



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 5, 2022 – 12:18 am GMT

PDB ID : 7OL4  
Title : Mouse contactin-1 neurofascin-155 immunoglobulin domains adhesion complex  
Authors : Chataigner, L.M.P.; Janssen, B.J.C.  
Deposited on : 2021-05-19  
Resolution : 4.80 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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.3  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

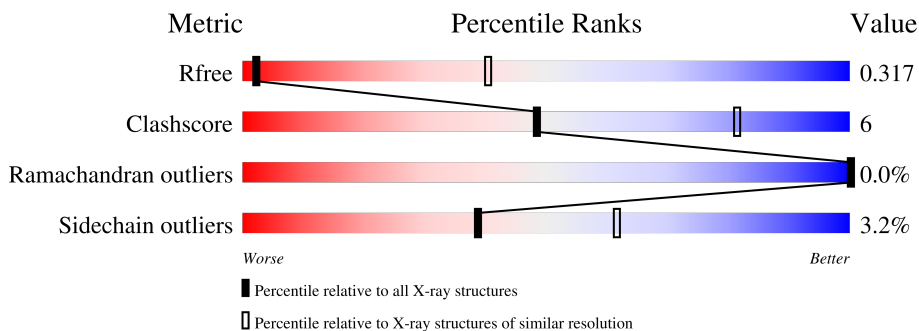
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.80 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 <sub>free</sub>	130704	1096 (5.80-3.80)
Clashscore	141614	1170 (5.80-3.80)
Ramachandran outliers	138981	1105 (5.80-3.80)
Sidechain outliers	138945	1085 (5.80-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	592	79% (green), 17% (yellow), 4% (orange), 2% (grey)
1	B	592	80% (green), 15% (yellow), 5% (orange), 0% (grey)
2	C	617	79% (green), 16% (yellow), 5% (orange), 0% (grey)
2	D	617	82% (green), 13% (yellow), 5% (orange), 0% (grey)
3	E	3	100% (green)
3	F	3	33% (green), 33% (yellow), 33% (orange)
3	H	3	100% (green)

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Mol	Chain	Length	Quality of chain
4	G	4	 75% 25%
4	P	4	 100%
5	I	4	 25% 50% 25%
6	J	6	 100%
7	K	6	 67% 17% 17%
8	L	5	 40% 20% 40%
9	M	7	 43% 57%
10	N	5	 40% 60%
10	R	5	 40% 40% 20%
11	O	5	 80% 20%
11	S	5	 60% 40%
12	Q	8	 25% 75%
13	T	4	 75% 25%

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 19300 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 Contactin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	570	Total	C	N	O	S	0	0	0
			4515	2879	759	852	25			
1	B	568	Total	C	N	O	S	0	0	0
			4498	2870	757	846	25			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP P12960
A	20	SER	-	expression tag	UNP P12960
A	433	VAL	ILE	conflict	UNP P12960
A	605	HIS	-	expression tag	UNP P12960
A	606	HIS	-	expression tag	UNP P12960
A	607	HIS	-	expression tag	UNP P12960
A	608	HIS	-	expression tag	UNP P12960
A	609	HIS	-	expression tag	UNP P12960
A	610	HIS	-	expression tag	UNP P12960
B	19	GLY	-	expression tag	UNP P12960
B	20	SER	-	expression tag	UNP P12960
B	433	VAL	ILE	conflict	UNP P12960
B	605	HIS	-	expression tag	UNP P12960
B	606	HIS	-	expression tag	UNP P12960
B	607	HIS	-	expression tag	UNP P12960
B	608	HIS	-	expression tag	UNP P12960
B	609	HIS	-	expression tag	UNP P12960
B	610	HIS	-	expression tag	UNP P12960

- Molecule 2 is a protein called Neurofascin.

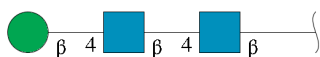
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	587	Total	C	N	O	S	0	0	0
			4648	2917	825	878	28			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	590	4668	2927	828	885	28	0	0	0

- Molecule 3 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
			Total	C	N	O			
3	E	3	39	22	2	15	0	0	0
3	F	3	39	22	2	15	0	0	0
3	H	3	39	22	2	15	0	0	0

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



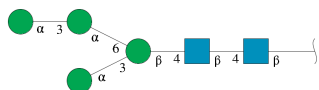
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	4	50	28	2	20	0	0	0
4	P	4	50	28	2	20	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



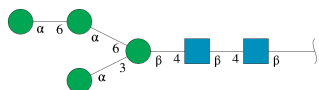
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	I	4	50	28	2	20	0	0	0

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



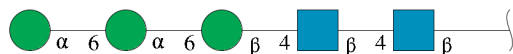
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	J	6	72	40	2	30	0	0	0

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



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

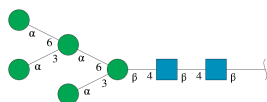
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

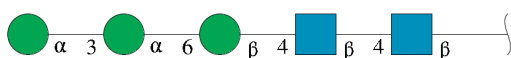
- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glu

copyranose.



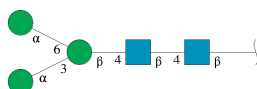
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	M	7	83	46	2	35	0	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



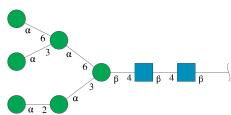
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	N	5	61	34	2	25	0	0	0
10	R	5	61	34	2	25	0	0	0

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



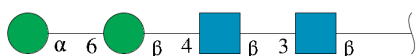
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	O	5	61	34	2	25	0	0	0
11	S	5	61	34	2	25	0	0	0

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



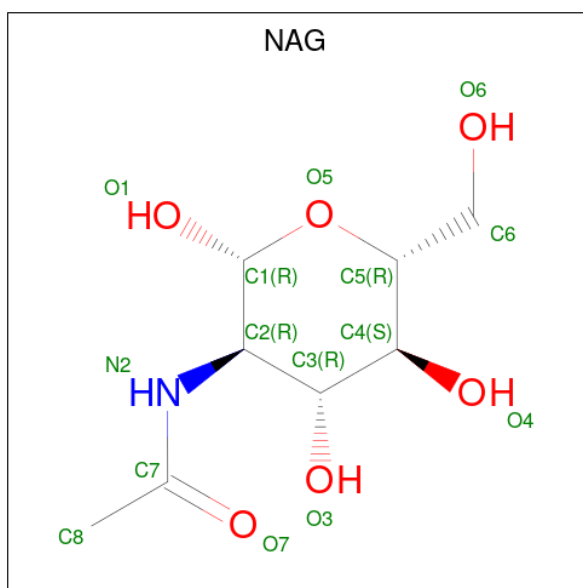
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	Q	8	94	52	2	40	0	0	0

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



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

- Molecule 14 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
			Total	C	N	O		
14	A	1	14	8	1	5	0	0
14	B	1	14	8	1	5	0	0

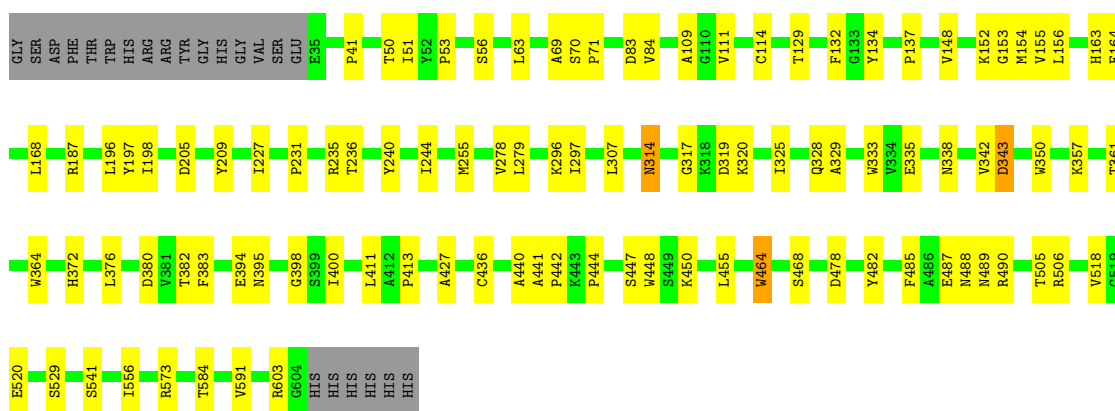


### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

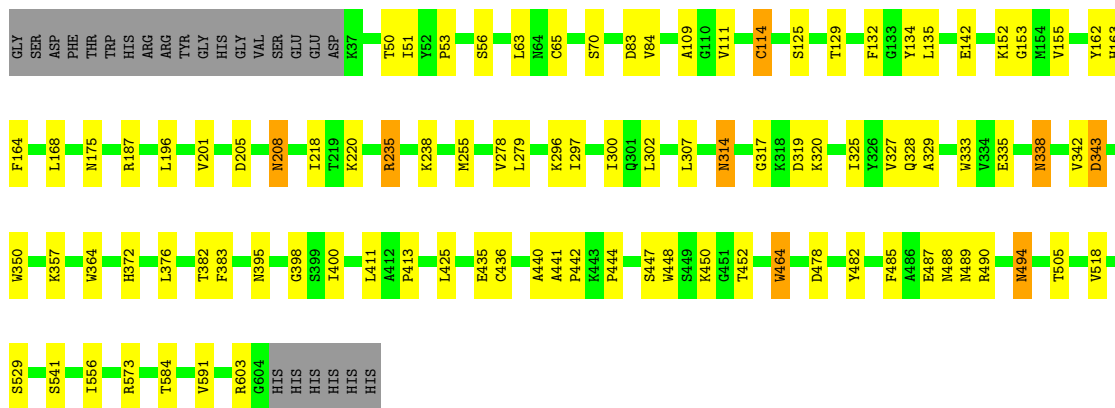
- Molecule 1: Contactin-1

Chain A:  79% 17%




- Molecule 1: Contactin-1

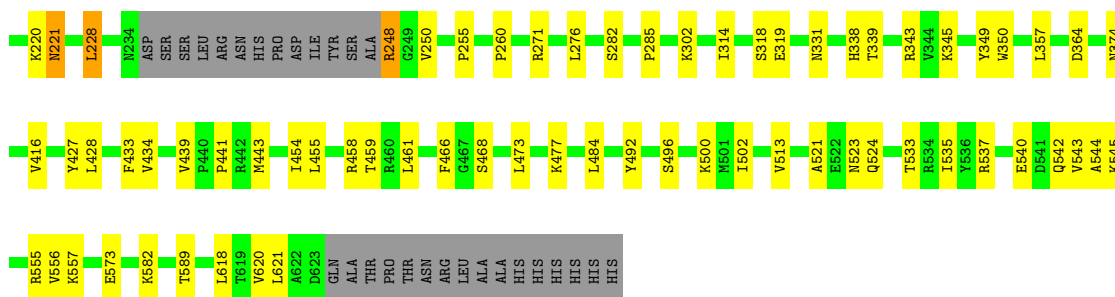
Chain B:  80% 15%



- Molecule 2: Neurofascin

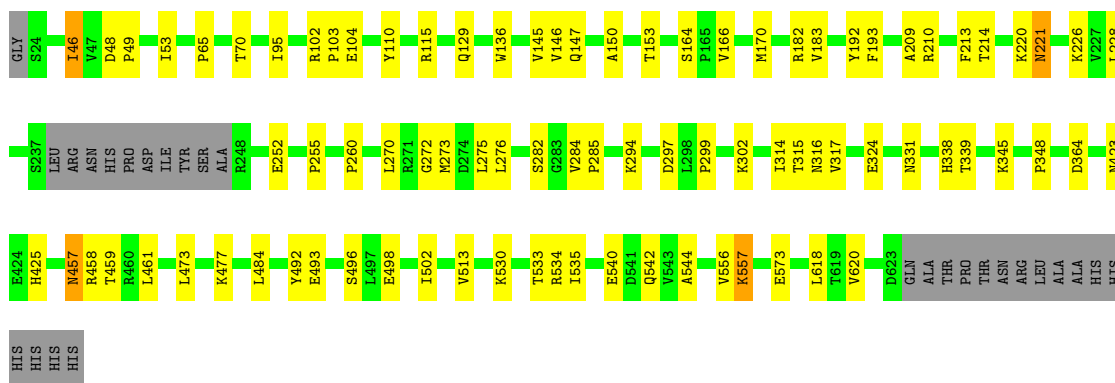
Chain C:  79% 16% 5%





- Molecule 2: Neurofascin

Chain D: 82% 13%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 33% 33% 33%

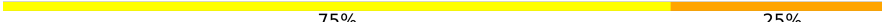


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 100%



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

Chain G:  75% 25%

MAG1  
MAG2  
BMA3  
MAN4

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

Chain P:  100%

MAG1  
MAG2  
BMA3  
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  25% 50% 25%

MAG1  
MAG2  
BMA3  
MAN4

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

Chain J:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

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

Chain K:  67% 17% 17%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

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

Chain L:  40% 20% 40%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  43% 57%



- Molecule 10: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  40% 60%




- Molecule 10: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  40% 40% 20%



- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  80% 20%

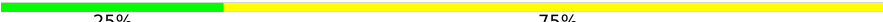


- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  60% 40%



- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  25% 75%



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

Chain T:



MAG1  
MAG2  
BMA3  
MAN4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.77Å 151.78Å 162.34Å 90.00° 111.78° 90.00°	Depositor
Resolution (Å)	75.38 – 4.80 75.89 – 4.80	Depositor EDS
% Data completeness (in resolution range)	48.0 (75.38-4.80) 48.1 (75.89-4.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 4.87Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, $R_{free}$	0.288 , 0.326 0.288 , 0.317	Depositor DCC
$R_{free}$ test set	794 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	103.8	Xtriage
Anisotropy	1.170	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.77	EDS
Total number of atoms	19300	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	259.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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, MAN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/4628	0.51	0/6291
1	B	0.25	0/4611	0.50	0/6268
2	C	0.25	0/4754	0.52	0/6450
2	D	0.25	0/4774	0.51	0/6477
All	All	0.25	0/18767	0.51	0/25486

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	4515	0	4412	60	1
1	B	4498	0	4402	54	0
2	C	4648	0	4577	56	0
2	D	4668	0	4591	48	0
3	E	39	0	34	0	0
3	F	39	0	34	1	0
3	H	39	0	34	0	0
4	G	50	0	43	2	0
4	P	50	0	43	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	50	0	43	3	0
6	J	72	0	61	0	0
7	K	72	0	61	4	0
8	L	61	0	52	1	0
9	M	83	0	70	0	0
10	N	61	0	52	1	0
10	R	61	0	52	1	0
11	O	61	0	52	2	0
11	S	61	0	52	0	0
12	Q	94	0	79	0	0
13	T	50	0	43	2	0
14	A	14	0	13	0	0
14	B	14	0	13	0	0
All	All	19300	0	18813	230	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (230) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:PRO:HD3	1:B:488:ASN:HD22	1.46	0.80
1:B:425:LEU:HB3	1:B:591:VAL:HG12	1.64	0.79
1:A:427:ALA:HB2	1:A:591:VAL:HB	1.64	0.78
1:A:413:PRO:HD3	1:A:488:ASN:HD22	1.47	0.78
11:O:1:NAG:H3	11:O:1:NAG:H83	1.71	0.71
7:K:2:NAG:H3	7:K:2:NAG:H83	1.77	0.67
2:C:147:GLN:HG2	2:C:228:LEU:HD12	1.75	0.67
1:B:300:ILE:HD11	1:B:327:VAL:HG22	1.80	0.64
1:A:154:MET:HG3	1:A:155:VAL:H	1.63	0.63
2:C:477:LYS:HB2	2:C:484:LEU:HD11	1.81	0.63
2:C:458:ARG:HG2	2:C:500:LYS:O	1.99	0.62
1:A:488:ASN:OD1	1:A:489:ASN:N	2.32	0.62
1:B:338:ASN:OD1	1:B:338:ASN:N	2.33	0.62
1:B:488:ASN:OD1	1:B:489:ASN:N	2.33	0.62
1:B:111:VAL:HG22	1:B:129:THR:HG22	1.82	0.62
1:B:314:ASN:HD21	1:B:317:GLY:H	1.46	0.62
1:A:314:ASN:HD21	1:A:317:GLY:H	1.46	0.61
1:A:342:VAL:HG12	1:A:343:ASP:H	1.64	0.61
1:B:342:VAL:HG12	1:B:343:ASP:H	1.66	0.60
1:A:109:ALA:HB2	1:A:132:PHE:HE2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:ASP:O	1:B:482:TYR:OH	2.16	0.59
2:C:416:VAL:HG22	2:C:433:PHE:HB3	1.84	0.59
1:A:111:VAL:HG22	1:A:129:THR:HG22	1.85	0.58
2:C:345:LYS:HB3	2:C:374:ASN:O	2.04	0.58
2:D:182:ARG:HG2	2:D:183:VAL:HG23	1.85	0.58
2:C:182:ARG:HG2	2:C:183:VAL:HG23	1.85	0.58
1:A:478:ASP:O	1:A:482:TYR:OH	2.15	0.58
1:B:135:LEU:HD13	1:B:220:LYS:HG2	1.84	0.58
2:C:461:LEU:O	2:C:496:SER:HA	2.03	0.58
2:D:270:LEU:HA	2:D:345:LYS:O	2.04	0.57
1:B:494:ASN:OD1	1:B:494:ASN:N	2.36	0.57
2:D:285:PRO:HD2	2:D:331:ASN:HD21	1.68	0.57
1:A:464:TRP:HA	4:G:1:NAG:H5	1.86	0.56
1:B:464:TRP:HA	7:K:1:NAG:H5	1.87	0.56
1:B:135:LEU:HD12	1:B:218:ILE:HD11	1.87	0.56
2:C:166:VAL:HB	2:C:210:ARG:HB3	1.87	0.56
1:A:137:PRO:HG2	2:C:50:ARG:HD3	1.88	0.56
1:A:156:LEU:HD13	1:A:227:ILE:HD12	1.87	0.56
2:C:285:PRO:HD2	2:C:331:ASN:HD21	1.71	0.56
2:C:535:ILE:HG12	2:C:556:VAL:HG22	1.86	0.55
1:B:411:LEU:H	1:B:441:ALA:HB2	1.72	0.55
5:I:1:NAG:H4	5:I:2:NAG:N2	2.22	0.55
1:A:235:ARG:HH11	1:A:236:THR:H	1.53	0.54
1:B:109:ALA:HB2	1:B:132:PHE:HE1	1.72	0.54
8:L:2:NAG:H3	8:L:5:MAN:H2	1.89	0.54
2:D:459:THR:HB	2:D:502:ILE:HD11	1.89	0.54
1:B:413:PRO:HB3	1:B:440:ALA:HB2	1.90	0.54
2:D:477:LYS:HB2	2:D:484:LEU:HD11	1.90	0.53
2:C:533:THR:HA	2:C:557:LYS:O	2.09	0.53
2:D:275:LEU:HD23	2:D:314:ILE:HD12	1.90	0.53
1:A:413:PRO:HB3	1:A:440:ALA:HB2	1.89	0.52
2:C:248:ARG:NH1	2:C:248:ARG:HA	2.24	0.52
2:D:535:ILE:HG12	2:D:556:VAL:HG22	1.90	0.52
1:A:411:LEU:H	1:A:441:ALA:HB2	1.74	0.52
2:C:492:TYR:OH	4:P:2:NAG:H82	2.09	0.52
2:D:49:PRO:HA	2:D:103:PRO:HG2	1.92	0.52
1:A:109:ALA:HB2	1:A:132:PHE:CE2	2.44	0.52
2:C:260:PRO:HB2	2:C:338:HIS:CE1	2.46	0.51
2:C:459:THR:HB	2:C:502:ILE:HD11	1.93	0.51
2:D:166:VAL:HB	2:D:210:ARG:HB3	1.92	0.51
2:C:345:LYS:HA	2:C:374:ASN:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:THR:O	2:D:110:TYR:HA	2.10	0.51
1:A:148:VAL:O	1:A:231:PRO:HA	2.12	0.50
1:B:364:TRP:CE3	1:B:376:LEU:HD22	2.46	0.50
2:C:443:MET:HG2	2:C:521:ALA:HB1	1.94	0.50
2:D:260:PRO:HB2	2:D:338:HIS:CE1	2.47	0.50
5:I:2:NAG:H3	5:I:2:NAG:H83	1.93	0.50
2:C:146:VAL:CG2	2:C:150:ALA:HB3	2.42	0.50
1:A:134:TYR:O	1:A:163:HIS:HA	2.12	0.50
2:C:248:ARG:HA	2:C:248:ARG:CZ	2.42	0.50
1:B:278:VAL:HG23	1:B:279:LEU:H	1.77	0.49
2:D:348:PRO:HD3	2:D:423:ASN:ND2	2.27	0.49
4:P:2:NAG:O7	4:P:2:NAG:O3	2.28	0.49
1:A:464:TRP:CE3	4:G:2:NAG:H82	2.48	0.49
10:R:3:BMA:H5	10:R:4:MAN:H5	1.94	0.49
1:A:278:VAL:HG23	1:A:279:LEU:H	1.78	0.49
7:K:1:NAG:H61	7:K:2:NAG:C7	2.42	0.48
1:B:505:THR:HA	1:B:529:SER:O	2.13	0.48
1:A:464:TRP:NE1	1:A:468:SER:OG	2.46	0.48
2:C:343:ARG:HD2	2:C:345:LYS:HE3	1.94	0.48
1:A:333:TRP:CE2	1:A:400:ILE:HD12	2.48	0.48
1:A:441:ALA:HB3	1:A:442:PRO:HD3	1.95	0.48
2:D:145:VAL:HG13	2:D:226:LYS:HB3	1.96	0.48
1:B:109:ALA:HB2	1:B:132:PHE:CE1	2.48	0.48
1:B:208:ASN:N	1:B:208:ASN:HD22	2.12	0.48
1:B:464:TRP:HE3	7:K:2:NAG:O7	1.96	0.48
2:C:544:ALA:O	2:C:620:VAL:HA	2.13	0.48
2:D:221:ASN:OD1	2:D:221:ASN:N	2.47	0.48
1:A:395:ASN:OD1	1:A:398:GLY:N	2.45	0.48
1:A:505:THR:HA	1:A:529:SER:O	2.14	0.48
2:C:146:VAL:O	2:C:228:LEU:HG	2.14	0.47
2:D:147:GLN:HG2	2:D:228:LEU:HD12	1.95	0.47
3:F:1:NAG:H62	3:F:2:NAG:C7	2.44	0.47
1:A:154:MET:HG3	1:A:155:VAL:N	2.28	0.47
1:B:278:VAL:HG21	1:B:307:LEU:HB2	1.97	0.47
2:D:146:VAL:CG2	2:D:150:ALA:HB3	2.44	0.47
2:D:166:VAL:O	2:D:209:ALA:HA	2.14	0.47
1:A:235:ARG:O	1:A:236:THR:OG1	2.32	0.47
1:B:333:TRP:CE2	1:B:400:ILE:HD12	2.49	0.47
2:C:43:LYS:NZ	2:C:427:TYR:O	2.48	0.47
1:A:447:SER:OG	1:A:485:PHE:HB2	2.13	0.47
1:B:328:GLN:HA	1:B:357:LYS:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:ALA:HB3	1:B:442:PRO:HD3	1.96	0.47
2:C:70:THR:O	2:C:110:TYR:HA	2.15	0.47
1:B:255:MET:N	1:B:328:GLN:O	2.48	0.47
1:A:361:THR:OG1	1:A:394:GLU:O	2.31	0.47
13:T:1:NAG:O7	13:T:1:NAG:H3	2.15	0.47
1:B:447:SER:OG	1:B:485:PHE:HB2	2.14	0.46
2:C:46:ILE:HD12	2:C:213:PHE:CE1	2.50	0.46
2:C:136:TRP:CH2	2:C:220:LYS:HD2	2.50	0.46
2:D:275:LEU:HB2	2:D:317:VAL:HG11	1.95	0.46
1:A:319:ASP:OD1	1:A:320:LYS:N	2.48	0.46
2:C:454:ILE:HD12	2:C:455:LEU:N	2.31	0.46
2:D:136:TRP:CH2	2:D:220:LYS:HD2	2.50	0.46
1:B:436:CYS:HB2	1:B:448:TRP:CZ2	2.51	0.46
1:A:278:VAL:HG21	1:A:307:LEU:HB2	1.96	0.46
2:C:302:LYS:HD3	2:C:314:ILE:HG23	1.98	0.46
1:A:83:ASP:OD1	1:A:84:VAL:N	2.49	0.46
1:B:485:PHE:CD1	1:B:494:ASN:HB3	2.51	0.46
2:C:271:ARG:HD3	2:C:349:TYR:CE2	2.49	0.46
1:A:53:PRO:HB2	1:A:56:SER:HB2	1.98	0.46
1:B:153:GLY:HA2	1:B:201:VAL:HG23	1.98	0.46
2:C:439:VAL:H	2:C:468:SER:HB2	1.81	0.46
2:D:345:LYS:HB3	2:D:425:HIS:NE2	2.30	0.45
11:O:1:NAG:H3	11:O:1:NAG:C8	2.43	0.45
1:B:83:ASP:OD1	1:B:84:VAL:N	2.48	0.45
1:A:328:GLN:HA	1:A:357:LYS:HG2	1.96	0.45
1:A:163:HIS:CD2	1:A:168:LEU:HD11	2.51	0.45
1:A:255:MET:N	1:A:328:GLN:O	2.48	0.45
2:C:49:PRO:HA	2:C:103:PRO:HG2	1.98	0.45
2:D:252:GLU:HA	2:D:284:VAL:HG11	1.98	0.45
2:D:544:ALA:O	2:D:620:VAL:HA	2.16	0.45
2:C:166:VAL:O	2:C:209:ALA:HA	2.16	0.45
2:C:473:LEU:HA	2:C:513:VAL:O	2.17	0.45
2:D:473:LEU:HA	2:D:513:VAL:O	2.17	0.45
1:B:235:ARG:CZ	1:B:235:ARG:HA	2.47	0.45
2:C:318:SER:HB3	10:N:1:NAG:H81	1.99	0.45
1:B:395:ASN:OD1	1:B:398:GLY:N	2.46	0.45
1:A:152:LYS:HE2	1:A:240:TYR:CZ	2.53	0.44
1:B:329:ALA:HB3	1:B:357:LYS:H	1.81	0.44
2:C:183:VAL:HG22	2:C:193:PHE:HA	1.99	0.44
2:C:350:TRP:NE1	2:C:428:LEU:HD13	2.31	0.44
1:A:244:ILE:HG13	1:A:319:ASP:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ARG:NH2	1:A:205:ASP:OD1	2.49	0.44
1:B:319:ASP:OD1	1:B:320:LYS:N	2.50	0.44
2:D:299:PRO:HB2	2:D:302:LYS:HG2	1.99	0.44
2:C:543:VAL:HG12	2:C:621:LEU:HD11	1.99	0.44
2:D:492:TYR:CD2	13:T:1:NAG:H61	2.52	0.44
2:D:542:GLN:HG3	2:D:618:LEU:HD13	2.00	0.44
1:A:70:SER:OG	1:A:71:PRO:HD3	2.18	0.44
1:A:329:ALA:HB3	1:A:357:LYS:H	1.82	0.44
2:D:294:LYS:HB2	2:D:324:GLU:HB2	1.99	0.44
1:A:364:TRP:CE3	1:A:376:LEU:HD22	2.53	0.44
2:D:183:VAL:HG22	2:D:193:PHE:HA	1.99	0.44
2:C:248:ARG:NH1	2:C:250:VAL:HG12	2.33	0.44
2:C:542:GLN:HG3	2:C:618:LEU:HD13	1.99	0.44
2:D:46:ILE:HA	2:D:129:GLN:O	2.18	0.44
1:A:63:LEU:HD23	1:A:63:LEU:HA	1.83	0.43
1:B:53:PRO:HB2	1:B:56:SER:HB2	2.00	0.43
2:C:357:LEU:HB2	2:C:434:VAL:HG22	2.00	0.43
1:A:153:GLY:HA3	1:A:198:ILE:O	2.19	0.43
2:C:221:ASN:OD1	2:C:221:ASN:N	2.49	0.43
2:D:533:THR:HA	2:D:557:LYS:O	2.19	0.43
1:B:556:ILE:O	1:B:573:ARG:NH2	2.51	0.43
1:B:134:TYR:O	1:B:163:HIS:HA	2.19	0.43
2:D:270:LEU:O	2:D:273:MET:HB2	2.19	0.43
1:B:187:ARG:NH2	1:B:205:ASP:OD1	2.50	0.43
2:C:35:PRO:HA	2:C:60:LYS:O	2.19	0.43
1:A:444:PRO:HB3	1:A:488:ASN:HA	2.00	0.43
1:B:63:LEU:HD23	1:B:63:LEU:HA	1.83	0.43
2:D:48:ASP:OD2	2:D:214:THR:HA	2.19	0.43
2:D:65:PRO:HA	2:D:115:ARG:O	2.18	0.43
1:A:155:VAL:HG22	1:A:197:TYR:HA	2.01	0.42
1:A:444:PRO:HB2	1:A:487:GLU:O	2.19	0.42
1:A:436:CYS:HB2	1:A:448:TRP:CZ2	2.53	0.42
2:C:72:ASN:HD22	2:C:109:GLU:HB2	1.84	0.42
1:A:518:VAL:HG13	1:A:603:ARG:O	2.19	0.42
1:A:556:ILE:O	1:A:573:ARG:NH2	2.53	0.42
2:D:53:ILE:HG22	2:D:95:ILE:HB	2.02	0.42
1:B:114:CYS:HB3	1:B:125:SER:OG	2.20	0.42
2:D:255:PRO:HA	2:D:282:SER:O	2.19	0.42
1:A:205:ASP:O	1:A:209:TYR:OH	2.31	0.42
2:C:71:ARG:HA	2:C:109:GLU:O	2.20	0.42
2:C:153:THR:HG23	2:C:192:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:272:GLY:HA2	2:D:316:ASN:HB2	2.00	0.42
2:D:348:PRO:HD3	2:D:423:ASN:HD21	1.84	0.42
5:I:1:NAG:O4	5:I:2:NAG:H2	2.20	0.42
1:A:450:LYS:HB2	1:A:455:LEU:HD11	2.01	0.42
2:D:458:ARG:NH1	2:D:498:GLU:OE2	2.52	0.42
1:A:155:VAL:HA	1:A:196:LEU:O	2.19	0.42
1:B:163:HIS:CD2	1:B:168:LEU:HD11	2.54	0.42
2:C:65:PRO:HA	2:C:115:ARG:O	2.20	0.42
1:A:296:LYS:O	1:A:297:ILE:HD13	2.19	0.42
2:D:153:THR:HG23	2:D:192:TYR:CE1	2.53	0.42
1:B:444:PRO:HB3	1:B:488:ASN:HA	2.02	0.42
1:B:518:VAL:HG13	1:B:603:ARG:O	2.20	0.42
2:D:457:ASN:HD22	2:D:457:ASN:HA	1.45	0.42
1:A:541:SER:OG	1:A:584:THR:HB	2.20	0.41
2:C:53:ILE:HG22	2:C:95:ILE:HB	2.01	0.41
4:P:3:BMA:H61	4:P:4:MAN:H2	1.79	0.41
1:A:325:ILE:HD13	1:A:325:ILE:HA	1.85	0.41
2:C:165:PRO:HB2	2:C:209:ALA:HB1	2.02	0.41
1:A:278:VAL:HG23	1:A:279:LEU:N	2.35	0.41
2:D:46:ILE:HD12	2:D:213:PHE:HE2	1.85	0.41
1:B:296:LYS:O	1:B:297:ILE:HD13	2.20	0.41
2:D:535:ILE:HG23	2:D:556:VAL:HG22	2.03	0.41
1:A:50:THR:C	1:A:51:ILE:HG13	2.41	0.41
2:D:294:LYS:HD2	2:D:324:GLU:HG3	2.03	0.41
2:D:458:ARG:HD2	2:D:498:GLU:OE2	2.20	0.41
1:B:541:SER:OG	1:B:584:THR:HB	2.20	0.41
1:A:154:MET:CG	1:A:155:VAL:H	2.31	0.41
1:B:325:ILE:HD13	1:B:325:ILE:HA	1.86	0.41
2:C:136:TRP:CH2	2:C:158:PRO:HA	2.56	0.41
1:B:278:VAL:HG23	1:B:279:LEU:N	2.36	0.41
2:C:255:PRO:HA	2:C:282:SER:O	2.20	0.41
1:B:50:THR:C	1:B:51:ILE:HG13	2.41	0.41
2:C:537:ARG:HB2	2:C:555:ARG:HB2	2.03	0.41
2:D:314:ILE:HG22	2:D:315:THR:N	2.36	0.41
2:D:461:LEU:O	2:D:496:SER:HA	2.21	0.41
1:B:155:VAL:HA	1:B:196:LEU:O	2.20	0.40
2:D:297:ASP:OD1	2:D:297:ASP:N	2.54	0.40
1:A:41:PRO:HA	1:A:69:ALA:HB2	2.02	0.40
2:C:441:PRO:HA	2:C:466:PHE:O	2.21	0.40
2:D:102:ARG:NH2	2:D:104:GLU:OE2	2.54	0.40
1:B:134:TYR:CE1	1:B:162:TYR:HB2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:319:GLU:OE1	2:C:319:GLU:N	2.52	0.40
2:C:582:LYS:HB3	2:C:589:THR:OG1	2.22	0.40
1:B:450:LYS:O	1:B:452:THR:N	2.52	0.40
2:C:523:ASN:OD1	2:C:524:GLN:N	2.55	0.40
1:B:444:PRO:HB2	1:B:487:GLU:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LYS:NZ	1:A:380:ASP:OD2[2_656]	2.17	0.03

## 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	568/592 (96%)	521 (92%)	47 (8%)	0	100	100
1	B	566/592 (96%)	520 (92%)	45 (8%)	1 (0%)	47	81
2	C	583/617 (94%)	546 (94%)	37 (6%)	0	100	100
2	D	586/617 (95%)	556 (95%)	30 (5%)	0	100	100
All	All	2303/2418 (95%)	2143 (93%)	159 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	175	ASN

### 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	494/513 (96%)	480 (97%)	14 (3%)	43	65
1	B	492/513 (96%)	470 (96%)	22 (4%)	27	53
2	C	520/545 (95%)	506 (97%)	14 (3%)	44	66
2	D	523/545 (96%)	509 (97%)	14 (3%)	44	66
All	All	2029/2116 (96%)	1965 (97%)	64 (3%)	39	61

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	CYS
1	A	164	PHE
1	A	314	ASN
1	A	335	GLU
1	A	338	ASN
1	A	343	ASP
1	A	350	TRP
1	A	372	HIS
1	A	382	THR
1	A	383	PHE
1	A	464	TRP
1	A	490	ARG
1	A	506	ARG
1	A	520	GLU
1	B	65	CYS
1	B	70	SER
1	B	114	CYS
1	B	142	GLU
1	B	152	LYS
1	B	164	PHE
1	B	208	ASN
1	B	235	ARG
1	B	238	LYS
1	B	302	LEU

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Mol	Chain	Res	Type
1	B	314	ASN
1	B	335	GLU
1	B	338	ASN
1	B	343	ASP
1	B	350	TRP
1	B	372	HIS
1	B	382	THR
1	B	383	PHE
1	B	435	GLU
1	B	464	TRP
1	B	490	ARG
1	B	494	ASN
2	C	46	ILE
2	C	72	ASN
2	C	155	GLN
2	C	164	SER
2	C	170	MET
2	C	221	ASN
2	C	228	LEU
2	C	248	ARG
2	C	276	LEU
2	C	339	THR
2	C	364	ASP
2	C	540	GLU
2	C	545	LYS
2	C	573	GLU
2	D	46	ILE
2	D	164	SER
2	D	170	MET
2	D	221	ASN
2	D	276	LEU
2	D	339	THR
2	D	364	ASP
2	D	457	ASN
2	D	493	GLU
2	D	530	LYS
2	D	534	ARG
2	D	540	GLU
2	D	557	LYS
2	D	573	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:



Mol	Chain	Res	Type
2	C	72	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

77 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	$\# Z  > 2$
3	NAG	E	1	1,3	14,14,15	0.30	0	17,19,21	0.54	0
3	NAG	E	2	3	14,14,15	0.49	0	17,19,21	0.52	0
3	BMA	E	3	3	11,11,12	0.70	0	15,15,17	0.74	0
3	NAG	F	1	1,3	14,14,15	0.23	0	17,19,21	0.52	0
3	NAG	F	2	3	14,14,15	0.39	0	17,19,21	1.00	1 (5%)
3	BMA	F	3	3	11,11,12	0.76	0	15,15,17	0.82	0
4	NAG	G	1	4,1	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	G	2	4	14,14,15	0.42	0	17,19,21	0.91	1 (5%)
4	BMA	G	3	4	11,11,12	1.05	1 (9%)	15,15,17	1.61	1 (6%)
4	MAN	G	4	4	11,11,12	0.91	1 (9%)	15,15,17	0.98	0
3	NAG	H	1	1,3	14,14,15	0.29	0	17,19,21	0.67	0
3	NAG	H	2	3	14,14,15	0.59	0	17,19,21	0.54	0
3	BMA	H	3	3	11,11,12	0.59	0	15,15,17	0.73	0
5	NAG	I	1	5,1	14,14,15	0.59	0	17,19,21	0.83	0
5	NAG	I	2	5	14,14,15	1.63	2 (14%)	17,19,21	1.38	2 (11%)
5	BMA	I	3	5	11,11,12	0.99	0	15,15,17	0.92	0
5	MAN	I	4	5	11,11,12	0.73	0	15,15,17	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	J	1	1,6	14,14,15	1.31	1 (7%)	17,19,21	1.24	1 (5%)
6	NAG	J	2	6	14,14,15	0.80	0	17,19,21	1.57	2 (11%)
6	BMA	J	3	6	11,11,12	1.68	4 (36%)	15,15,17	1.01	1 (6%)
6	MAN	J	4	6	11,11,12	1.35	1 (9%)	15,15,17	1.31	2 (13%)
6	MAN	J	5	6	11,11,12	0.83	1 (9%)	15,15,17	0.94	1 (6%)
6	MAN	J	6	6	11,11,12	0.92	1 (9%)	15,15,17	0.87	1 (6%)
7	NAG	K	1	7,1	14,14,15	0.22	0	17,19,21	0.37	0
7	NAG	K	2	7	14,14,15	0.55	0	17,19,21	1.13	1 (5%)
7	BMA	K	3	7	11,11,12	0.65	0	15,15,17	0.87	0
7	MAN	K	4	7	11,11,12	0.78	0	15,15,17	0.81	0
7	MAN	K	5	7	11,11,12	0.71	0	15,15,17	0.83	0
7	MAN	K	6	7	11,11,12	0.69	0	15,15,17	0.80	0
8	NAG	L	1	8,1	14,14,15	0.30	0	17,19,21	0.60	0
8	NAG	L	2	8	14,14,15	0.29	0	17,19,21	0.66	1 (5%)
8	BMA	L	3	8	11,11,12	0.68	0	15,15,17	0.68	0
8	MAN	L	4	8	11,11,12	0.63	0	15,15,17	1.02	1 (6%)
8	MAN	L	5	8	11,11,12	0.91	1 (9%)	15,15,17	0.98	0
9	NAG	M	1	9,2	14,14,15	0.20	0	17,19,21	0.32	0
9	NAG	M	2	9	14,14,15	0.56	0	17,19,21	0.76	1 (5%)
9	BMA	M	3	9	11,11,12	1.24	2 (18%)	15,15,17	0.77	0
9	MAN	M	4	9	11,11,12	0.58	0	15,15,17	0.85	1 (6%)
9	MAN	M	5	9	11,11,12	0.70	0	15,15,17	0.76	0
9	MAN	M	6	9	11,11,12	0.78	0	15,15,17	0.85	1 (6%)
9	MAN	M	7	9	11,11,12	0.70	0	15,15,17	0.70	0
10	NAG	N	1	10,2	14,14,15	0.24	0	17,19,21	0.43	0
10	NAG	N	2	10	14,14,15	0.42	0	17,19,21	0.81	1 (5%)
10	BMA	N	3	10	11,11,12	0.75	0	15,15,17	0.73	0
10	MAN	N	4	10	11,11,12	0.72	0	15,15,17	0.82	1 (6%)
10	MAN	N	5	10	11,11,12	0.67	0	15,15,17	0.83	0
11	NAG	O	1	11,2	14,14,15	0.96	1 (7%)	17,19,21	1.22	1 (5%)
11	NAG	O	2	11	14,14,15	0.45	0	17,19,21	0.79	1 (5%)
11	BMA	O	3	11	11,11,12	1.05	0	15,15,17	1.09	1 (6%)
11	MAN	O	4	11	11,11,12	0.94	1 (9%)	15,15,17	1.10	2 (13%)
11	MAN	O	5	11	11,11,12	0.98	0	15,15,17	1.01	1 (6%)
4	NAG	P	1	4,2	14,14,15	0.91	1 (7%)	17,19,21	0.51	0
4	NAG	P	2	4	14,14,15	0.49	0	17,19,21	0.67	0
4	BMA	P	3	4	11,11,12	0.50	0	15,15,17	0.59	0
4	MAN	P	4	4	11,11,12	0.70	0	15,15,17	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	NAG	Q	1	12,2	14,14,15	0.31	0	17,19,21	0.41	0
12	NAG	Q	2	12	14,14,15	0.75	1 (7%)	17,19,21	0.85	1 (5%)
12	BMA	Q	3	12	11,11,12	2.15	3 (27%)	15,15,17	1.48	3 (20%)
12	MAN	Q	4	12	11,11,12	1.02	0	15,15,17	1.30	1 (6%)
12	MAN	Q	5	12	11,11,12	0.74	0	15,15,17	1.03	1 (6%)
12	MAN	Q	6	12	11,11,12	1.18	1 (9%)	15,15,17	1.45	4 (26%)
12	MAN	Q	7	12	11,11,12	0.82	1 (9%)	15,15,17	0.81	1 (6%)
12	MAN	Q	8	12	11,11,12	0.76	0	15,15,17	0.94	0
10	NAG	R	1	10,2	14,14,15	0.20	0	17,19,21	0.78	1 (5%)
10	NAG	R	2	10	14,14,15	0.51	0	17,19,21	0.49	0
10	BMA	R	3	10	11,11,12	0.55	0	15,15,17	0.81	0
10	MAN	R	4	10	11,11,12	0.88	0	15,15,17	1.02	1 (6%)
10	MAN	R	5	10	11,11,12	0.65	0	15,15,17	0.86	0
11	NAG	S	1	11,2	14,14,15	0.31	0	17,19,21	0.48	0
11	NAG	S	2	11	14,14,15	0.56	0	17,19,21	0.65	1 (5%)
11	BMA	S	3	11	11,11,12	0.71	0	15,15,17	0.70	0
11	MAN	S	4	11	11,11,12	0.68	0	15,15,17	0.75	0
11	MAN	S	5	11	11,11,12	0.62	0	15,15,17	0.80	1 (6%)
13	NAG	T	1	2,13	14,14,15	1.07	2 (14%)	17,19,21	1.26	3 (17%)
13	NAG	T	2	13	14,14,15	0.79	0	17,19,21	0.94	2 (11%)
13	BMA	T	3	13	11,11,12	0.93	0	15,15,17	1.15	1 (6%)
13	MAN	T	4	13	11,11,12	0.95	1 (9%)	15,15,17	0.93	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
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
5	NAG	I	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	I	2	5	-	5/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	MAN	I	4	5	-	0/2/19/22	0/1/1/1
6	NAG	J	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
6	MAN	J	5	6	-	0/2/19/22	0/1/1/1
6	MAN	J	6	6	-	0/2/19/22	0/1/1/1
7	NAG	K	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	3/6/23/26	0/1/1/1
7	BMA	K	3	7	-	0/2/19/22	0/1/1/1
7	MAN	K	4	7	-	2/2/19/22	0/1/1/1
7	MAN	K	5	7	-	0/2/19/22	0/1/1/1
7	MAN	K	6	7	-	0/2/19/22	0/1/1/1
8	NAG	L	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	L	2	8	-	1/6/23/26	0/1/1/1
8	BMA	L	3	8	-	2/2/19/22	0/1/1/1
8	MAN	L	4	8	-	2/2/19/22	0/1/1/1
8	MAN	L	5	8	-	1/2/19/22	0/1/1/1
9	NAG	M	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	M	2	9	-	0/6/23/26	0/1/1/1
9	BMA	M	3	9	-	0/2/19/22	0/1/1/1
9	MAN	M	4	9	-	0/2/19/22	0/1/1/1
9	MAN	M	5	9	-	0/2/19/22	0/1/1/1
9	MAN	M	6	9	-	0/2/19/22	0/1/1/1
9	MAN	M	7	9	-	0/2/19/22	0/1/1/1
10	NAG	N	1	10,2	-	0/6/23/26	0/1/1/1
10	NAG	N	2	10	-	0/6/23/26	0/1/1/1
10	BMA	N	3	10	-	2/2/19/22	0/1/1/1
10	MAN	N	4	10	-	0/2/19/22	0/1/1/1
10	MAN	N	5	10	-	1/2/19/22	0/1/1/1
11	NAG	O	1	11,2	-	3/6/23/26	0/1/1/1
11	NAG	O	2	11	-	2/6/23/26	0/1/1/1
11	BMA	O	3	11	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	O	4	11	-	1/2/19/22	0/1/1/1
11	MAN	O	5	11	-	0/2/19/22	0/1/1/1
4	NAG	P	1	4,2	-	1/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	BMA	P	3	4	-	0/2/19/22	0/1/1/1
4	MAN	P	4	4	-	1/2/19/22	0/1/1/1
12	NAG	Q	1	12,2	-	0/6/23/26	0/1/1/1
12	NAG	Q	2	12	-	1/6/23/26	0/1/1/1
12	BMA	Q	3	12	-	0/2/19/22	0/1/1/1
12	MAN	Q	4	12	-	1/2/19/22	0/1/1/1
12	MAN	Q	5	12	-	0/2/19/22	0/1/1/1
12	MAN	Q	6	12	-	2/2/19/22	0/1/1/1
12	MAN	Q	7	12	-	0/2/19/22	0/1/1/1
12	MAN	Q	8	12	-	0/2/19/22	0/1/1/1
10	NAG	R	1	10,2	-	0/6/23/26	0/1/1/1
10	NAG	R	2	10	-	1/6/23/26	0/1/1/1
10	BMA	R	3	10	-	1/2/19/22	0/1/1/1
10	MAN	R	4	10	-	0/2/19/22	0/1/1/1
10	MAN	R	5	10	-	0/2/19/22	0/1/1/1
11	NAG	S	1	11,2	-	0/6/23/26	0/1/1/1
11	NAG	S	2	11	-	0/6/23/26	0/1/1/1
11	BMA	S	3	11	-	0/2/19/22	0/1/1/1
11	MAN	S	4	11	-	0/2/19/22	0/1/1/1
11	MAN	S	5	11	-	0/2/19/22	0/1/1/1
13	NAG	T	1	2,13	-	2/6/23/26	0/1/1/1
13	NAG	T	2	13	-	3/6/23/26	0/1/1/1
13	BMA	T	3	13	-	1/2/19/22	0/1/1/1
13	MAN	T	4	13	-	1/2/19/22	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	2	NAG	C1-C2	4.71	1.59	1.52
12	Q	3	BMA	O5-C1	-4.41	1.36	1.43
6	J	1	NAG	O5-C1	-4.16	1.37	1.43
5	I	2	NAG	O5-C1	3.74	1.49	1.43
12	Q	3	BMA	C2-C3	3.72	1.58	1.52
12	Q	3	BMA	O3-C3	3.56	1.51	1.43
6	J	4	MAN	O5-C1	-3.55	1.38	1.43
4	P	1	NAG	O5-C1	-3.20	1.38	1.43
12	Q	6	MAN	O5-C1	-3.15	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	O	1	NAG	C1-C2	2.83	1.56	1.52
13	T	1	NAG	C1-C2	2.80	1.56	1.52
6	J	3	BMA	O5-C1	-2.78	1.39	1.43
6	J	3	BMA	O5-C5	-2.66	1.38	1.43
8	L	5	MAN	C1-C2	2.64	1.58	1.52
13	T	4	MAN	C1-C2	2.59	1.58	1.52
4	G	4	MAN	C1-C2	2.34	1.57	1.52
9	M	3	BMA	O5-C1	-2.34	1.40	1.43
6	J	5	MAN	C1-C2	2.33	1.57	1.52
11	O	4	MAN	C1-C2	2.32	1.57	1.52
12	Q	2	NAG	C1-C2	2.32	1.55	1.52
6	J	3	BMA	C1-C2	2.29	1.57	1.52
9	M	3	BMA	C2-C3	2.22	1.55	1.52
6	J	3	BMA	C2-C3	2.12	1.55	1.52
6	J	6	MAN	C1-C2	2.06	1.56	1.52
4	G	3	BMA	C6-C5	2.06	1.58	1.51
13	T	1	NAG	O5-C1	-2.05	1.40	1.43
12	Q	7	MAN	O5-C1	-2.02	1.40	1.43

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	3	BMA	O5-C5-C6	5.59	115.97	107.20
6	J	2	NAG	C1-O5-C5	5.07	119.06	112.19
5	I	2	NAG	C2-N2-C7	4.44	129.22	122.90
11	O	1	NAG	C2-N2-C7	4.04	128.66	122.90
7	K	2	NAG	C2-N2-C7	3.78	128.29	122.90
13	T	3	BMA	O5-C5-C6	3.77	113.12	107.20
12	Q	3	BMA	C1-O5-C5	3.62	117.09	112.19
3	F	2	NAG	C1-O5-C5	3.10	116.40	112.19
12	Q	4	MAN	O2-C2-C3	-2.95	104.24	110.14
5	I	2	NAG	C1-C2-N2	2.73	115.16	110.49
12	Q	6	MAN	C1-C2-C3	2.71	113.00	109.67
6	J	2	NAG	O4-C4-C5	-2.62	102.80	109.30
8	L	4	MAN	O5-C5-C6	2.62	111.31	107.20
12	Q	2	NAG	O4-C4-C5	-2.58	102.89	109.30
6	J	1	NAG	O3-C3-C2	-2.52	104.26	109.47
10	R	1	NAG	O4-C4-C3	-2.38	104.86	110.35
13	T	1	NAG	C3-C4-C5	2.36	114.45	110.24
6	J	4	MAN	C1-C2-C3	-2.34	106.78	109.67
10	N	2	NAG	C1-O5-C5	2.29	115.30	112.19
13	T	1	NAG	O4-C4-C5	-2.26	103.70	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	Q	5	MAN	O5-C5-C6	2.24	110.72	107.20
12	Q	6	MAN	O6-C6-C5	-2.24	103.62	111.29
13	T	2	NAG	O5-C1-C2	-2.22	107.78	111.29
9	M	6	MAN	O2-C2-C3	-2.22	105.69	110.14
11	O	3	BMA	C6-C5-C4	2.21	118.19	113.00
12	Q	3	BMA	O6-C6-C5	-2.21	103.72	111.29
8	L	2	NAG	C1-O5-C5	2.19	115.16	112.19
11	O	2	NAG	C1-O5-C5	2.19	115.16	112.19
9	M	4	MAN	O2-C2-C3	-2.18	105.76	110.14
6	J	4	MAN	O3-C3-C2	2.16	114.14	109.99
12	Q	6	MAN	O3-C3-C4	-2.14	105.41	110.35
6	J	3	BMA	C1-C2-C3	-2.13	107.05	109.67
10	N	4	MAN	O2-C2-C3	-2.12	105.89	110.14
13	T	2	NAG	C1-C2-N2	2.12	114.11	110.49
12	Q	3	BMA	O3-C3-C2	2.12	114.05	109.99
10	R	4	MAN	O2-C2-C3	-2.11	105.91	110.14
12	Q	7	MAN	O2-C2-C3	-2.11	105.91	110.14
11	S	5	MAN	O2-C2-C3	-2.10	105.94	110.14
6	J	6	MAN	O2-C2-C3	-2.08	105.97	110.14
11	O	4	MAN	O2-C2-C3	-2.08	105.98	110.14
5	I	4	MAN	O2-C2-C3	-2.07	105.98	110.14
12	Q	6	MAN	O3-C3-C2	-2.07	106.04	109.99
4	G	2	NAG	C1-C2-N2	2.06	114.00	110.49
6	J	5	MAN	O2-C2-C3	-2.03	106.06	110.14
11	S	2	NAG	C1-O5-C5	2.03	114.95	112.19
11	O	4	MAN	C1-O5-C5	2.03	114.94	112.19
11	O	5	MAN	O2-C2-C3	-2.02	106.10	110.14
13	T	1	NAG	C2-N2-C7	2.02	125.77	122.90
9	M	2	NAG	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	T	2	NAG	O5-C5-C6-O6
4	P	2	NAG	C1-C2-N2-C7
6	J	3	BMA	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
13	T	2	NAG	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
6	J	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
6	J	2	NAG	C8-C7-N2-C2
6	J	2	NAG	O7-C7-N2-C2
7	K	1	NAG	C8-C7-N2-C2
7	K	1	NAG	O7-C7-N2-C2
7	K	2	NAG	C8-C7-N2-C2
7	K	2	NAG	O7-C7-N2-C2
11	O	1	NAG	C8-C7-N2-C2
11	O	1	NAG	O7-C7-N2-C2
10	N	3	BMA	C4-C5-C6-O6
8	L	4	MAN	O5-C5-C6-O6
12	Q	4	MAN	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
12	Q	6	MAN	O5-C5-C6-O6
5	I	1	NAG	C1-C2-N2-C7
10	N	3	BMA	O5-C5-C6-O6
8	L	3	BMA	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
8	L	4	MAN	C4-C5-C6-O6
10	N	5	MAN	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
4	P	4	MAN	O5-C5-C6-O6
12	Q	6	MAN	C4-C5-C6-O6
13	T	1	NAG	O5-C5-C6-O6
10	R	3	BMA	O5-C5-C6-O6
13	T	4	MAN	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
8	L	5	MAN	O5-C5-C6-O6
11	O	4	MAN	O5-C5-C6-O6
8	L	2	NAG	O5-C5-C6-O6
12	Q	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
13	T	1	NAG	C3-C2-N2-C7
5	I	2	NAG	C4-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
13	T	3	BMA	C4-C5-C6-O6
7	K	4	MAN	O5-C5-C6-O6

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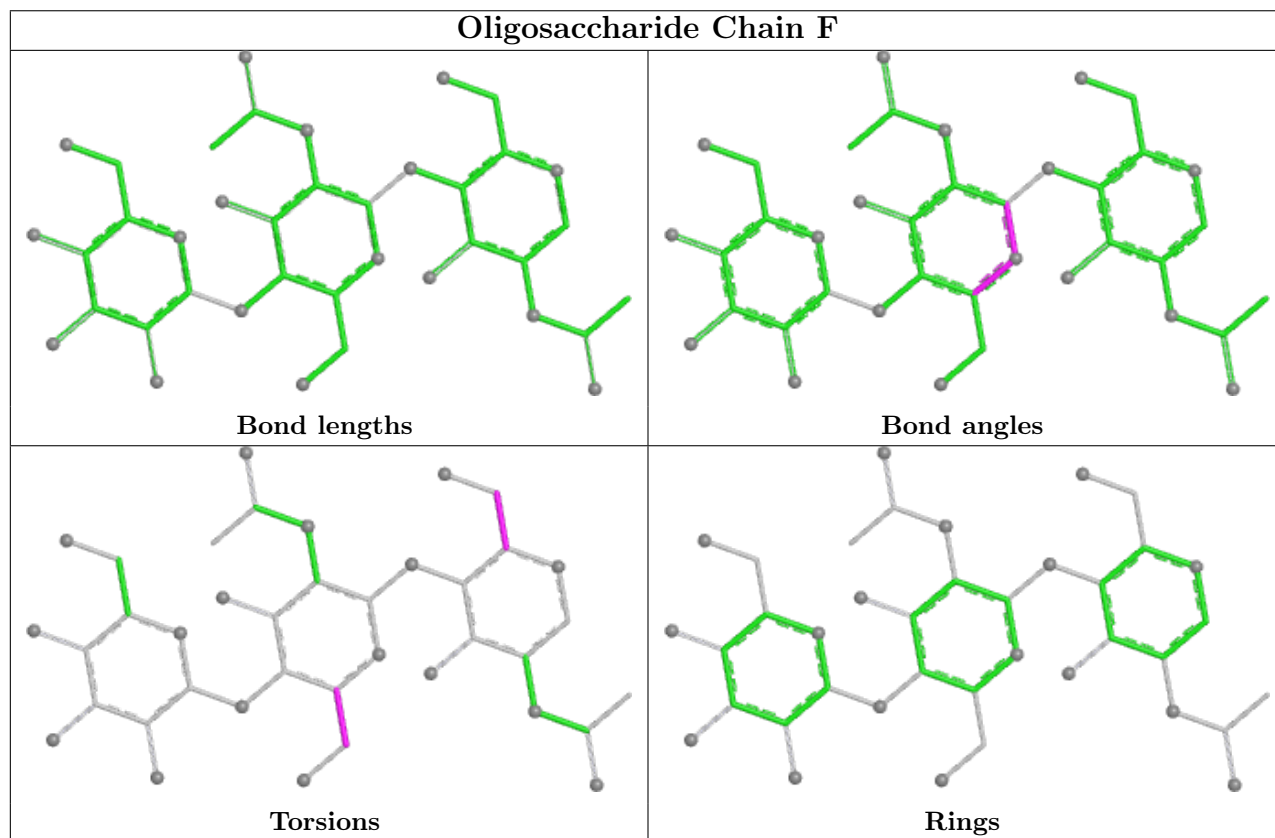
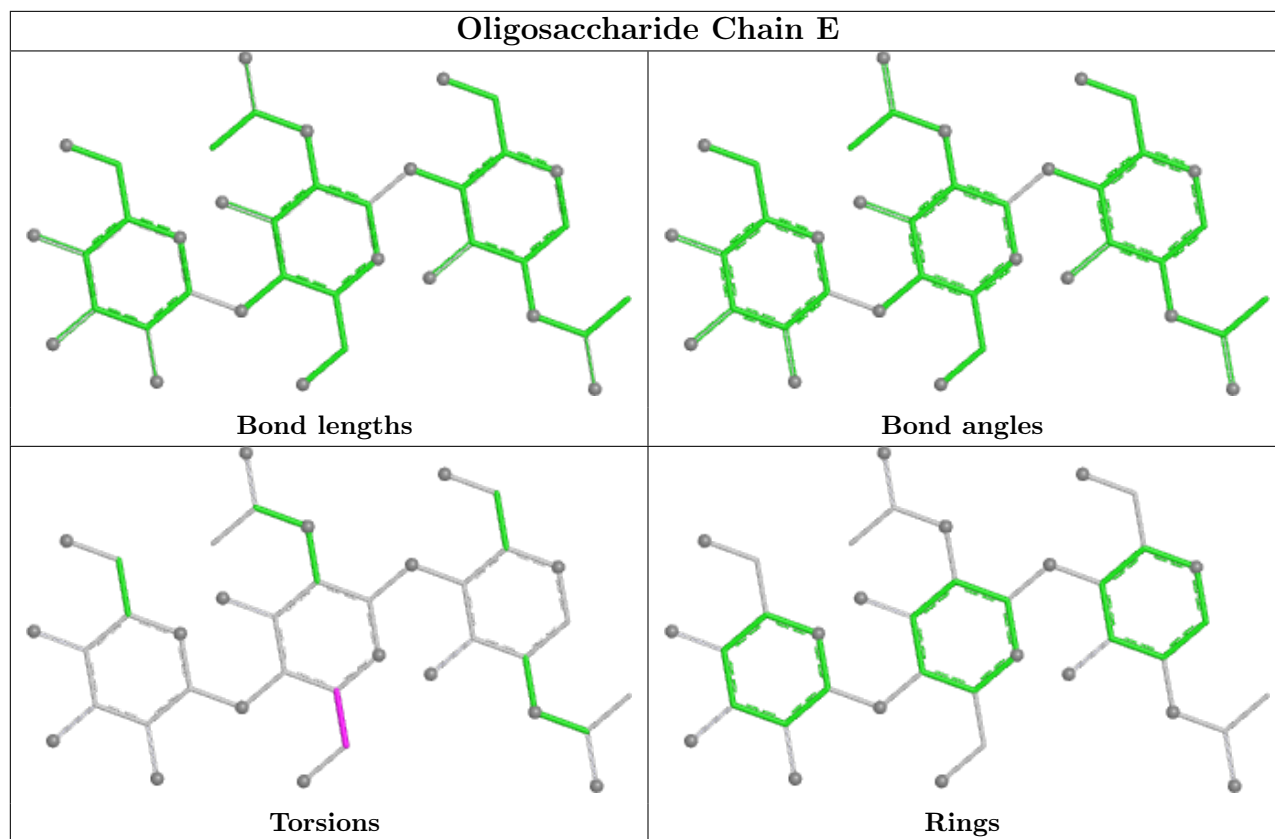
Mol	Chain	Res	Type	Atoms
7	K	4	MAN	C4-C5-C6-O6
3	H	1	NAG	C3-C2-N2-C7
4	P	2	NAG	C3-C2-N2-C7
5	I	2	NAG	C3-C2-N2-C7
7	K	2	NAG	C3-C2-N2-C7
11	O	1	NAG	C3-C2-N2-C7
3	H	1	NAG	C1-C2-N2-C7
13	T	2	NAG	C1-C2-N2-C7
3	H	2	NAG	C1-C2-N2-C7
8	L	3	BMA	C4-C5-C6-O6
10	R	2	NAG	C1-C2-N2-C7
9	M	1	NAG	O5-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
11	O	2	NAG	C3-C2-N2-C7
6	J	1	NAG	C1-C2-N2-C7
11	O	2	NAG	C1-C2-N2-C7

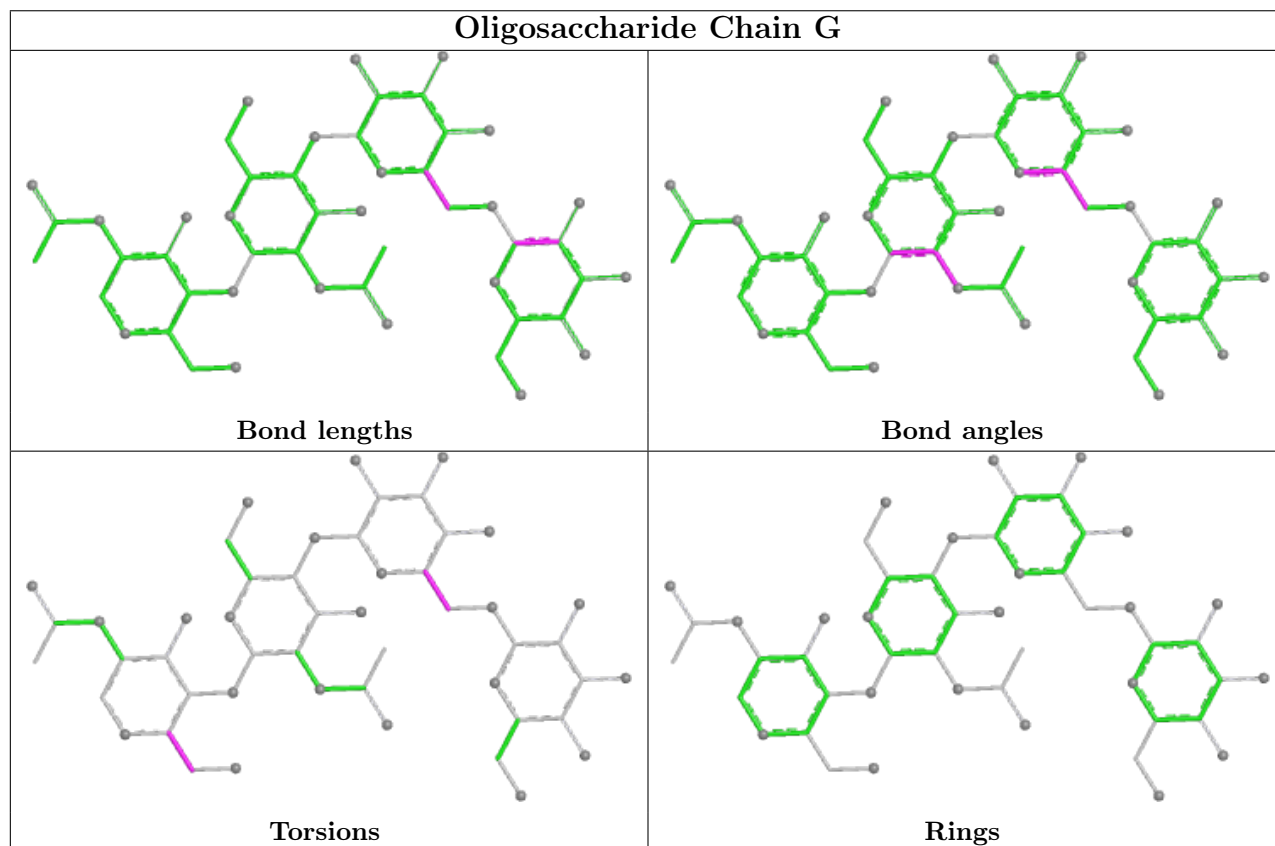
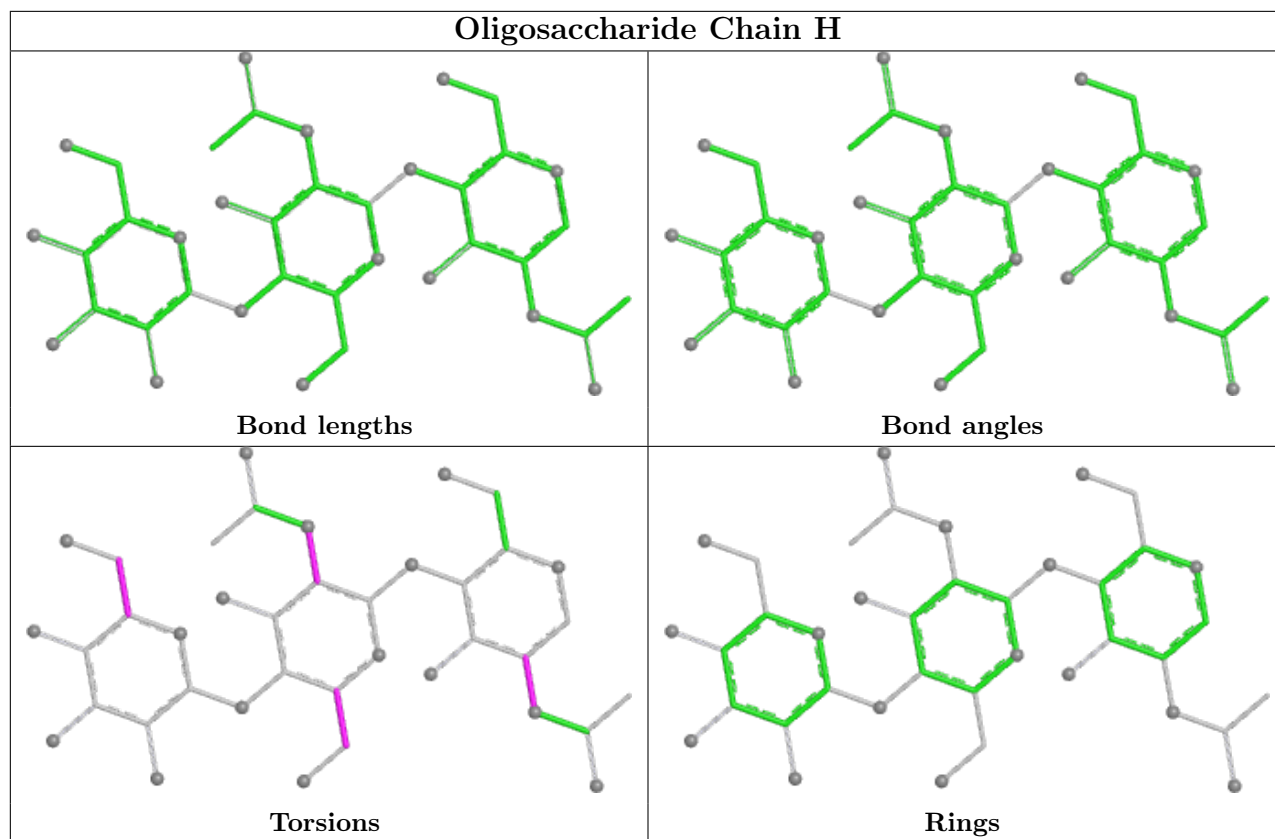
There are no ring outliers.

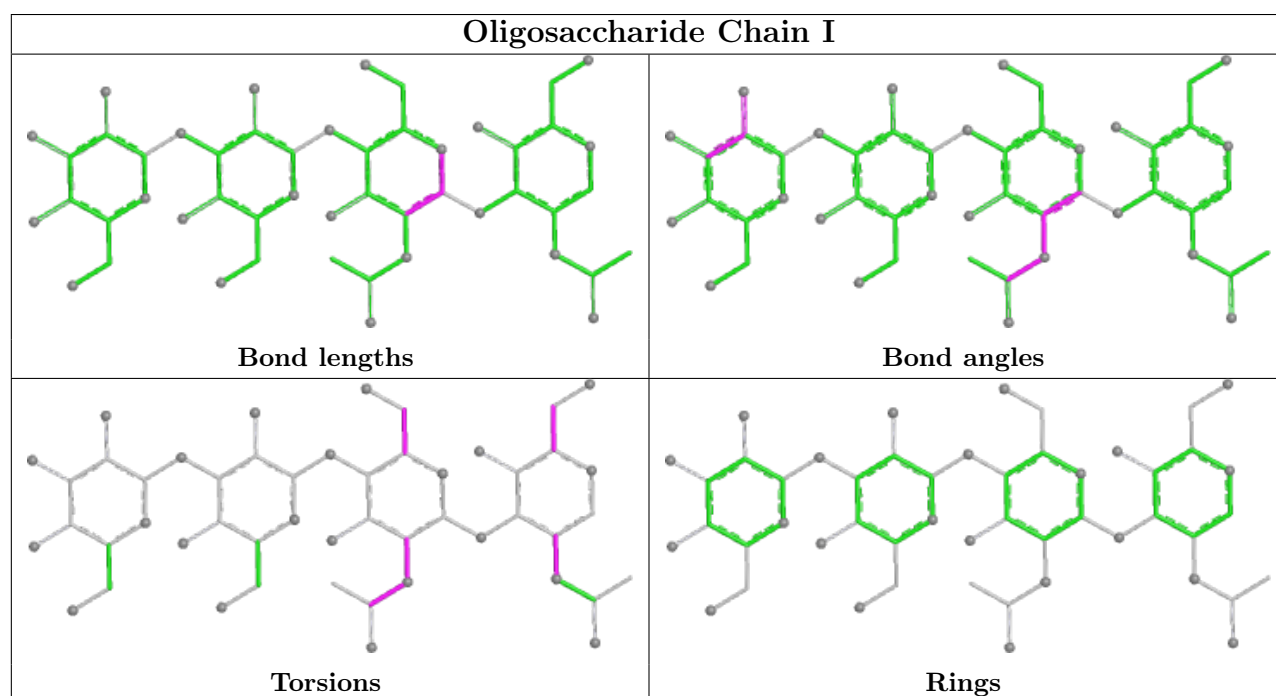
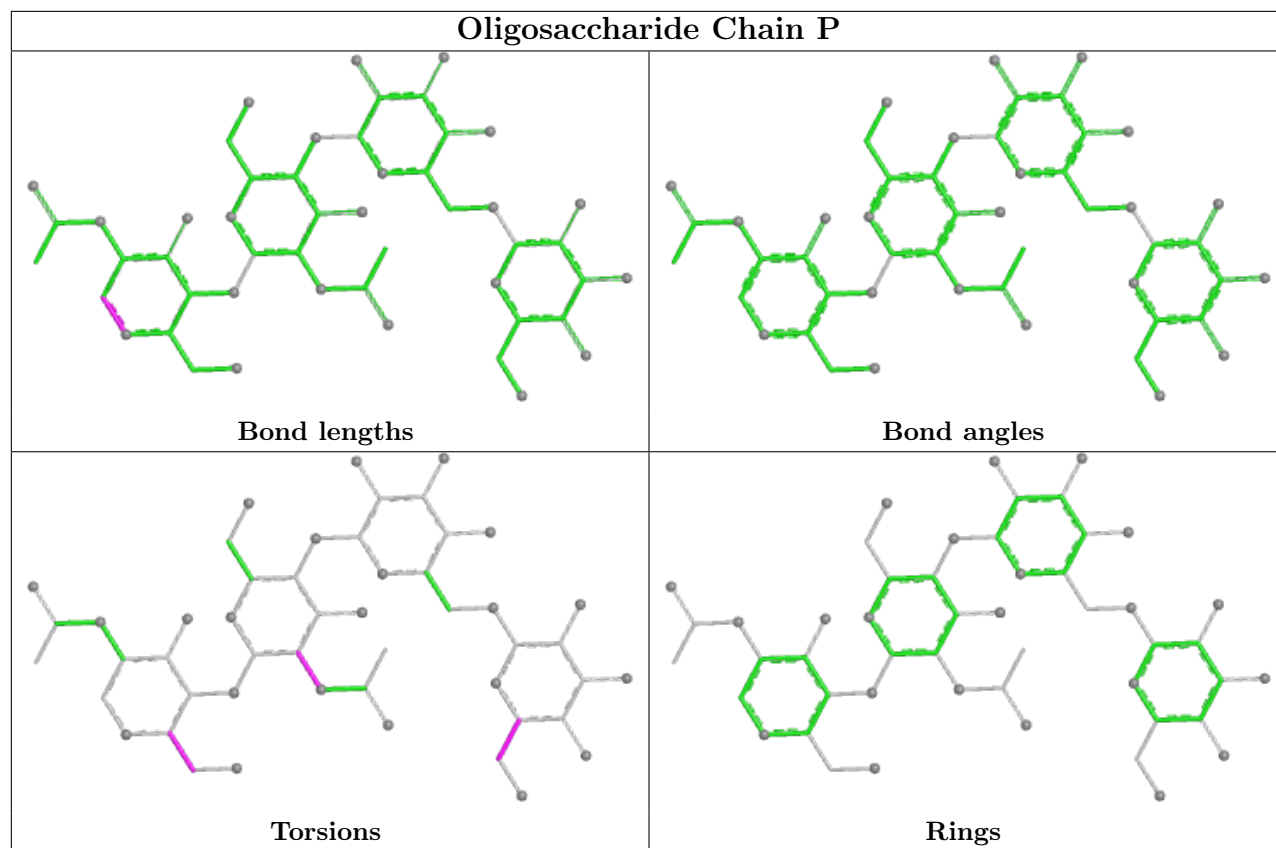
18 monomers are involved in 20 short contacts:

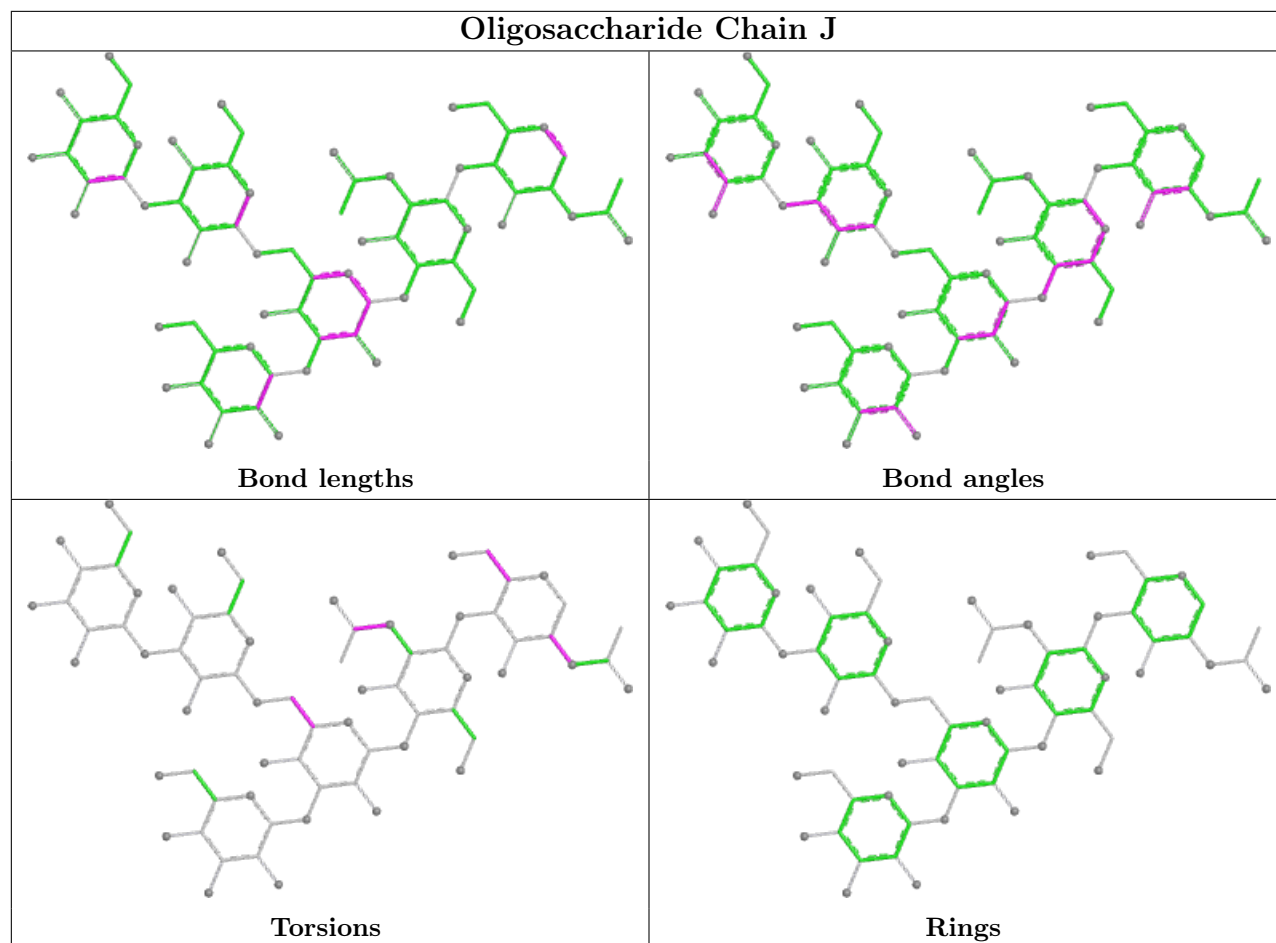
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	3	BMA	1	0
8	L	5	MAN	1	0
3	F	2	NAG	1	0
13	T	1	NAG	2	0
4	G	2	NAG	1	0
5	I	2	NAG	3	0
4	G	1	NAG	1	0
8	L	2	NAG	1	0
7	K	1	NAG	2	0
4	P	4	MAN	1	0
4	P	2	NAG	2	0
5	I	1	NAG	2	0
3	F	1	NAG	1	0
7	K	2	NAG	3	0
10	R	3	BMA	1	0
10	R	4	MAN	1	0
11	O	1	NAG	2	0
10	N	1	NAG	1	0

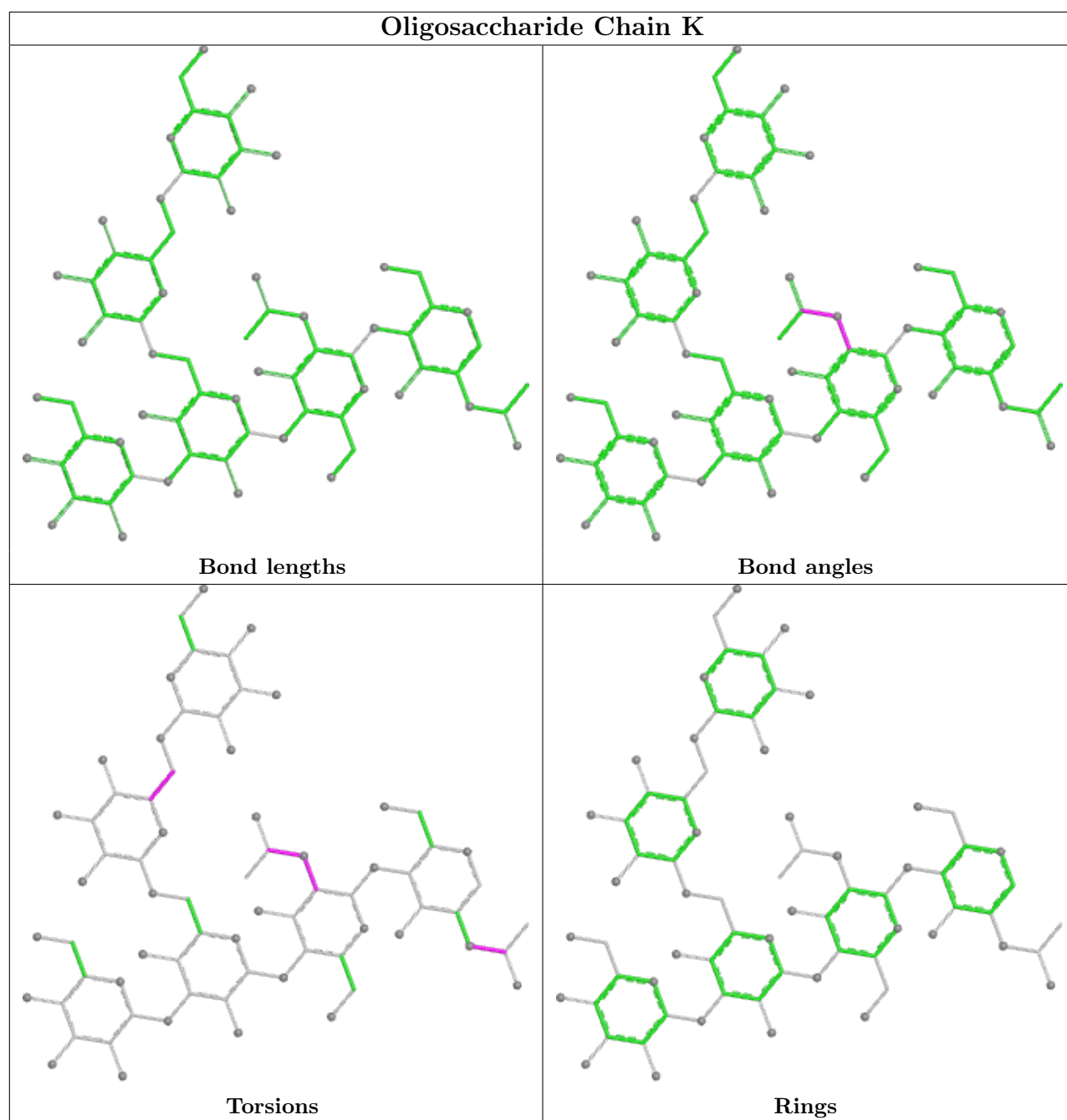
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

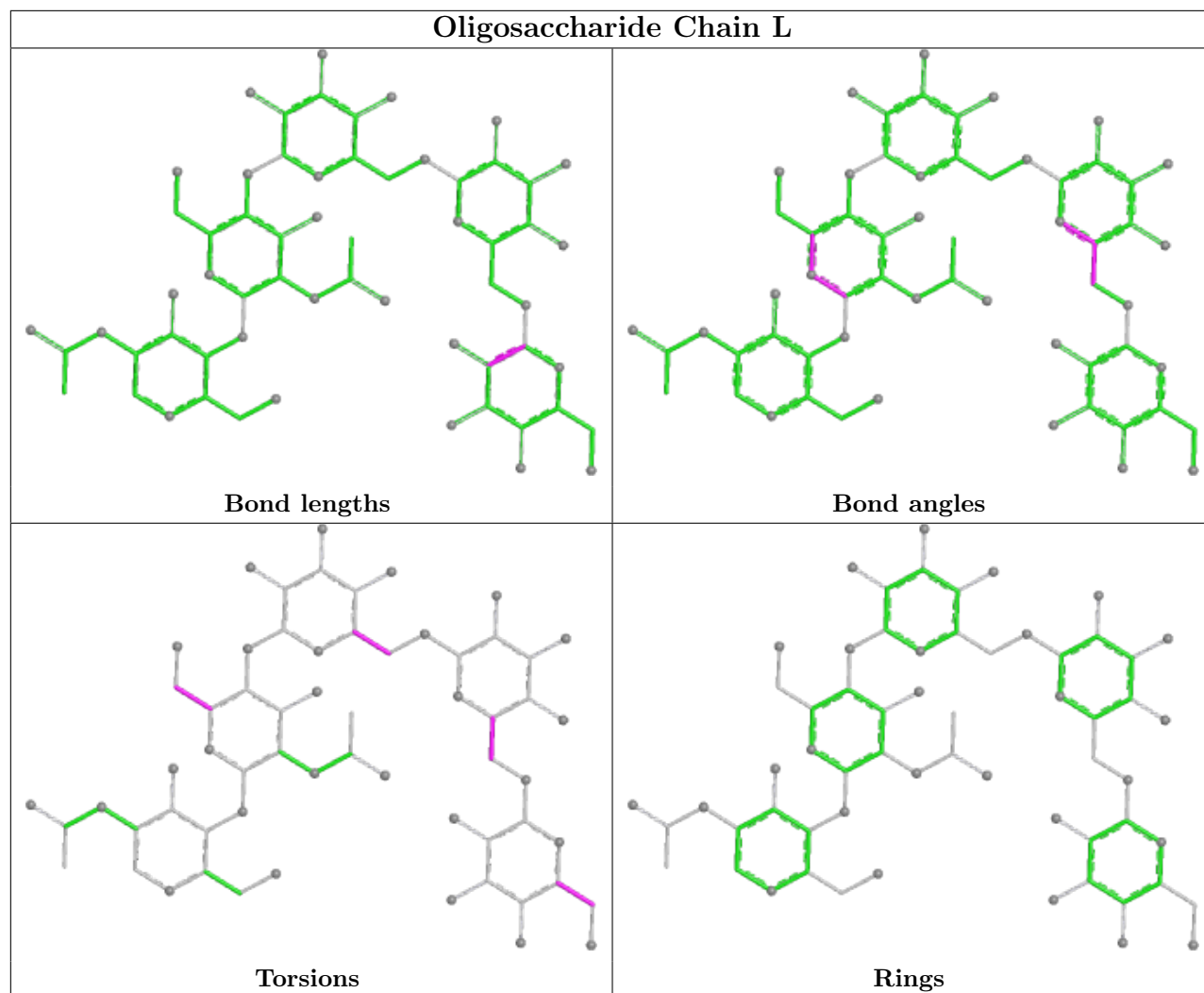


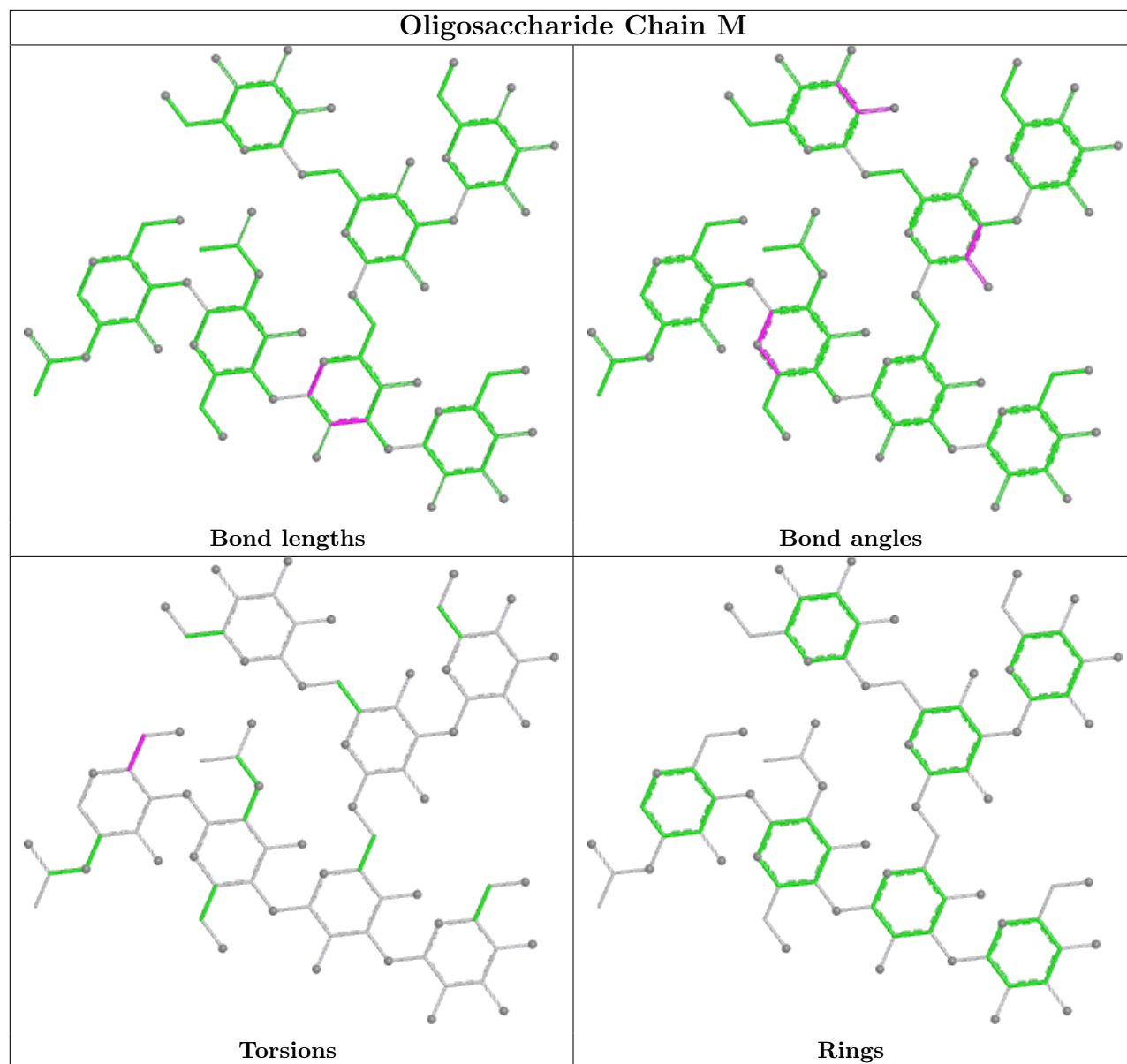




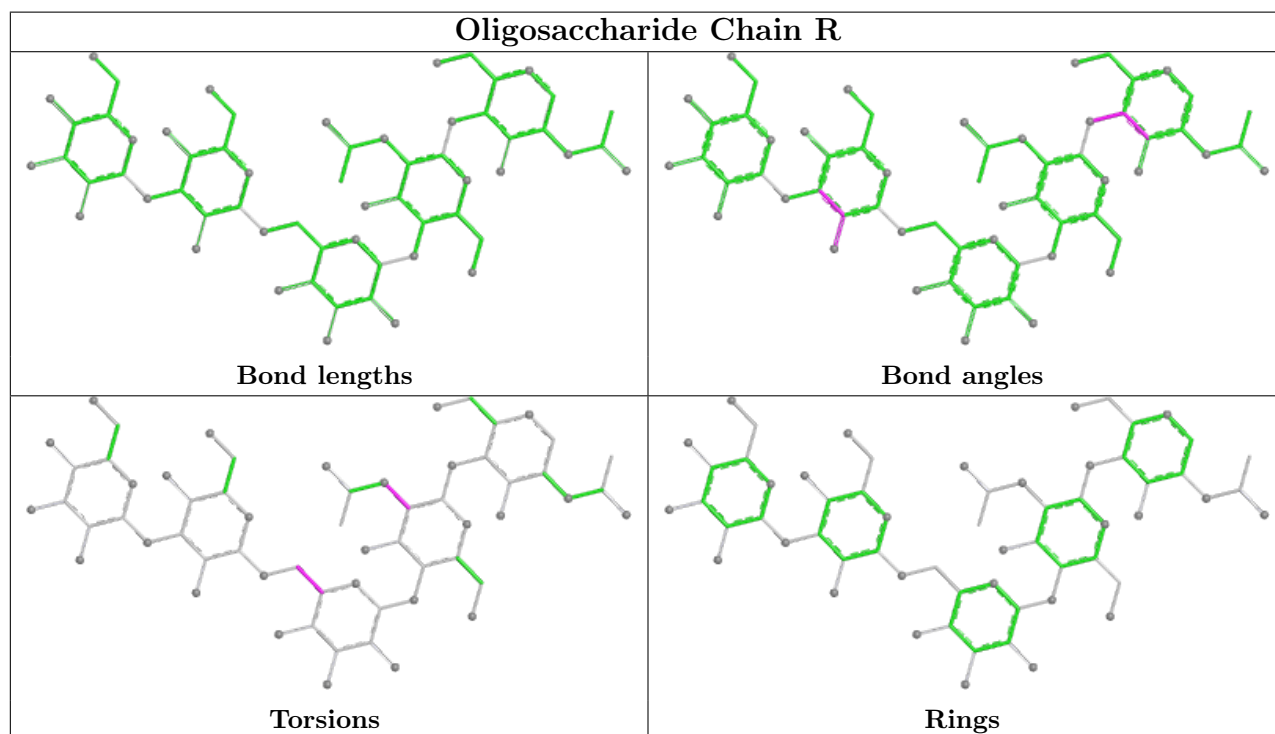
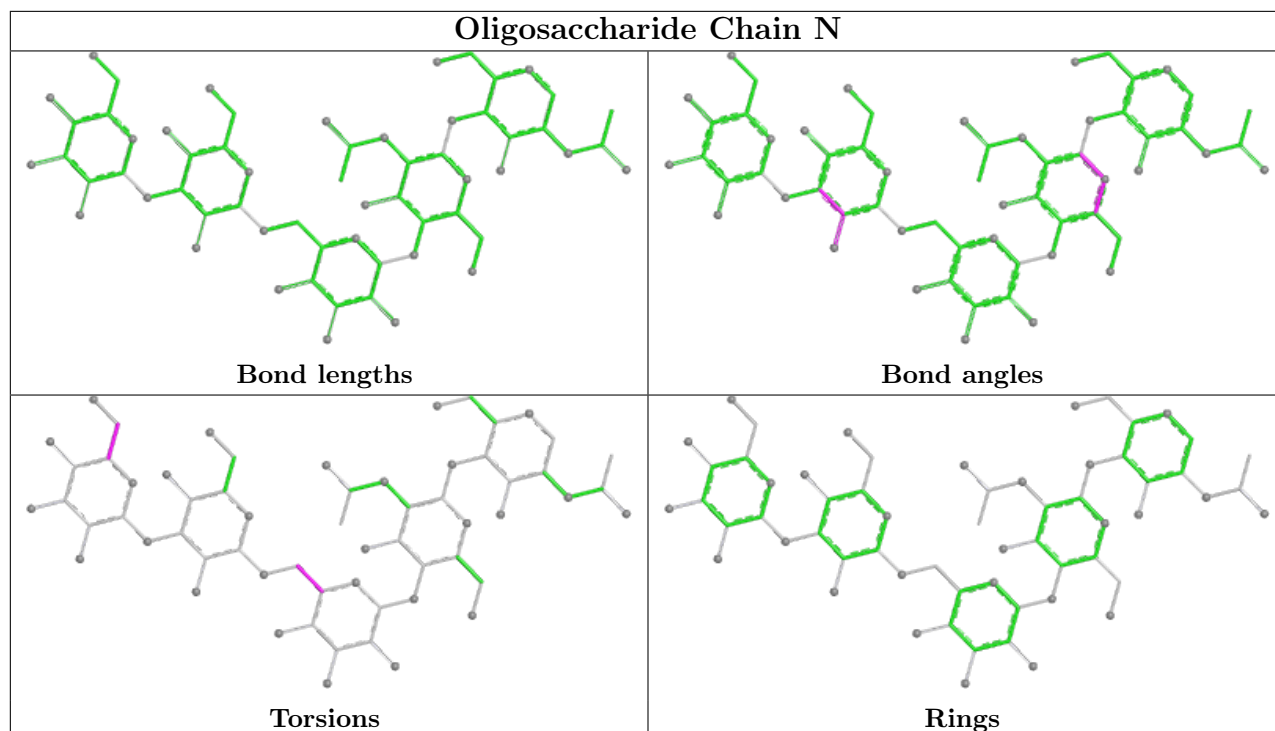


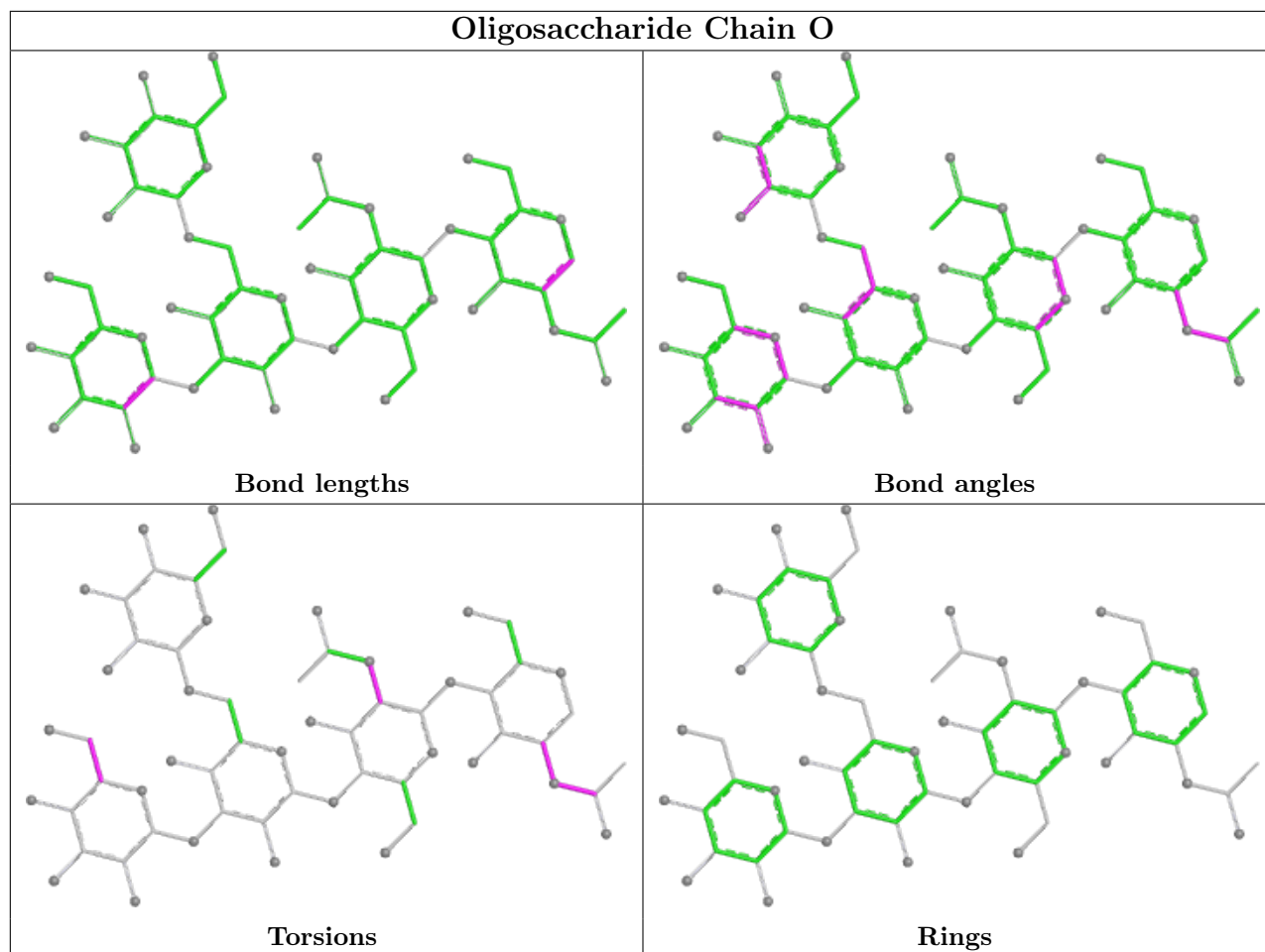


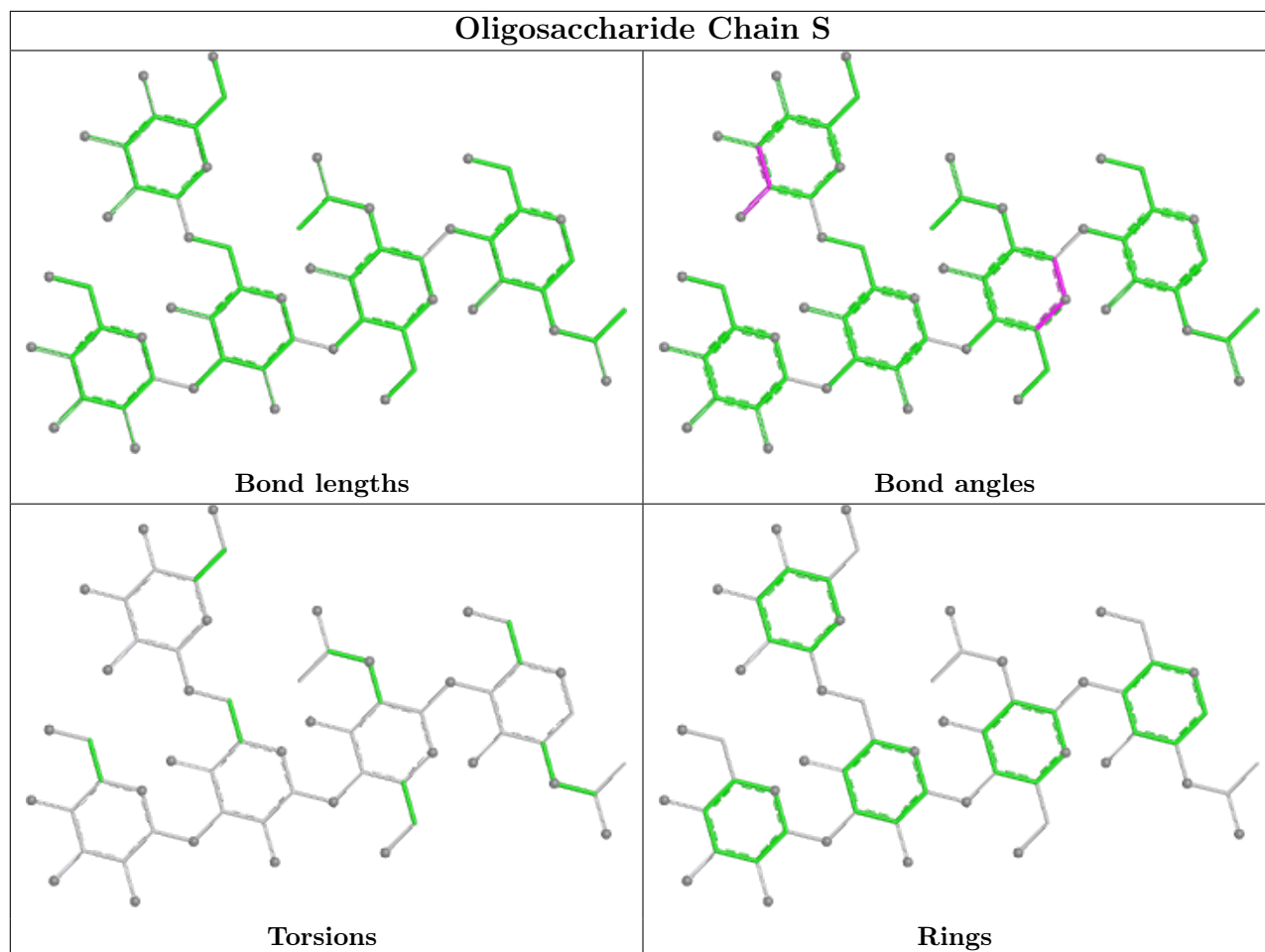


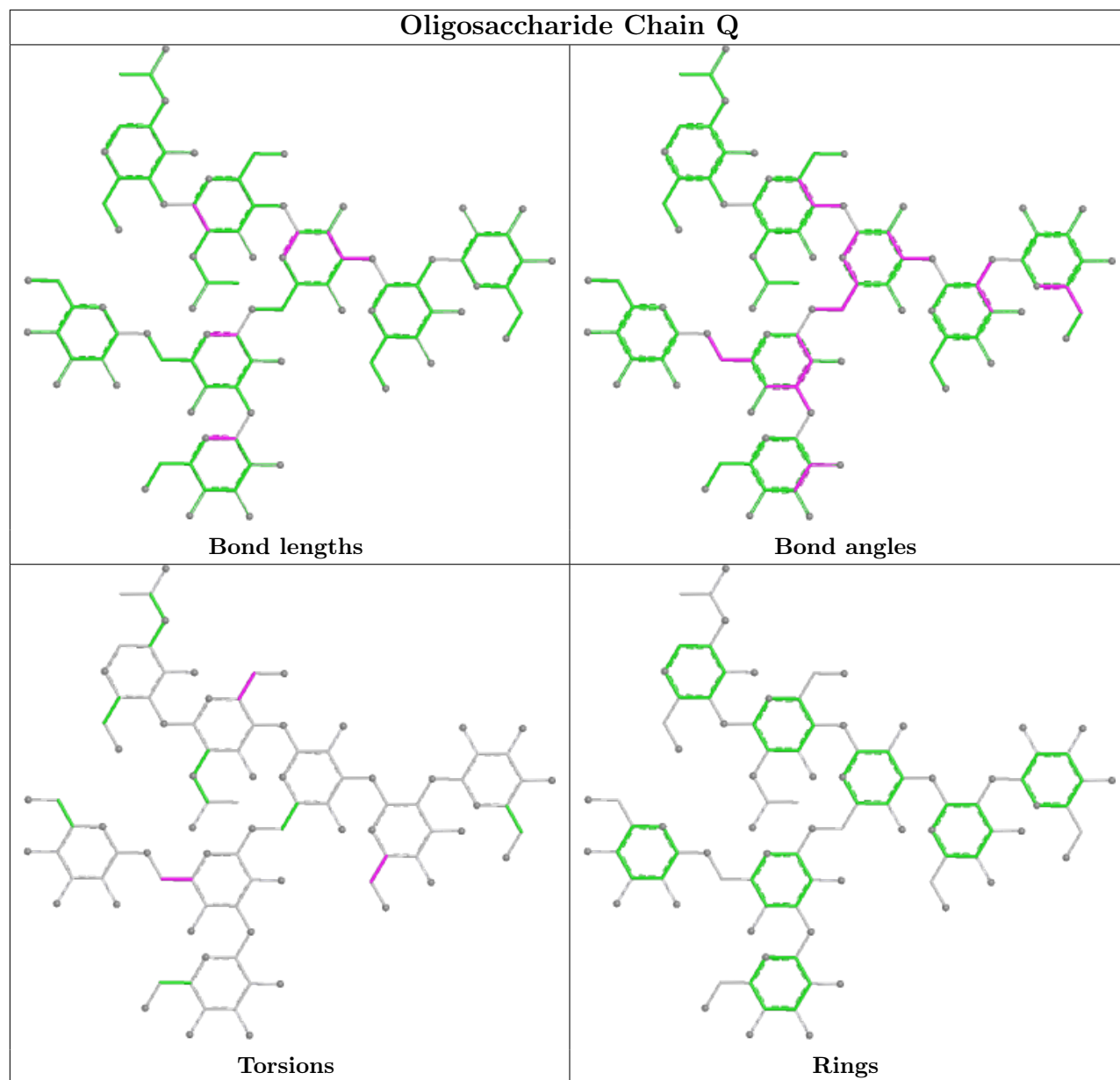


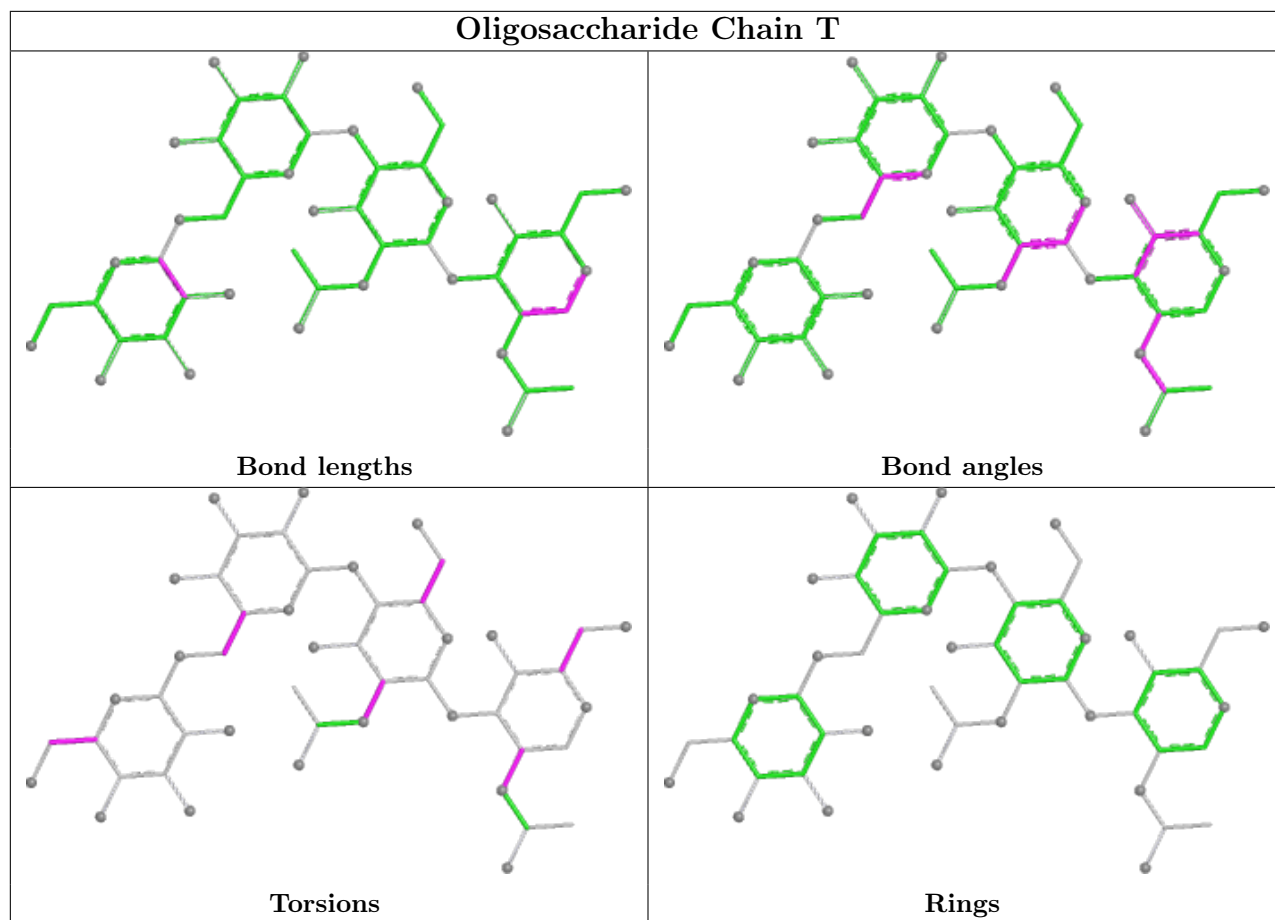












## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
14	NAG	A	701	1	14,14,15	0.22	0	17,19,21	0.82	0
14	NAG	B	701	1	14,14,15	0.20	0	17,19,21	0.51	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	A	701	1	-	3/6/23/26	0/1/1/1
14	NAG	B	701	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

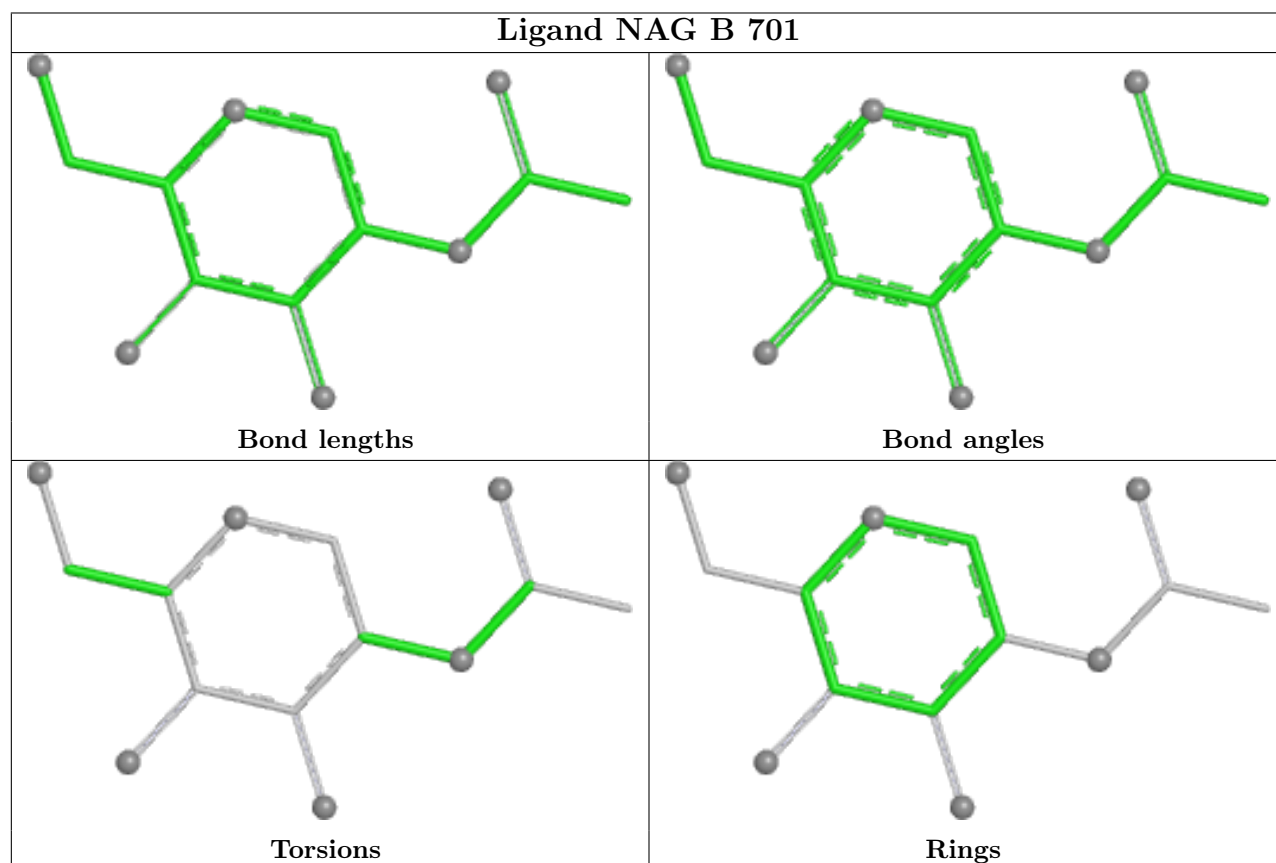
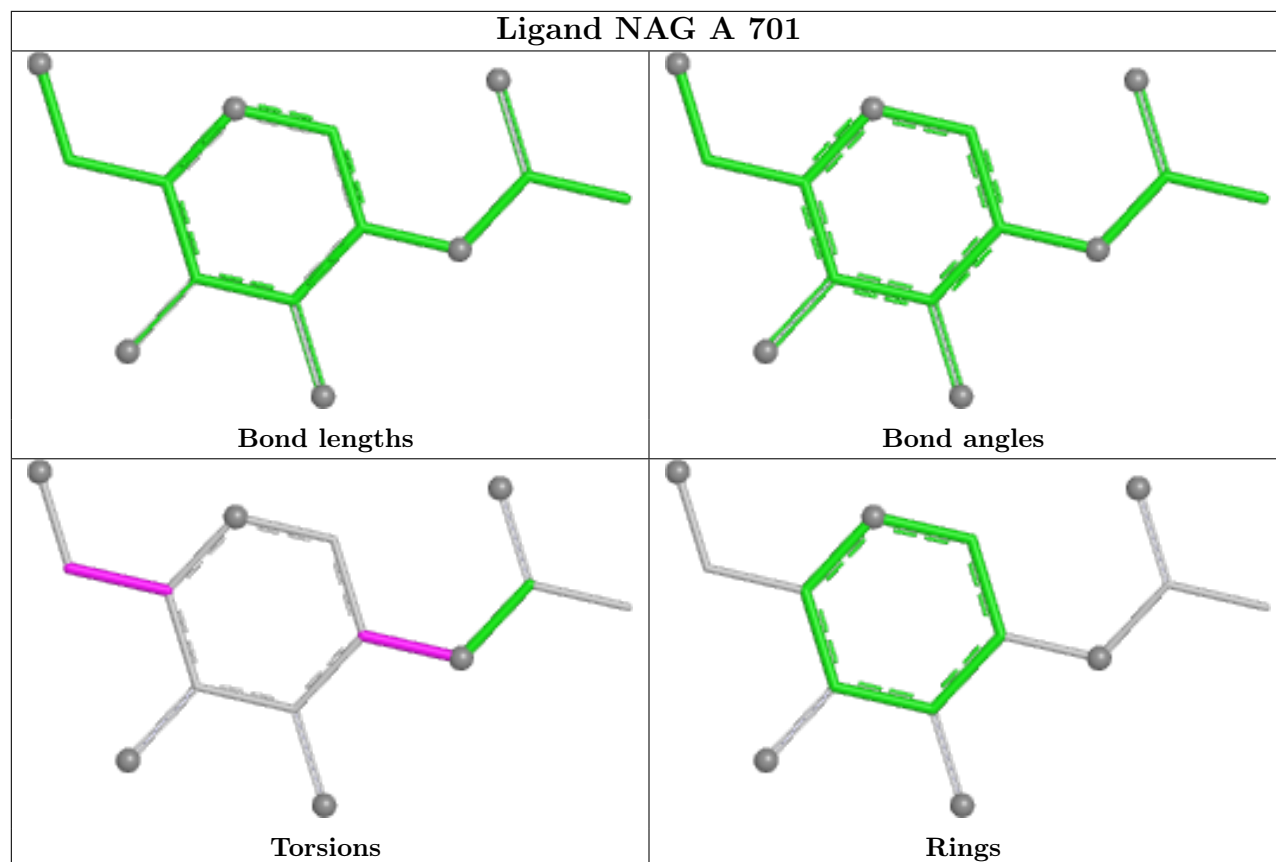
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	701	NAG	C4-C5-C6-O6
14	A	701	NAG	O5-C5-C6-O6
14	A	701	NAG	C3-C2-N2-C7

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.



## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

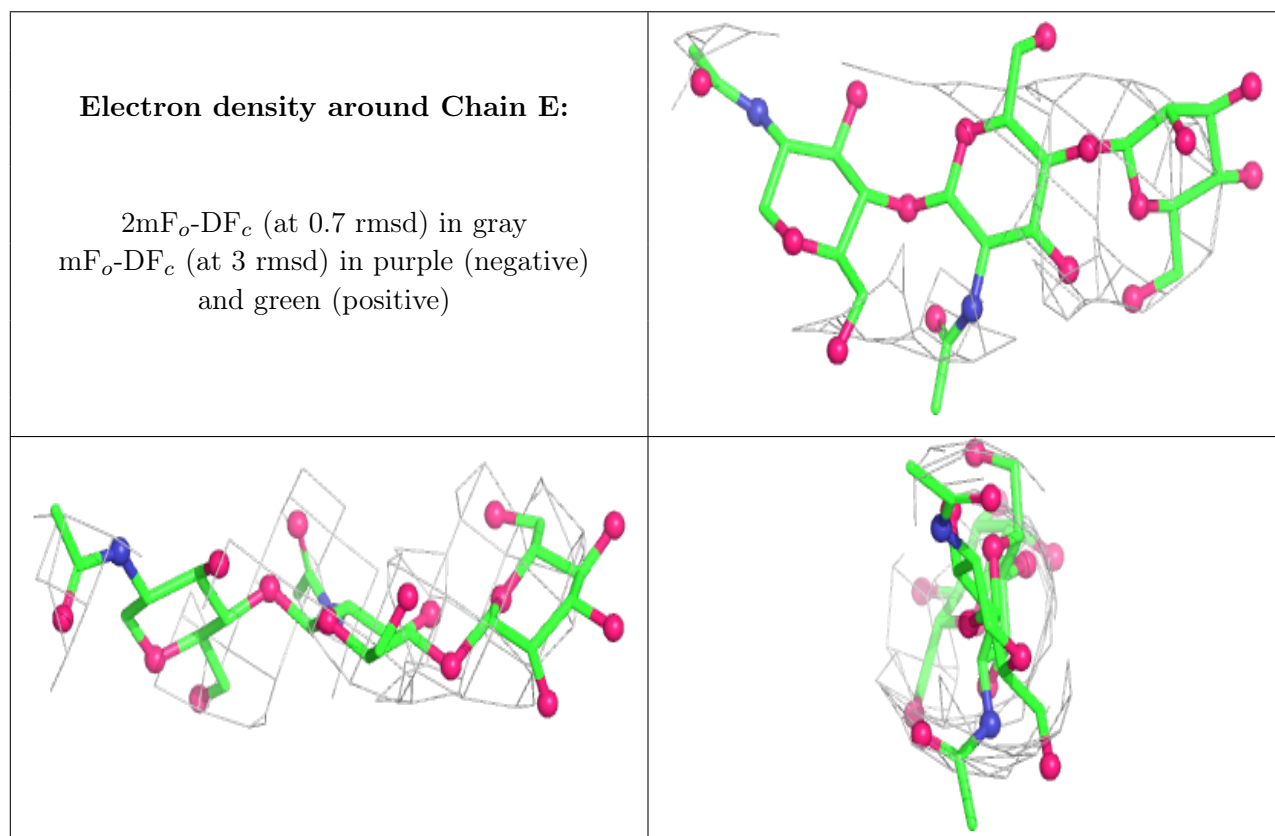
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

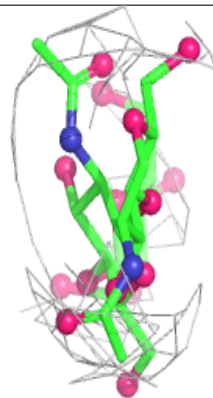
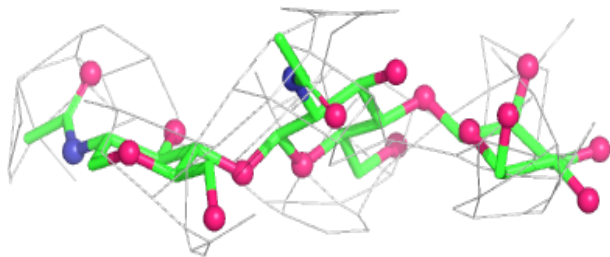
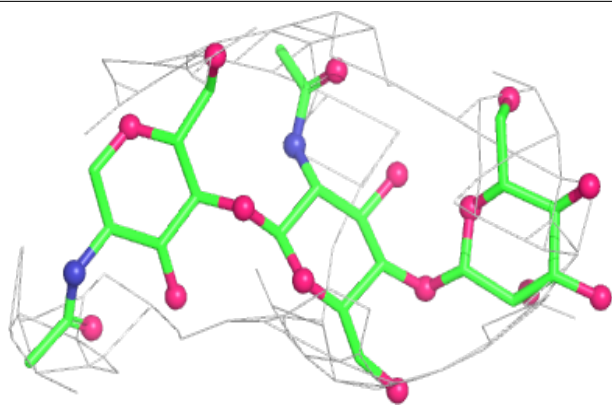
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

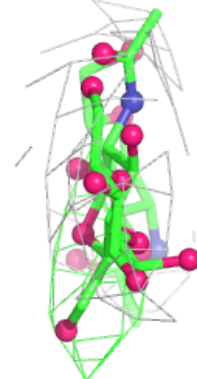
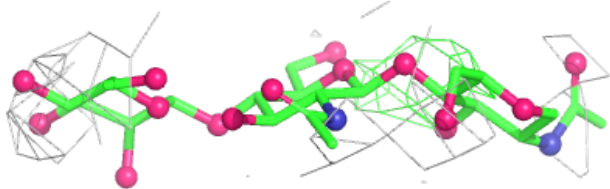
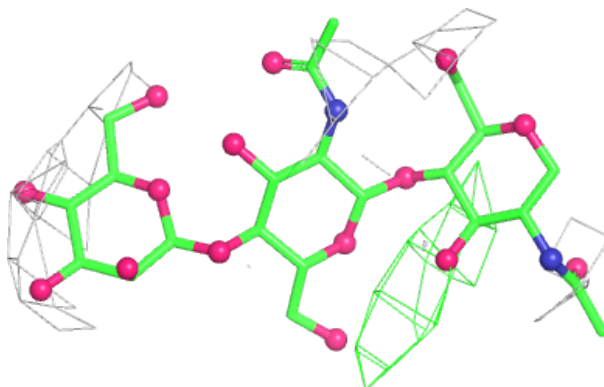


**Electron density around Chain F:**

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

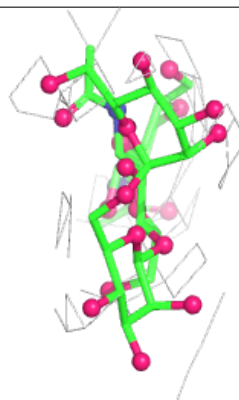
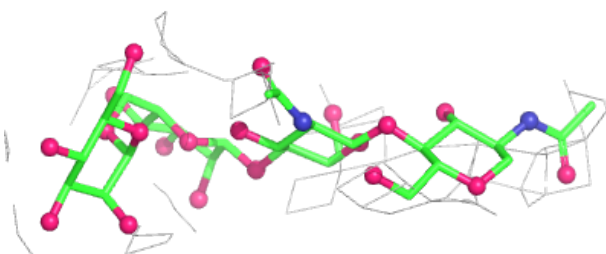
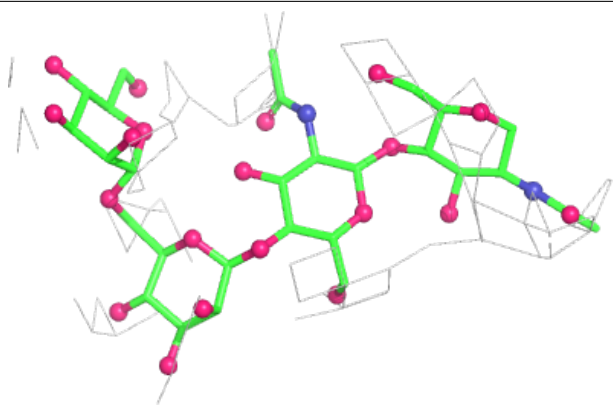
**Electron density around Chain H:**

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

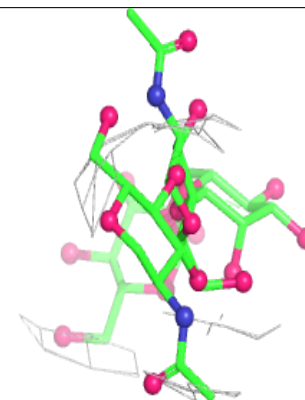
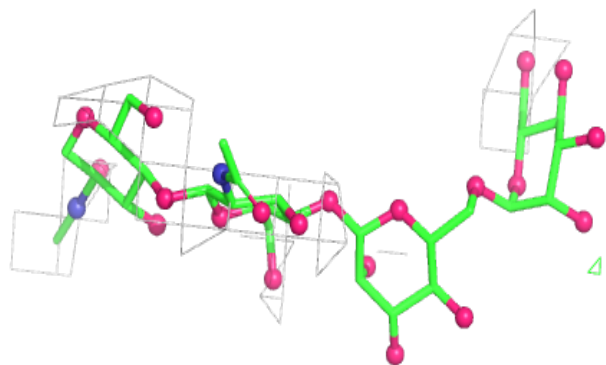
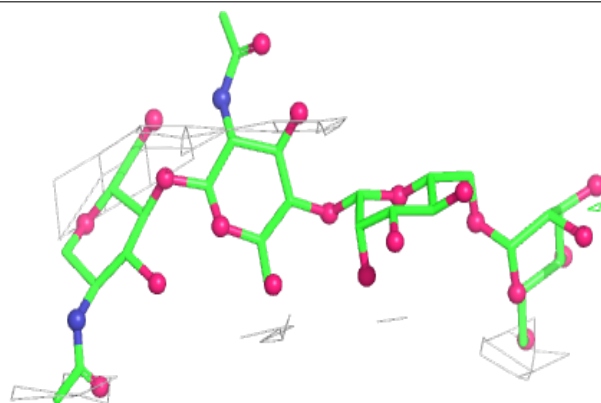


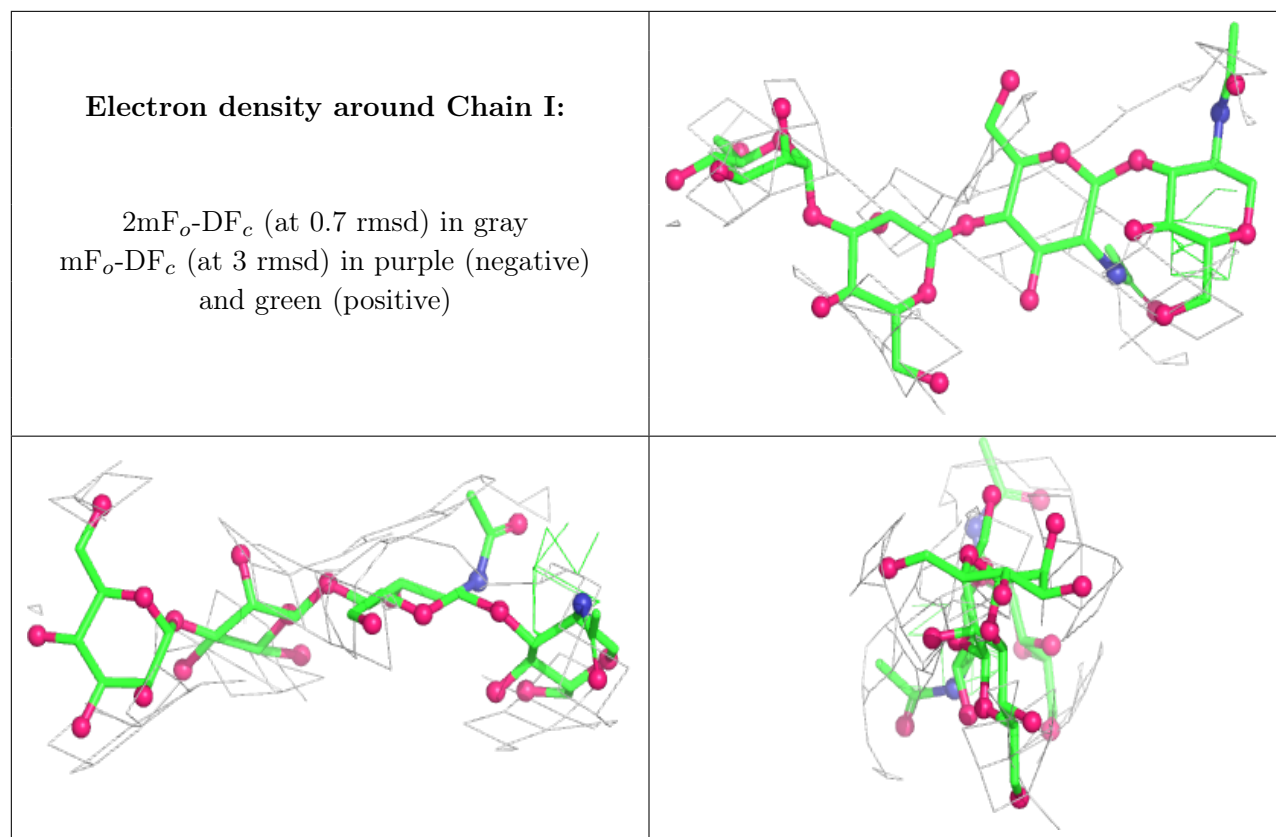
**Electron density around Chain G:**

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

**Electron density around Chain P:**

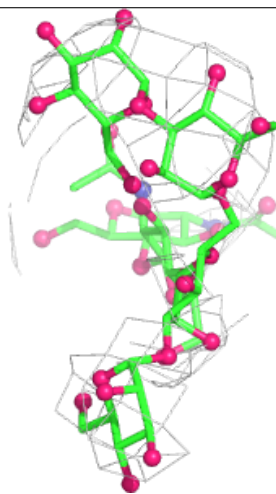
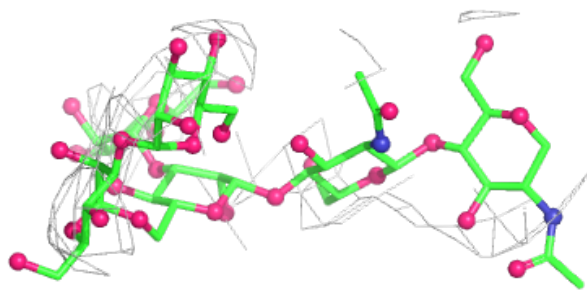
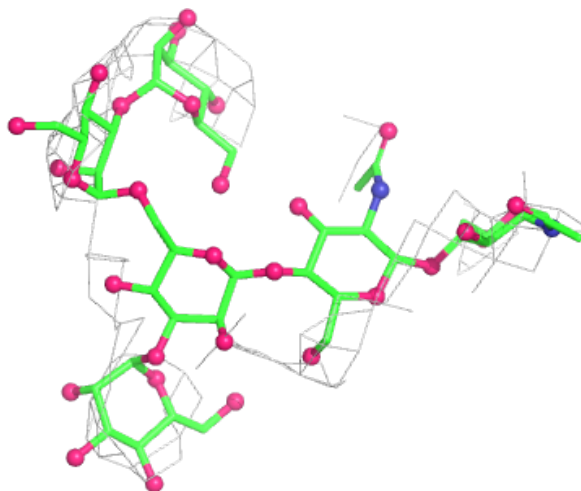
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





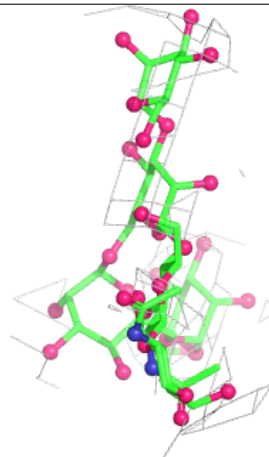
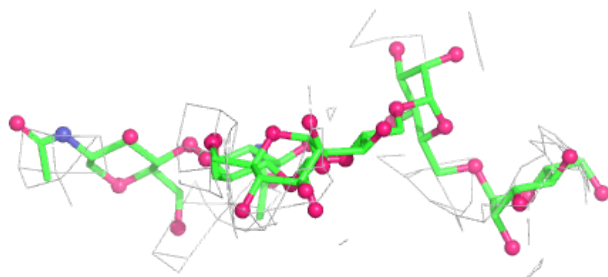
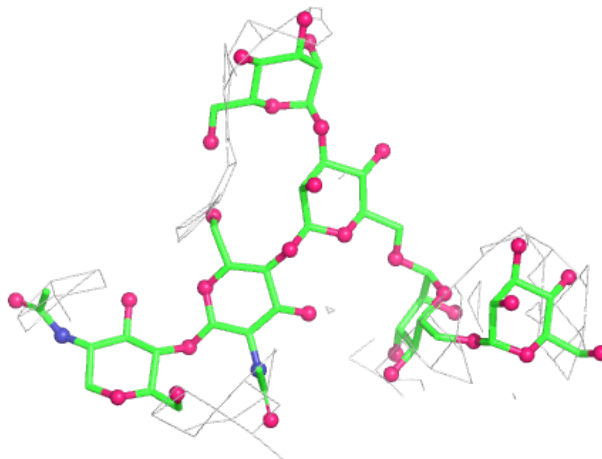
**Electron density around Chain J:**

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



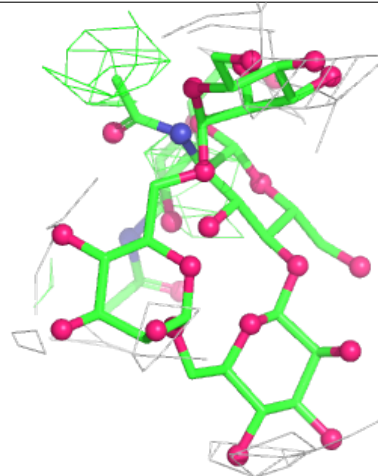
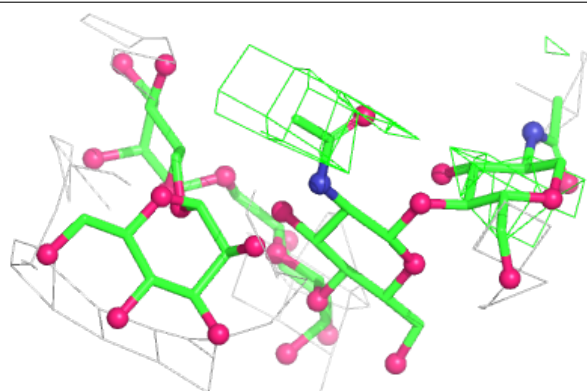
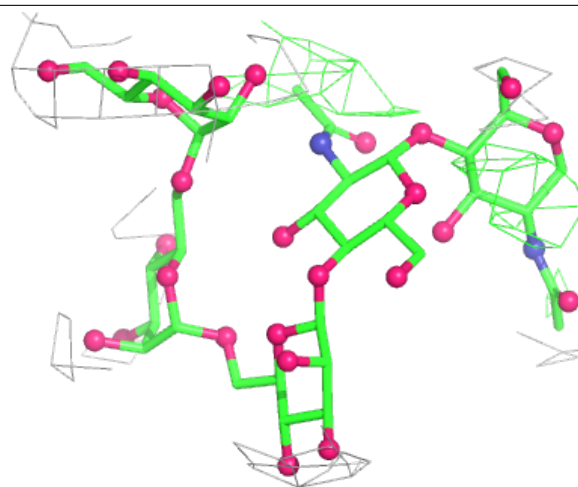
**Electron density around Chain K:**

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



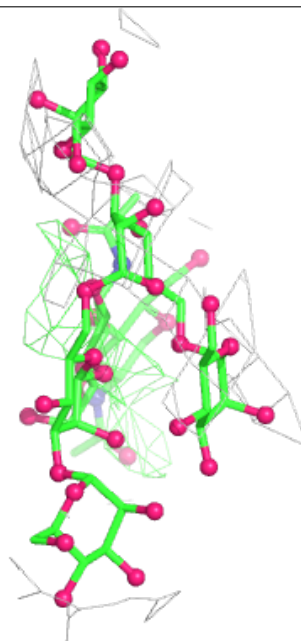
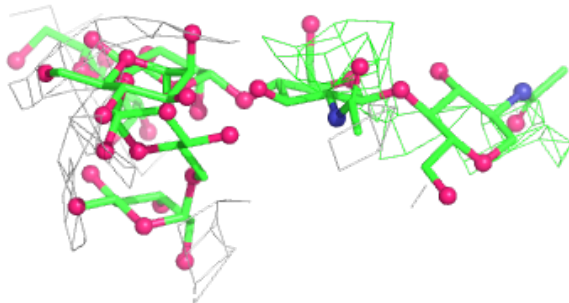
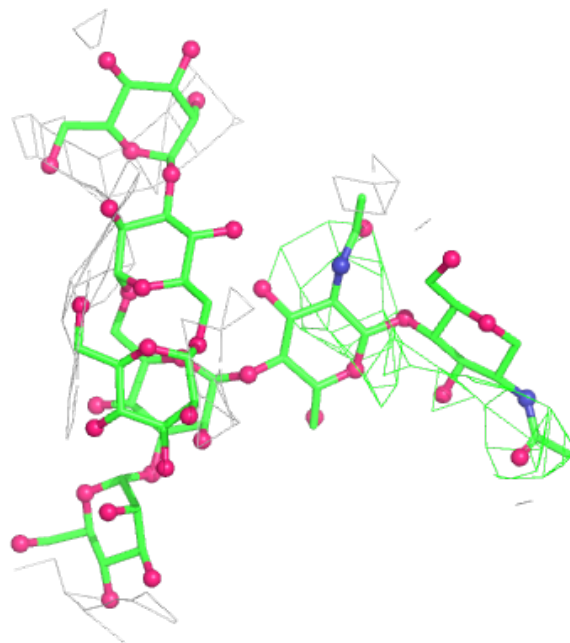
**Electron density around Chain L:**

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



**Electron density around Chain M:**

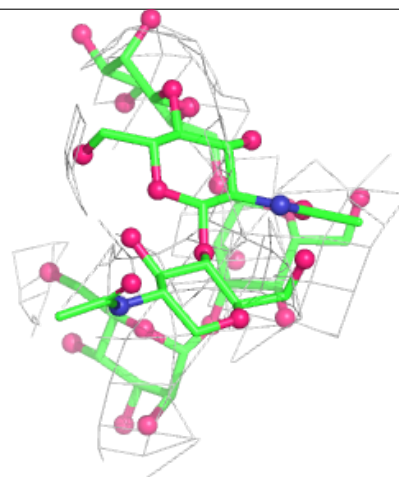
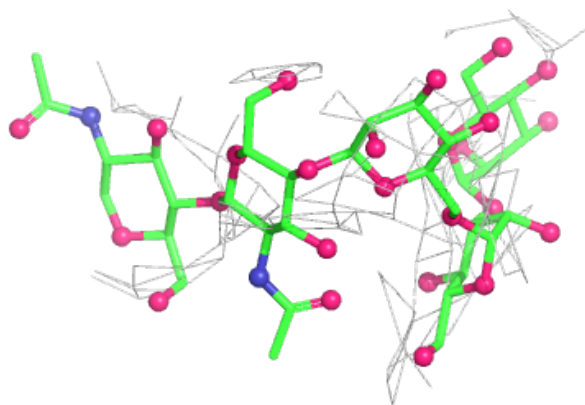
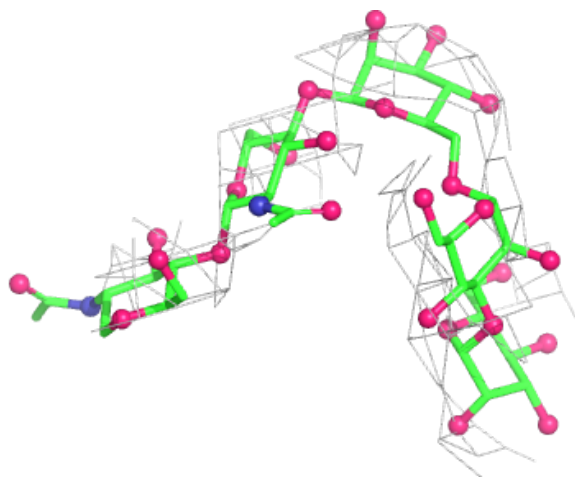
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

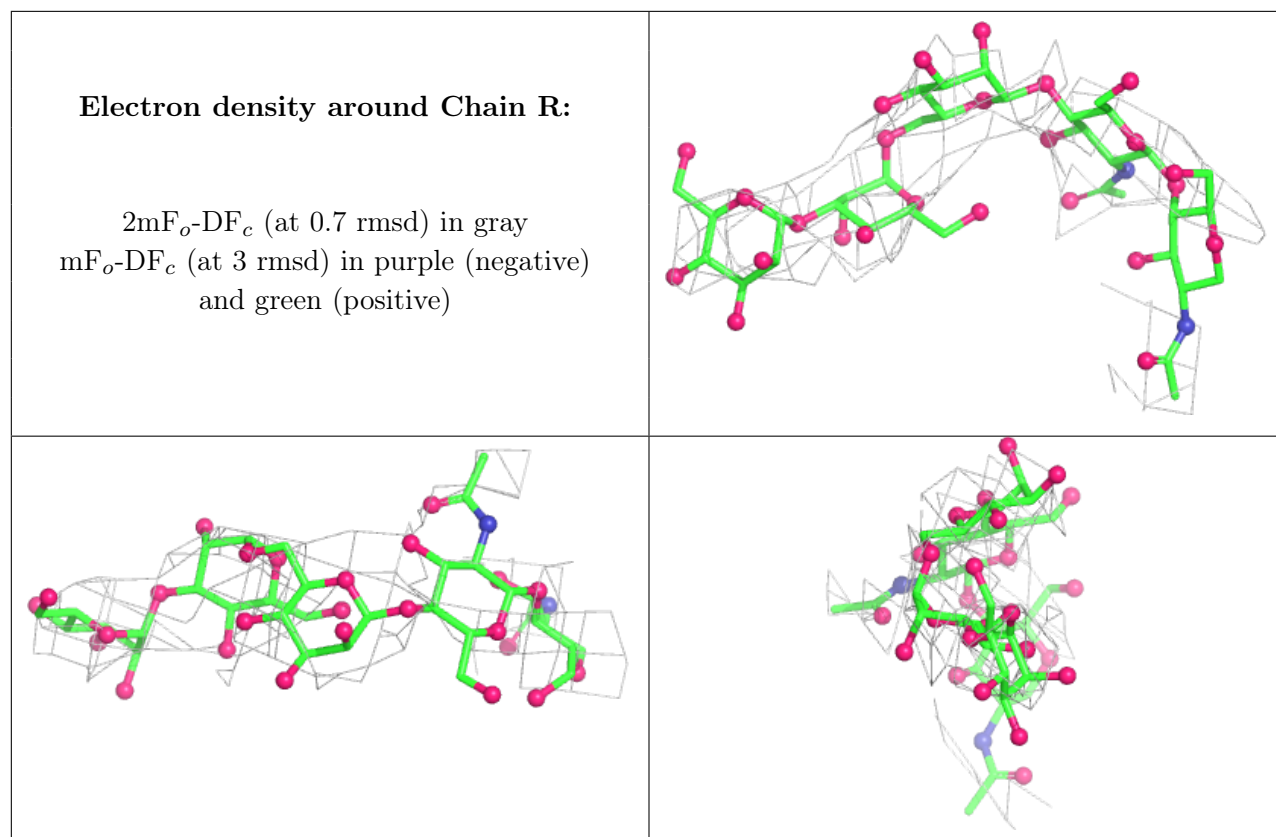




**Electron density around Chain N:**

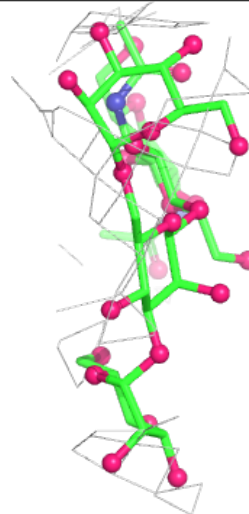
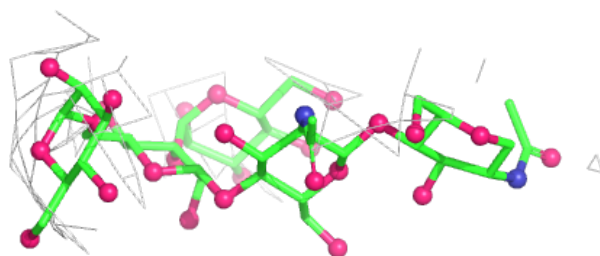
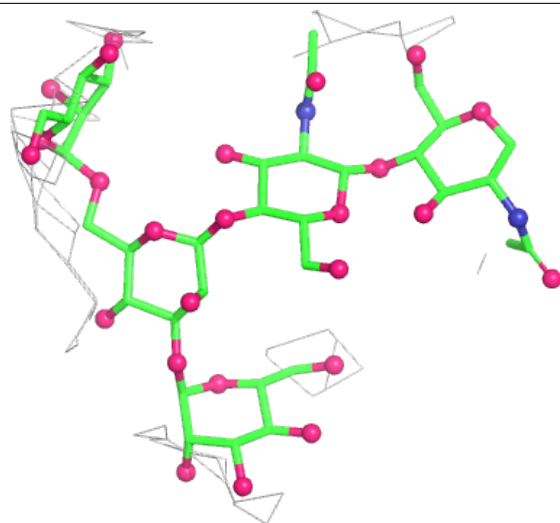
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

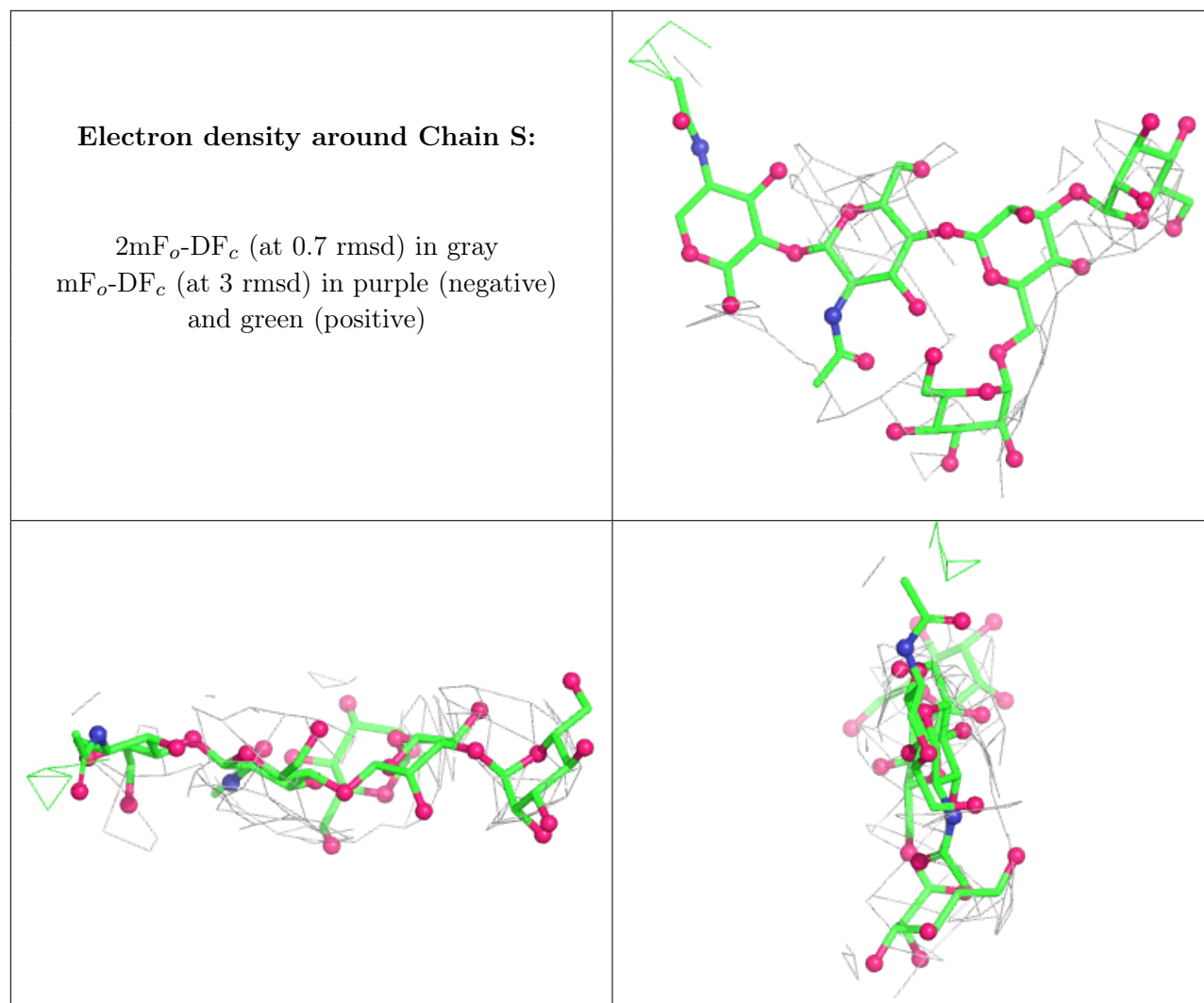


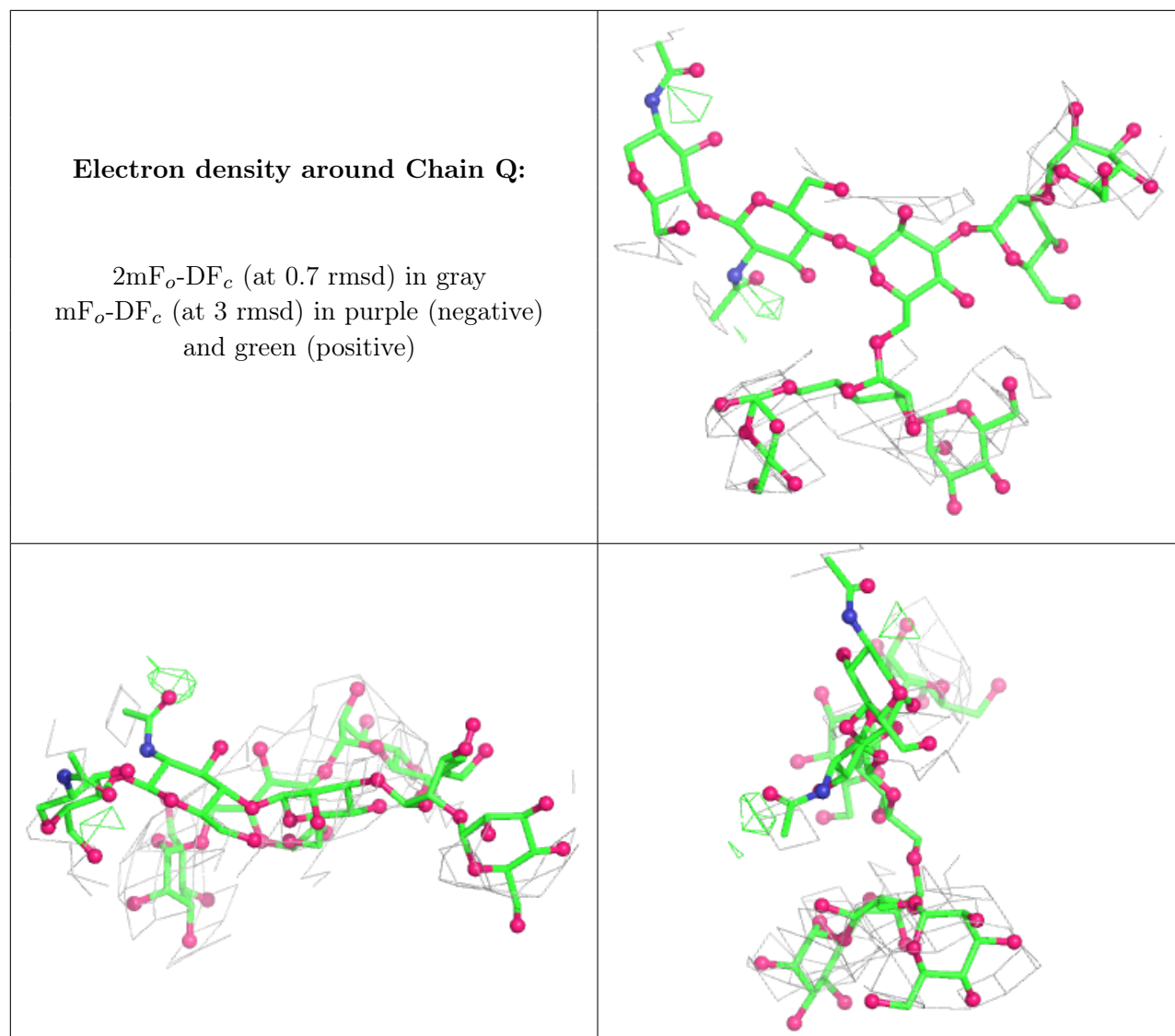


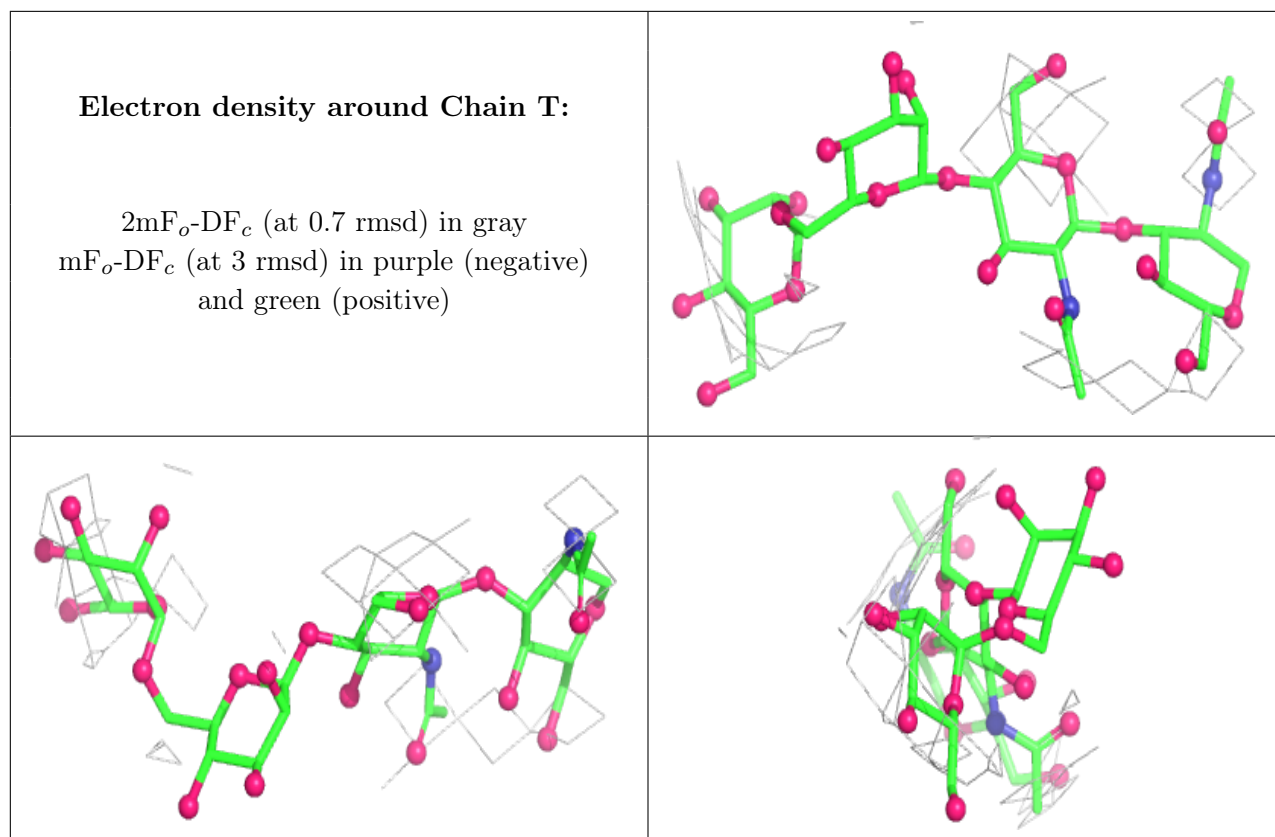
**Electron density around Chain O:**

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









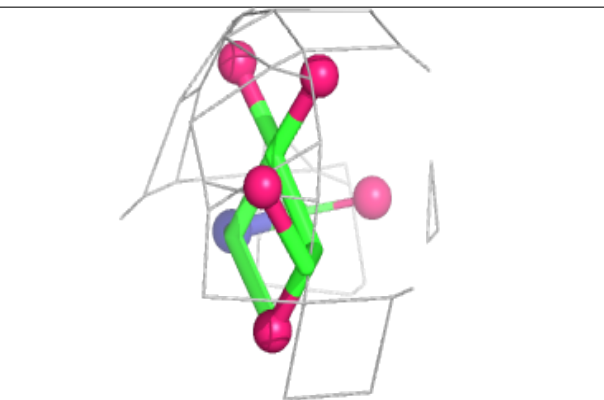
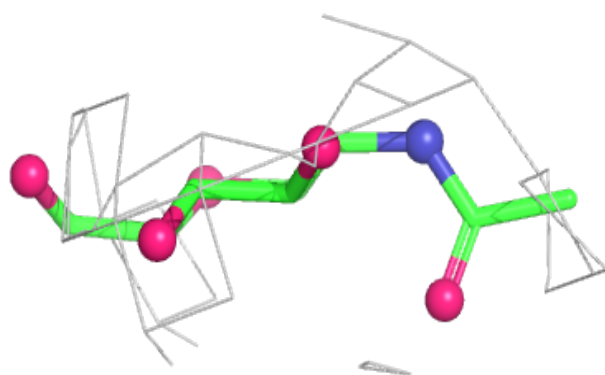
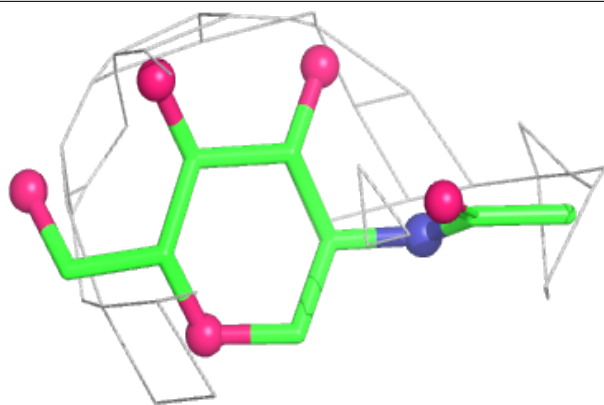
## 6.4 Ligands [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.

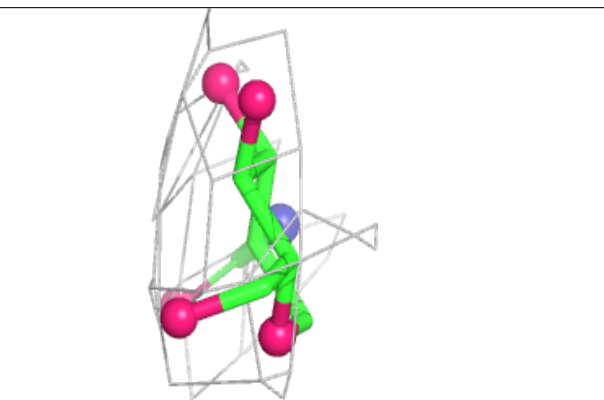
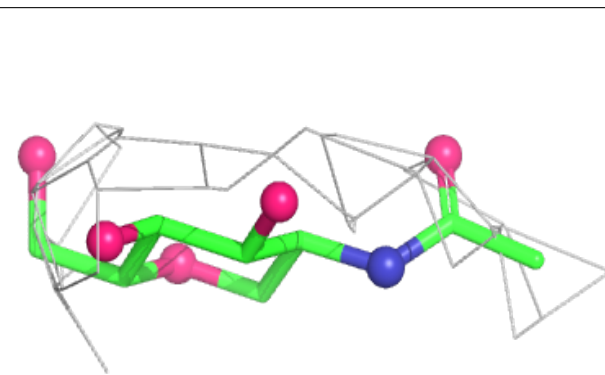
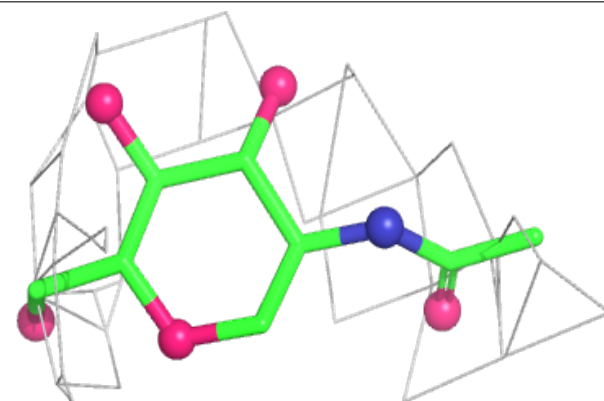
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAG A 701:**

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

**Electron density around NAG B 701:**

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



## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.