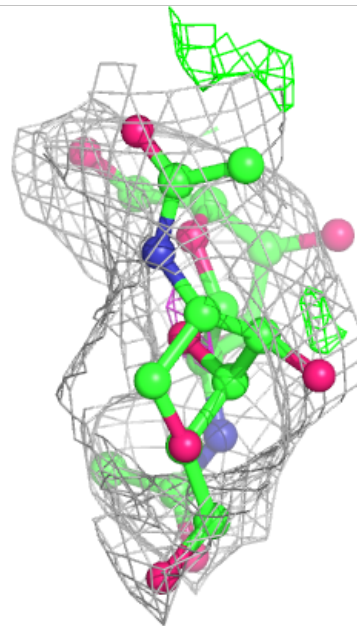
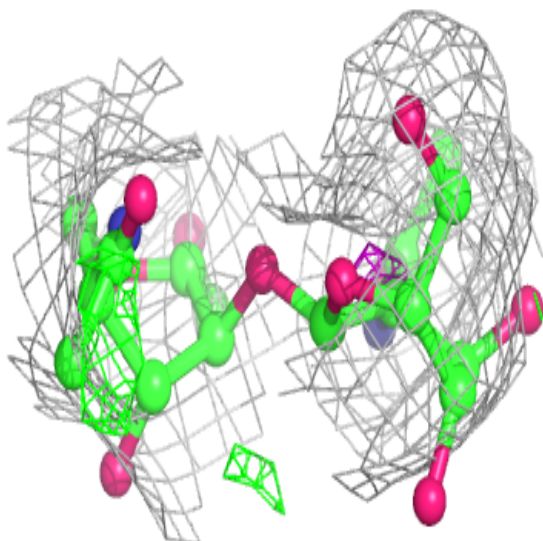
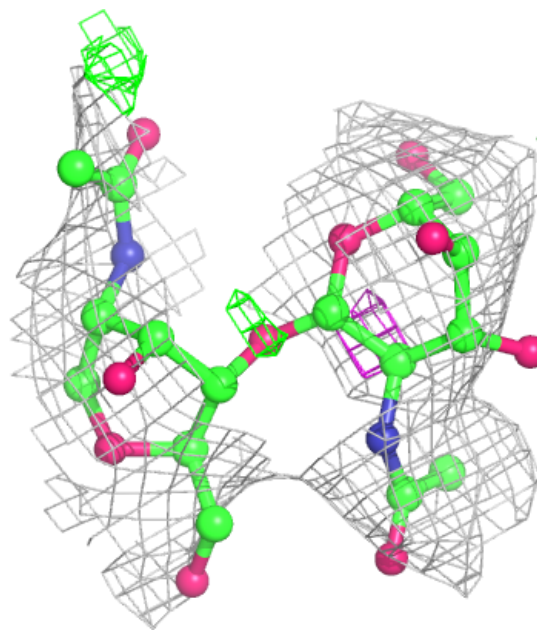
**Electron density around Chain R:**

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



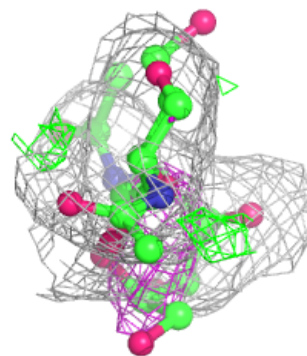
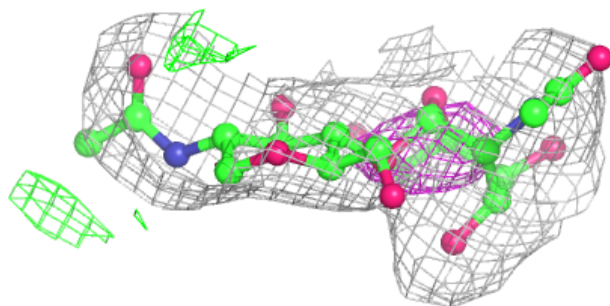
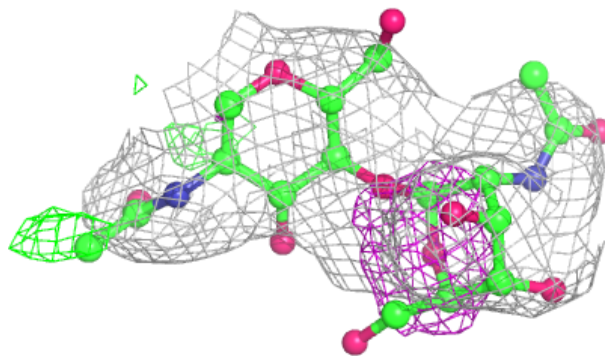
**Electron density around Chain S:**

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



**Electron density around Chain W:**

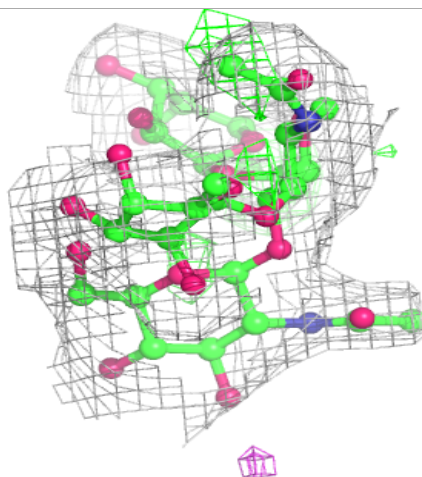
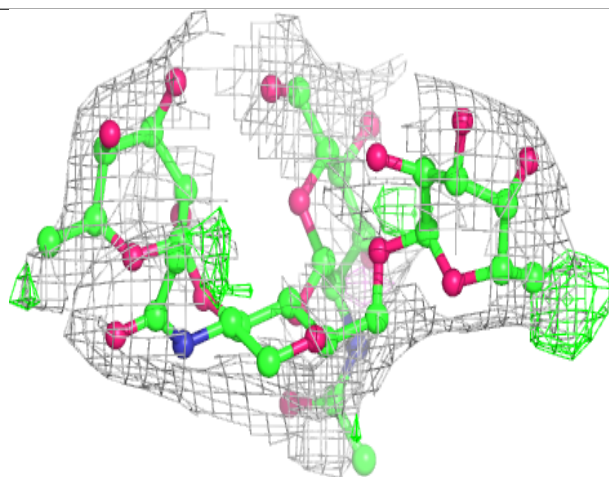
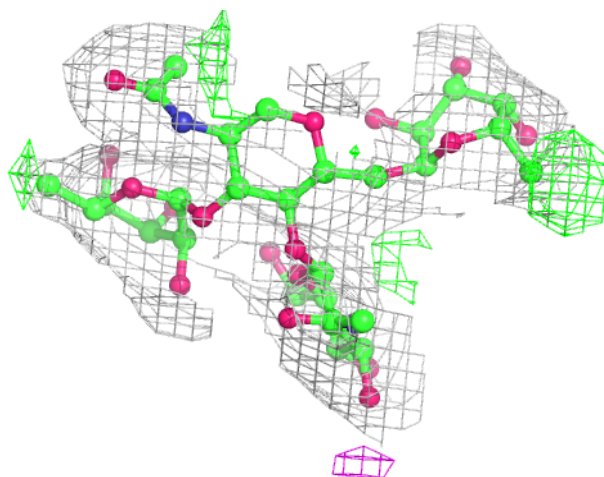
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





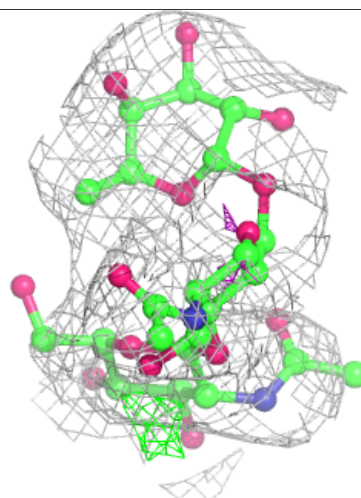
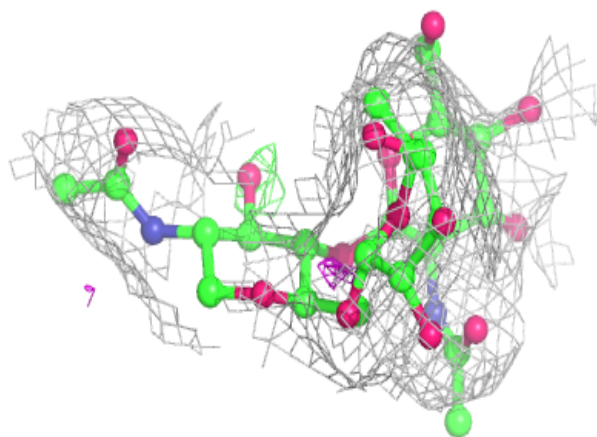
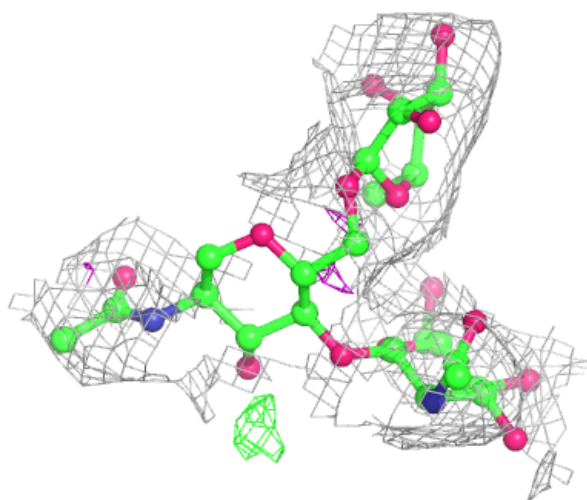
**Electron density around Chain H:**

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



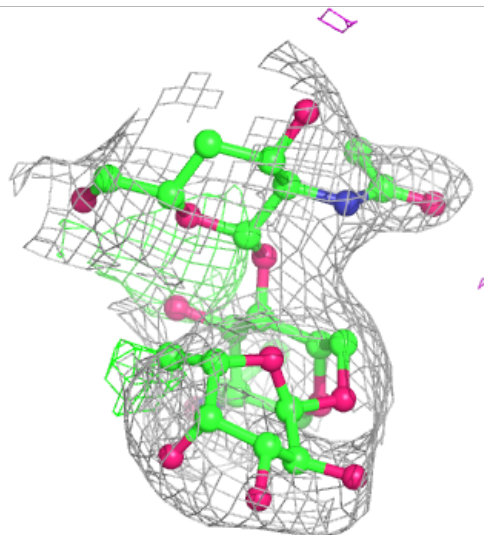
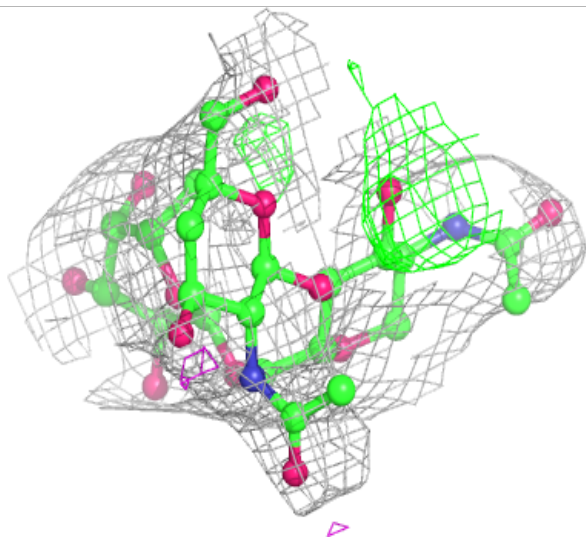
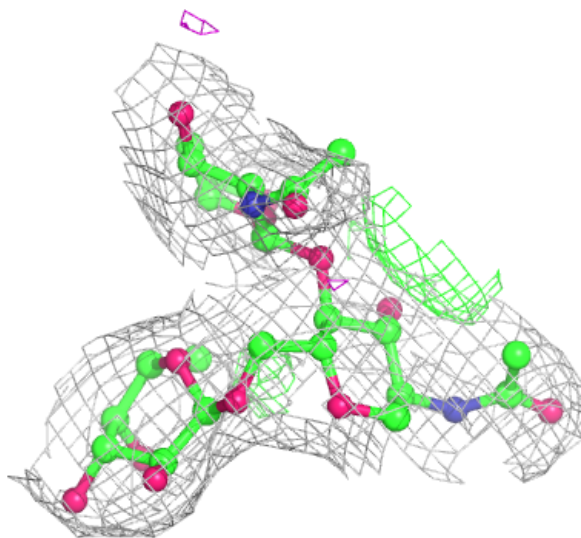
**Electron density around Chain M:**

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



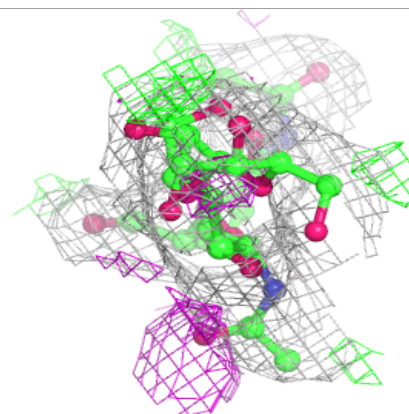
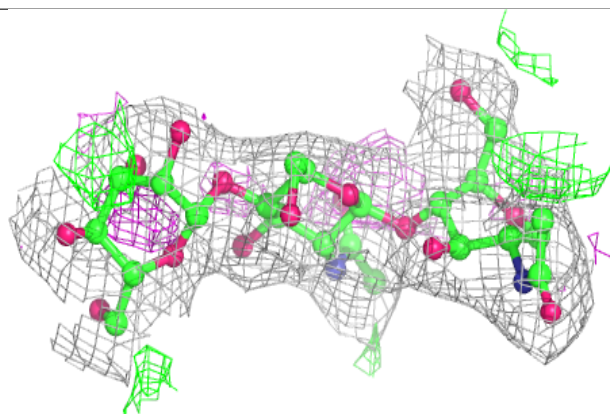
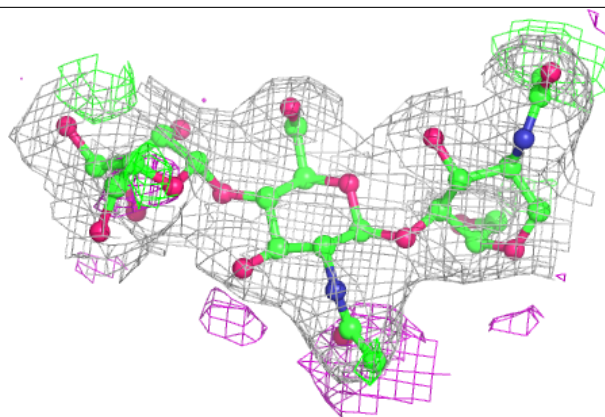
**Electron density around Chain O:**

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

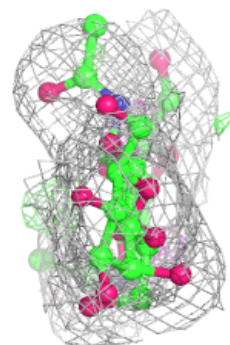
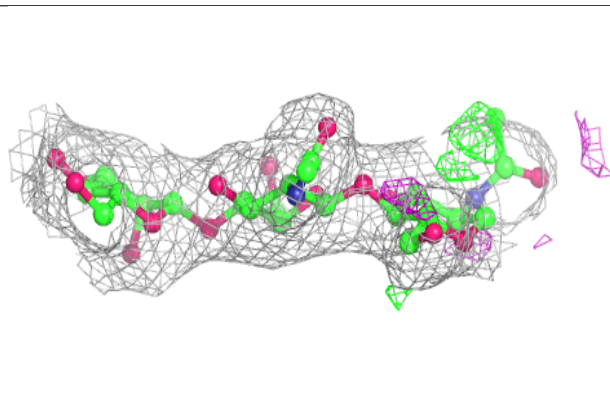
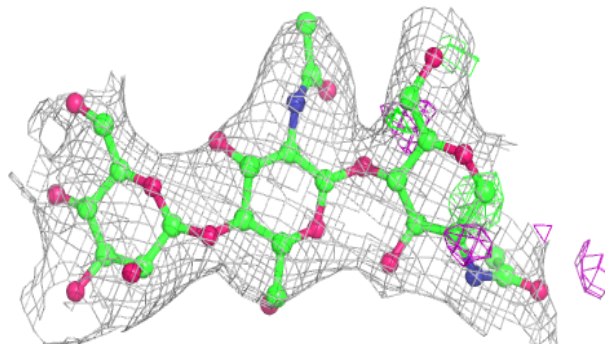


**Electron density around Chain N:**

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

**Electron density around Chain T:**

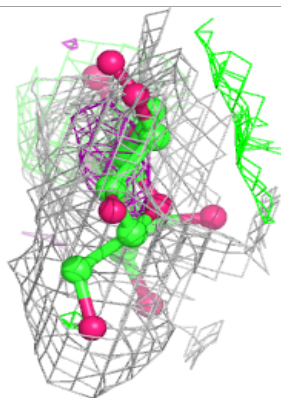
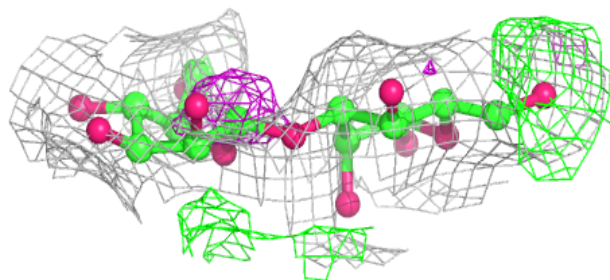
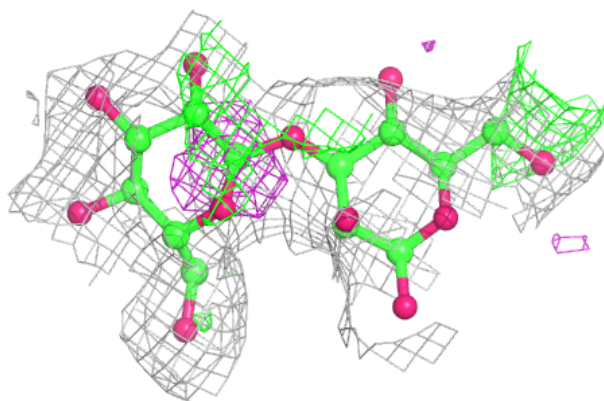
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



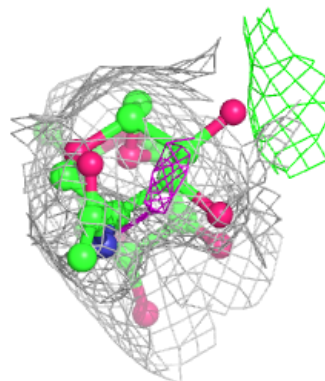
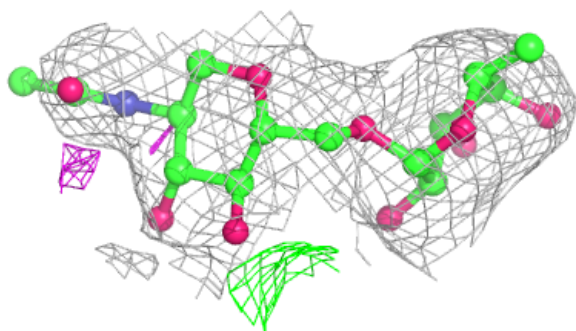
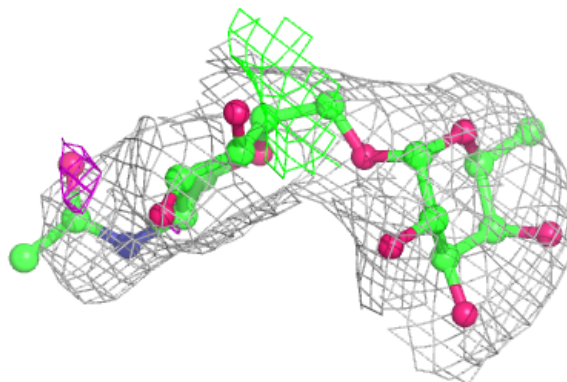


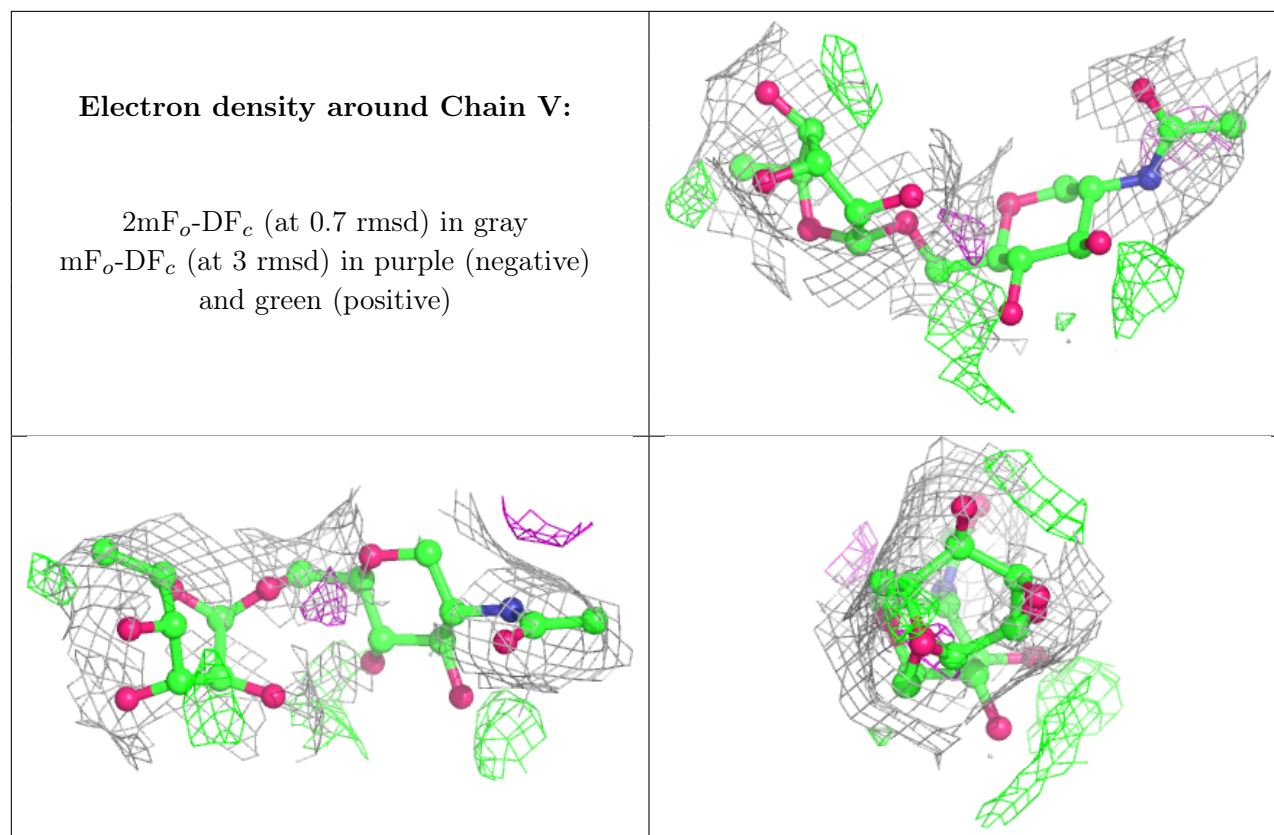
**Electron density around Chain P:**

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

**Electron density around Chain U:**

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





## 6.4 Ligands [i](#)

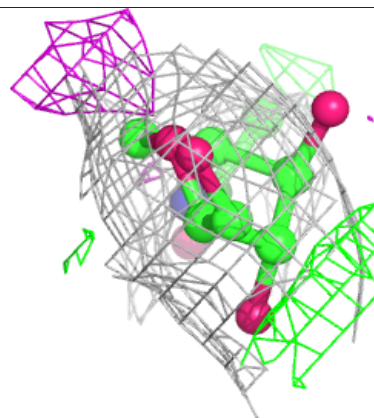
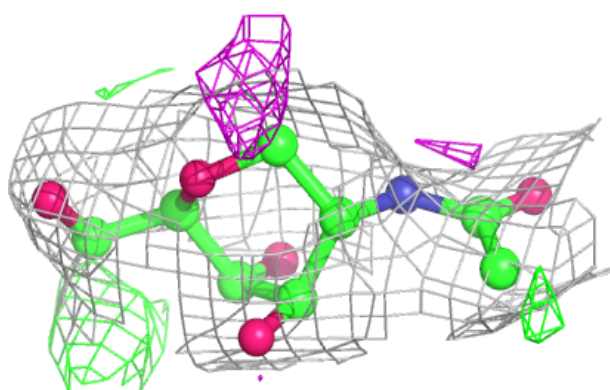
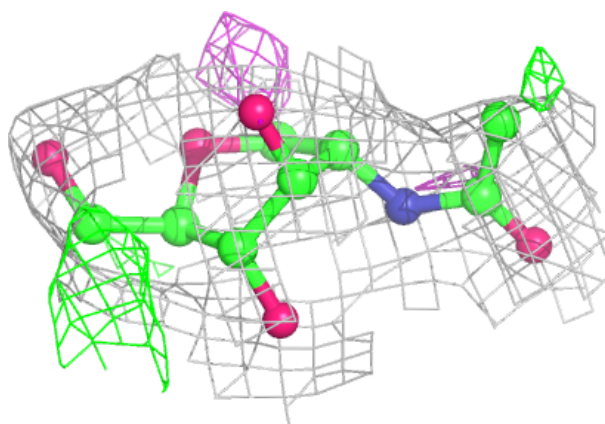
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
10	NAG	D	1403	14/15	0.50	0.20	76,92,101,101	0
10	NAG	D	1402	14/15	0.57	0.21	76,92,109,127	0
10	NAG	A	1603	14/15	0.58	0.19	98,107,113,130	0
11	BMA	B	301	12/12	0.60	0.14	82,82,82,82	0
10	NAG	A	1602	14/15	0.64	0.15	87,98,106,106	0
10	NAG	D	1405	14/15	0.74	0.14	72,82,94,96	0
10	NAG	D	1404	14/15	0.76	0.11	85,96,98,103	0
10	NAG	A	1601	14/15	0.77	0.15	86,99,105,110	0
10	NAG	D	1401	14/15	0.88	0.12	51,62,81,102	0

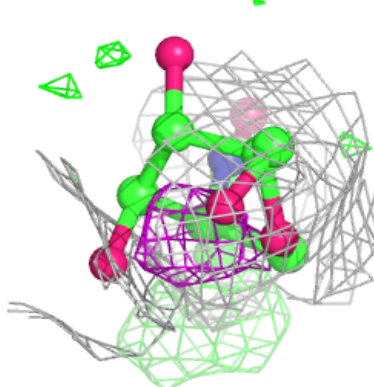
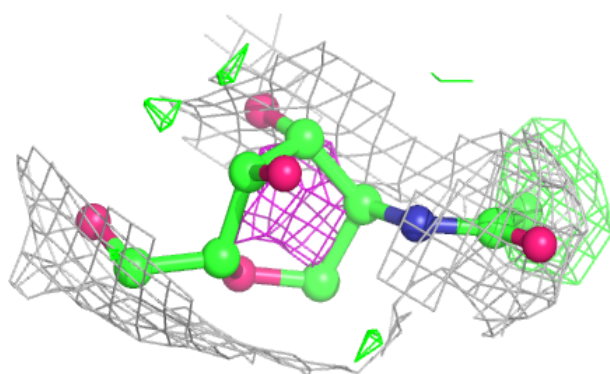
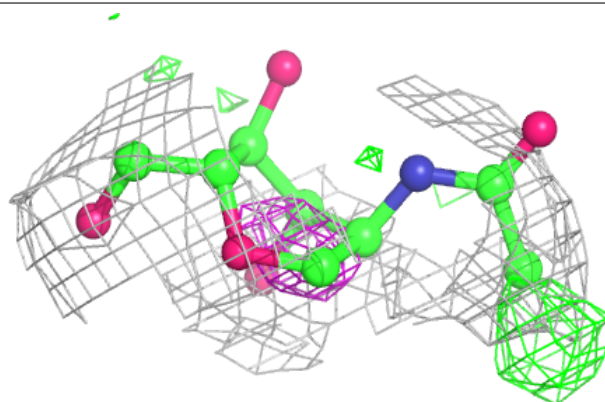
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAG D 1403:**

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

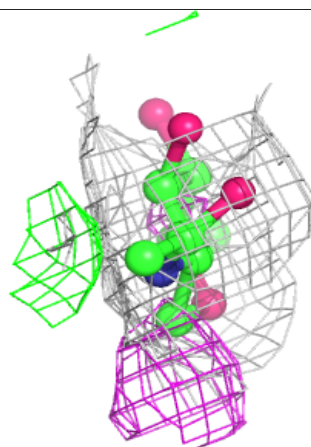
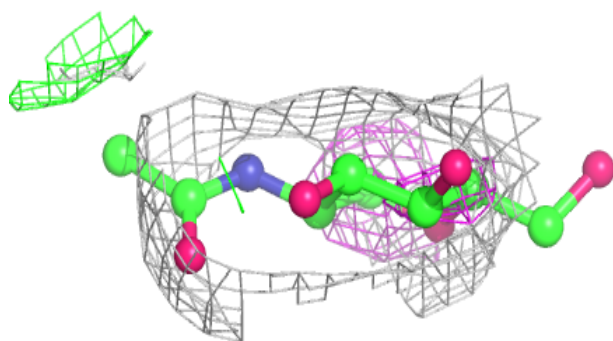
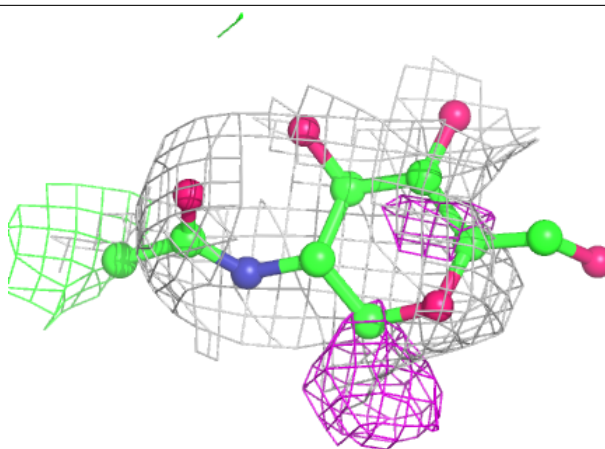
**Electron density around NAG D 1402:**

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



**Electron density around NAG A 1603:**

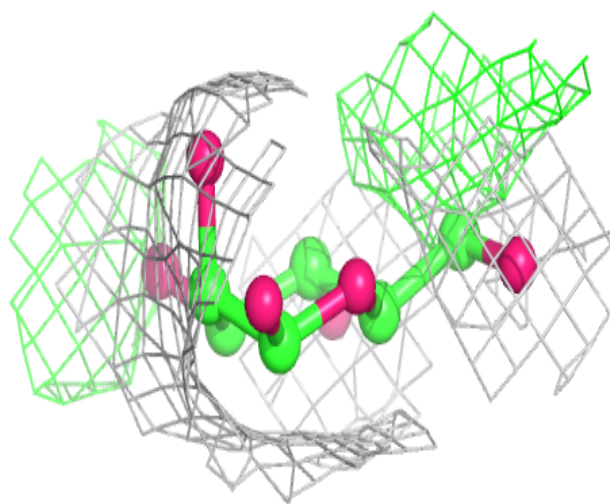
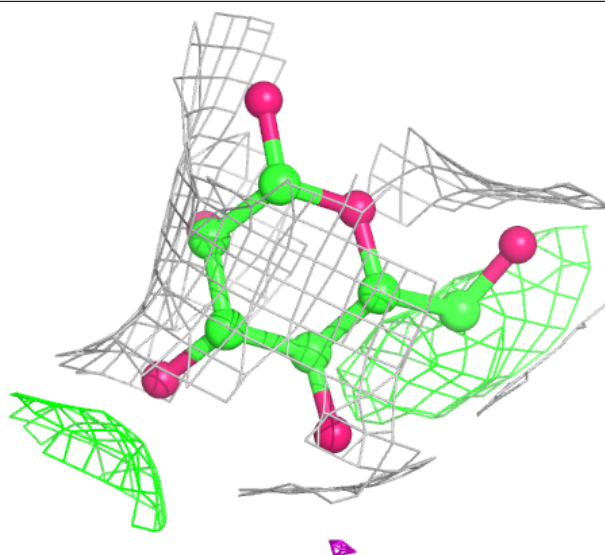
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





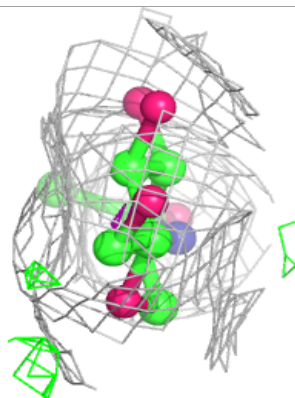
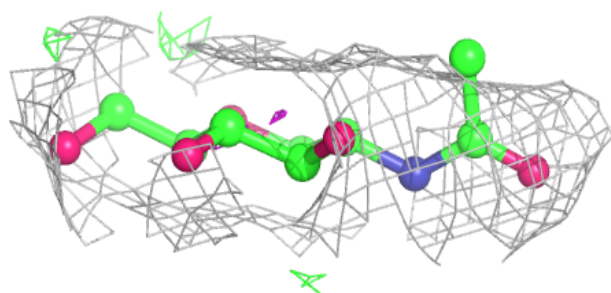
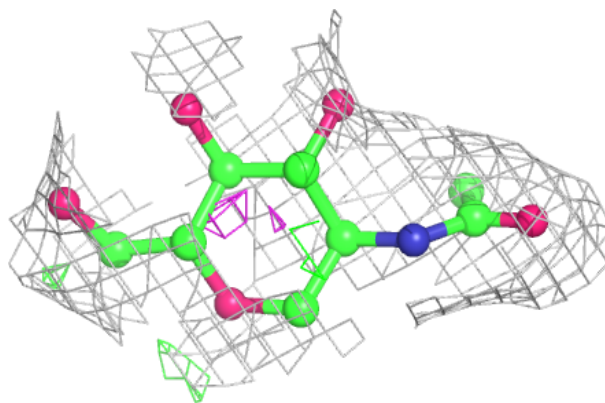
**Electron density around BMA B 301:**

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

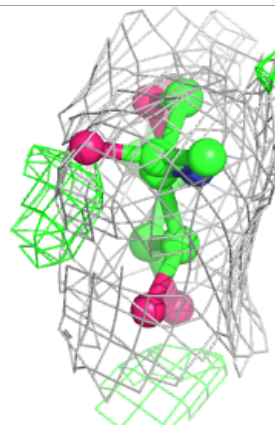
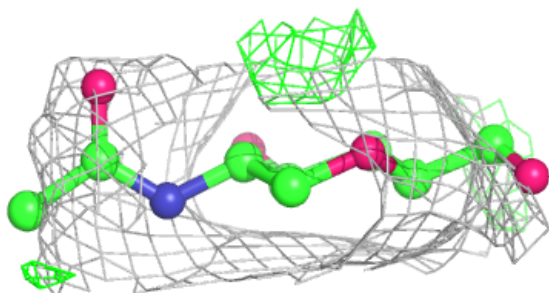
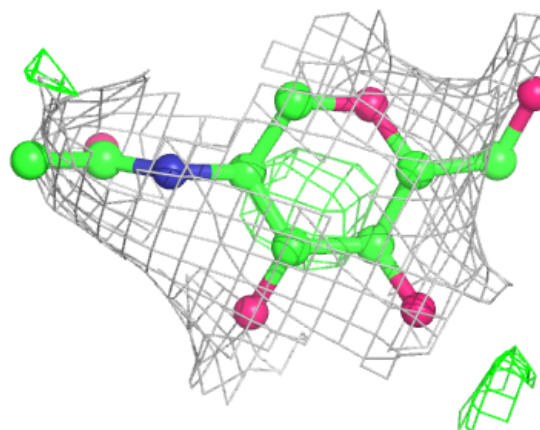


**Electron density around NAG A 1602:**

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

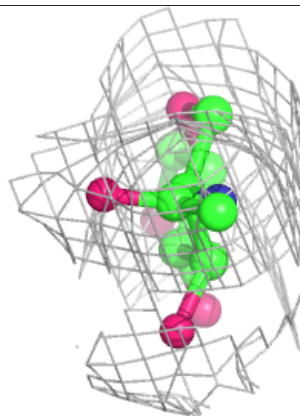
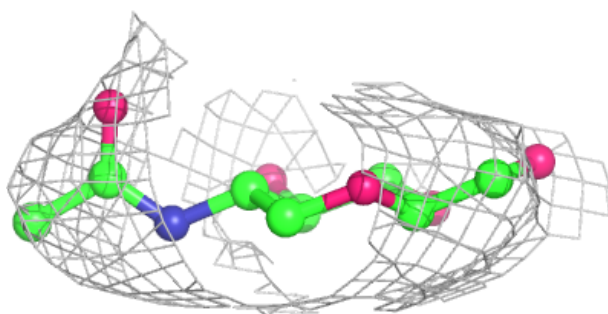
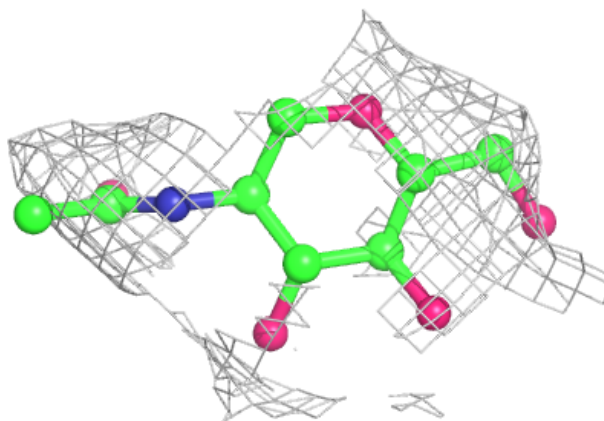
**Electron density around NAG D 1405:**

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



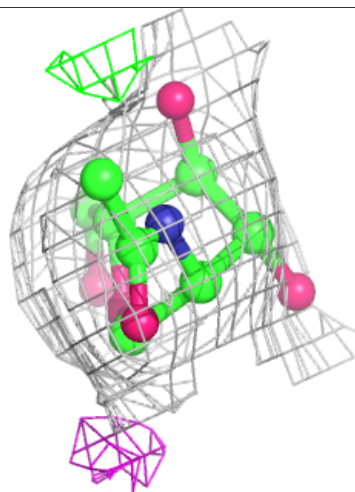
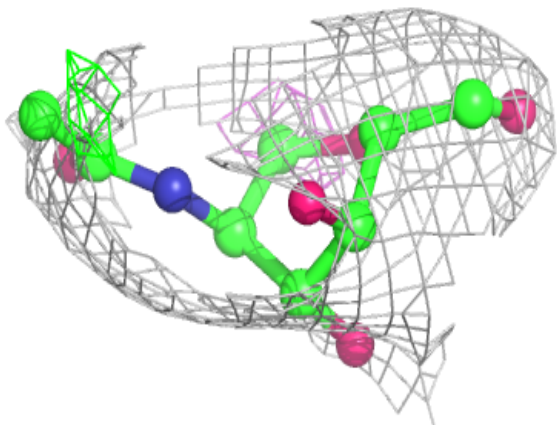
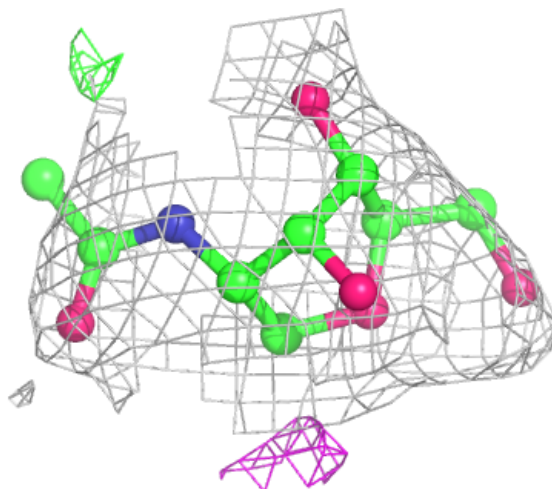
**Electron density around NAG D 1404:**

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



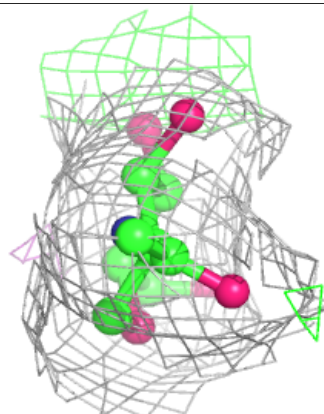
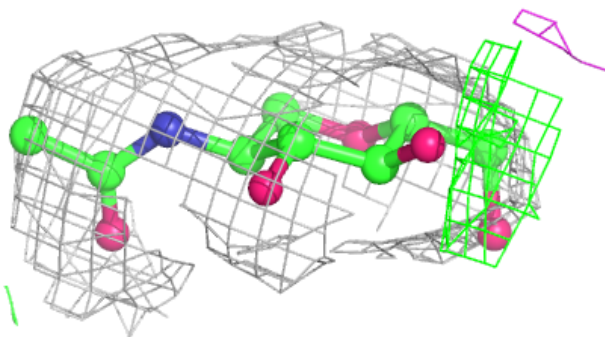
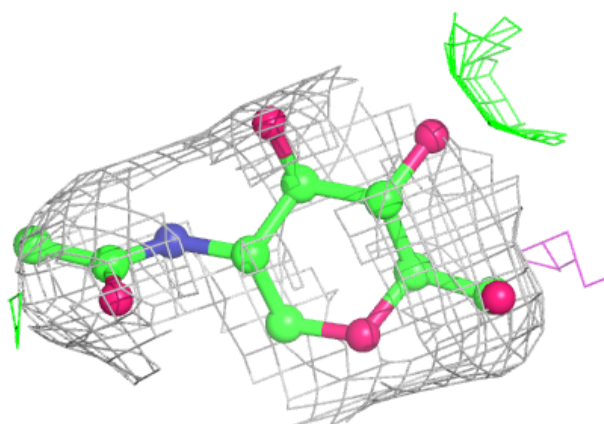
**Electron density around NAG A 1601:**

$2mF_o-DF_c$  (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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.