



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2025 – 11:09 AM EST

PDB ID : 5T3Z  
Title : 3.5 Angstrom Crystal Structure of a Fully and Natively Glycosylated BG505  
SOSIP.664 HIV-1 Env Trimer in Complex with the Broadly Neutralizing An-  
tibodies IOMA and 10-1074  
Authors : Gristick, H.B.; Bjorkman, P.J.  
Deposited on : 2016-08-26  
Resolution : 3.50 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:

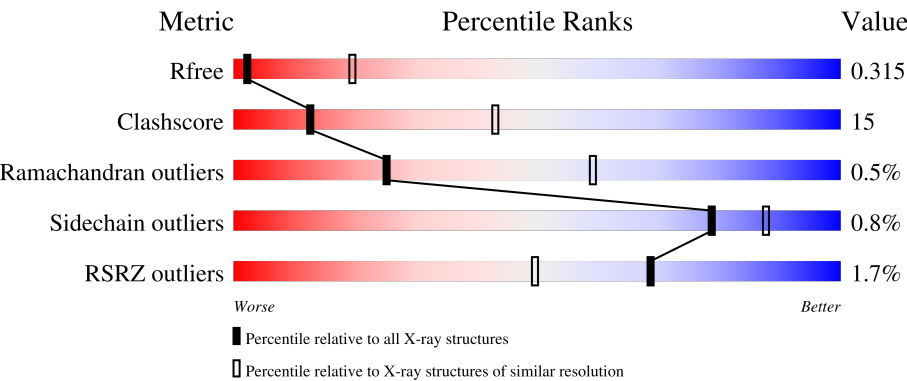
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (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 3.50 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>	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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	B	153	<div><div></div><div></div><div></div><div></div><div></div></div> <div>56%26%18%</div>
2	G	481	<div><div></div><div></div><div></div><div></div><div></div></div> <div>%62%32%6%</div>
3	H	238	<div><div></div><div></div><div></div><div></div><div></div></div> <div>%60%37%. </div>
4	L	214	<div><div></div><div></div><div></div><div></div><div></div></div> <div>63%35%. </div>

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Mol	Chain	Length	Quality of chain
5	D	232	
6	E	214	
7	A	2	
8	C	3	
8	W	3	
9	F	2	
9	I	2	
9	N	2	
9	Q	2	
10	J	11	
11	K	5	
11	P	5	
11	U	5	
12	M	8	
13	O	7	
14	R	6	
15	S	10	
16	T	7	
17	V	4	

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 12265 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein gp160.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S6
B	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	450	Total	C	N	O	S	0	0	0
			3538	2221	624	666	27			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6
G	509	ARG	GLU	conflict	UNP Q2N0S6
G	510	ARG	LYS	conflict	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 3 is a protein called 10-1074 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	230	Total	C	N	O	S	0	0	0
			1753	1108	293	345	7			

- Molecule 4 is a protein called 10-1074 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	211	Total	C	N	O	S	0	0	0
			1607	1006	281	314	6			

- Molecule 5 is a protein called IOMA Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	229	Total	C	N	O	S	0	0	0
			1742	1100	298	332	12			

- Molecule 6 is a protein called IOMA Light Chain.

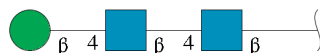
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	210	Total	C	N	O	S	0	0	0
			1558	976	261	317	4			

- Molecule 7 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



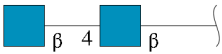
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	A	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 8 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.



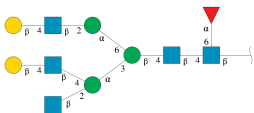
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
8	W	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



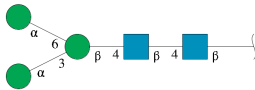
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	11	Total	C	N	O	0	0	0
			135	76	5	54			

- 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.



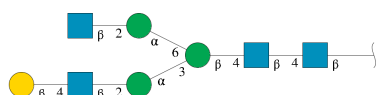
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	K	5	Total	C	N	O	0	0	0
			61	34	2	25			
11	P	5	Total	C	N	O	0	0	0
			61	34	2	25			

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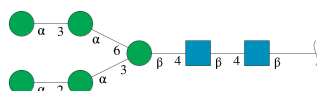
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	U	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



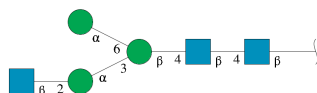
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	M	8	Total	C	N	O	0	0	0
			100	56	4	40			

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



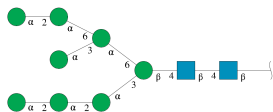
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 14 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



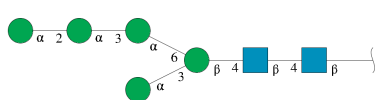
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	R	6	Total	C	N	O	0	0	0
			75	42	3	30			

- Molecule 15 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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.



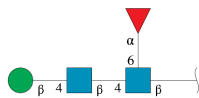
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	S	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 16 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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
16	T	7	Total	C	N	O	0	0	0
			83	46	2	35			

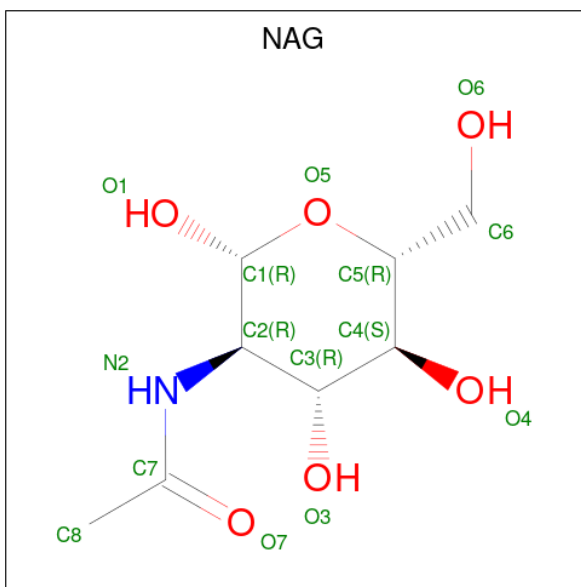
- Molecule 17 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 18 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).



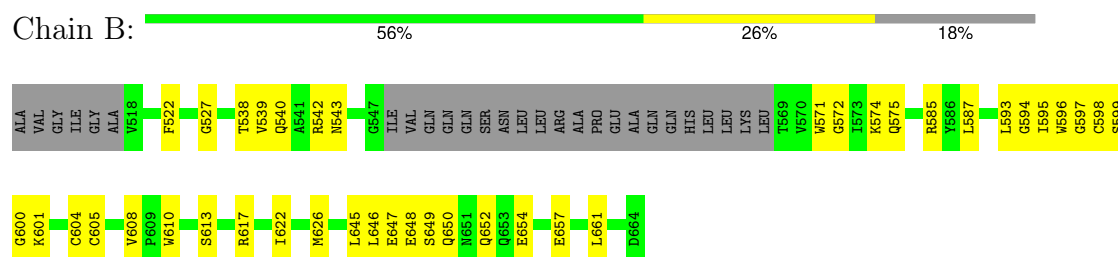


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	G	1	Total	C	N	O	0	0
			14	8	1	5		
18	G	1	Total	C	N	O	0	0
			14	8	1	5		

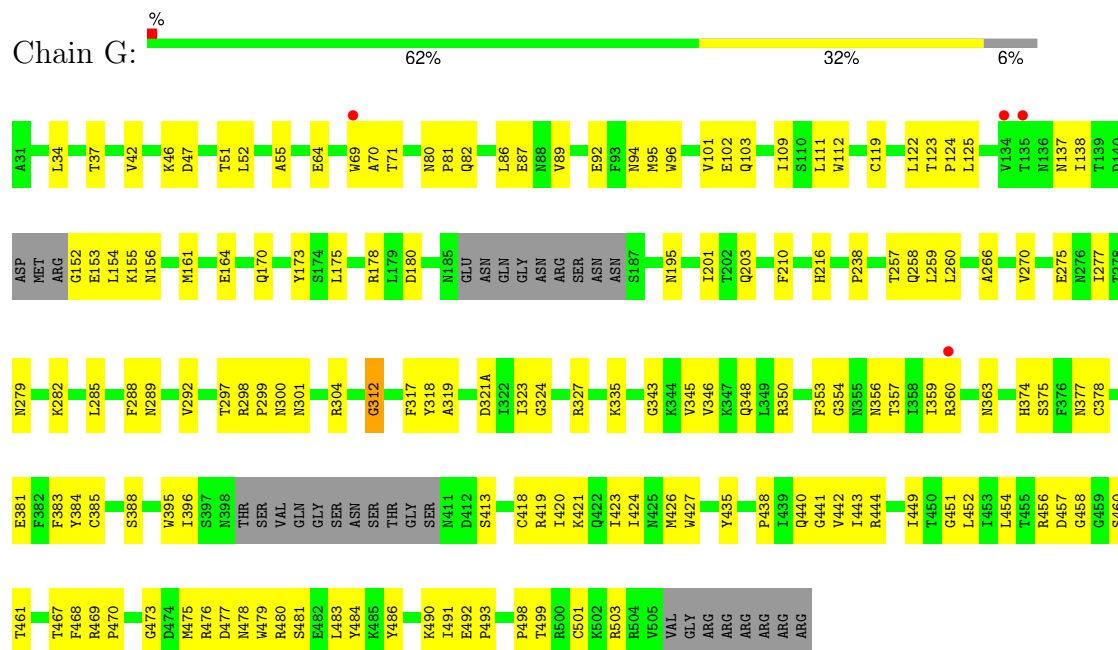
### 3 Residue-property plots

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

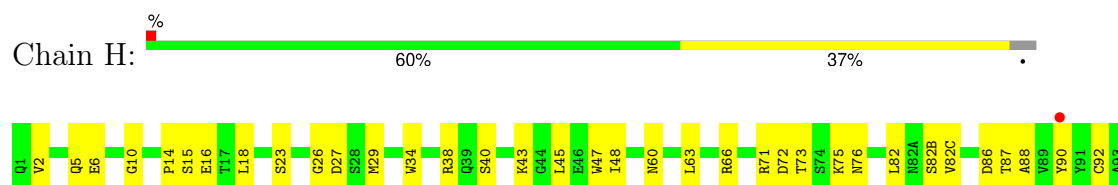
#### • Molecule 1: Envelope glycoprotein gp160

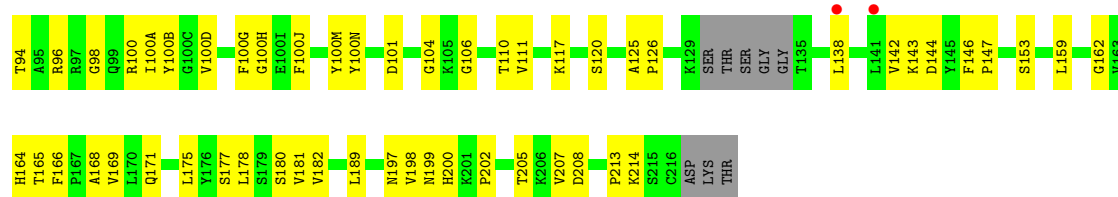


#### • Molecule 2: Envelope glycoprotein gp160



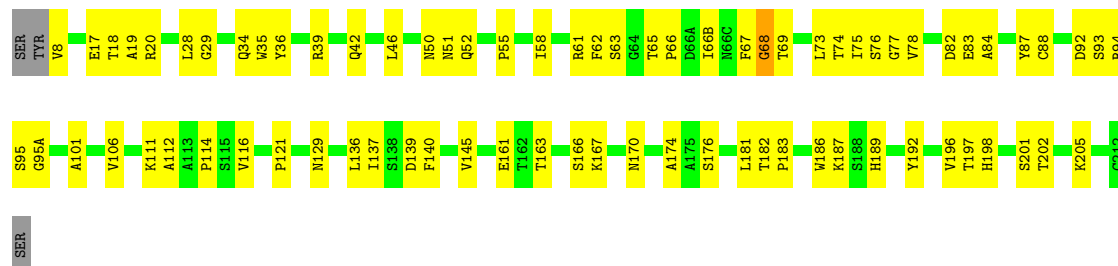
#### • Molecule 3: 10-1074 Heavy Chain





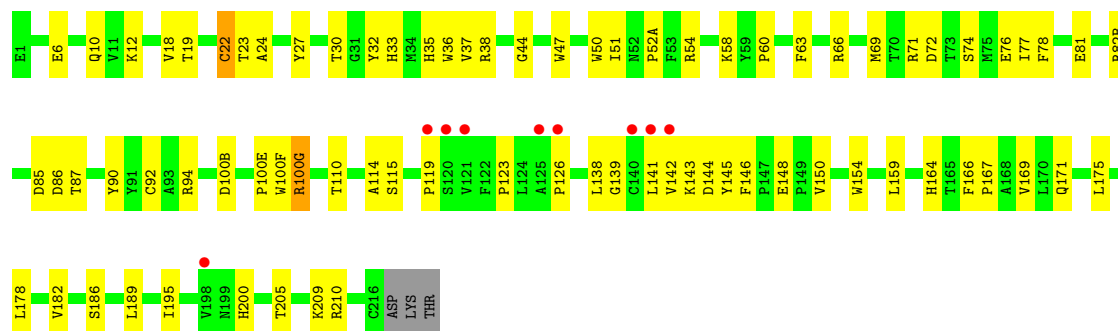
• Molecule 4: 10-1074 Light Chain

Chain L: 63% 35%



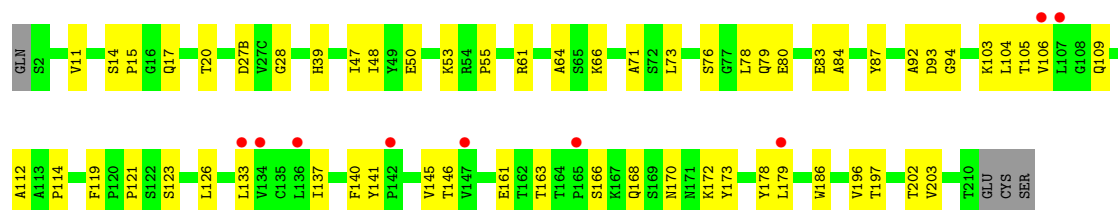
• Molecule 5: IOMA Heavy Chain

Chain D: 4% 65% 33%



• Molecule 6: IOMA Light Chain

Chain E: 4% 71% 28%



• Molecule 7: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 50% 50%



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



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



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



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



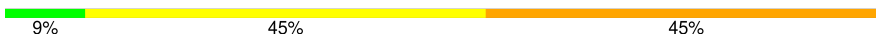
- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

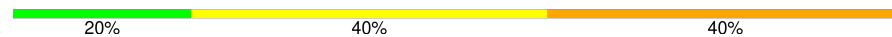


- Molecule 10: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)]alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 



- 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 K: 

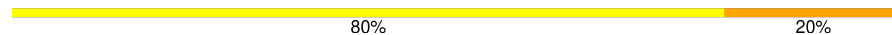


- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 

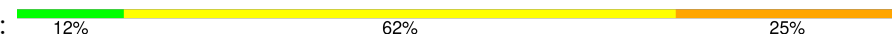


- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U: 



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




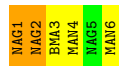
- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  71% 29%

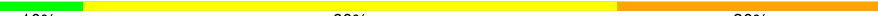


- Molecule 14: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  17% 50% 33%



- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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:  10% 60% 30%



- Molecule 16: alpha-D-mannopyranose-(1-2)-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 T:  14% 86%



- Molecule 17: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	217.26Å 217.26Å 154.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.63 – 3.50 64.63 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.63-3.50) 94.8 (64.63-3.50)	Depositor EDS
$R_{merge}$	0.68	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.265 , 0.306 0.281 , 0.315	Depositor DCC
$R_{free}$ test set	1755 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	112.0	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 152.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.130 for k,h,-l	Depositor
Outliers	0 of 34373 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	12265	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	189.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: NAG, FUC, MAN, GAL, BMA

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	B	0.26	0/1019	0.49	0/1382
2	G	0.30	0/3611	0.54	0/4903
3	H	0.27	0/1796	0.51	0/2450
4	L	0.27	0/1649	0.50	0/2250
5	D	0.30	0/1790	0.55	0/2437
6	E	0.26	0/1596	0.49	0/2175
All	All	0.28	0/11461	0.52	0/15597

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	B	1001	0	976	28	0
2	G	3538	0	3469	111	0
3	H	1753	0	1719	67	0
4	L	1607	0	1550	56	0
5	D	1742	0	1698	69	0
6	E	1558	0	1511	44	0
7	A	24	0	22	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	39	0	34	1	0
8	W	39	0	34	0	0
9	F	28	0	25	1	0
9	I	28	0	25	0	0
9	N	28	0	25	0	0
9	Q	28	0	25	0	0
10	J	135	0	115	5	0
11	K	61	0	52	1	0
11	P	61	0	52	4	0
11	U	61	0	52	1	0
12	M	100	0	85	1	0
13	O	83	0	70	1	0
14	R	75	0	64	1	0
15	S	116	0	97	3	0
16	T	83	0	70	6	0
17	V	49	0	43	0	0
18	G	28	0	26	0	0
All	All	12265	0	11839	361	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 15.

All (361) 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)
5:D:82(B):ARG:HH22	16:T:5:MAN:H5	1.26	0.98
5:D:119:PRO:HD2	5:D:205:THR:HB	1.58	0.84
1:B:605:CYS:HA	2:G:37:THR:HG22	1.68	0.76
4:L:51:ASN:ND2	15:S:5:MAN:O3	2.18	0.76
2:G:95:MET:HB3	2:G:484:TYR:HA	1.68	0.75
2:G:92:GLU:HA	2:G:238:PRO:HA	1.70	0.74
2:G:266:ALA:N	2:G:288:PHE:O	2.15	0.74
5:D:52(A):PRO:HG3	5:D:78:PHE:HZ	1.53	0.74
2:G:292:VAL:HB	2:G:449:ILE:HB	1.71	0.72
1:B:647:GLU:HG3	1:B:648:GLU:HG3	1.72	0.71
4:L:83:GLU:HG2	4:L:106:VAL:H	1.57	0.70
4:L:29:GLY:H	4:L:67:PHE:HZ	1.38	0.69
5:D:19:THR:HG22	5:D:81:GLU:HB2	1.75	0.69
3:H:200:HIS:HB3	3:H:205:THR:HB	1.74	0.69
2:G:46:LYS:HG3	2:G:492:GLU:HG3	1.76	0.68
2:G:279:ASN:OD1	5:D:100(F):TRP:NE1	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:87:GLU:HB3	9:F:1:NAG:H82	1.75	0.68
4:L:19:ALA:HB3	4:L:75:ILE:HB	1.76	0.68
4:L:8:VAL:HG12	4:L:101:ALA:HB3	1.77	0.67
3:H:15:SER:HA	3:H:82(B):SER:HA	1.77	0.66
5:D:12:LYS:HG3	5:D:18:VAL:HG21	1.77	0.66
5:D:87:THR:HG23	5:D:110:THR:HA	1.76	0.66
2:G:457:ASP:OD2	2:G:467:THR:HB	1.96	0.66
3:H:88:ALA:HB3	3:H:90:TYR:HE1	1.60	0.66
6:E:133:LEU:HD12	6:E:179:LEU:HD23	1.77	0.66
5:D:6:GLU:HG2	5:D:22:CYS:HB2	1.78	0.66
5:D:72:ASP:O	5:D:76:GLU:N	2.27	0.65
6:E:66:LYS:HA	6:E:71:ALA:HA	1.79	0.65
2:G:321(A):ASP:HB2	10:J:11:FUC:H63	1.78	0.64
3:H:169:VAL:HG21	4:L:161:GLU:HB3	1.78	0.64
6:E:145:VAL:HG12	6:E:146:THR:H	1.63	0.64
3:H:197:ASN:ND2	3:H:208:ASP:OD2	2.30	0.63
11:K:1:NAG:H61	11:K:2:NAG:H82	1.78	0.63
2:G:301:ASN:HB3	2:G:323:ILE:HB	1.81	0.62
2:G:304:ARG:HD3	2:G:318:TYR:HB3	1.81	0.62
2:G:153:GLU:H	2:G:178:ARG:HH21	1.47	0.62
5:D:82(B):ARG:NH2	16:T:5:MAN:H5	2.07	0.62
5:D:33:HIS:CG	5:D:100(E):PRO:HB3	2.35	0.62
2:G:424:ILE:HG22	2:G:426:MET:H	1.64	0.61
6:E:15:PRO:HD3	6:E:106:VAL:HG13	1.82	0.61
5:D:144:ASP:HA	5:D:175:LEU:HB3	1.80	0.61
5:D:186:SER:HA	5:D:189:LEU:HG	1.83	0.61
2:G:86:LEU:HB3	2:G:89:VAL:HG21	1.81	0.61
2:G:259:LEU:HD23	2:G:452:LEU:HD21	1.82	0.61
2:G:456:ARG:NH2	6:E:93:ASP:OD1	2.25	0.61
2:G:298:ARG:HD2	2:G:300:ASN:HB2	1.83	0.61
4:L:83:GLU:OE1	4:L:167:LYS:NZ	2.32	0.61
3:H:117:LYS:HD3	3:H:175:LEU:HD22	1.83	0.60
5:D:30:THR:HA	5:D:52(A):PRO:HB2	1.82	0.60
2:G:335:LYS:H	2:G:413:SER:HA	1.66	0.60
5:D:82(B):ARG:NH2	16:T:4:MAN:O2	2.35	0.60
6:E:48:ILE:HG21	6:E:64:ALA:HB3	1.83	0.60
2:G:101:VAL:HG13	2:G:479:TRP:HB2	1.84	0.60
4:L:39:ARG:NH1	4:L:83:GLU:O	2.34	0.59
3:H:2:VAL:HG22	3:H:27:ASP:HB2	1.84	0.59
2:G:353:PHE:HE2	2:G:357:THR:HG1	1.50	0.59
2:G:456:ARG:HG2	2:G:457:ASP:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:144:ASP:OD1	3:H:171:GLN:NE2	2.31	0.59
2:G:70:ALA:HA	2:G:111:LEU:HD21	1.84	0.59
2:G:499:THR:HG23	2:G:501:CYS:H	1.68	0.58
13:O:3:BMA:O4	13:O:5:MAN:O6	2.14	0.58
3:H:38:ARG:HH12	3:H:86:ASP:HA	1.68	0.58
1:B:648:GLU:O	1:B:652:GLN:HB3	2.04	0.57
1:B:539:VAL:HG22	1:B:542:ARG:HH22	1.69	0.57
2:G:378:CYS:HB3	2:G:383:PHE:CE1	2.39	0.57
5:D:23:THR:HG22	5:D:77:ILE:HG23	1.86	0.57
3:H:66:ARG:HD2	3:H:82(B):SER:HB2	1.85	0.57
4:L:19:ALA:O	4:L:75:ILE:N	2.31	0.57
2:G:161:MET:N	2:G:170:GLN:O	2.34	0.57
4:L:139:ASP:OD1	4:L:170:ASN:ND2	2.38	0.57
5:D:195:ILE:HG12	5:D:210:ARG:HG2	1.87	0.57
4:L:39:ARG:HB2	4:L:42:GLN:HB2	1.85	0.57
2:G:299:PRO:HG2	2:G:327:ARG:HB2	1.85	0.56
2:G:478:ASN:O	2:G:481:SER:OG	2.21	0.56
3:H:117:LYS:HB3	3:H:146:PHE:N	2.20	0.56
4:L:67:PHE:O	4:L:69:THR:N	2.38	0.56
6:E:50:GLU:OE1	6:E:53:LYS:NZ	2.34	0.56
2:G:297:THR:HG22	2:G:444:ARG:HG3	1.87	0.56
2:G:321(A):ASP:HB2	10:J:11:FUC:C6	2.34	0.56
3:H:10:GLY:HA3	3:H:202:PRO:HG3	1.86	0.56
6:E:166:SER:O	6:E:168:GLN:NE2	2.39	0.56
3:H:18:LEU:HB3	3:H:82:LEU:HB3	1.88	0.56
3:H:142:VAL:HB	3:H:178:LEU:HG	1.87	0.56
6:E:123:SER:HA	6:E:126:LEU:HB2	1.88	0.56
3:H:100(D):VAL:HG13	3:H:100(G):PHE:HB2	1.89	0.55
4:L:61:ARG:NH1	4:L:77:GLY:O	2.40	0.55
4:L:55:PRO:HD2	4:L:58:ILE:HG13	1.87	0.55
2:G:55:ALA:HB3	2:G:216:HIS:HB2	1.88	0.55
3:H:16:GLU:H	3:H:82(C):VAL:HG22	1.72	0.55
6:E:121:PRO:HD2	6:E:186:TRP:CZ2	2.42	0.55
2:G:304:ARG:HB3	2:G:440:GLN:HE21	1.72	0.55
5:D:38:ARG:NH2	5:D:85:ASP:O	2.39	0.54
2:G:299:PRO:HA	2:G:442:VAL:HG13	1.88	0.54
10:J:5:NAG:H81	10:J:9:NAG:H82	1.89	0.54
5:D:169:VAL:HG21	6:E:163:THR:HA	1.88	0.54
1:B:613:SER:HB2	7:A:2:FUC:H5	1.88	0.54
3:H:165:THR:HA	3:H:180:SER:HA	1.90	0.54
2:G:298:ARG:NH2	2:G:441:GLY:O	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:ARG:NH2	2:G:491:ILE:O	2.38	0.54
5:D:6:GLU:OE2	5:D:92:CYS:N	2.40	0.54
5:D:60:PRO:HD2	5:D:63:PHE:HB2	1.90	0.53
5:D:24:ALA:HB1	5:D:27:TYR:HE1	1.72	0.53
3:H:100(D):VAL:HA	15:S:2:NAG:H2	1.90	0.53
4:L:112:ALA:HB3	4:L:140:PHE:HA	1.89	0.53
5:D:119:PRO:HB3	5:D:145:TYR:HB3	1.91	0.53
2:G:153:GLU:O	2:G:178:ARG:N	2.42	0.53
3:H:6:GLU:N	3:H:6:GLU:OE1	2.41	0.52
3:H:98:GLY:N	3:H:100(M):TYR:O	2.42	0.52
3:H:125:ALA:HB3	3:H:214:LYS:HE3	1.91	0.52
2:G:152:GLY:C	2:G:154:LEU:H	2.12	0.52
2:G:259:LEU:HB2	2:G:374:HIS:CE1	2.44	0.52
2:G:260:LEU:HD12	2:G:451:GLY:HA3	1.91	0.52
2:G:343:GLY:HA2	2:G:346:VAL:HG12	1.91	0.52
2:G:304:ARG:HG3	2:G:438:PRO:HG2	1.92	0.52
2:G:460:SER:OG	2:G:461:THR:N	2.43	0.52
3:H:14:PRO:HA	3:H:82(C):VAL:HG23	1.91	0.52
4:L:50:ASN:O	4:L:52:GLN:N	2.38	0.52
2:G:51:THR:HA	2:G:103:GLN:HE22	1.74	0.52
2:G:350:ARG:NH2	2:G:396:ILE:O	2.43	0.52
3:H:5:GLN:O	3:H:23:SER:N	2.43	0.51
3:H:153:SER:O	3:H:197:ASN:N	2.36	0.51
12:M:2:NAG:H61	12:M:7:MAN:H3	1.92	0.51
11:P:3:BMA:H2	11:P:4:MAN:H5	1.92	0.51
2:G:359:ILE:O	2:G:395:TRP:N	2.42	0.51
2:G:363:ASN:HB3	2:G:388:SER:HA	1.93	0.51
5:D:72:ASP:OD1	5:D:74:SER:OG	2.27	0.51
6:E:109:GLN:HE22	6:E:172:LYS:HG2	1.76	0.51
3:H:168:ALA:HB2	3:H:178:LEU:HB3	1.91	0.51
6:E:92:ALA:O	6:E:94:GLY:N	2.42	0.51
3:H:171:GLN:NE2	3:H:177:SER:OG	2.43	0.51
3:H:200:HIS:N	3:H:205:THR:O	2.37	0.51
5:D:60:PRO:HG2	5:D:63:PHE:HD2	1.75	0.51
3:H:71:ARG:HH21	3:H:73:THR:HG22	1.76	0.51
3:H:72:ASP:HB3	3:H:75:LYS:HB2	1.93	0.51
4:L:34:GLN:HB3	4:L:36:TYR:CE1	2.46	0.51
2:G:300:ASN:ND2	2:G:327:ARG:O	2.36	0.51
6:E:20:THR:HA	6:E:73:LEU:O	2.11	0.51
1:B:571:TRP:HH2	2:G:71:THR:HA	1.75	0.51
2:G:34:LEU:HB3	2:G:498:PRO:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:270:VAL:HG12	2:G:289:ASN:H	1.76	0.50
5:D:159:LEU:HD21	5:D:182:VAL:HG21	1.94	0.50
6:E:61:ARG:HB3	6:E:76:SER:O	2.11	0.50
6:E:197:THR:HA	6:E:202:THR:HA	1.91	0.50
6:E:196:VAL:O	6:E:203:VAL:N	2.26	0.50
4:L:181:LEU:HG	4:L:182:THR:H	1.76	0.50
5:D:143:LYS:HG2	5:D:144:ASP:H	1.76	0.50
3:H:100(H):GLY:HA2	3:H:100(J):PHE:CE2	2.47	0.50
4:L:111:LYS:HG3	4:L:198:HIS:HE1	1.75	0.50
5:D:10:GLN:HB3	5:D:12:LYS:NZ	2.27	0.50
5:D:27:TYR:CZ	5:D:94:ARG:HD3	2.47	0.50
5:D:142:VAL:HG11	5:D:150:VAL:HG11	1.93	0.50
11:P:1:NAG:H62	11:P:2:NAG:C7	2.42	0.50
2:G:266:ALA:O	2:G:289:ASN:ND2	2.43	0.49
1:B:646:LEU:O	1:B:650:GLN:HB2	2.11	0.49
2:G:164:GLU:HA	2:G:312:GLY:O	2.12	0.49
3:H:40:SER:HB3	3:H:43:LYS:HD2	1.94	0.49
6:E:39:HIS:CD2	6:E:84:ALA:HB2	2.47	0.49
4:L:137:ILE:HG22	4:L:140:PHE:CE1	2.48	0.49
4:L:51:ASN:HB3	4:L:65:THR:O	2.12	0.49
6:E:27(B):ASP:HB3	6:E:92:ALA:HB2	1.94	0.49
3:H:92:CYS:O	3:H:104:GLY:N	2.45	0.49
5:D:119:PRO:HD3	5:D:200:HIS:ND1	2.27	0.49
2:G:210:PHE:HB2	2:G:377:ASN:ND2	2.27	0.49
4:L:198:HIS:N	4:L:201:SER:O	2.38	0.49
5:D:146:PHE:H	5:D:200:HIS:HE1	1.60	0.49
2:G:298:ARG:HB3	2:G:443:ILE:HB	1.94	0.49
4:L:18:THR:HG23	4:L:76:SER:HA	1.95	0.48
3:H:159:LEU:HG	3:H:182:VAL:HG21	1.94	0.48
4:L:17:GLU:O	4:L:78:VAL:HG23	2.14	0.48
2:G:155:LYS:O	2:G:175:LEU:HA	2.14	0.48
2:G:477:ASP:OD1	2:G:480:ARG:NH1	2.46	0.48
5:D:178:LEU:HD23	5:D:178:LEU:HA	1.48	0.48
2:G:384:TYR:O	2:G:419:ARG:N	2.46	0.48
3:H:18:LEU:N	3:H:82:LEU:O	2.45	0.48
3:H:60:ASN:HB3	3:H:63:LEU:HD13	1.96	0.48
5:D:27:TYR:HE2	5:D:32:TYR:HB2	1.78	0.48
5:D:38:ARG:HB3	5:D:90:TYR:CD2	2.49	0.48
5:D:146:PHE:H	5:D:200:HIS:CE1	2.32	0.48
5:D:146:PHE:HB2	5:D:175:LEU:HD23	1.96	0.48
1:B:522:PHE:CE1	1:B:540:GLN:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:TRP:CD2	2:G:498:PRO:HB3	2.49	0.47
5:D:141:LEU:HD12	5:D:178:LEU:O	2.13	0.47
6:E:47:ILE:O	6:E:55:PRO:HD2	2.14	0.47
10:J:4:MAN:O3	10:J:7:NAG:O5	2.24	0.47
5:D:44:GLY:HA2	6:E:87:TYR:HE2	1.79	0.47
3:H:126:PRO:HD2	3:H:213:PRO:HA	1.96	0.47
5:D:167:PRO:C	5:D:178:LEU:HD21	2.35	0.47
2:G:277:ILE:HB	11:P:1:NAG:H82	1.95	0.47
3:H:90:TYR:O	3:H:106:GLY:HA2	2.14	0.47
6:E:39:HIS:HD2	6:E:84:ALA:HB2	1.79	0.47
11:P:1:NAG:H62	11:P:2:NAG:H82	1.97	0.47
2:G:161:MET:HB3	2:G:170:GLN:HB3	1.96	0.47
4:L:39:ARG:HD2	4:L:84:ALA:HB2	1.96	0.47
2:G:173:TYR:OH	10:J:11:FUC:H5	2.15	0.47
3:H:166:PHE:CG	4:L:136:LEU:HD22	2.50	0.47
4:L:63:SER:O	4:L:74:THR:N	2.47	0.47
5:D:38:ARG:HB3	5:D:90:TYR:CE2	2.50	0.47
6:E:161:GLU:HG2	6:E:178:TYR:HD2	1.79	0.47
2:G:203:GLN:HG3	2:G:435:TYR:HD2	1.79	0.47
4:L:163:THR:HG1	4:L:176:SER:H	1.57	0.47
5:D:139:GLY:HA2	5:D:154:TRP:HH2	1.79	0.47
16:T:1:NAG:H62	16:T:2:NAG:H82	1.95	0.47
3:H:45:LEU:HG	4:L:87:TYR:CZ	2.49	0.47
3:H:87:THR:OG1	3:H:111:VAL:N	2.48	0.47
5:D:37:VAL:HG22	5:D:47:TRP:HA	1.97	0.47
6:E:112:ALA:HB3	6:E:140:PHE:HA	1.95	0.47
4:L:82:ASP:HB2	4:L:106:VAL:HG21	1.97	0.47
5:D:47:TRP:CE3	5:D:60:PRO:HG3	2.50	0.47
3:H:100:ARG:NH2	15:S:4:MAN:O6	2.48	0.46
1:B:522:PHE:CE1	1:B:543:ASN:HB2	2.50	0.46
6:E:103:LYS:HZ3	6:E:173:TYR:HE2	1.63	0.46
2:G:476:ARG:HA	2:G:479:TRP:CD1	2.50	0.46
5:D:38:ARG:HH22	5:D:86:ASP:HA	1.80	0.46
5:D:115:SER:O	5:D:146:PHE:HB3	2.16	0.46
2:G:301:ASN:OD1	2:G:441:GLY:HA2	2.16	0.46
5:D:52(A):PRO:HG3	5:D:78:PHE:CZ	2.43	0.46
2:G:282:LYS:HA	2:G:282:LYS:HD3	1.64	0.46
3:H:169:VAL:HG12	3:H:177:SER:HB2	1.98	0.46
4:L:186:TRP:CD1	4:L:187:LYS:HG3	2.50	0.46
2:G:427:TRP:H	5:D:54:ARG:NH2	2.13	0.46
2:G:475:MET:HB3	2:G:479:TRP:CZ2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:117:LYS:HB3	3:H:146:PHE:H	1.81	0.46
5:D:44:GLY:HA2	6:E:87:TYR:CE2	2.51	0.46
5:D:119:PRO:HG3	5:D:200:HIS:HB2	1.98	0.46
6:E:121:PRO:HD2	6:E:186:TRP:CH2	2.50	0.46
2:G:96:TRP:HH2	2:G:285:LEU:HG	1.80	0.46
2:G:360:ARG:NH2	2:G:467:THR:OG1	2.48	0.46
4:L:67:PHE:HB3	4:L:68:GLY:H	1.40	0.46
5:D:38:ARG:HD3	5:D:63:PHE:CE1	2.51	0.46
2:G:96:TRP:CG	2:G:275:GLU:HB2	2.50	0.46
3:H:153:SER:OG	3:H:197:ASN:HB2	2.16	0.45
6:E:140:PHE:CE1	6:E:173:TYR:HB2	2.50	0.45
1:B:587:LEU:HD23	1:B:587:LEU:HA	1.82	0.45
5:D:145:TYR:HE2	5:D:148:GLU:HA	1.81	0.45
2:G:80:ASN:O	2:G:82:GLN:N	2.49	0.45
2:G:137:ASN:HB2	4:L:95(A):GLY:HA2	1.98	0.45
2:G:257:THR:HG23	2:G:375:SER:HB2	1.97	0.45
6:E:11:VAL:HG23	6:E:104:LEU:HD13	1.97	0.45
6:E:14:SER:HB3	6:E:17:GLN:HG3	1.98	0.45
2:G:385:CYS:HA	2:G:418:CYS:HA	1.98	0.45
3:H:164:HIS:N	3:H:181:VAL:O	2.32	0.45
6:E:83:GLU:HG3	6:E:104:LEU:O	2.17	0.45
6:E:79:GLN:HG2	6:E:80:GLU:H	1.81	0.45
2:G:298:ARG:NH1	2:G:381:GLU:HG3	2.32	0.45
3:H:162:GLY:O	3:H:182:VAL:HA	2.17	0.45
5:D:51:ILE:HD13	5:D:78:PHE:CD1	2.52	0.45
1:B:598:CYS:C	1:B:600:GLY:H	2.20	0.45
2:G:122:LEU:HG	2:G:203:GLN:HB2	1.98	0.45
3:H:120:SER:HB2	3:H:143:LYS:HB3	1.98	0.45
5:D:38:ARG:NH2	5:D:86:ASP:HA	2.32	0.45
2:G:69:TRP:CG	2:G:70:ALA:N	2.83	0.44
4:L:121:PRO:HD2	4:L:186:TRP:CZ2	2.52	0.44
4:L:137:ILE:HG12	4:L:196:VAL:HG21	2.00	0.44
1:B:608:VAL:HG21	1:B:646:LEU:HD23	1.98	0.44
3:H:18:LEU:HB2	3:H:82(C):VAL:HG11	1.99	0.44
4:L:20:ARG:HA	4:L:73:LEU:O	2.17	0.44
2:G:123:THR:N	2:G:124:PRO:HD2	2.33	0.44
2:G:153:GLU:HG3	2:G:419:ARG:HH21	1.83	0.44
3:H:198:VAL:HB	3:H:207:VAL:HB	2.00	0.44
4:L:145:VAL:HG11	4:L:196:VAL:HG13	1.99	0.44
3:H:146:PHE:HA	3:H:147:PRO:HA	1.80	0.44
5:D:100(B):ASP:O	5:D:100(G):ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:201:ILE:HD13	2:G:423:ILE:HG23	2.00	0.43
5:D:126:PRO:HA	6:E:119:PHE:HE1	1.82	0.43
2:G:94:ASN:OD1	2:G:96:TRP:N	2.51	0.43
2:G:298:ARG:NH2	2:G:443:ILE:HG13	2.33	0.43
4:L:35:TRP:CZ3	4:L:88:CYS:HB2	2.53	0.43
3:H:100:ARG:NH1	3:H:100(A):ILE:O	2.51	0.43
5:D:66:ARG:NH1	5:D:86:ASP:OD2	2.52	0.43
1:B:617:ARG:HB2	1:B:622:ILE:HD11	2.00	0.43
2:G:324:GLY:O	4:L:94:ARG:NH1	2.46	0.43
2:G:454:LEU:HD23	2:G:470:PRO:HA	2.00	0.43
3:H:29:MET:HA	3:H:34:TRP:HZ2	1.84	0.43
5:D:143:LYS:HG2	5:D:144:ASP:N	2.34	0.43
2:G:457:ASP:HB3	2:G:458:GLY:H	1.72	0.43
4:L:29:GLY:N	4:L:67:PHE:CZ	2.85	0.43
4:L:137:ILE:HG22	4:L:140:PHE:CD1	2.54	0.43
5:D:164:HIS:CD2	6:E:168:GLN:HG3	2.54	0.43
1:B:657:GLU:O	1:B:661:LEU:HG	2.18	0.43
3:H:101:ASP:OD1	3:H:101:ASP:N	2.40	0.43
4:L:116:VAL:O	4:L:205:LYS:HE3	2.19	0.43
5:D:143:LYS:HE3	5:D:171:GLN:NE2	2.34	0.43
1:B:572:GLY:O	1:B:575:GLN:NE2	2.50	0.43
1:B:594:GLY:HA2	1:B:599:SER:HB2	2.01	0.43
3:H:96:ARG:O	3:H:100(N):TYR:HA	2.19	0.42
3:H:100(B):TYR:CZ	4:L:93:SER:HB2	2.54	0.42
4:L:166:SER:O	4:L:174:ALA:N	2.47	0.42
4:L:189:HIS:ND1	4:L:192:TYR:OH	2.51	0.42
5:D:123:PRO:HG3	5:D:209:LYS:HE2	2.00	0.42
6:E:28:GLY:O	6:E:66:LYS:NZ	2.51	0.42
2:G:122:LEU:O	2:G:125:LEU:HB2	2.19	0.42
6:E:78:LEU:H	6:E:78:LEU:HG	1.70	0.42
14:R:1:NAG:H61	14:R:2:NAG:N2	2.34	0.42
1:B:574:LYS:HG3	2:G:52:LEU:O	2.19	0.42
2:G:203:GLN:HG3	2:G:435:TYR:CD2	2.54	0.42
1:B:596:TRP:CD1	1:B:646:LEU:HB2	2.54	0.42
4:L:62:PHE:HB3	4:L:73:LEU:HD11	2.02	0.42
5:D:114:ALA:HB3	5:D:146:PHE:CD1	2.55	0.42
2:G:473:GLY:O	5:D:54:ARG:NH1	2.52	0.42
3:H:88:ALA:HB3	3:H:90:TYR:CE1	2.48	0.42
4:L:92:ASP:OD1	4:L:95:SER:N	2.44	0.42
16:T:3:BMA:H3	16:T:7:MAN:C5	2.50	0.42
1:B:593:LEU:HD21	1:B:601:LYS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:180:ASP:OD1	2:G:421:LYS:HG2	2.20	0.42
4:L:129:ASN:HA	4:L:183:PRO:HG2	2.02	0.42
4:L:114:PRO:HG3	4:L:198:HIS:HB2	2.02	0.42
16:T:2:NAG:O7	11:U:1:NAG:O3	2.29	0.42
1:B:622:ILE:O	1:B:626:MET:HB2	2.20	0.42
2:G:42:VAL:HG22	2:G:493:PRO:O	2.20	0.42
2:G:92:GLU:HG2	2:G:238:PRO:HB3	2.02	0.42
3:H:126:PRO:HB3	3:H:138:LEU:HB3	2.01	0.42
3:H:189:LEU:HD23	3:H:189:LEU:HA	1.89	0.42
5:D:58:LYS:HB2	5:D:58:LYS:HE3	1.83	0.42
2:G:345:VAL:O	2:G:348:GLN:N	2.53	0.42
3:H:34:TRP:CD1	3:H:71:ARG:HD2	2.54	0.42
5:D:36:TRP:HB2	5:D:69:MET:CE	2.50	0.42
2:G:161:MET:O	2:G:170:GLN:N	2.51	0.41
2:G:298:ARG:HG3	2:G:420:ILE:HD12	2.02	0.41
4:L:36:TYR:CE2	4:L:46:LEU:HD13	2.54	0.41
1:B:538:THR:O	1:B:542:ARG:NH1	2.53	0.41
2:G:381:GLU:HB3	2:G:420:ILE:HD13	2.02	0.41
2:G:456:ARG:NH1	6:E:93:ASP:OD2	2.31	0.41
2:G:46:LYS:N	2:G:490:LYS:O	2.45	0.41
3:H:2:VAL:HA	3:H:26:GLY:HA3	2.03	0.41
5:D:166:PHE:HA	5:D:167:PRO:HD3	1.91	0.41
2:G:270:VAL:HG12	2:G:289:ASN:N	2.36	0.41
5:D:35:HIS:ND1	5:D:50:TRP:HB3	2.35	0.41
6:E:170:ASN:C	6:E:172:LYS:H	2.24	0.41
8:C:1:NAG:H61	8:C:2:NAG:O7	2.20	0.41
2:G:119:CYS:HB3	2:G:203:GLN:O	2.20	0.41
2:G:195:ASN:ND2	2:G:201:ILE:HB	2.36	0.41
2:G:483:LEU:HA	2:G:486:TYR:HD2	1.85	0.41
3:H:47:TRP:HD1	3:H:48:ILE:H	1.69	0.41
3:H:87:THR:HG23	3:H:110:THR:HA	2.02	0.41
6:E:105:THR:HB	6:E:106:VAL:H	1.65	0.41
1:B:645:LEU:O	1:B:649:SER:N	2.54	0.41
5:D:35:HIS:O	5:D:92:CYS:HA	2.21	0.41
3:H:166:PHE:CD1	4:L:136:LEU:HD13	2.56	0.41
4:L:197:THR:HA	4:L:202:THR:HA	2.02	0.41
2:G:96:TRP:CD2	2:G:275:GLU:HB2	2.56	0.41
3:H:199:ASN:HA	3:H:205:THR:O	2.21	0.41
6:E:48:ILE:HA	6:E:53:LYS:O	2.21	0.41
6:E:114:PRO:HB3	6:E:137:ILE:HG23	2.03	0.41
6:E:170:ASN:OD1	6:E:170:ASN:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:GLY:HA3	2:G:503:ARG:CZ	2.52	0.40
1:B:654:GLU:OE2	2:G:503:ARG:NH2	2.47	0.40
2:G:298:ARG:O	2:G:300:ASN:N	2.47	0.40
3:H:94:THR:OG1	3:H:101:ASP:OD1	2.34	0.40
4:L:28:LEU:HD23	4:L:28:LEU:HA	1.84	0.40
1:B:527:GLY:HA3	2:G:87:GLU:O	2.22	0.40
2:G:317:PHE:CE2	2:G:319:ALA:HB2	2.56	0.40
3:H:29:MET:SD	3:H:76:ASN:HA	2.62	0.40
3:H:166:PHE:CZ	4:L:136:LEU:HB3	2.57	0.40
4:L:189:HIS:CG	4:L:192:TYR:HH	2.39	0.40
2:G:456:ARG:HG3	2:G:468:PHE:CE2	2.56	0.40
4:L:66:PRO:HG2	4:L:66(B):ILE:HD11	2.03	0.40
5:D:164:HIS:CE1	6:E:168:GLN:HB3	2.56	0.40
1:B:595:ILE:HG13	1:B:596:TRP:CD1	2.56	0.40
2:G:109:ILE:O	2:G:112:TRP:HB3	2.22	0.40
2:G:156:ASN:HA	2:G:175:LEU:HD12	2.02	0.40
6:E:140:PHE:H	6:E:172:LYS:HB3	1.86	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	B	122/153 (80%)	108 (88%)	14 (12%)	0	100	100
2	G	442/481 (92%)	404 (91%)	32 (7%)	6 (1%)	9	40
3	H	226/238 (95%)	212 (94%)	14 (6%)	0	100	100
4	L	209/214 (98%)	200 (96%)	8 (4%)	1 (0%)	25	59
5	D	227/232 (98%)	214 (94%)	13 (6%)	0	100	100
6	E	208/214 (97%)	188 (90%)	20 (10%)	0	100	100
All	All	1434/1532 (94%)	1326 (92%)	101 (7%)	7 (0%)	25	59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	68	GLY
2	G	64	GLU
2	G	138	ILE
2	G	258	GLN
2	G	81	PRO
2	G	312	GLY
2	G	354	GLY

### 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	B	108/129 (84%)	107 (99%)	1 (1%)	75	86
2	G	401/428 (94%)	397 (99%)	4 (1%)	73	84
3	H	202/208 (97%)	202 (100%)	0	100	100
4	L	175/178 (98%)	175 (100%)	0	100	100
5	D	194/197 (98%)	190 (98%)	4 (2%)	48	71
6	E	173/177 (98%)	172 (99%)	1 (1%)	84	91
All	All	1253/1317 (95%)	1243 (99%)	10 (1%)	79	88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	604	CYS
2	G	47	ASP
2	G	102	GLU
2	G	356	ASN
2	G	469	ARG
5	D	22	CYS
5	D	71	ARG
5	D	100(G)	ARG
5	D	138	LEU
6	E	141	TYR

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

Mol	Chain	Res	Type
1	B	650	GLN
2	G	280	ASN
4	L	198	HIS
5	D	39	GLN
5	D	155	ASN
6	E	38	GLN
6	E	109	GLN

### 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](#)

84 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	NAG	A	1	1,7	14,14,15	0.67	0	17,19,21	0.95	0
7	FUC	A	2	7	10,10,11	0.76	0	14,14,16	0.93	0
8	NAG	C	1	1,8	14,14,15	0.76	0	17,19,21	1.48	2 (11%)
8	NAG	C	2	8	14,14,15	0.65	0	17,19,21	1.20	1 (5%)
8	BMA	C	3	8	11,11,12	0.88	0	15,15,17	2.59	5 (33%)
9	NAG	F	1	2,9	14,14,15	0.75	0	17,19,21	1.05	1 (5%)
9	NAG	F	2	9	14,14,15	0.68	0	17,19,21	0.86	0
9	NAG	I	1	2,9	14,14,15	0.66	0	17,19,21	2.54	4 (23%)
9	NAG	I	2	9	14,14,15	0.67	0	17,19,21	1.05	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	NAG	J	1	2,10	14,14,15	0.72	0	17,19,21	1.71	4 (23%)
10	GAL	J	10	10	11,11,12	0.68	0	15,15,17	0.94	1 (6%)
10	FUC	J	11	10	10,10,11	0.87	0	14,14,16	1.29	2 (14%)
10	NAG	J	2	10	14,14,15	0.80	0	17,19,21	1.66	2 (11%)
10	BMA	J	3	10	11,11,12	0.87	0	15,15,17	2.72	6 (40%)
10	MAN	J	4	10	11,11,12	0.65	0	15,15,17	2.42	3 (20%)
10	NAG	J	5	10	14,14,15	0.80	0	17,19,21	1.25	2 (11%)
10	GAL	J	6	10	11,11,12	0.68	0	15,15,17	0.92	0
10	NAG	J	7	10	14,14,15	0.63	0	17,19,21	1.30	1 (5%)
10	MAN	J	8	10	11,11,12	0.89	0	15,15,17	1.94	2 (13%)
10	NAG	J	9	10	14,14,15	0.70	0	17,19,21	1.03	1 (5%)
11	NAG	K	1	2,11	14,14,15	0.79	0	17,19,21	1.55	2 (11%)
11	NAG	K	2	11	14,14,15	0.75	0	17,19,21	2.48	3 (17%)
11	BMA	K	3	11	11,11,12	0.85	0	15,15,17	2.65	6 (40%)
11	MAN	K	4	11	11,11,12	0.57	0	15,15,17	1.61	1 (6%)
11	MAN	K	5	11	11,11,12	0.81	0	15,15,17	0.90	0
12	NAG	M	1	2,12	14,14,15	0.91	1 (7%)	17,19,21	1.85	2 (11%)
12	NAG	M	2	12	14,14,15	0.93	0	17,19,21	2.24	4 (23%)
12	BMA	M	3	12	11,11,12	1.11	1 (9%)	15,15,17	1.72	4 (26%)
12	MAN	M	4	12	11,11,12	0.61	0	15,15,17	2.60	2 (13%)
12	NAG	M	5	12	14,14,15	0.68	0	17,19,21	1.08	1 (5%)
12	GAL	M	6	12	11,11,12	0.67	0	15,15,17	0.95	1 (6%)
12	MAN	M	7	12	11,11,12	0.59	0	15,15,17	2.21	5 (33%)
12	NAG	M	8	12	14,14,15	0.64	0	17,19,21	0.98	0
9	NAG	N	1	2,9	14,14,15	0.84	0	17,19,21	0.99	1 (5%)
9	NAG	N	2	9	14,14,15	0.69	0	17,19,21	1.13	1 (5%)
13	NAG	O	1	2,13	14,14,15	0.80	0	17,19,21	1.22	2 (11%)
13	NAG	O	2	13	14,14,15	0.80	0	17,19,21	1.58	4 (23%)
13	BMA	O	3	13	11,11,12	0.83	0	15,15,17	2.30	6 (40%)
13	MAN	O	4	13	11,11,12	0.57	0	15,15,17	1.88	1 (6%)
13	MAN	O	5	13	11,11,12	0.74	0	15,15,17	1.17	1 (6%)
13	MAN	O	6	13	11,11,12	0.65	0	15,15,17	1.23	1 (6%)
13	MAN	O	7	13	11,11,12	0.75	0	15,15,17	0.95	1 (6%)
11	NAG	P	1	2,11	14,14,15	0.85	1 (7%)	17,19,21	1.58	4 (23%)
11	NAG	P	2	11	14,14,15	0.96	0	17,19,21	2.02	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	BMA	P	3	11	11,11,12	0.66	0	15,15,17	2.20	5 (33%)
11	MAN	P	4	11	11,11,12	0.52	0	15,15,17	2.36	1 (6%)
11	MAN	P	5	11	11,11,12	0.70	0	15,15,17	1.15	1 (6%)
9	NAG	Q	1	2,9	14,14,15	0.75	0	17,19,21	0.84	0
9	NAG	Q	2	9	14,14,15	0.73	0	17,19,21	0.77	0
14	NAG	R	1	14,2	14,14,15	0.78	0	17,19,21	1.12	2 (11%)
14	NAG	R	2	14	14,14,15	0.74	0	17,19,21	1.12	1 (5%)
14	BMA	R	3	14	11,11,12	0.85	0	15,15,17	2.23	4 (26%)
14	MAN	R	4	14	11,11,12	0.55	0	15,15,17	1.96	1 (6%)
14	NAG	R	5	14	14,14,15	0.73	0	17,19,21	0.87	0
14	MAN	R	6	14	11,11,12	0.64	0	15,15,17	1.32	1 (6%)
15	NAG	S	1	2,15	14,14,15	0.81	0	17,19,21	0.81	0
15	MAN	S	10	15	11,11,12	0.85	1 (9%)	15,15,17	0.86	0
15	NAG	S	2	15	14,14,15	0.70	0	17,19,21	1.51	3 (17%)
15	BMA	S	3	15	11,11,12	0.80	0	15,15,17	2.50	6 (40%)
15	MAN	S	4	15	11,11,12	0.60	0	15,15,17	1.98	2 (13%)
15	MAN	S	5	15	11,11,12	0.72	0	15,15,17	1.52	2 (13%)
15	MAN	S	6	15	11,11,12	0.89	1 (9%)	15,15,17	1.35	3 (20%)
15	MAN	S	7	15	11,11,12	0.76	0	15,15,17	0.98	1 (6%)
15	MAN	S	8	15	11,11,12	0.71	0	15,15,17	1.62	2 (13%)
15	MAN	S	9	15	11,11,12	0.89	1 (9%)	15,15,17	0.77	0
16	NAG	T	1	16,2	14,14,15	0.85	1 (7%)	17,19,21	1.61	3 (17%)
16	NAG	T	2	16	14,14,15	0.77	0	17,19,21	1.11	1 (5%)
16	BMA	T	3	16	11,11,12	0.77	0	15,15,17	2.98	3 (20%)
16	MAN	T	4	16	11,11,12	0.74	0	15,15,17	1.75	2 (13%)
16	MAN	T	5	16	11,11,12	0.81	0	15,15,17	1.05	1 (6%)
16	MAN	T	6	16	11,11,12	0.61	0	15,15,17	1.30	1 (6%)
16	MAN	T	7	16	11,11,12	0.63	0	15,15,17	3.06	2 (13%)
11	NAG	U	1	2,11	14,14,15	0.70	0	17,19,21	1.30	1 (5%)
11	NAG	U	2	11	14,14,15	0.64	0	17,19,21	1.24	1 (5%)
11	BMA	U	3	11	11,11,12	0.93	0	15,15,17	3.15	6 (40%)
11	MAN	U	4	11	11,11,12	0.60	0	15,15,17	1.84	2 (13%)
11	MAN	U	5	11	11,11,12	0.52	0	15,15,17	2.87	1 (6%)
17	NAG	V	1	17,2	14,14,15	0.77	0	17,19,21	1.05	2 (11%)
17	NAG	V	2	17	14,14,15	0.67	0	17,19,21	1.23	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	BMA	V	3	17	11,11,12	0.94	0	15,15,17	2.37	5 (33%)
17	FUC	V	4	17	10,10,11	0.83	0	14,14,16	1.30	2 (14%)
8	NAG	W	1	2,8	14,14,15	0.70	0	17,19,21	1.07	2 (11%)
8	NAG	W	2	8	14,14,15	0.68	0	17,19,21	0.97	2 (11%)
8	BMA	W	3	8	11,11,12	0.85	0	15,15,17	2.99	6 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1	1,7	-	0/6/23/26	0/1/1/1
7	FUC	A	2	7	-	-	0/1/1/1
8	NAG	C	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	C	2	8	-	4/6/23/26	0/1/1/1
8	BMA	C	3	8	-	1/2/19/22	0/1/1/1
9	NAG	F	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	F	2	9	-	0/6/23/26	0/1/1/1
9	NAG	I	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	I	2	9	-	1/6/23/26	0/1/1/1
10	NAG	J	1	2,10	-	2/6/23/26	0/1/1/1
10	GAL	J	10	10	-	0/2/19/22	0/1/1/1
10	FUC	J	11	10	-	-	0/1/1/1
10	NAG	J	2	10	-	1/6/23/26	0/1/1/1
10	BMA	J	3	10	-	1/2/19/22	0/1/1/1
10	MAN	J	4	10	-	0/2/19/22	0/1/1/1
10	NAG	J	5	10	-	1/6/23/26	0/1/1/1
10	GAL	J	6	10	-	0/2/19/22	0/1/1/1
10	NAG	J	7	10	-	1/6/23/26	0/1/1/1
10	MAN	J	8	10	-	0/2/19/22	0/1/1/1
10	NAG	J	9	10	-	0/6/23/26	0/1/1/1
11	NAG	K	1	2,11	-	2/6/23/26	0/1/1/1
11	NAG	K	2	11	-	3/6/23/26	0/1/1/1
11	BMA	K	3	11	-	0/2/19/22	0/1/1/1
11	MAN	K	4	11	-	0/2/19/22	0/1/1/1
11	MAN	K	5	11	-	0/2/19/22	0/1/1/1
12	NAG	M	1	2,12	-	0/6/23/26	0/1/1/1
12	NAG	M	2	12	-	2/6/23/26	0/1/1/1
12	BMA	M	3	12	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	M	4	12	-	2/2/19/22	0/1/1/1
12	NAG	M	5	12	-	2/6/23/26	0/1/1/1
12	GAL	M	6	12	-	2/2/19/22	0/1/1/1
12	MAN	M	7	12	-	0/2/19/22	0/1/1/1
12	NAG	M	8	12	-	2/6/23/26	0/1/1/1
9	NAG	N	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	N	2	9	-	1/6/23/26	0/1/1/1
13	NAG	O	1	2,13	-	2/6/23/26	0/1/1/1
13	NAG	O	2	13	-	2/6/23/26	0/1/1/1
13	BMA	O	3	13	-	2/2/19/22	0/1/1/1
13	MAN	O	4	13	-	1/2/19/22	0/1/1/1
13	MAN	O	5	13	-	0/2/19/22	0/1/1/1
13	MAN	O	6	13	-	2/2/19/22	0/1/1/1
13	MAN	O	7	13	-	0/2/19/22	0/1/1/1
11	NAG	P	1	2,11	-	1/6/23/26	0/1/1/1
11	NAG	P	2	11	-	1/6/23/26	0/1/1/1
11	BMA	P	3	11	-	2/2/19/22	0/1/1/1
11	MAN	P	4	11	-	2/2/19/22	0/1/1/1
11	MAN	P	5	11	-	2/2/19/22	0/1/1/1
9	NAG	Q	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	0/6/23/26	0/1/1/1
14	NAG	R	1	14,2	-	1/6/23/26	0/1/1/1
14	NAG	R	2	14	-	0/6/23/26	0/1/1/1
14	BMA	R	3	14	-	1/2/19/22	0/1/1/1
14	MAN	R	4	14	-	0/2/19/22	0/1/1/1
14	NAG	R	5	14	-	2/6/23/26	0/1/1/1
14	MAN	R	6	14	-	0/2/19/22	0/1/1/1
15	NAG	S	1	2,15	-	0/6/23/26	0/1/1/1
15	MAN	S	10	15	-	1/2/19/22	0/1/1/1
15	NAG	S	2	15	-	2/6/23/26	0/1/1/1
15	BMA	S	3	15	-	0/2/19/22	0/1/1/1
15	MAN	S	4	15	-	0/2/19/22	0/1/1/1
15	MAN	S	5	15	-	0/2/19/22	0/1/1/1
15	MAN	S	6	15	-	0/2/19/22	0/1/1/1
15	MAN	S	7	15	-	2/2/19/22	0/1/1/1
15	MAN	S	8	15	-	0/2/19/22	0/1/1/1
15	MAN	S	9	15	-	2/2/19/22	0/1/1/1
16	NAG	T	1	16,2	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	NAG	T	2	16	-	1/6/23/26	0/1/1/1
16	BMA	T	3	16	-	0/2/19/22	0/1/1/1
16	MAN	T	4	16	-	0/2/19/22	0/1/1/1
16	MAN	T	5	16	-	0/2/19/22	0/1/1/1
16	MAN	T	6	16	-	2/2/19/22	0/1/1/1
16	MAN	T	7	16	-	2/2/19/22	0/1/1/1
11	NAG	U	1	2,11	-	0/6/23/26	0/1/1/1
11	NAG	U	2	11	-	1/6/23/26	0/1/1/1
11	BMA	U	3	11	-	2/2/19/22	0/1/1/1
11	MAN	U	4	11	-	0/2/19/22	0/1/1/1
11	MAN	U	5	11	-	2/2/19/22	0/1/1/1
17	NAG	V	1	17,2	-	1/6/23/26	0/1/1/1
17	NAG	V	2	17	-	1/6/23/26	0/1/1/1
17	BMA	V	3	17	-	0/2/19/22	0/1/1/1
17	FUC	V	4	17	-	-	0/1/1/1
8	NAG	W	1	2,8	-	3/6/23/26	0/1/1/1
8	NAG	W	2	8	-	0/6/23/26	0/1/1/1
8	BMA	W	3	8	-	1/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	3	BMA	C2-C3	2.40	1.56	1.52
15	S	6	MAN	O5-C1	-2.39	1.39	1.43
15	S	9	MAN	O5-C1	-2.38	1.39	1.43
12	M	1	NAG	O5-C1	-2.37	1.39	1.43
11	P	1	NAG	O5-C1	-2.12	1.40	1.43
16	T	1	NAG	O5-C1	-2.02	1.40	1.43
15	S	10	MAN	O5-C1	-2.00	1.40	1.43

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	7	MAN	C1-O5-C5	10.70	126.53	112.19
16	T	3	BMA	C1-O5-C5	10.57	126.35	112.19
11	U	5	MAN	C1-O5-C5	10.16	125.81	112.19
11	U	3	BMA	C1-O5-C5	9.96	125.54	112.19
8	W	3	BMA	C1-O5-C5	9.48	124.89	112.19
12	M	4	MAN	C1-O5-C5	9.37	124.75	112.19
11	P	4	MAN	C1-O5-C5	8.52	123.61	112.19
11	K	2	NAG	C2-N2-C7	8.38	134.13	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	S	3	BMA	C1-O5-C5	7.88	122.75	112.19
9	I	1	NAG	C1-O5-C5	7.83	122.68	112.19
10	J	3	BMA	C1-O5-C5	7.58	122.35	112.19
8	C	3	BMA	C1-O5-C5	7.56	122.32	112.19
11	K	3	BMA	C1-O5-C5	7.43	122.14	112.19
13	O	3	BMA	C1-O5-C5	7.01	121.58	112.19
14	R	4	MAN	C1-O5-C5	6.64	121.08	112.19
12	M	2	NAG	C4-C3-C2	6.61	120.70	111.02
17	V	3	BMA	C1-O5-C5	6.47	120.86	112.19
10	J	4	MAN	C1-C2-C3	-6.37	100.36	109.64
13	O	4	MAN	C1-O5-C5	6.37	120.72	112.19
12	M	1	NAG	C1-O5-C5	6.28	120.61	112.19
14	R	3	BMA	C1-O5-C5	6.23	120.53	112.19
11	U	4	MAN	C1-O5-C5	6.12	120.38	112.19
10	J	8	MAN	O2-C2-C3	6.11	122.81	110.15
15	S	4	MAN	C1-O5-C5	6.00	120.22	112.19
11	P	3	BMA	C1-O5-C5	5.74	119.88	112.19
11	P	2	NAG	C1-O5-C5	5.48	119.53	112.19
11	K	4	MAN	C1-O5-C5	5.46	119.50	112.19
12	M	7	MAN	C1-O5-C5	5.38	119.40	112.19
9	I	1	NAG	O4-C4-C5	5.05	121.76	109.32
10	J	2	NAG	O5-C1-C2	-4.97	103.59	111.29
10	J	4	MAN	C1-O5-C5	4.63	118.39	112.19
11	P	2	NAG	O4-C4-C3	-4.47	99.83	110.38
10	J	7	NAG	C1-O5-C5	4.41	118.10	112.19
16	T	4	MAN	C1-C2-C3	4.35	115.97	109.64
16	T	1	NAG	C1-O5-C5	-4.34	106.37	112.19
15	S	8	MAN	C1-O5-C5	4.17	117.78	112.19
14	R	6	MAN	C1-O5-C5	4.12	117.71	112.19
11	U	2	NAG	O5-C1-C2	-4.01	105.08	111.29
16	T	6	MAN	C1-O5-C5	3.94	117.47	112.19
12	M	2	NAG	O5-C1-C2	-3.94	105.19	111.29
15	S	5	MAN	C1-O5-C5	3.94	117.47	112.19
12	M	7	MAN	C3-C4-C5	-3.93	103.10	110.23
8	C	1	NAG	O4-C4-C3	-3.89	101.21	110.38
10	J	3	BMA	O3-C3-C2	-3.79	102.31	110.05
10	J	1	NAG	C1-O5-C5	-3.77	107.13	112.19
11	U	1	NAG	C1-O5-C5	3.73	117.18	112.19
8	W	3	BMA	C3-C4-C5	3.71	116.96	110.23
12	M	3	BMA	O3-C3-C4	3.69	119.09	110.38
16	T	4	MAN	C1-O5-C5	3.68	117.11	112.19
13	O	6	MAN	C1-O5-C5	3.65	117.08	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	1	NAG	C1-O5-C5	3.65	117.08	112.19
11	K	3	BMA	C2-C3-C4	3.60	117.19	110.86
9	N	2	NAG	C1-O5-C5	3.58	116.99	112.19
17	V	3	BMA	C2-C3-C4	3.54	117.08	110.86
10	J	4	MAN	O4-C4-C5	3.54	118.03	109.32
12	M	7	MAN	C2-C3-C4	-3.48	104.74	110.86
10	J	3	BMA	C3-C4-C5	3.34	116.29	110.23
8	C	3	BMA	C3-C4-C5	3.33	116.27	110.23
13	O	2	NAG	C2-N2-C7	3.29	127.31	122.90
16	T	7	MAN	C1-C2-C3	3.28	114.42	109.64
13	O	2	NAG	O5-C1-C2	-3.28	106.21	111.29
11	U	3	BMA	C3-C4-C5	3.27	116.16	110.23
16	T	2	NAG	O5-C1-C2	-3.26	106.25	111.29
11	K	1	NAG	O5-C1-C2	-3.23	106.29	111.29
8	C	3	BMA	C2-C3-C4	3.20	116.49	110.86
10	J	2	NAG	C1-C2-N2	3.19	115.46	110.43
11	K	2	NAG	C1-C2-N2	3.19	115.46	110.43
8	C	2	NAG	C2-N2-C7	3.18	127.16	122.90
10	J	1	NAG	O4-C4-C3	-3.17	102.89	110.38
15	S	2	NAG	C2-N2-C7	3.09	127.04	122.90
10	J	3	BMA	C2-C3-C4	3.04	116.21	110.86
17	V	3	BMA	C3-C4-C5	3.02	115.71	110.23
11	P	1	NAG	O5-C1-C2	-3.02	106.62	111.29
11	P	1	NAG	C1-C2-N2	3.01	115.18	110.43
11	P	3	BMA	O3-C3-C2	-2.97	104.00	110.05
11	P	1	NAG	O4-C4-C3	-2.92	103.49	110.38
10	J	1	NAG	C4-C3-C2	2.92	115.29	111.02
10	J	5	NAG	C1-O5-C5	2.90	116.08	112.19
15	S	2	NAG	O5-C1-C2	-2.90	106.80	111.29
11	K	3	BMA	O3-C3-C2	-2.90	104.13	110.05
15	S	8	MAN	C1-C2-C3	-2.89	105.44	109.64
11	P	1	NAG	C3-C4-C5	2.86	115.41	110.23
10	J	1	NAG	O5-C1-C2	-2.82	106.93	111.29
12	M	7	MAN	O4-C4-C5	2.80	116.21	109.32
8	C	1	NAG	O5-C1-C2	-2.79	106.97	111.29
10	J	11	FUC	C1-C2-C3	2.78	113.70	109.64
11	U	3	BMA	C1-C2-C3	2.78	113.69	109.64
9	I	2	NAG	C1-O5-C5	2.77	115.90	112.19
12	M	5	NAG	O5-C1-C2	-2.73	107.06	111.29
12	M	3	BMA	O5-C5-C6	2.72	112.96	107.66
14	R	3	BMA	O3-C3-C2	-2.72	104.50	110.05
11	P	3	BMA	O3-C3-C4	2.71	116.77	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	1	NAG	C1-O5-C5	2.70	115.81	112.19
11	K	3	BMA	C3-C4-C5	2.69	115.11	110.23
15	S	4	MAN	C1-C2-C3	2.68	113.55	109.64
14	R	3	BMA	C3-C4-C5	2.68	115.09	110.23
13	O	5	MAN	C1-O5-C5	2.68	115.77	112.19
9	F	1	NAG	O4-C4-C3	-2.68	104.07	110.38
13	O	2	NAG	C4-C3-C2	2.67	114.94	111.02
11	U	3	BMA	O3-C3-C2	-2.67	104.60	110.05
11	K	2	NAG	C8-C7-N2	2.66	120.52	116.12
11	P	5	MAN	C1-O5-C5	2.65	115.74	112.19
17	V	2	NAG	C1-C2-N2	2.64	114.60	110.43
10	J	9	NAG	C1-O5-C5	2.64	115.72	112.19
9	I	1	NAG	C4-C3-C2	-2.63	107.16	111.02
8	W	3	BMA	C2-C3-C4	2.59	115.42	110.86
16	T	3	BMA	O3-C3-C4	2.57	116.44	110.38
15	S	5	MAN	O2-C2-C1	-2.56	103.36	109.22
10	J	5	NAG	C2-N2-C7	2.56	126.33	122.90
8	W	3	BMA	O5-C5-C4	2.56	117.05	110.83
11	U	3	BMA	C2-C3-C4	2.54	115.33	110.86
9	N	1	NAG	O5-C1-C2	-2.54	107.36	111.29
12	M	1	NAG	O4-C4-C3	-2.52	104.44	110.38
11	P	3	BMA	O5-C5-C6	2.52	112.56	107.66
15	S	6	MAN	C1-O5-C5	2.50	115.54	112.19
8	W	2	NAG	O5-C1-C2	-2.49	107.43	111.29
9	I	1	NAG	O5-C5-C6	-2.49	102.82	107.66
14	R	1	NAG	O5-C1-C2	-2.47	107.48	111.29
17	V	3	BMA	O3-C3-C2	-2.46	105.04	110.05
11	U	3	BMA	O5-C5-C4	2.45	116.79	110.83
15	S	6	MAN	C1-C2-C3	-2.44	106.09	109.64
14	R	3	BMA	C2-C3-C4	2.44	115.16	110.86
10	J	11	FUC	C3-C4-C5	-2.44	106.11	109.81
17	V	1	NAG	O5-C1-C2	-2.42	107.54	111.29
15	S	3	BMA	C2-C3-C4	2.41	115.11	110.86
8	C	3	BMA	O3-C3-C2	-2.40	105.16	110.05
13	O	1	NAG	O5-C1-C2	-2.39	107.59	111.29
15	S	2	NAG	C1-C2-N2	2.39	114.20	110.43
10	J	3	BMA	O5-C5-C4	2.39	116.63	110.83
16	T	5	MAN	C1-C2-C3	2.33	113.04	109.64
8	C	3	BMA	O4-C4-C3	-2.30	104.96	110.38
8	W	1	NAG	C1-O5-C5	2.30	115.27	112.19
15	S	7	MAN	C1-O5-C5	2.29	115.26	112.19
17	V	4	FUC	O2-C2-C3	2.29	114.90	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	2	NAG	C1-C2-N2	2.27	114.01	110.43
10	J	8	MAN	C1-O5-C5	2.27	115.22	112.19
17	V	2	NAG	C4-C3-C2	-2.25	107.72	111.02
14	R	2	NAG	O5-C1-C2	-2.24	107.82	111.29
13	O	3	BMA	C3-C4-C5	2.24	114.29	110.23
14	R	1	NAG	C1-O5-C5	2.23	115.17	112.19
11	P	3	BMA	O4-C4-C3	-2.22	105.13	110.38
12	M	3	BMA	O5-C1-C2	-2.21	105.52	110.79
15	S	3	BMA	O3-C3-C2	-2.21	105.55	110.05
11	U	4	MAN	C1-C2-C3	2.21	112.86	109.64
16	T	1	NAG	O5-C1-C2	-2.19	107.90	111.29
13	O	7	MAN	C1-O5-C5	2.19	115.11	112.19
12	M	3	BMA	C3-C4-C5	2.17	114.17	110.23
15	S	3	BMA	C3-C4-C5	2.17	114.16	110.23
13	O	2	NAG	O4-C4-C3	-2.16	105.28	110.38
8	W	3	BMA	O4-C4-C3	-2.16	105.28	110.38
11	P	2	NAG	C2-N2-C7	2.13	125.76	122.90
17	V	4	FUC	O5-C1-C2	-2.13	105.70	110.79
8	W	2	NAG	O3-C3-C2	-2.12	104.99	109.40
11	K	3	BMA	O5-C5-C4	2.12	115.99	110.83
16	T	3	BMA	O5-C5-C4	2.12	115.98	110.83
11	K	3	BMA	O4-C4-C3	-2.11	105.40	110.38
17	V	3	BMA	O4-C4-C3	-2.11	105.41	110.38
13	O	3	BMA	O3-C3-C4	2.11	115.34	110.38
16	T	1	NAG	C1-C2-N2	-2.10	107.12	110.43
12	M	2	NAG	O4-C4-C3	-2.09	105.46	110.38
10	J	3	BMA	O4-C4-C3	-2.09	105.46	110.38
13	O	3	BMA	C1-C2-C3	2.09	112.68	109.64
15	S	6	MAN	O4-C4-C3	-2.08	105.47	110.38
12	M	6	GAL	C1-O5-C5	2.08	114.97	112.19
12	M	4	MAN	C2-C3-C4	-2.06	107.24	110.86
15	S	3	BMA	O3-C3-C4	2.05	115.21	110.38
10	J	10	GAL	C1-O5-C5	2.05	114.93	112.19
13	O	3	BMA	O4-C4-C3	-2.04	105.58	110.38
13	O	3	BMA	O5-C5-C4	2.03	115.78	110.83
17	V	1	NAG	C3-C4-C5	2.03	113.91	110.23
8	W	1	NAG	C4-C3-C2	-2.01	108.07	111.02
8	W	3	BMA	O3-C3-C2	-2.01	105.96	110.05
12	M	7	MAN	O2-C2-C1	-2.01	104.63	109.22
15	S	3	BMA	O4-C4-C3	-2.00	105.65	110.38

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	O	2	NAG	C1-C2-N2-C7
9	Q	1	NAG	O5-C5-C6-O6
11	P	3	BMA	O5-C5-C6-O6
11	U	5	MAN	O5-C5-C6-O6
12	M	4	MAN	O5-C5-C6-O6
11	U	3	BMA	C4-C5-C6-O6
12	M	3	BMA	O5-C5-C6-O6
9	Q	1	NAG	C4-C5-C6-O6
12	M	6	GAL	C4-C5-C6-O6
12	M	2	NAG	O5-C5-C6-O6
11	P	3	BMA	C4-C5-C6-O6
11	U	3	BMA	O5-C5-C6-O6
16	T	7	MAN	O5-C5-C6-O6
12	M	6	GAL	O5-C5-C6-O6
11	U	5	MAN	C4-C5-C6-O6
12	M	4	MAN	C4-C5-C6-O6
14	R	5	NAG	O5-C5-C6-O6
10	J	1	NAG	O5-C5-C6-O6
10	J	1	NAG	C4-C5-C6-O6
14	R	5	NAG	C4-C5-C6-O6
13	O	3	BMA	O5-C5-C6-O6
12	M	2	NAG	C4-C5-C6-O6
8	W	1	NAG	C8-C7-N2-C2
8	W	1	NAG	O7-C7-N2-C2
11	K	1	NAG	C8-C7-N2-C2
11	K	1	NAG	O7-C7-N2-C2
11	K	2	NAG	C8-C7-N2-C2
11	K	2	NAG	O7-C7-N2-C2
12	M	5	NAG	C8-C7-N2-C2
12	M	5	NAG	O7-C7-N2-C2
12	M	8	NAG	C8-C7-N2-C2
12	M	8	NAG	O7-C7-N2-C2
8	C	2	NAG	C4-C5-C6-O6
15	S	9	MAN	C4-C5-C6-O6
13	O	1	NAG	O5-C5-C6-O6
11	P	4	MAN	O5-C5-C6-O6
13	O	1	NAG	C4-C5-C6-O6
13	O	3	BMA	C4-C5-C6-O6
11	P	5	MAN	C4-C5-C6-O6
15	S	9	MAN	O5-C5-C6-O6
15	S	7	MAN	O5-C5-C6-O6
11	P	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
15	S	7	MAN	C4-C5-C6-O6
16	T	7	MAN	C4-C5-C6-O6
12	M	3	BMA	C4-C5-C6-O6
8	C	2	NAG	O5-C5-C6-O6
8	W	3	BMA	O5-C5-C6-O6
16	T	2	NAG	O5-C5-C6-O6
16	T	6	MAN	C4-C5-C6-O6
11	P	1	NAG	O5-C5-C6-O6
10	J	2	NAG	O5-C5-C6-O6
9	I	2	NAG	O5-C5-C6-O6
8	W	1	NAG	O5-C5-C6-O6
15	S	10	MAN	O5-C5-C6-O6
15	S	2	NAG	C1-C2-N2-C7
17	V	1	NAG	C4-C5-C6-O6
13	O	4	MAN	O5-C5-C6-O6
14	R	3	BMA	O5-C5-C6-O6
13	O	6	MAN	C4-C5-C6-O6
8	C	2	NAG	C3-C2-N2-C7
11	K	2	NAG	C3-C2-N2-C7
13	O	6	MAN	O5-C5-C6-O6
8	C	3	BMA	O5-C5-C6-O6
10	J	3	BMA	O5-C5-C6-O6
16	T	6	MAN	O5-C5-C6-O6
17	V	2	NAG	O5-C5-C6-O6
8	C	2	NAG	C1-C2-N2-C7
10	J	7	NAG	C1-C2-N2-C7
14	R	1	NAG	C1-C2-N2-C7
11	P	2	NAG	C4-C5-C6-O6
13	O	2	NAG	C3-C2-N2-C7
15	S	2	NAG	C3-C2-N2-C7
11	P	4	MAN	C4-C5-C6-O6
9	N	2	NAG	C4-C5-C6-O6
10	J	5	NAG	O5-C5-C6-O6
11	U	2	NAG	O5-C5-C6-O6
16	T	1	NAG	O5-C5-C6-O6

There are no ring outliers.

31 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	2	NAG	1	0
15	S	4	MAN	1	0

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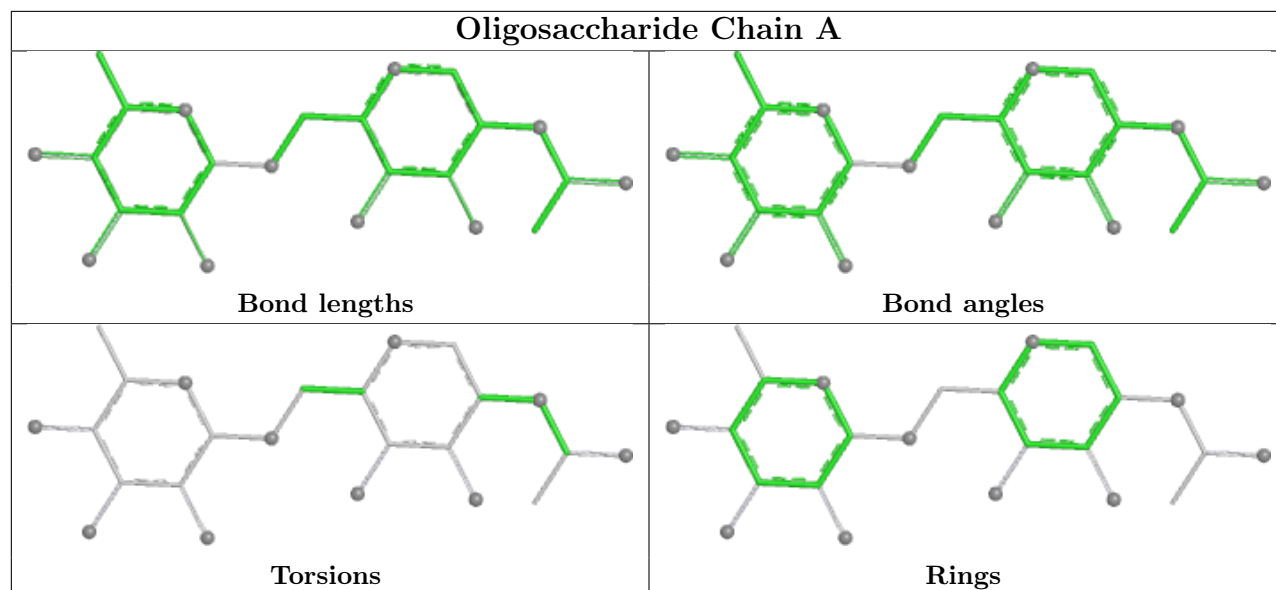
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	T	4	MAN	1	0
11	U	1	NAG	1	0
8	C	1	NAG	1	0
11	P	4	MAN	1	0
10	J	7	NAG	1	0
16	T	2	NAG	2	0
16	T	3	BMA	1	0
9	F	1	NAG	1	0
10	J	4	MAN	1	0
12	M	7	MAN	1	0
15	S	2	NAG	1	0
8	C	2	NAG	1	0
10	J	11	FUC	3	0
14	R	2	NAG	1	0
16	T	7	MAN	1	0
7	A	2	FUC	1	0
15	S	5	MAN	1	0
11	P	3	BMA	1	0
16	T	5	MAN	2	0
12	M	2	NAG	1	0
14	R	1	NAG	1	0
13	O	5	MAN	1	0
16	T	1	NAG	1	0
10	J	9	NAG	1	0
10	J	5	NAG	1	0
11	P	1	NAG	3	0
11	K	1	NAG	1	0
11	P	2	NAG	2	0
13	O	3	BMA	1	0

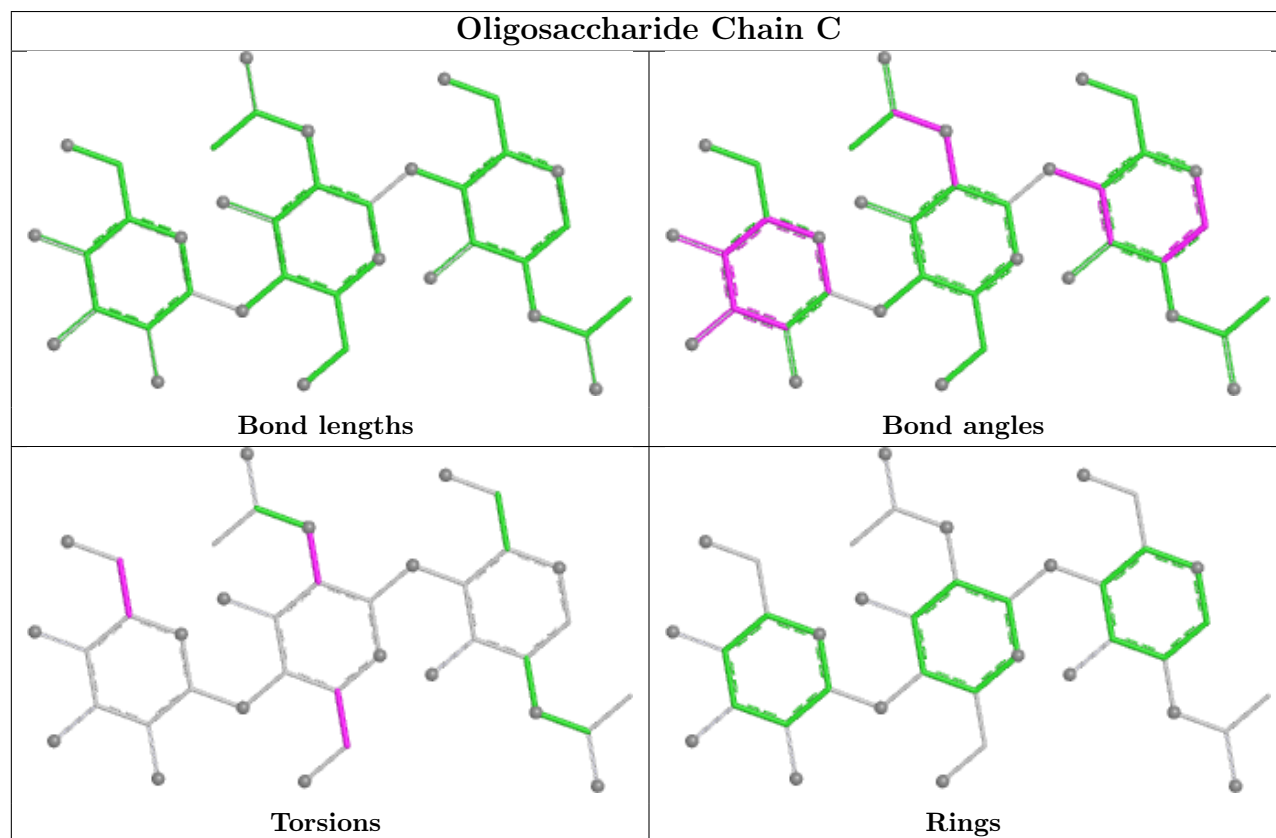
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

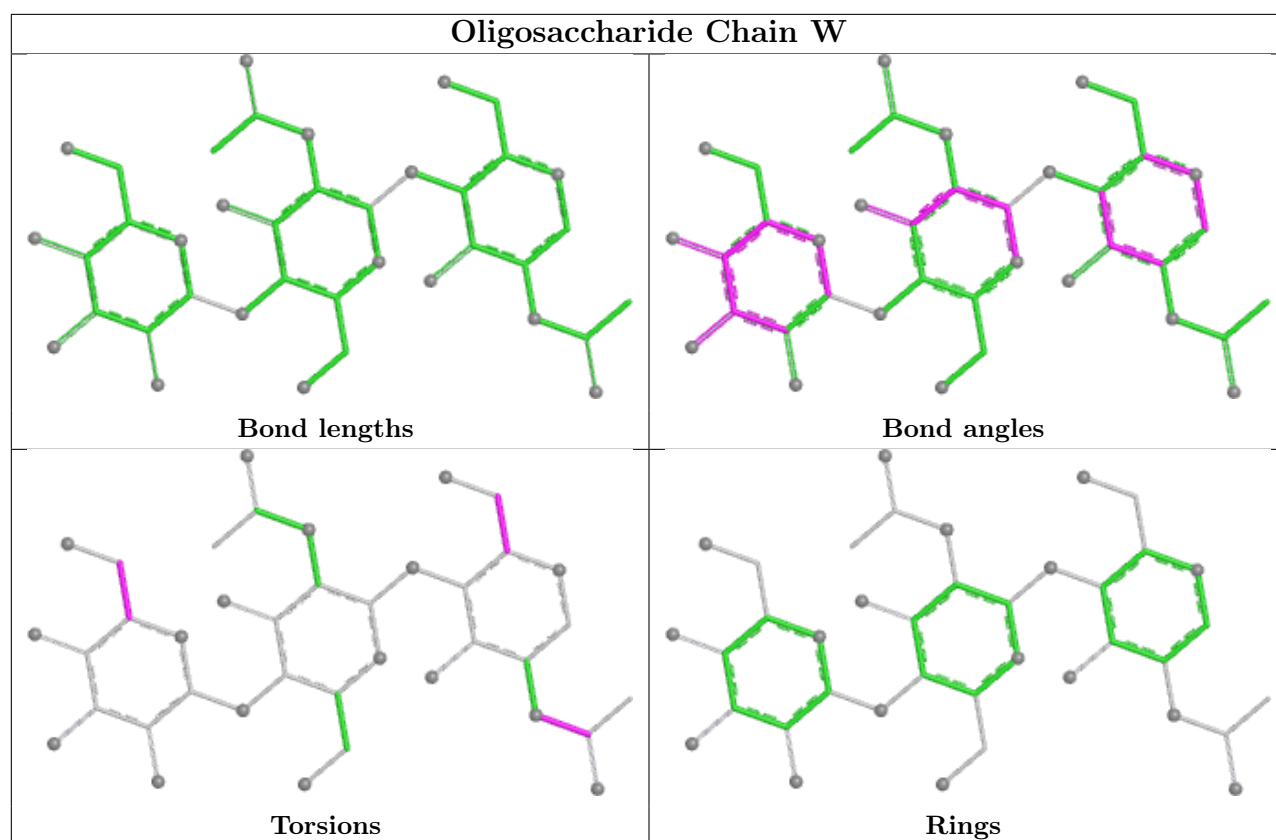


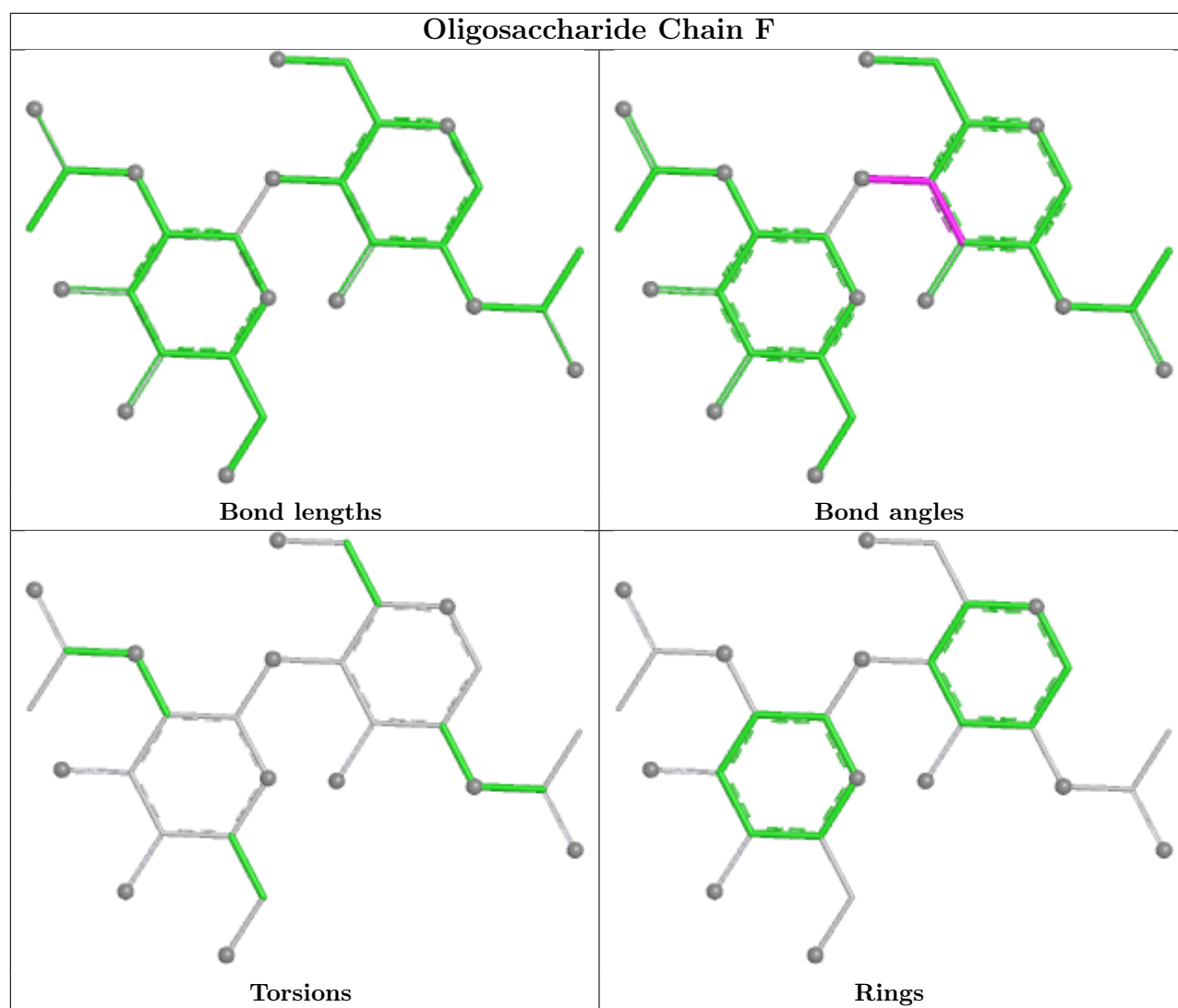
## Oligosaccharide Chain A

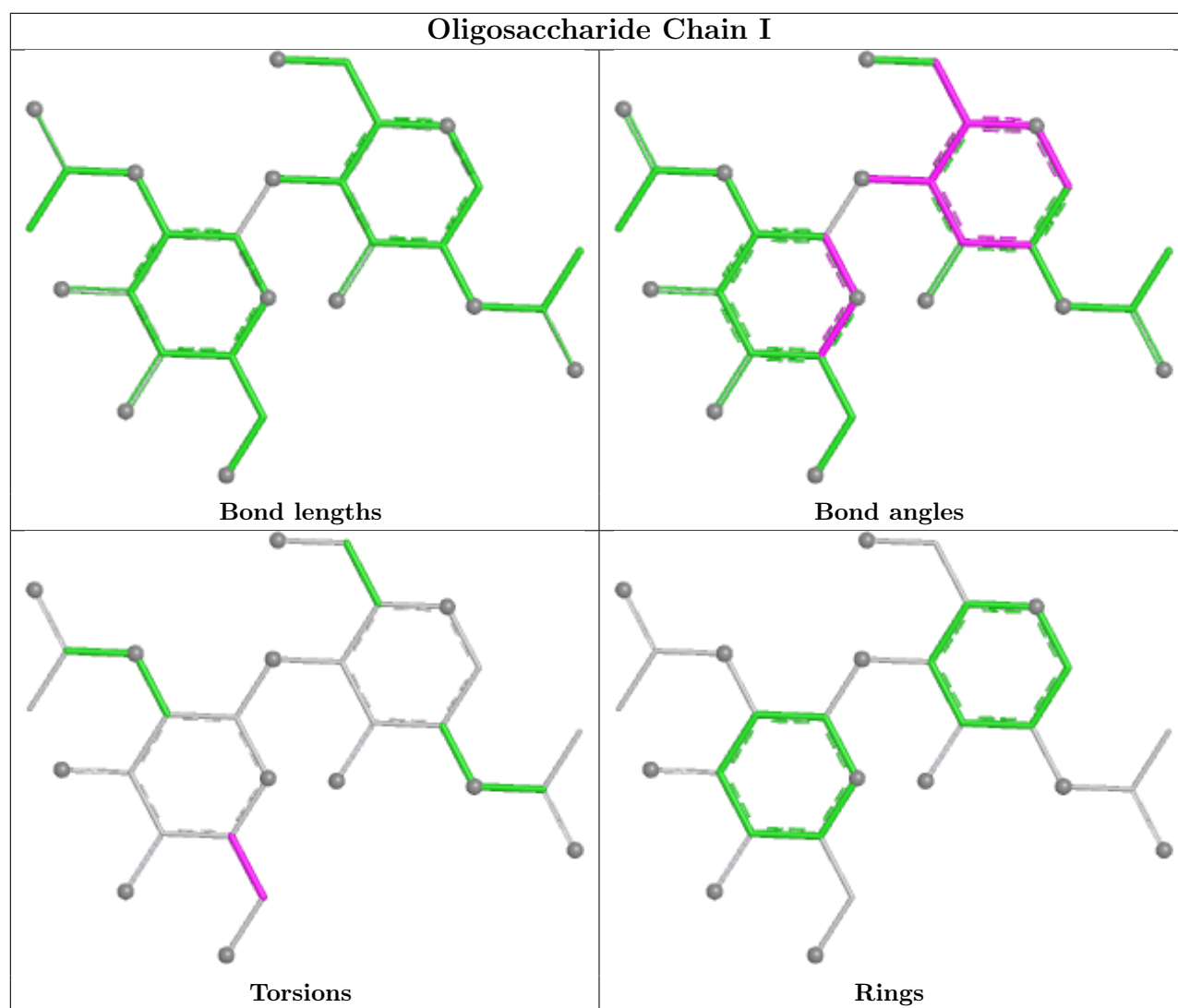


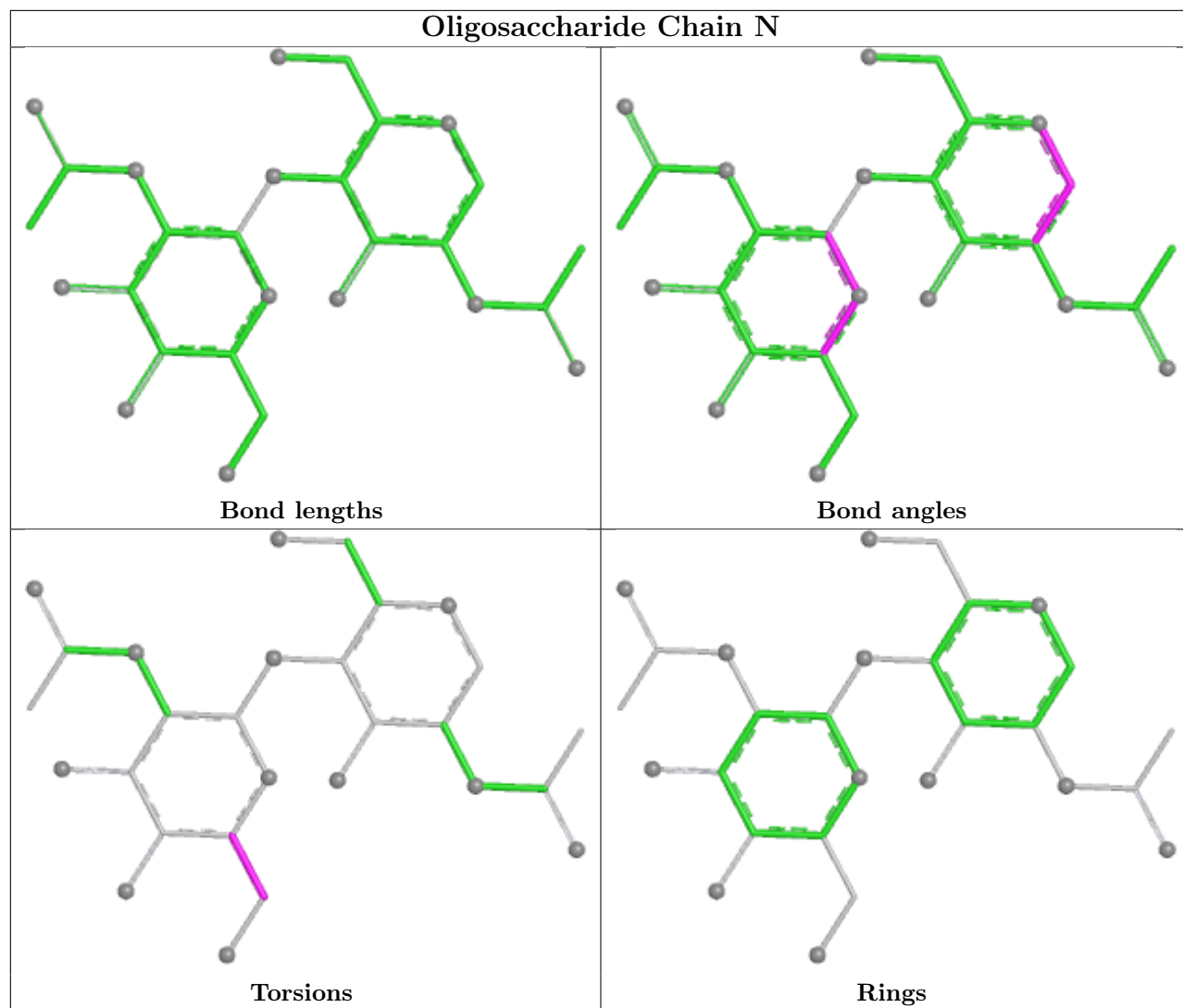
## Oligosaccharide Chain C

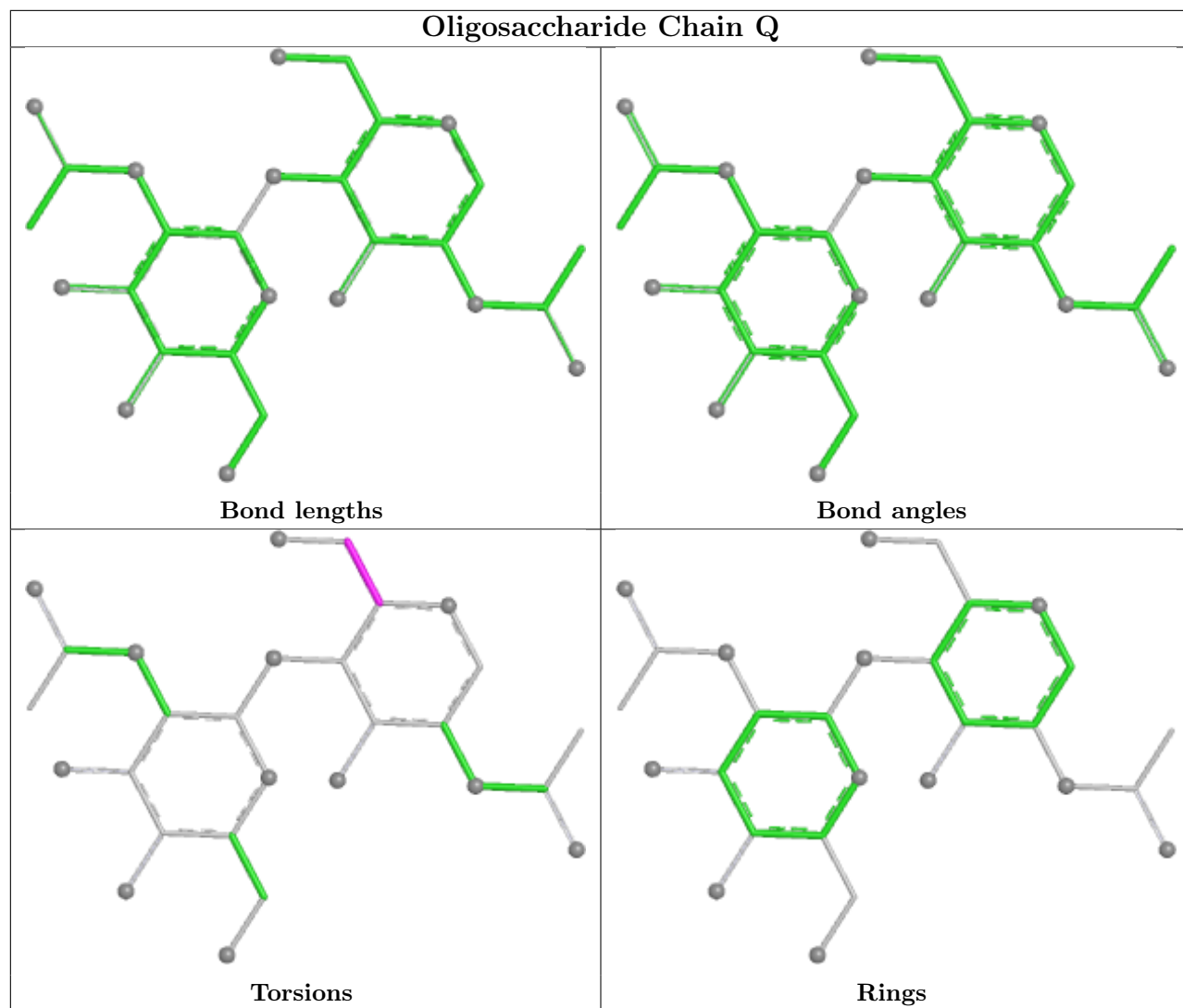


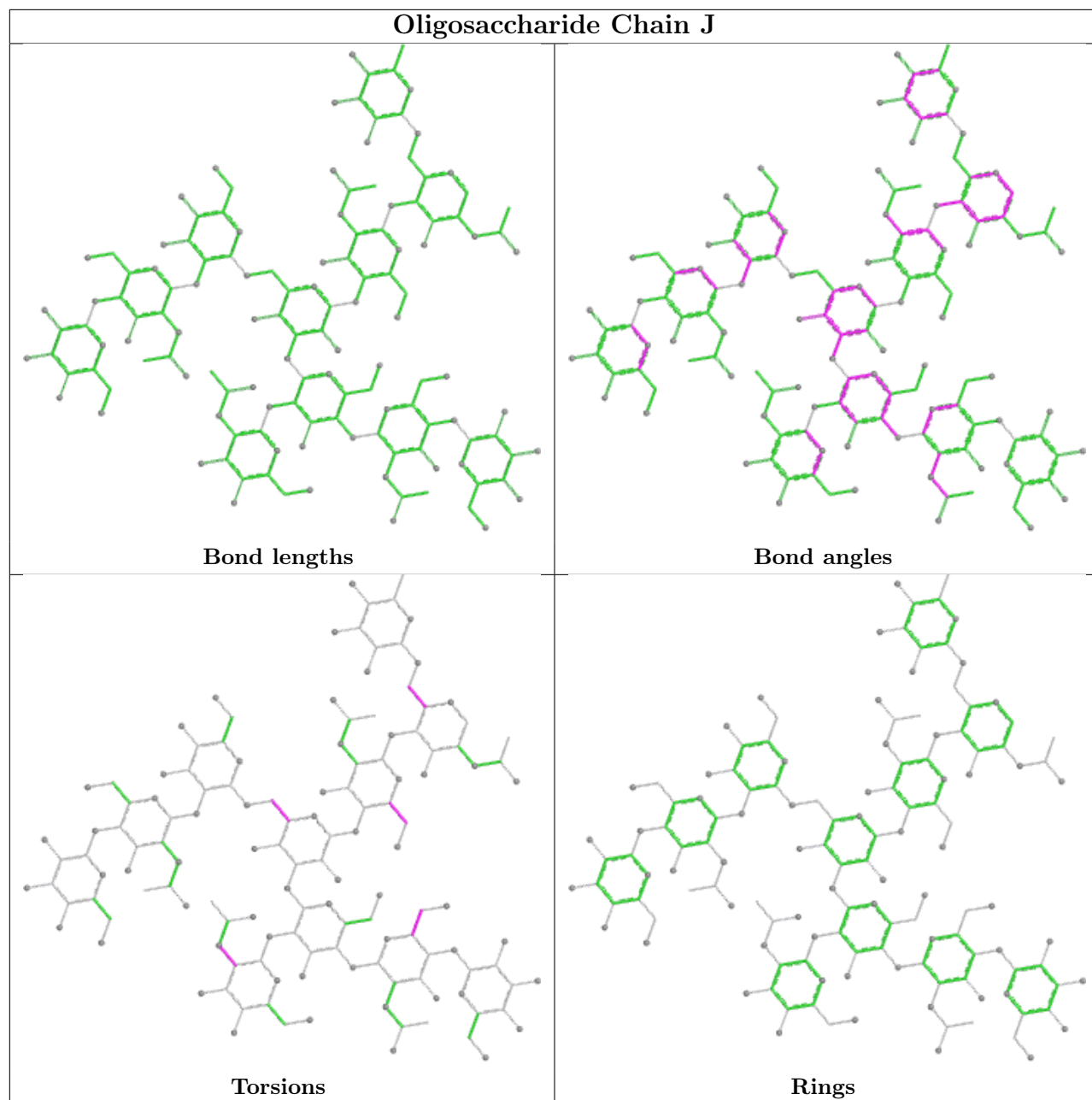


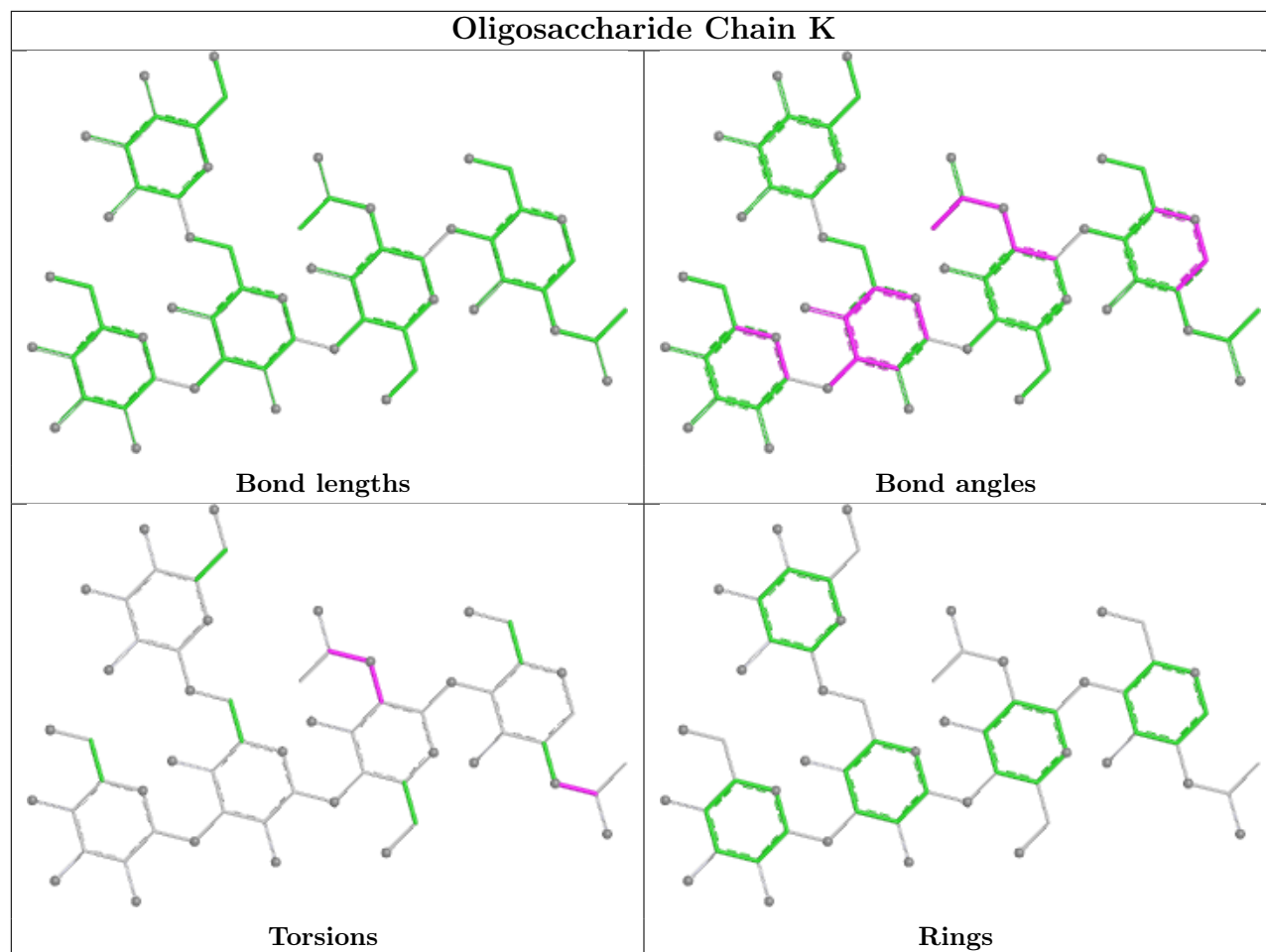




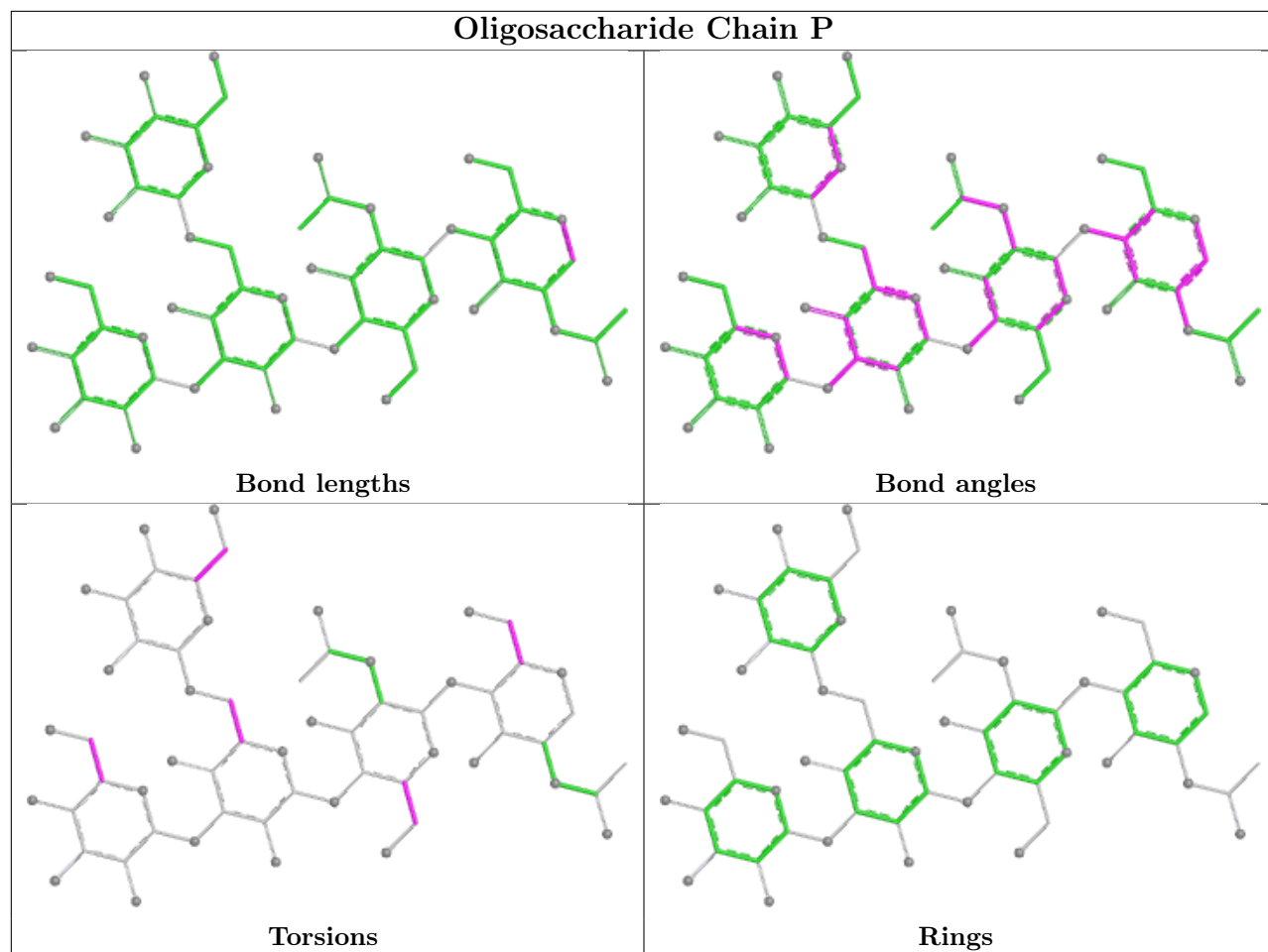


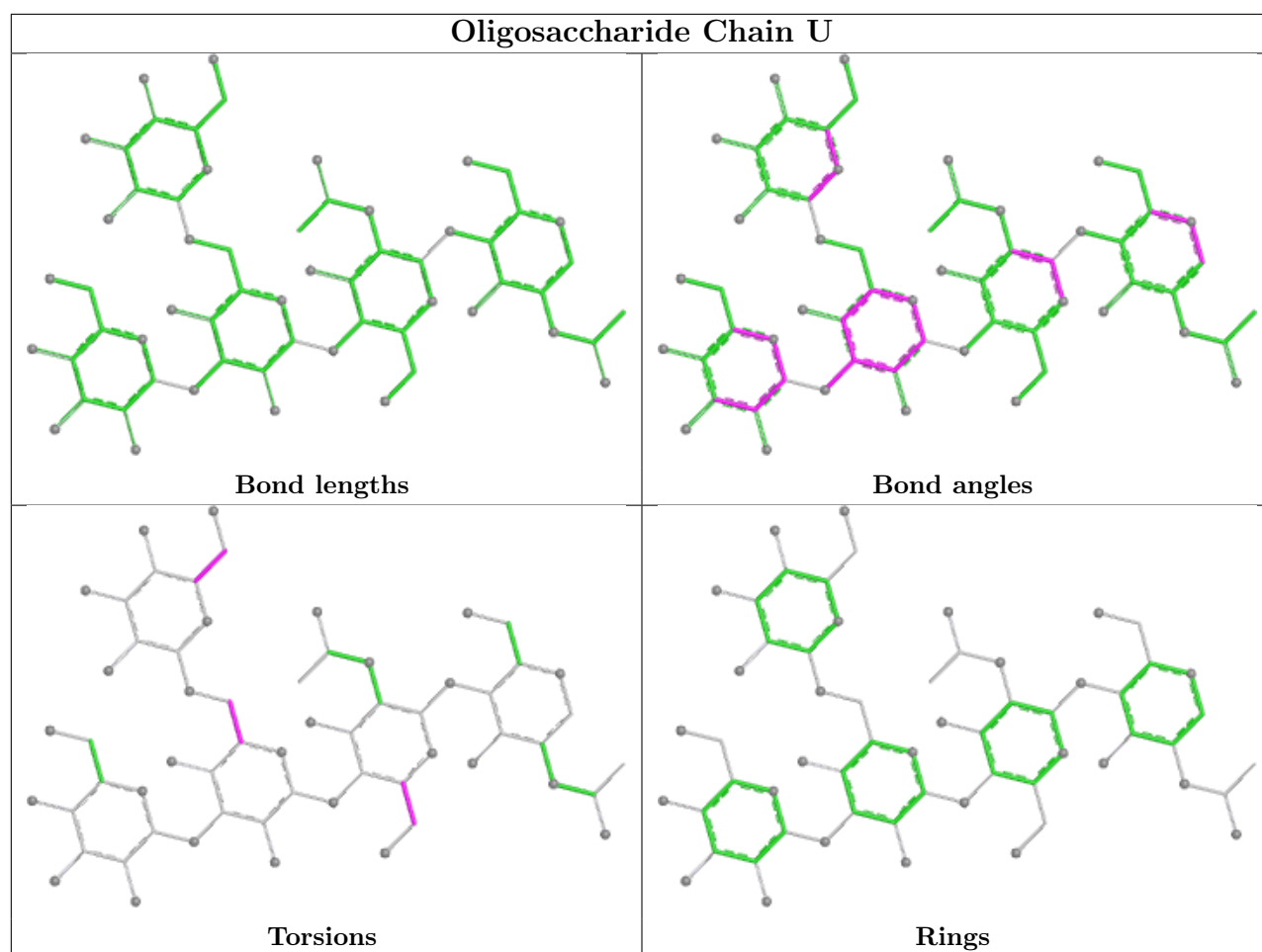




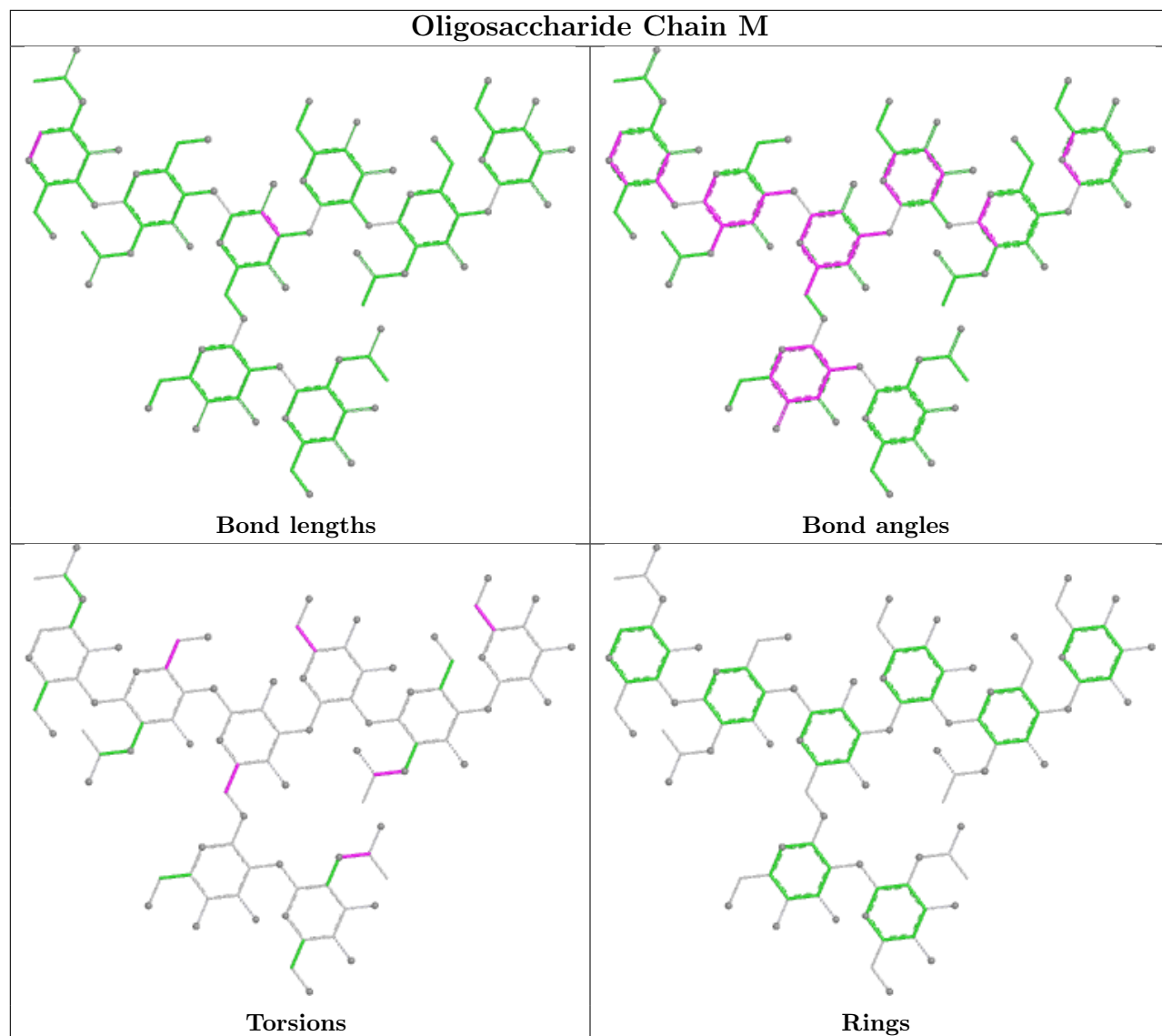


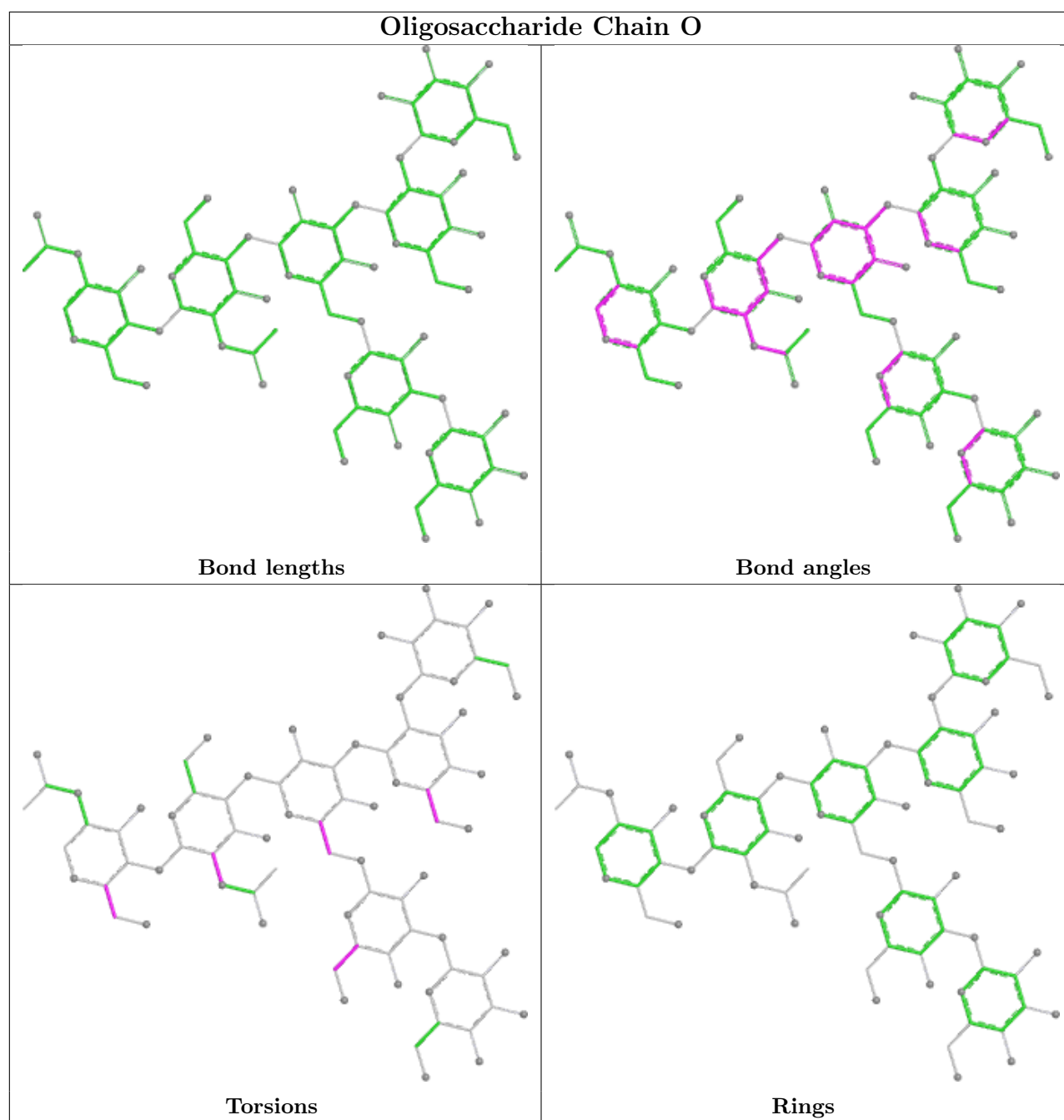


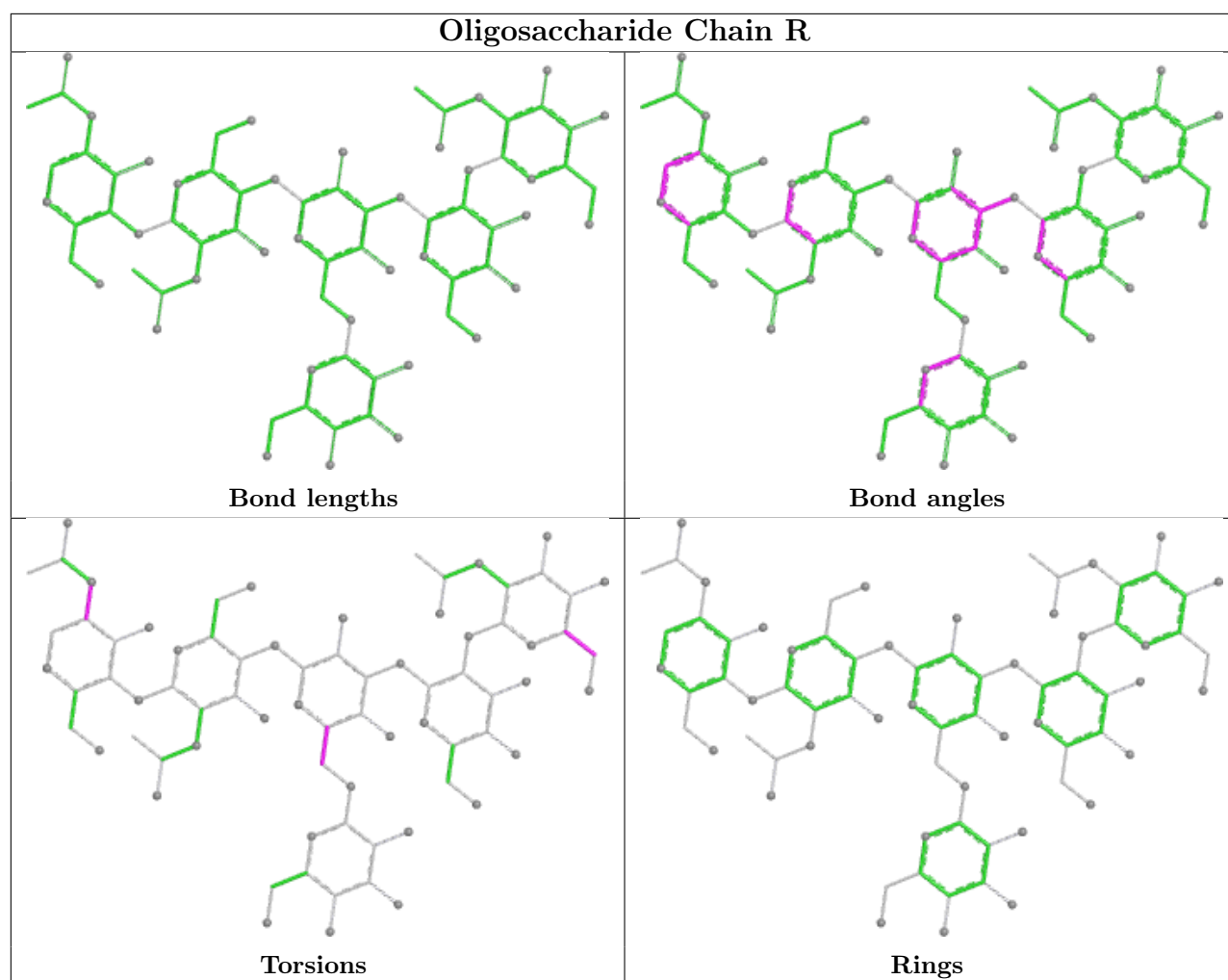


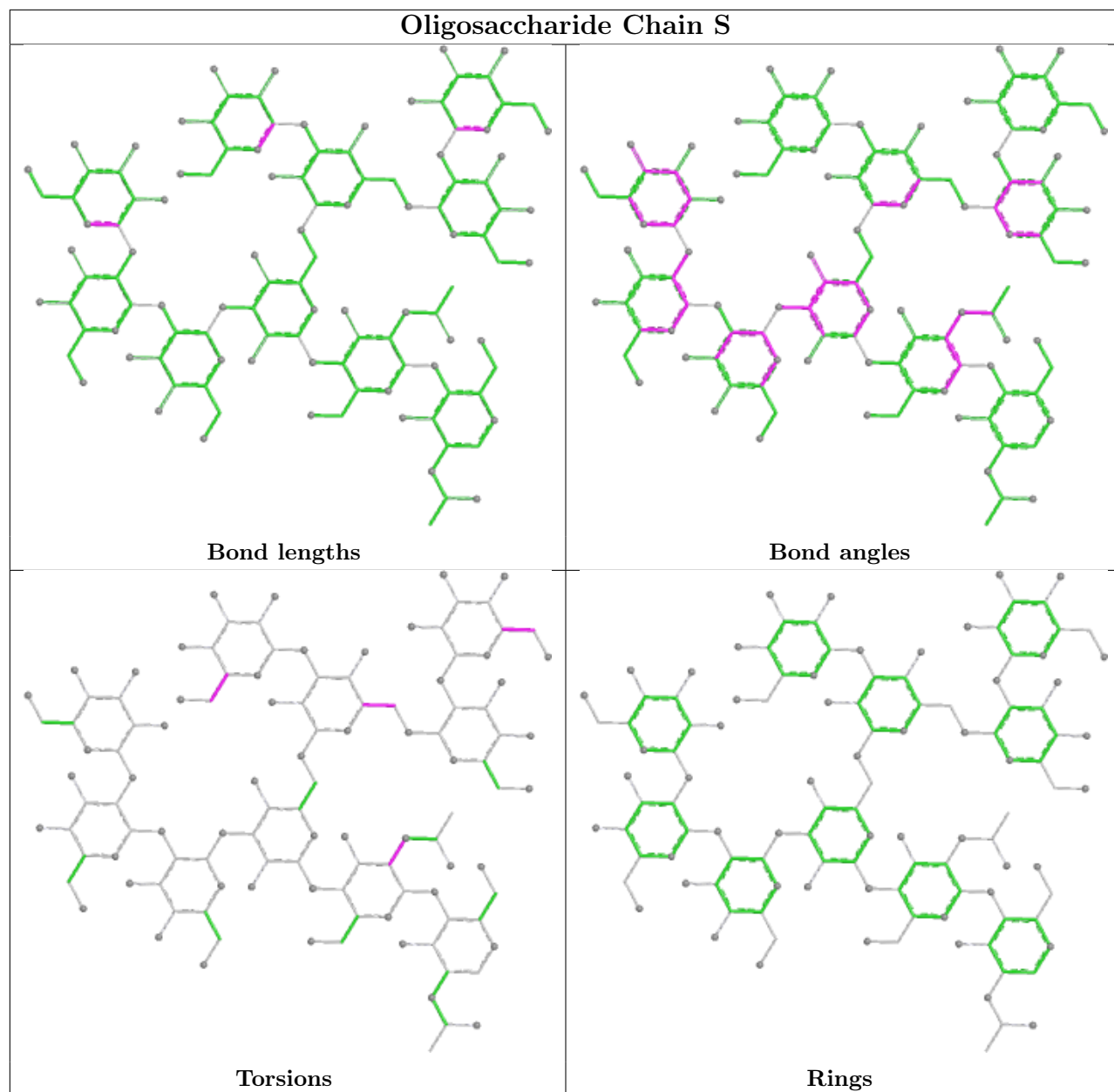


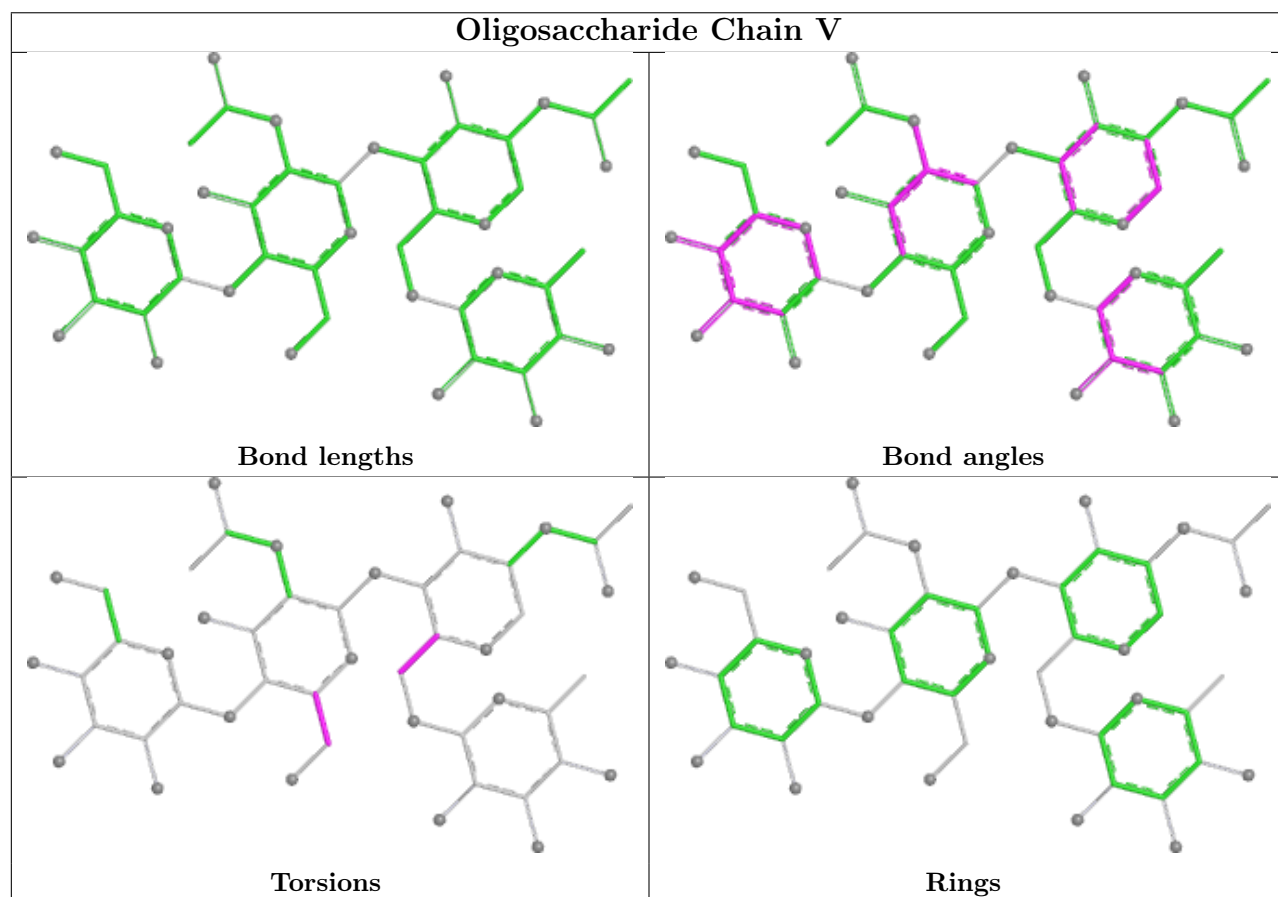
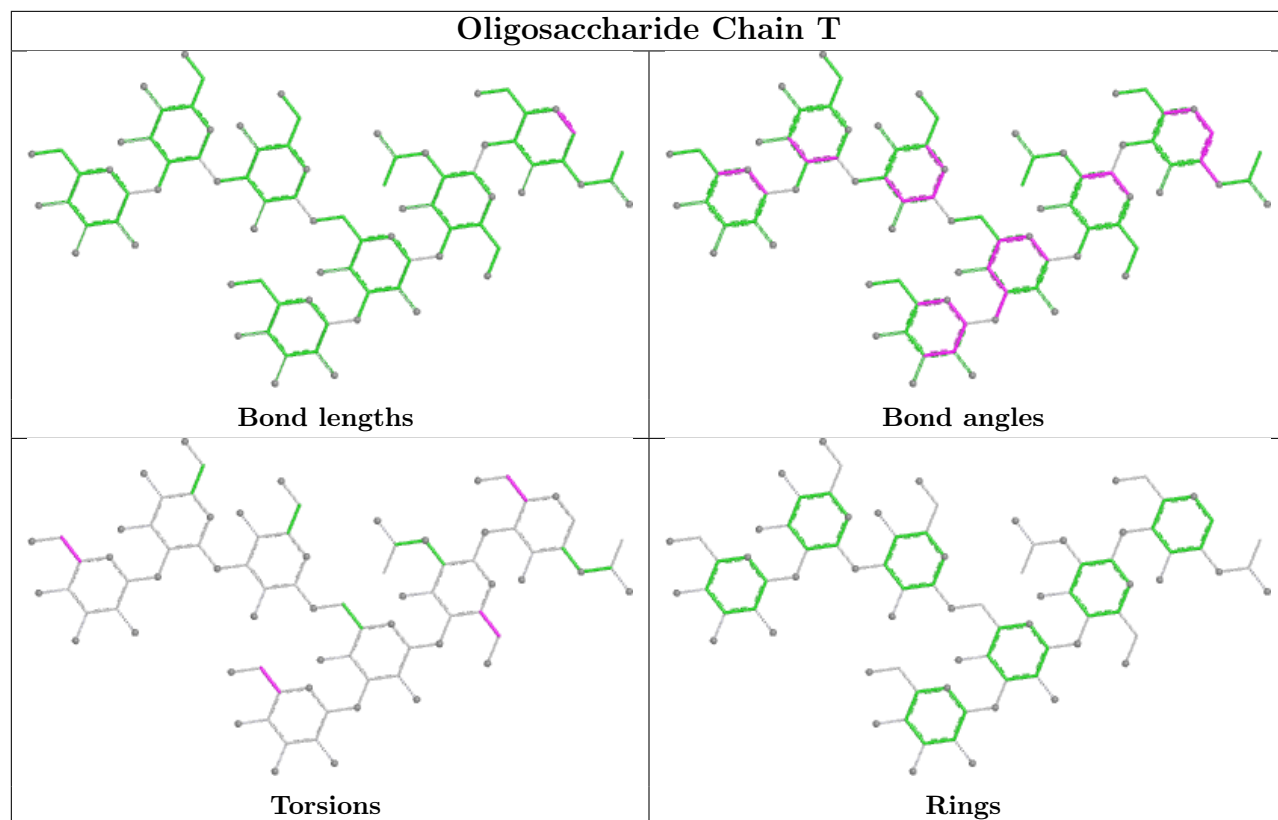
## Oligosaccharide Chain M











## 5.6 Ligand geometry

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$
18	NAG	G	601	2	14,14,15	0.71	0	17,19,21	0.91	1 (5%)
18	NAG	G	602	2	14,14,15	0.68	0	17,19,21	0.86	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
18	NAG	G	601	2	-	0/6/23/26	0/1/1/1
18	NAG	G	602	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
18	G	601	NAG	C1-O5-C5	2.24	115.19	112.19
18	G	602	NAG	O5-C1-C2	-2.02	108.17	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

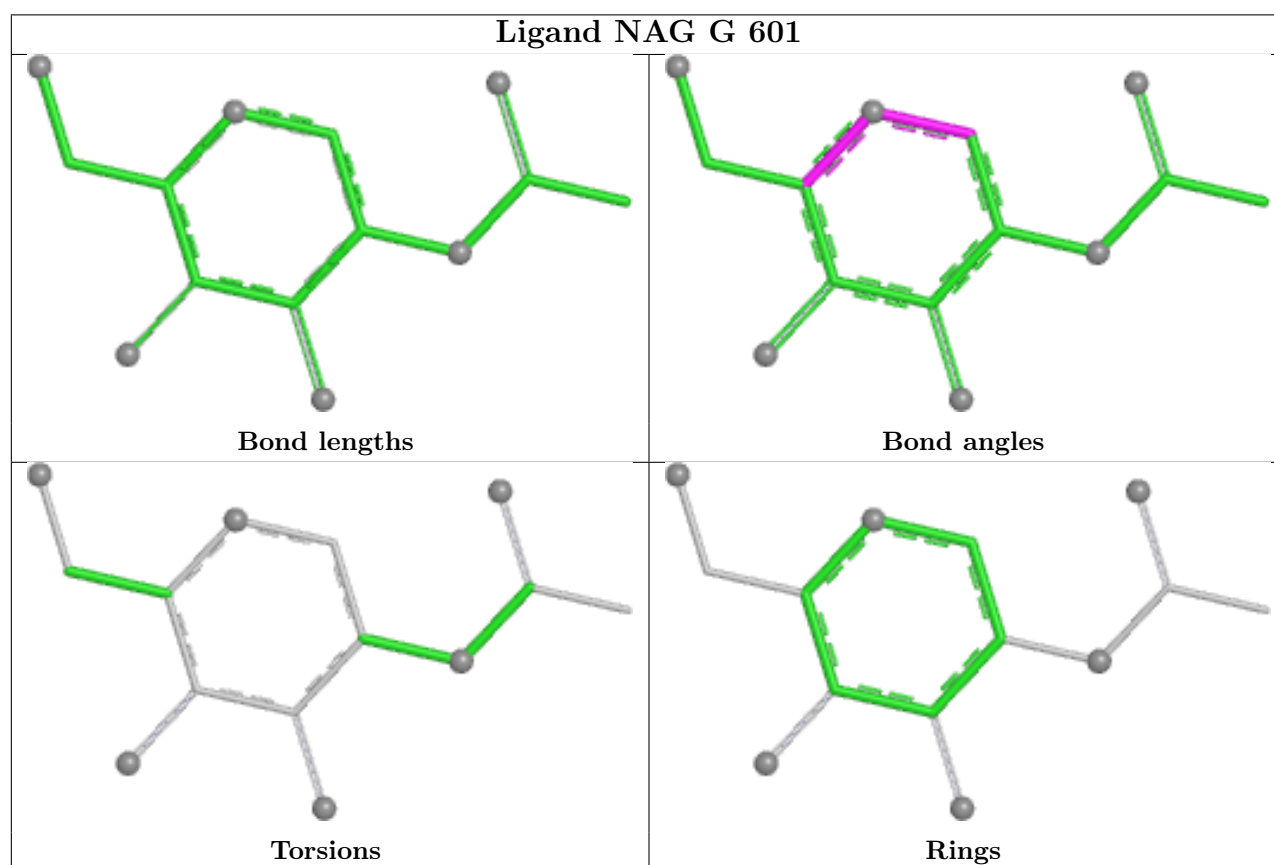
Mol	Chain	Res	Type	Atoms
18	G	602	NAG	C8-C7-N2-C2
18	G	602	NAG	O7-C7-N2-C2
18	G	602	NAG	C4-C5-C6-O6
18	G	602	NAG	O5-C5-C6-O6

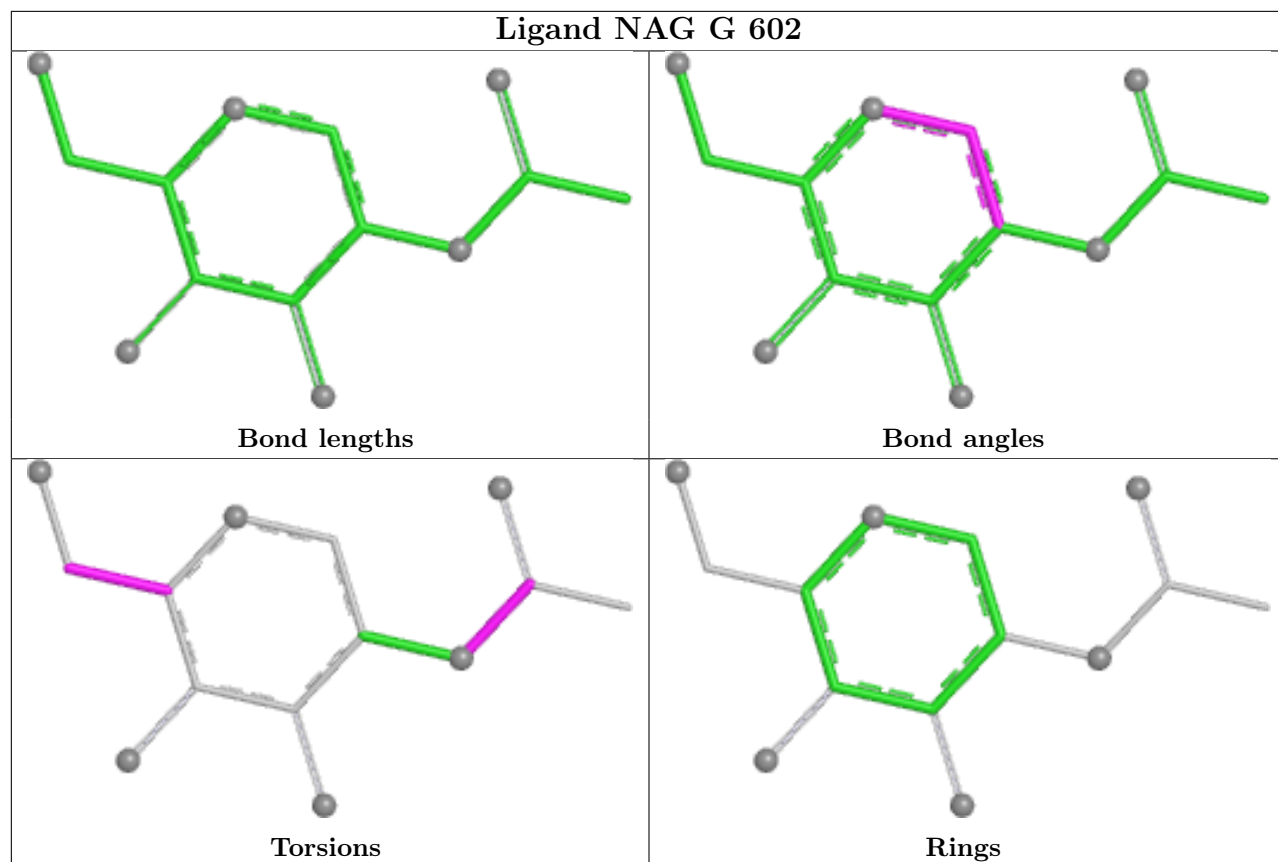
There are no ring outliers.



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.





## 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	B	126/153 (82%)	-0.13	0 100 100	126, 179, 216, 231	0
2	G	450/481 (93%)	-0.06	4 (0%) 81 64	74, 127, 211, 286	0
3	H	230/238 (96%)	0.08	3 (1%) 74 56	105, 203, 312, 369	0
4	L	211/214 (98%)	-0.03	0 100 100	118, 224, 343, 371	0
5	D	229/232 (98%)	0.15	9 (3%) 44 30	92, 147, 379, 418	0
6	E	210/214 (98%)	0.24	9 (4%) 40 27	108, 192, 346, 369	0
All	All	1456/1532 (95%)	0.04	25 (1%) 69 49	74, 169, 340, 418	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	E	134	VAL	4.5
5	D	126	PRO	4.3
5	D	141	LEU	3.8
5	D	140	CYS	3.5
6	E	106	VAL	3.2
6	E	142	PRO	3.2
5	D	198	VAL	3.1
5	D	120	SER	3.0
6	E	165	PRO	3.0
5	D	142	VAL	2.9
6	E	136	LEU	2.8
6	E	133	LEU	2.7
6	E	107	LEU	2.7
5	D	119	PRO	2.6
2	G	360	ARG	2.5
3	H	138	LEU	2.4
6	E	179	LEU	2.3
5	D	125	ALA	2.3
3	H	90	TYR	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	H	141	LEU	2.1
2	G	134	VAL	2.1
5	D	121	VAL	2.1
2	G	135	THR	2.0
2	G	69	TRP	2.0
6	E	147	VAL	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](#)

SUGAR-RSR INFOmissingINFO

## 6.4 Ligands [i](#)

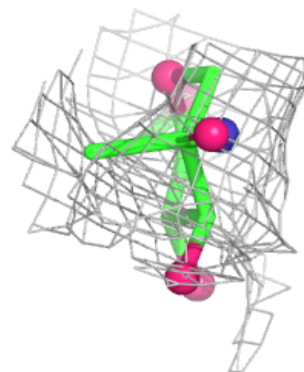
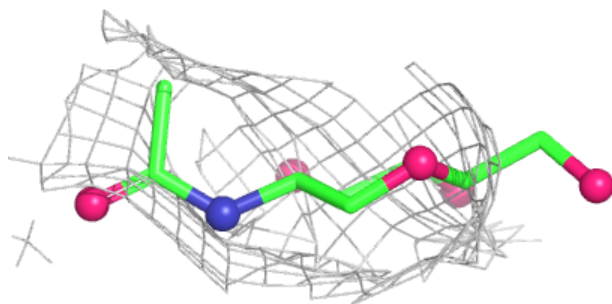
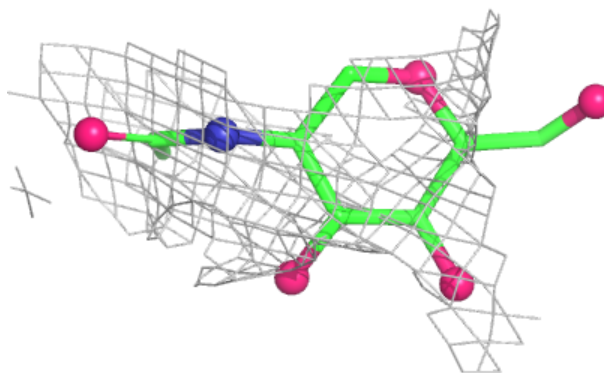
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
18	NAG	G	602	14/15	0.25	0.10	233,249,256,258	0
18	NAG	G	601	14/15	0.80	0.10	179,197,204,209	0

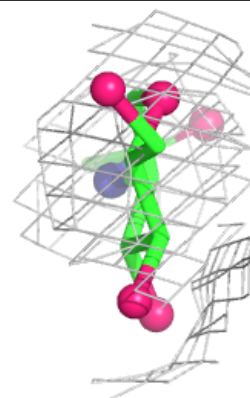
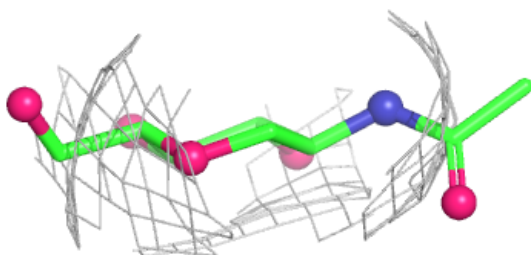
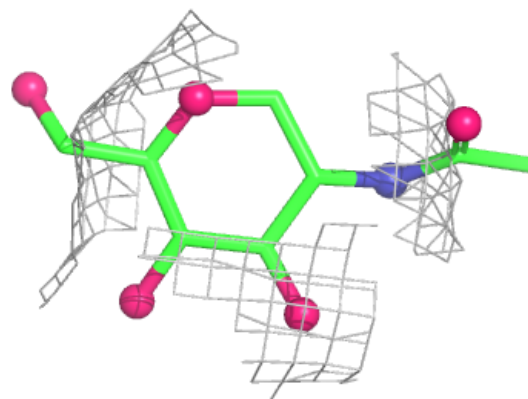
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAG G 602:**

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

**Electron density around NAG G 601:**

$2mF_o-DF_c$  (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.