



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:49 AM EDT

PDB ID : 5T3X / pdb_00005t3x
Title : 3.9 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 : 3.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

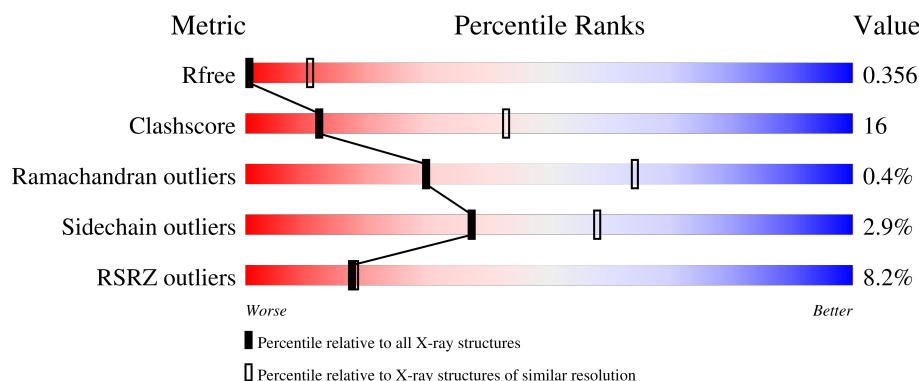
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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

Mol	Chain	Length	Quality of chain
1	B	153	
2	G	481	
3	H	238	
4	L	214	
5	D	232	

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

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 12620 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	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	449	Total	C	N	O	S	0	0	0
			3532	2217	623	665	27			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	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.

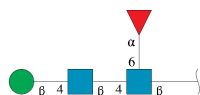
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	210	Total	C	N	O	S	0	0	0
			1558	976	261	317	4			

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



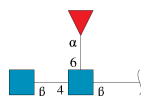
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	A	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



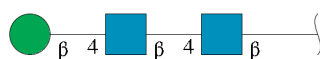
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	C	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



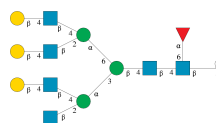
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	F	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 10 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.



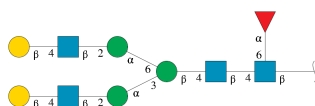
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 11 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-(1-4)]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.



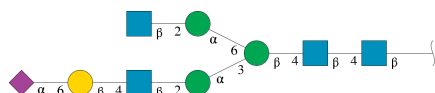
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	J	13	Total	C	N	O	0	0	0
			160	90	6	64			

- 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)-[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.



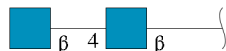
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	K	10	Total	C	N	O	0	0	0
			121	68	4	49			

- Molecule 13 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-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.



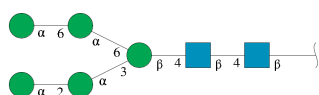
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	9	Total	C	N	O	0	0	0
			120	67	5	48			

- Molecule 14 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



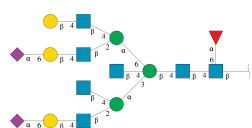
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
14	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
14	T	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



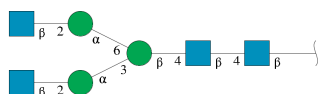
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 16 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-6)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]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.



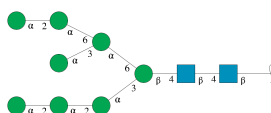
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	P	16	Total	C	N	O	0	0	0
			214	120	9	85			

- Molecule 17 is an oligosaccharide called 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.



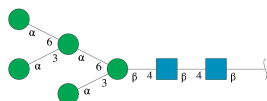
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	R	7	Total	C	N	O	0	0	0
			89	50	4	35			

- Molecule 18 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.



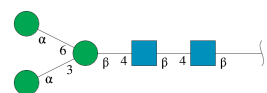
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	S	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 19 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-glucopyranose.



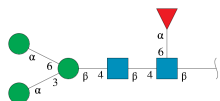
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	U	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 20 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
20	V	5	Total	C	N	O	0	0	0
			61	34	2	25			

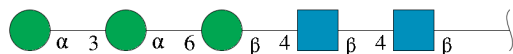
- Molecule 21 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	W	6	Total	C	N	O	0	0	0
			71	40	2	29			

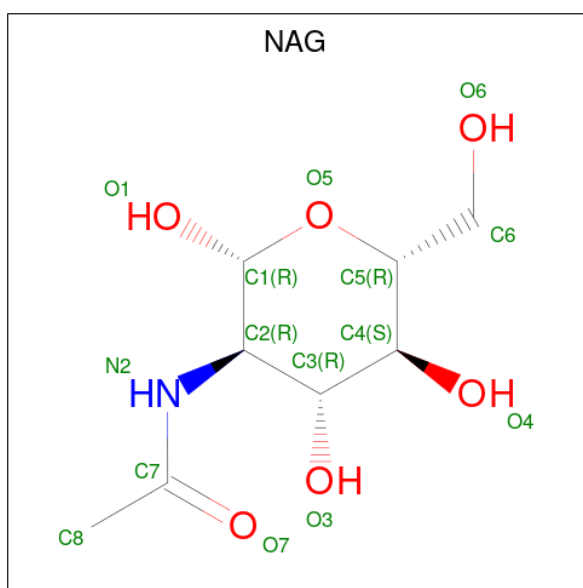
- Molecule 22 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-

acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 23 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

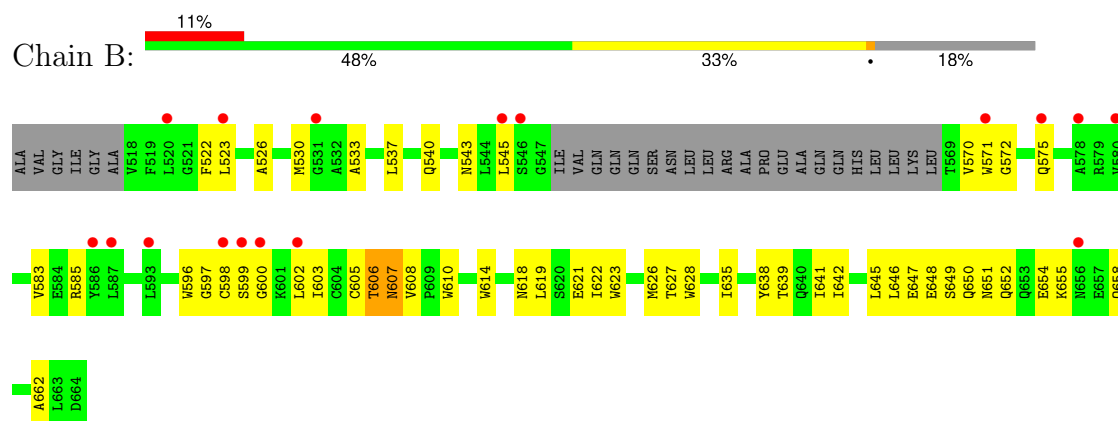


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
23	G	1	14	8	1	5	0	0

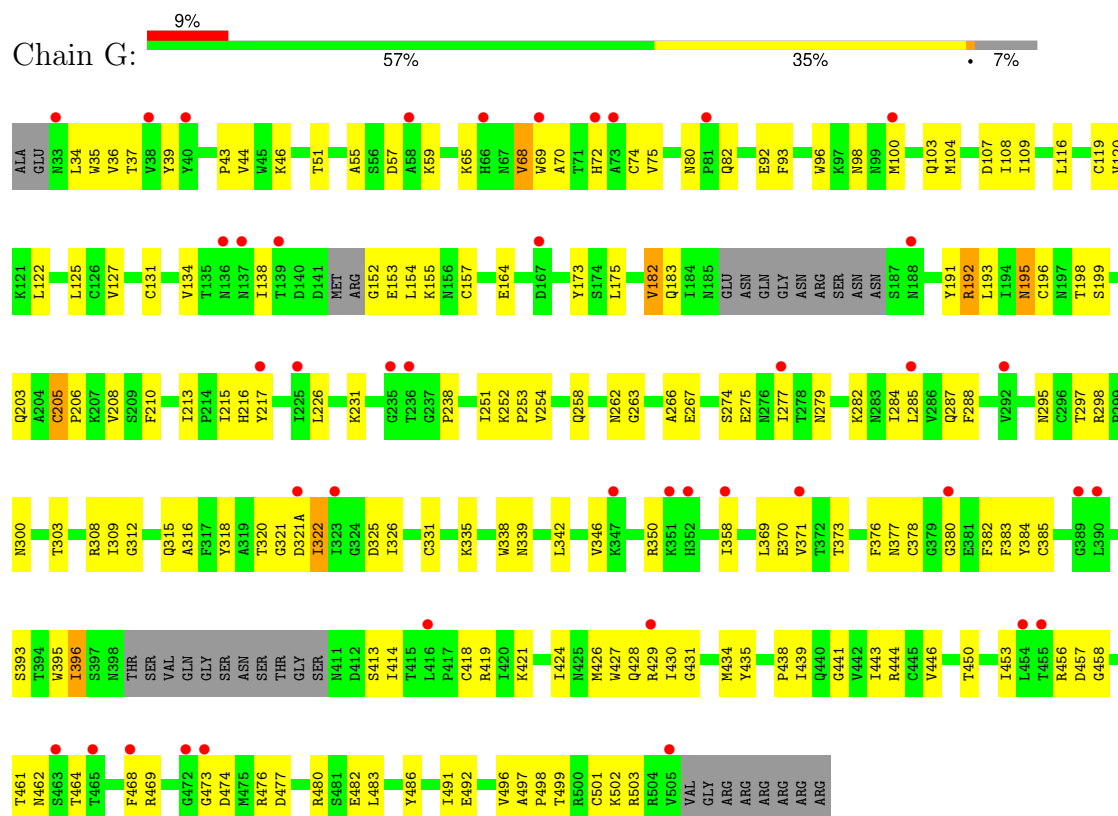
3 Residue-property plots

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.

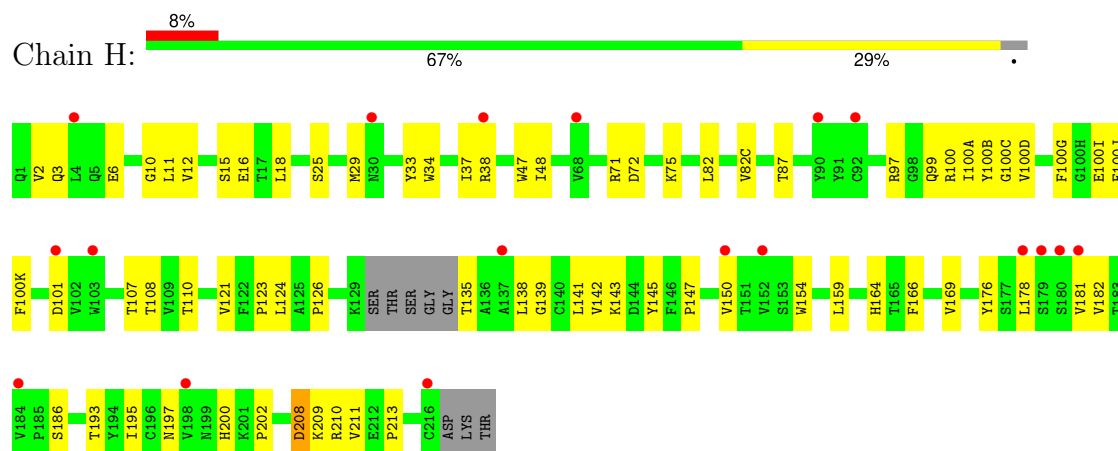
• Molecule 1: Envelope glycoprotein gp160



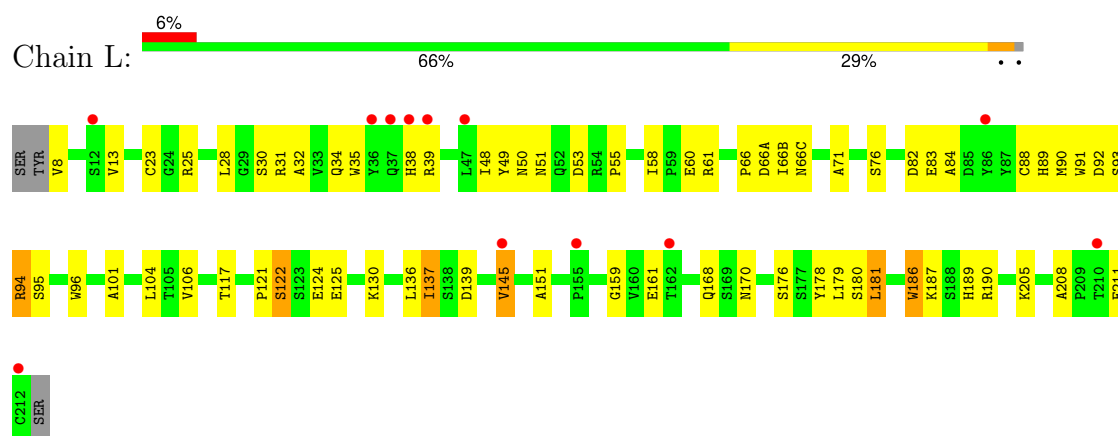
• Molecule 2: Envelope glycoprotein gp160



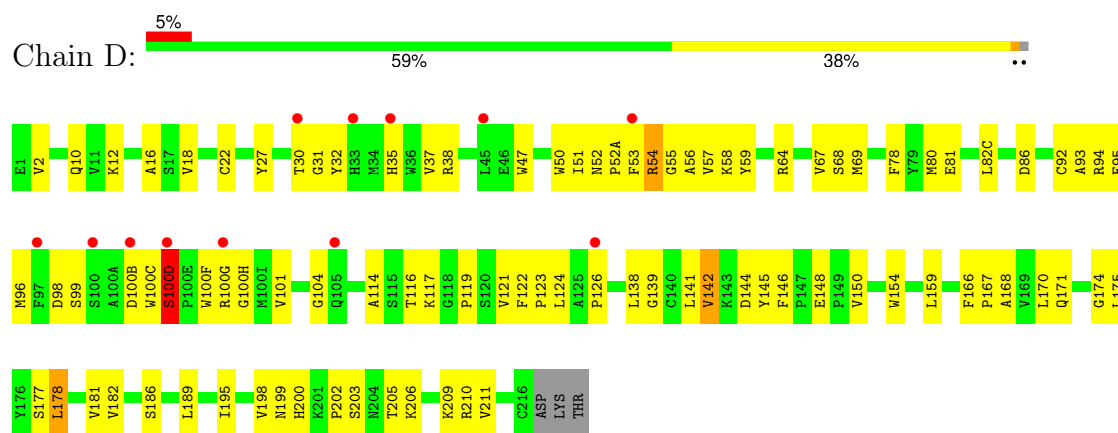
- Molecule 3: 10-1074 Heavy Chain



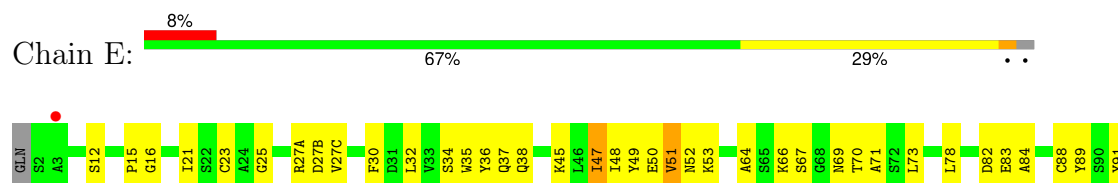
- Molecule 4: 10-1074 Light Chain

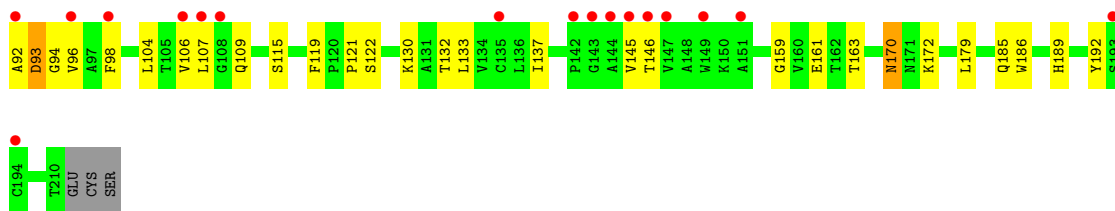


- Molecule 5: IOMA Heavy Chain

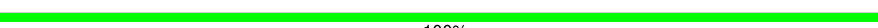


- Molecule 6: IOMA Light Chain





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

Chain A:  100%



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

Chain C:  50%

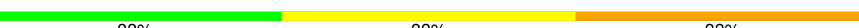


- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  67%

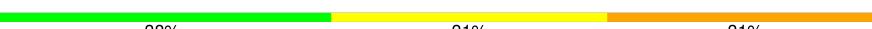


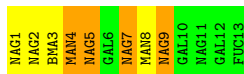
- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  33%



- Molecule 11: 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)]beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]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:  38%



- Molecule 12: beta-D-galactopyranose-(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



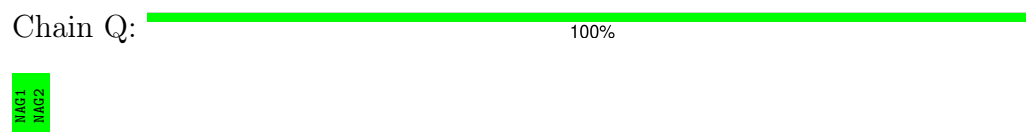
- Molecule 13: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



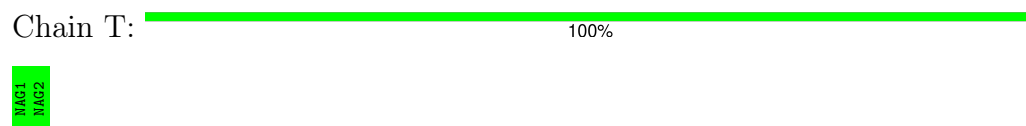
- Molecule 14: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 14: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 14: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



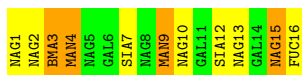
- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





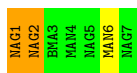
- Molecule 16: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-6)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]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 P:



- Molecule 17: 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 R:



- Molecule 18: 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:



- Molecule 19: 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 U:



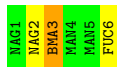
- Molecule 20: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

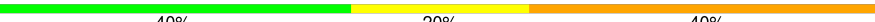


- Molecule 21: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  50% 33% 17%



- Molecule 22: 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 X:  40% 20% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	217.51Å 217.51Å 156.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.63 – 3.90 80.63 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (80.63-3.90) 95.6 (80.63-3.90)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 3.89Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.296 , 0.331 0.322 , 0.356	Depositor DCC
R_{free} test set	1276 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	134.0	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 410.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.075 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.160 for k,h,-l	Depositor
Outliers	0 of 25075 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	12620	wwPDB-VP
Average B, all atoms (Å ²)	302.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.15	0/1019	0.41	0/1382
2	G	0.17	0/3605	0.47	1/4895 (0.0%)
3	H	0.14	0/1796	0.37	0/2450
4	L	0.14	0/1649	0.39	0/2250
5	D	0.16	0/1790	0.46	2/2437 (0.1%)
6	E	0.16	0/1596	0.39	0/2175
All	All	0.16	0/11455	0.43	3/15589 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	458	GLY	O-C-N	-10.07	109.61	122.70
5	D	100(D)	SER	C-N-CD	-8.05	102.89	120.60
5	D	100(D)	SER	C-N-CA	6.31	148.50	122.00

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	53	0
2	G	3532	0	3462	135	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1753	0	1719	54	0
4	L	1607	0	1550	52	0
5	D	1742	0	1698	74	0
6	E	1558	0	1511	54	0
7	A	24	0	22	0	0
8	C	49	0	43	0	0
9	F	38	0	34	0	0
10	I	39	0	34	1	0
11	J	160	0	136	2	0
12	K	121	0	103	1	0
13	M	120	0	101	1	0
14	N	28	0	25	0	0
14	Q	28	0	25	0	0
14	T	28	0	25	0	0
15	O	83	0	70	2	0
16	P	214	0	180	4	0
17	R	89	0	76	2	0
18	S	116	0	97	4	0
19	U	83	0	70	0	0
20	V	61	0	52	1	0
21	W	71	0	61	1	0
22	X	61	0	52	1	0
23	G	14	0	13	1	0
All	All	12620	0	12135	385	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 16.

All (385) 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)
2:G:55:ALA:HB3	2:G:216:HIS:HB2	1.57	0.87
6:E:47:ILE:HG22	6:E:48:ILE:HG12	1.61	0.82
2:G:119:CYS:SG	2:G:205:CYS:N	2.50	0.81
5:D:199:ASN:OD1	5:D:206:LYS:NZ	2.13	0.80
2:G:297:THR:HG22	2:G:444:ARG:HG3	1.63	0.78
5:D:119:PRO:HB3	5:D:145:TYR:HB3	1.66	0.77
2:G:51:THR:HA	2:G:103:GLN:HE22	1.52	0.75
2:G:175:LEU:O	2:G:320:THR:OG1	2.06	0.73
5:D:119:PRO:HD2	5:D:205:THR:HB	1.70	0.72
1:B:642:ILE:HG21	2:G:496:VAL:HG11	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:100:ARG:NH2	4:L:66(A):ASP:OD2	2.22	0.72
1:B:606:THR:HG21	1:B:646:LEU:HD22	1.71	0.72
5:D:52(A):PRO:HG3	5:D:78:PHE:HZ	1.54	0.71
4:L:13:VAL:HG23	4:L:104:LEU:HD11	1.75	0.69
5:D:35:HIS:HD2	5:D:50:TRP:HB3	1.55	0.69
2:G:65:LYS:HB2	2:G:68:VAL:HG23	1.75	0.69
5:D:51:ILE:HG23	5:D:57:VAL:HG12	1.74	0.69
5:D:150:VAL:HG11	5:D:198:VAL:HG13	1.75	0.68
16:P:3:BMA:H2	16:P:4:MAN:H5	1.75	0.68
2:G:279:ASN:HD22	2:G:282:LYS:HG2	1.58	0.68
11:J:5:NAG:H81	11:J:9:NAG:H82	1.76	0.67
1:B:606:THR:OG1	2:G:36:VAL:O	2.11	0.67
2:G:69:TRP:HE1	2:G:253:PRO:HG2	1.60	0.67
4:L:39:ARG:NH1	4:L:83:GLU:O	2.27	0.67
2:G:303:THR:HB	2:G:321:GLY:HA3	1.75	0.67
2:G:131:CYS:HB3	2:G:155:LYS:HB3	1.77	0.66
2:G:92:GLU:HA	2:G:238:PRO:HA	1.77	0.66
4:L:25:ARG:HH21	4:L:90:MET:H	1.42	0.66
3:H:38:ARG:HG3	3:H:48:ILE:HD11	1.79	0.65
3:H:16:GLU:H	3:H:82(C):VAL:HG22	1.61	0.65
2:G:258:GLN:NE2	2:G:371:VAL:O	2.29	0.65
2:G:424:ILE:HG22	2:G:426:MET:H	1.63	0.64
6:E:48:ILE:HG21	6:E:64:ALA:HB3	1.78	0.64
3:H:195:ILE:HG12	3:H:210:ARG:HG2	1.79	0.64
3:H:11:LEU:HD13	3:H:147:PRO:HG3	1.80	0.64
5:D:37:VAL:HG22	5:D:47:TRP:HA	1.81	0.63
3:H:100(B):TYR:CE2	4:L:93:SER:HB2	2.34	0.63
4:L:159:GLY:O	4:L:180:SER:N	2.27	0.63
2:G:456:ARG:NH2	6:E:93:ASP:OD1	2.25	0.62
4:L:83:GLU:HG2	4:L:106:VAL:H	1.64	0.62
6:E:66:LYS:HA	6:E:71:ALA:HA	1.81	0.62
4:L:23:CYS:HB2	4:L:71:ALA:HB3	1.81	0.62
1:B:596:TRP:O	1:B:651:ASN:ND2	2.32	0.62
6:E:92:ALA:C	6:E:94:GLY:H	2.07	0.62
1:B:526:ALA:HA	2:G:43:PRO:HB2	1.82	0.62
1:B:598:CYS:C	1:B:600:GLY:H	2.08	0.62
4:L:61:ARG:NH1	4:L:76:SER:O	2.29	0.61
4:L:35:TRP:HB2	4:L:48:ILE:HB	1.81	0.61
3:H:3:GLN:HG3	3:H:25:SER:HB2	1.82	0.61
2:G:439:ILE:HB	2:G:443:ILE:HD11	1.81	0.61
1:B:654:GLU:OE1	2:G:503:ARG:NH1	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:123:PRO:HD3	5:D:209:LYS:HE2	1.82	0.60
2:G:251:ILE:HG23	2:G:482:GLU:HG3	1.83	0.60
5:D:27:TYR:HE2	5:D:32:TYR:HB2	1.65	0.60
2:G:266:ALA:N	2:G:288:PHE:O	2.31	0.60
6:E:23:CYS:HB3	6:E:71:ALA:HB3	1.81	0.60
2:G:477:ASP:OD1	2:G:480:ARG:NH1	2.34	0.60
1:B:540:GLN:HE22	2:G:43:PRO:HG3	1.66	0.60
1:B:537:LEU:HD13	1:B:602:LEU:O	2.02	0.60
4:L:137:ILE:HD13	4:L:145:VAL:HG11	1.83	0.60
3:H:47:TRP:HE3	4:L:96:TRP:HA	1.67	0.60
4:L:25:ARG:NH2	4:L:90:MET:H	2.00	0.59
5:D:95:GLU:HA	5:D:100(H):GLY:O	2.03	0.59
4:L:28:LEU:HB3	4:L:94:ARG:HB2	1.84	0.59
2:G:274:SER:HB3	2:G:277:ILE:HG12	1.85	0.59
1:B:533:ALA:HB1	2:G:43:PRO:HG2	1.85	0.58
5:D:35:HIS:CD2	5:D:50:TRP:HB3	2.37	0.58
5:D:142:VAL:HG11	5:D:150:VAL:HG21	1.85	0.58
20:V:1:NAG:O3	20:V:2:NAG:N2	2.35	0.58
6:E:34:SER:N	6:E:89:TYR:O	2.31	0.58
2:G:195:ASN:ND2	2:G:199:SER:O	2.34	0.58
5:D:2:VAL:HG11	5:D:94:ARG:HH12	1.67	0.58
5:D:141:LEU:HD12	5:D:178:LEU:O	2.03	0.58
1:B:638:TYR:HA	1:B:641:ILE:HD12	1.86	0.58
5:D:195:ILE:HG12	5:D:210:ARG:HG2	1.86	0.57
4:L:179:LEU:HG	4:L:181:LEU:HD13	1.86	0.57
5:D:150:VAL:HB	5:D:178:LEU:HD21	1.86	0.57
5:D:10:GLN:HB3	5:D:12:LYS:HE2	1.86	0.57
5:D:116:THR:HG23	5:D:203:SER:HA	1.86	0.57
5:D:145:TYR:HE1	5:D:148:GLU:HA	1.70	0.57
1:B:650:GLN:O	1:B:654:GLU:N	2.32	0.57
5:D:47:TRP:HZ2	5:D:50:TRP:HD1	1.52	0.57
1:B:647:GLU:HG3	1:B:648:GLU:HG3	1.87	0.57
3:H:100:ARG:NH1	3:H:100(A):ILE:O	2.37	0.57
6:E:109:GLN:HE22	6:E:172:LYS:HG2	1.68	0.57
2:G:370:GLU:OE1	2:G:428:GLN:NE2	2.38	0.56
22:X:1:NAG:O3	22:X:2:NAG:N2	2.38	0.56
2:G:182:VAL:HG13	2:G:192:ARG:HD3	1.87	0.56
1:B:606:THR:OG1	2:G:36:VAL:HG23	2.06	0.56
2:G:34:LEU:HB3	2:G:498:PRO:HB2	1.86	0.56
2:G:285:LEU:HD22	2:G:453:ILE:HG12	1.87	0.56
3:H:147:PRO:O	3:H:200:HIS:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:441:GLY:HA3	17:R:1:NAG:H82	1.88	0.56
5:D:68:SER:HB3	5:D:81:GLU:HB3	1.87	0.56
5:D:18:VAL:HG23	5:D:82(C):LEU:HD11	1.88	0.56
3:H:193:THR:HG21	3:H:210:ARG:CZ	2.36	0.56
11:J:4:MAN:O3	11:J:7:NAG:O5	2.20	0.56
2:G:155:LYS:O	2:G:175:LEU:HA	2.05	0.56
5:D:52(A):PRO:HG3	5:D:78:PHE:CZ	2.39	0.56
2:G:369:LEU:O	2:G:373:THR:OG1	2.23	0.55
5:D:159:LEU:HD21	5:D:182:VAL:HG21	1.88	0.55
4:L:32:ALA:N	4:L:91:TRP:O	2.32	0.55
2:G:385:CYS:HA	2:G:418:CYS:HA	1.87	0.55
6:E:21:ILE:HD12	6:E:73:LEU:HD23	1.88	0.55
2:G:380:GLY:HA3	2:G:439:ILE:HG13	1.89	0.54
4:L:117:THR:HA	4:L:205:LYS:HG3	1.89	0.54
4:L:186:TRP:CD1	4:L:187:LYS:HG3	2.42	0.54
5:D:142:VAL:O	5:D:177:SER:HA	2.06	0.54
6:E:15:PRO:HD3	6:E:106:VAL:HG13	1.88	0.54
2:G:193:LEU:HB2	2:G:196:CYS:SG	2.47	0.54
2:G:69:TRP:CG	2:G:70:ALA:N	2.75	0.54
2:G:325:ASP:OD1	4:L:30:SER:N	2.25	0.54
12:K:1:NAG:H62	12:K:2:NAG:H82	1.89	0.54
5:D:52:ASN:HB3	5:D:56:ALA:HB3	1.90	0.54
1:B:628:TRP:CD1	2:G:43:PRO:HD2	2.42	0.54
1:B:530:MET:HG2	1:B:628:TRP:CG	2.43	0.54
2:G:100:MET:HB2	2:G:483:LEU:HD13	1.90	0.54
5:D:69:MET:HG2	5:D:80:MET:HG2	1.90	0.54
2:G:119:CYS:HB3	2:G:203:GLN:O	2.08	0.53
1:B:545:LEU:HD11	1:B:583:VAL:HG12	1.89	0.53
6:E:92:ALA:O	6:E:94:GLY:N	2.34	0.53
3:H:143:LYS:HZ3	4:L:130:LYS:HD2	1.72	0.53
4:L:50:ASN:O	18:S:5:MAN:O3	2.24	0.53
3:H:166:PHE:HB3	4:L:176:SER:HB3	1.90	0.53
2:G:98:ASN:ND2	2:G:486:TYR:O	2.42	0.53
6:E:50:GLU:OE1	6:E:53:LYS:NZ	2.29	0.53
2:G:320:THR:HG22	2:G:438:PRO:HG3	1.91	0.52
3:H:142:VAL:HB	3:H:178:LEU:HG	1.92	0.52
6:E:121:PRO:HD2	6:E:186:TRP:CZ2	2.44	0.52
2:G:252:LYS:HE3	2:G:262:ASN:HB3	1.91	0.52
5:D:22:CYS:O	5:D:78:PHE:N	2.40	0.52
2:G:183:GLN:HA	2:G:191:TYR:HA	1.92	0.52
2:G:430:ILE:HG22	2:G:431:GLY:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:123:PRO:HD2	4:L:124:GLU:HB2	1.90	0.52
3:H:166:PHE:CZ	4:L:136:LEU:HB3	2.44	0.52
2:G:499:THR:HG23	2:G:501:CYS:H	1.75	0.52
3:H:169:VAL:HG21	4:L:161:GLU:HB3	1.90	0.52
1:B:610:TRP:NE1	1:B:614:TRP:O	2.42	0.52
2:G:358:ILE:HG12	2:G:396:ILE:HG23	1.91	0.52
2:G:69:TRP:CG	2:G:70:ALA:H	2.26	0.51
2:G:473:GLY:O	5:D:54:ARG:NH1	2.40	0.51
3:H:100(A):ILE:HG12	3:H:100(J):PHE:HB3	1.92	0.51
5:D:52:ASN:N	5:D:56:ALA:O	2.38	0.51
6:E:145:VAL:HG12	6:E:146:THR:N	2.25	0.51
1:B:523:LEU:HA	1:B:540:GLN:NE2	2.25	0.51
4:L:208:ALA:HB3	4:L:211:GLU:HG3	1.93	0.51
6:E:89:TYR:CE1	6:E:96:VAL:HG13	2.46	0.51
10:I:1:NAG:O6	10:I:2:NAG:N2	2.43	0.51
16:P:9:MAN:O5	16:P:15:NAG:H82	2.11	0.51
1:B:572:GLY:O	1:B:575:GLN:NE2	2.43	0.51
2:G:55:ALA:O	2:G:216:HIS:N	2.36	0.51
2:G:153:GLU:HG3	2:G:419:ARG:HH21	1.75	0.51
3:H:100(D):VAL:HA	18:S:2:NAG:H2	1.92	0.51
4:L:34:GLN:HE21	4:L:91:TRP:HD1	1.59	0.51
5:D:35:HIS:N	5:D:93:ALA:O	2.38	0.51
3:H:99:GLN:HG3	3:H:100(J):PHE:CD2	2.45	0.51
6:E:12:SER:HB2	6:E:107:LEU:HD13	1.91	0.51
4:L:31:ARG:NH2	4:L:66:PRO:O	2.43	0.51
1:B:523:LEU:HA	1:B:540:GLN:HE21	1.74	0.51
3:H:101:ASP:OD1	3:H:101:ASP:N	2.44	0.51
4:L:31:ARG:O	4:L:51:ASN:ND2	2.43	0.51
4:L:82:ASP:HB2	4:L:106:VAL:HG21	1.93	0.51
5:D:126:PRO:HA	6:E:119:PHE:CE1	2.46	0.51
2:G:263:GLY:O	2:G:450:THR:HG21	2.12	0.50
2:G:55:ALA:N	2:G:216:HIS:O	2.44	0.50
4:L:28:LEU:O	4:L:92:ASP:HB2	2.11	0.50
2:G:274:SER:HB2	2:G:284:ILE:HG23	1.94	0.50
1:B:610:TRP:CD2	2:G:498:PRO:HB3	2.47	0.50
2:G:266:ALA:HB2	2:G:287:GLN:HB3	1.92	0.50
5:D:67:VAL:HG11	5:D:69:MET:HE3	1.94	0.50
3:H:6:GLU:N	3:H:6:GLU:OE1	2.44	0.50
3:H:126:PRO:HD2	3:H:213:PRO:HA	1.94	0.50
5:D:31:GLY:O	5:D:98:ASP:HB3	2.12	0.50
1:B:610:TRP:CE3	2:G:36:VAL:HG12	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:186:SER:HA	5:D:189:LEU:HG	1.92	0.50
2:G:335:LYS:H	2:G:413:SER:HA	1.76	0.50
3:H:12:VAL:HG21	3:H:18:LEU:HD12	1.94	0.49
5:D:30:THR:HA	5:D:52(A):PRO:HB2	1.94	0.49
5:D:100(G):ARG:HA	6:E:89:TYR:CE2	2.47	0.49
2:G:164:GLU:HA	2:G:312:GLY:O	2.12	0.49
2:G:55:ALA:HA	2:G:75:VAL:O	2.13	0.49
5:D:144:ASP:HA	5:D:175:LEU:HB3	1.94	0.49
6:E:37:GLN:N	6:E:45:LYS:O	2.45	0.49
2:G:109:ILE:HG12	2:G:427:TRP:CD2	2.48	0.49
5:D:200:HIS:CE1	5:D:203:SER:HG	2.26	0.49
2:G:215:ILE:N	2:G:251:ILE:O	2.39	0.49
21:W:2:NAG:H4	21:W:3:BMA:O2	2.12	0.49
1:B:522:PHE:CD1	1:B:523:LEU:HG	2.47	0.48
3:H:29:MET:HA	3:H:34:TRP:HZ2	1.78	0.48
5:D:100(G):ARG:HE	6:E:49:TYR:HD2	1.61	0.48
1:B:522:PHE:CE2	1:B:540:GLN:HA	2.47	0.48
2:G:326:ILE:HG12	4:L:94:ARG:NE	2.28	0.48
5:D:100(C):TRP:O	5:D:100(D):SER:HB2	2.13	0.48
2:G:393:SER:HB3	2:G:395:TRP:HE1	1.77	0.48
4:L:35:TRP:CZ3	4:L:88:CYS:HB2	2.48	0.48
5:D:166:PHE:HE2	5:D:181:VAL:HG13	1.78	0.48
3:H:47:TRP:CD1	3:H:48:ILE:H	2.31	0.48
4:L:92:ASP:OD1	4:L:95:SER:OG	2.28	0.48
5:D:50:TRP:CE2	5:D:58:LYS:HB3	2.49	0.48
2:G:46:LYS:HG3	2:G:492:GLU:HG3	1.95	0.48
3:H:100(C):GLY:HA3	3:H:100(I):GLU:OE1	2.13	0.48
6:E:121:PRO:HD3	6:E:133:LEU:HD21	1.95	0.48
2:G:378:CYS:HB3	2:G:383:PHE:CE1	2.48	0.48
3:H:159:LEU:HG	3:H:182:VAL:HG21	1.96	0.48
5:D:167:PRO:HD2	6:E:163:THR:HB	1.95	0.48
5:D:59:TYR:O	5:D:64:ARG:NH2	2.47	0.48
6:E:36:TYR:HE1	6:E:89:TYR:HB3	1.79	0.48
2:G:279:ASN:HB2	16:P:16:FUC:H61	1.96	0.47
3:H:100(K):PHE:HE2	4:L:91:TRP:HB3	1.79	0.47
2:G:474:ASP:OD1	2:G:476:ARG:NH1	2.47	0.47
5:D:99:SER:OG	5:D:100(B):ASP:O	2.32	0.47
1:B:635:ILE:O	1:B:639:THR:HG23	2.14	0.47
3:H:121:VAL:HA	3:H:141:LEU:O	2.14	0.47
4:L:122:SER:OG	4:L:125:GLU:N	2.33	0.47
2:G:104:MET:HG2	2:G:217:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:55:PRO:HD2	4:L:58:ILE:HG13	1.97	0.47
1:B:605:CYS:HA	2:G:37:THR:HG22	1.95	0.47
2:G:107:ASP:OD2	2:G:217:TYR:OH	2.32	0.47
6:E:27(B):ASP:O	6:E:30:PHE:HB2	2.14	0.47
6:E:185:GLN:O	6:E:192:TYR:OH	2.33	0.47
1:B:522:PHE:CE2	1:B:543:ASN:HB2	2.50	0.47
1:B:607:ASN:OD1	1:B:607:ASN:N	2.47	0.46
1:B:571:TRP:CH2	2:G:74:CYS:HB2	2.50	0.46
2:G:279:ASN:ND2	2:G:282:LYS:HG2	2.25	0.46
2:G:298:ARG:HB2	2:G:383:PHE:HZ	1.79	0.46
2:G:338:TRP:O	2:G:342:LEU:HG	2.15	0.46
2:G:175:LEU:HD22	2:G:321(A):ASP:HA	1.97	0.46
3:H:38:ARG:HH12	3:H:82:LEU:HD22	1.79	0.46
3:H:124:LEU:HD23	4:L:122:SER:HB3	1.97	0.46
1:B:598:CYS:C	1:B:600:GLY:N	2.74	0.46
2:G:37:THR:OG1	2:G:497:ALA:O	2.33	0.46
2:G:206:PRO:HD3	2:G:318:TYR:CE2	2.51	0.46
1:B:645:LEU:HD12	1:B:649:SER:HB3	1.98	0.46
4:L:151:ALA:HB1	4:L:189:HIS:CD2	2.51	0.46
5:D:51:ILE:HD11	5:D:69:MET:HB3	1.98	0.46
6:E:27(B):ASP:OD1	6:E:27(C):VAL:N	2.43	0.46
13:M:4:MAN:H4	13:M:5:NAG:H83	1.97	0.46
5:D:168:ALA:HA	5:D:178:LEU:HB3	1.98	0.46
6:E:145:VAL:HG12	6:E:146:THR:H	1.80	0.46
2:G:192:ARG:NH2	2:G:193:LEU:O	2.44	0.46
4:L:8:VAL:HG12	4:L:101:ALA:HB3	1.98	0.45
1:B:651:ASN:O	1:B:655:LYS:HB2	2.15	0.45
3:H:166:PHE:CG	4:L:136:LEU:HD22	2.51	0.45
4:L:34:GLN:HB2	4:L:89:HIS:HB3	1.98	0.45
6:E:48:ILE:HA	6:E:53:LYS:O	2.16	0.45
2:G:122:LEU:O	2:G:125:LEU:HB2	2.16	0.45
5:D:138:LEU:HB2	5:D:211:VAL:HG11	1.98	0.45
4:L:49:TYR:O	4:L:53:ASP:HB2	2.16	0.45
4:L:66(A):ASP:O	18:S:4:MAN:O3	2.29	0.45
5:D:38:ARG:HH22	5:D:86:ASP:HA	1.81	0.45
2:G:384:TYR:CE1	2:G:421:LYS:HB3	2.51	0.45
1:B:658:GLN:O	1:B:662:ALA:N	2.50	0.45
2:G:44:VAL:HG12	2:G:492:GLU:HB2	1.98	0.45
2:G:152:GLY:C	2:G:154:LEU:H	2.25	0.45
3:H:135:THR:N	3:H:186:SER:HG	2.14	0.45
5:D:96:MET:HG2	5:D:101:VAL:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:TRP:HH2	2:G:39:TYR:CE1	2.35	0.45
5:D:121:VAL:HG21	5:D:198:VAL:HG11	1.99	0.45
3:H:29:MET:HE1	3:H:71:ARG:HB3	1.98	0.44
6:E:35:TRP:CZ3	6:E:88:CYS:HB3	2.52	0.44
2:G:80:ASN:O	2:G:82:GLN:N	2.49	0.44
3:H:142:VAL:HG11	3:H:150:VAL:HG11	1.99	0.44
1:B:571:TRP:HZ3	2:G:72:HIS:H	1.65	0.44
2:G:339:ASN:OD1	23:G:3390:NAG:N2	2.51	0.44
2:G:434:MET:HG2	2:G:435:TYR:N	2.33	0.44
2:G:35:TRP:O	2:G:498:PRO:HA	2.18	0.44
2:G:384:TYR:O	2:G:419:ARG:N	2.46	0.44
16:P:4:MAN:H2	16:P:15:NAG:H61	1.99	0.44
5:D:170:LEU:HD11	5:D:174:GLY:HA2	1.98	0.44
5:D:171:GLN:HG2	6:E:161:GLU:OE1	2.18	0.44
6:E:185:GLN:O	6:E:189:HIS:ND1	2.48	0.44
1:B:610:TRP:HE3	2:G:36:VAL:HG12	1.83	0.44
1:B:618:ASN:HB2	1:B:621:GLU:HG3	1.98	0.44
2:G:120:VAL:HG11	2:G:316:ALA:O	2.17	0.44
3:H:10:GLY:HA3	3:H:202:PRO:HG3	2.00	0.44
4:L:66(B):ILE:O	4:L:66(C):ASN:HB2	2.18	0.44
5:D:122:PHE:CE2	5:D:141:LEU:HD23	2.53	0.44
2:G:198:THR:OG1	2:G:199:SER:N	2.51	0.43
18:S:8:MAN:H2	18:S:9:MAN:H2	1.78	0.43
2:G:298:ARG:HB2	2:G:383:PHE:CZ	2.53	0.43
2:G:350:ARG:NH2	2:G:396:ILE:O	2.48	0.43
6:E:16:GLY:H	6:E:78:LEU:HB2	1.82	0.43
2:G:312:GLY:HA2	2:G:315:GLN:HB2	1.98	0.43
2:G:393:SER:HB3	2:G:395:TRP:NE1	2.32	0.43
3:H:139:GLY:HA2	3:H:154:TRP:CZ2	2.53	0.43
4:L:139:ASP:OD1	4:L:170:ASN:ND2	2.52	0.43
3:H:164:HIS:NE2	4:L:168:GLN:OE1	2.51	0.43
5:D:16:ALA:O	5:D:82(C):LEU:HG	2.18	0.43
5:D:92:CYS:O	5:D:104:GLY:N	2.48	0.43
5:D:124:LEU:HB3	6:E:119:PHE:CD2	2.53	0.43
2:G:69:TRP:CH2	2:G:108:ILE:HG23	2.54	0.43
5:D:122:PHE:HE2	5:D:141:LEU:HD23	1.83	0.43
6:E:170:ASN:OD1	6:E:170:ASN:N	2.39	0.43
2:G:279:ASN:OD1	5:D:100(F):TRP:NE1	2.48	0.43
2:G:321(A):ASP:OD1	2:G:322:ILE:N	2.51	0.43
3:H:87:THR:HG23	3:H:110:THR:HA	2.00	0.43
5:D:100(G):ARG:HA	6:E:89:TYR:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:209:LYS:HE2	3:H:209:LYS:HB2	1.78	0.43
6:E:30:PHE:HB3	6:E:32:LEU:HG	2.00	0.43
6:E:50:GLU:HB2	6:E:53:LYS:HG2	1.99	0.43
6:E:83:GLU:HG3	6:E:104:LEU:O	2.19	0.43
17:R:2:NAG:H61	17:R:6:MAN:H3	2.01	0.43
2:G:96:TRP:CG	2:G:275:GLU:HB2	2.54	0.43
2:G:157:CYS:O	2:G:173:TYR:HA	2.18	0.43
2:G:231:LYS:HD2	2:G:267:GLU:HG3	2.01	0.43
2:G:380:GLY:HA3	2:G:439:ILE:CG1	2.48	0.43
2:G:462:ASN:OD1	6:E:27(A):ARG:NH1	2.52	0.43
6:E:89:TYR:HB2	6:E:98:PHE:CD1	2.53	0.43
2:G:93:PHE:HZ	2:G:226:LEU:HB2	1.84	0.42
2:G:210:PHE:HB2	2:G:377:ASN:CG	2.44	0.42
2:G:252:LYS:O	2:G:254:VAL:N	2.52	0.42
2:G:300:ASN:HB3	2:G:322:ILE:HD13	2.01	0.42
5:D:141:LEU:HD11	5:D:177:SER:OG	2.19	0.42
3:H:100(G):PHE:HB2	3:H:100(I):GLU:HG3	2.01	0.42
5:D:145:TYR:HD1	5:D:200:HIS:NE2	2.17	0.42
5:D:200:HIS:CD2	5:D:202:PRO:HD2	2.54	0.42
6:E:25:GLY:O	6:E:69:ASN:HB3	2.19	0.42
1:B:610:TRP:CH2	2:G:498:PRO:HD3	2.53	0.42
1:B:614:TRP:CD1	1:B:638:TYR:CG	3.08	0.42
1:B:622:ILE:O	1:B:626:MET:HB2	2.20	0.42
3:H:107:THR:OG1	3:H:108:THR:N	2.50	0.42
6:E:32:LEU:HD12	6:E:91:TYR:HB3	2.02	0.42
1:B:607:ASN:HA	2:G:502:LYS:HG3	2.02	0.42
5:D:145:TYR:CE1	5:D:150:VAL:HG23	2.55	0.42
1:B:597:GLY:HA3	2:G:503:ARG:CZ	2.50	0.42
1:B:608:VAL:HB	2:G:36:VAL:CG2	2.50	0.42
2:G:226:LEU:O	2:G:486:TYR:HA	2.20	0.42
6:E:115:SER:O	6:E:137:ILE:HA	2.20	0.42
1:B:614:TRP:CZ3	1:B:642:ILE:HG12	2.55	0.42
2:G:427:TRP:O	2:G:429:ARG:N	2.53	0.42
4:L:32:ALA:HA	4:L:51:ASN:ND2	2.35	0.42
2:G:376:PHE:O	2:G:382:PHE:HA	2.19	0.42
3:H:138:LEU:HD13	3:H:211:VAL:HG11	2.02	0.42
4:L:38:HIS:O	4:L:84:ALA:HB1	2.19	0.42
4:L:161:GLU:HB2	4:L:178:TYR:HB2	2.01	0.42
5:D:100(G):ARG:HG3	5:D:100(H):GLY:N	2.35	0.42
5:D:139:GLY:HA2	5:D:154:TRP:CH2	2.55	0.42
1:B:596:TRP:CD1	1:B:646:LEU:HB2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:116:LEU:HD22	2:G:434:MET:HG3	2.02	0.41
3:H:197:ASN:ND2	3:H:208:ASP:OD2	2.53	0.41
2:G:134:VAL:HB	2:G:154:LEU:O	2.20	0.41
3:H:15:SER:N	3:H:82(C):VAL:O	2.37	0.41
5:D:145:TYR:CE1	5:D:148:GLU:HA	2.52	0.41
6:E:35:TRP:CD1	6:E:48:ILE:HB	2.56	0.41
1:B:523:LEU:HD11	2:G:491:ILE:HD11	2.02	0.41
1:B:540:GLN:HE22	2:G:43:PRO:CG	2.33	0.41
3:H:126:PRO:HB3	3:H:138:LEU:HB3	2.01	0.41
1:B:570:VAL:C	1:B:572:GLY:H	2.27	0.41
2:G:59:LYS:HA	2:G:59:LYS:HD2	1.84	0.41
3:H:72:ASP:HB3	3:H:75:LYS:HB2	2.02	0.41
3:H:150:VAL:HB	3:H:178:LEU:HD21	2.02	0.41
4:L:121:PRO:HD2	4:L:186:TRP:CE2	2.56	0.41
5:D:117:LYS:HZ1	6:E:130:LYS:HE2	1.84	0.41
2:G:468:PHE:C	2:G:469:ARG:HG3	2.46	0.41
2:G:164:GLU:HG3	2:G:308:ARG:HB3	2.02	0.41
3:H:200:HIS:CD2	3:H:202:PRO:HD2	2.56	0.41
5:D:53:PHE:C	5:D:55:GLY:H	2.29	0.41
2:G:461:THR:HB	2:G:464:THR:HG21	2.02	0.41
3:H:33:TYR:HE2	3:H:97:ARG:HD3	1.86	0.41
3:H:100(D):VAL:HG13	3:H:100(G):PHE:HB2	2.01	0.41
1:B:646:LEU:O	1:B:650:GLN:HB2	2.19	0.41
2:G:346:VAL:O	2:G:350:ARG:HG3	2.20	0.41
6:E:23:CYS:O	6:E:71:ALA:N	2.32	0.41
1:B:585:ARG:NE	2:G:491:ILE:O	2.41	0.41
1:B:648:GLU:O	1:B:652:GLN:HB3	2.20	0.41
2:G:282:LYS:HA	2:G:282:LYS:HD3	1.84	0.41
2:G:295:ASN:O	2:G:331:CYS:HA	2.21	0.41
3:H:145:TYR:CZ	3:H:176:TYR:HB2	2.55	0.41
5:D:12:LYS:HG3	5:D:18:VAL:CG2	2.51	0.41
5:D:122:PHE:HB2	6:E:122:SER:OG	2.21	0.41
6:E:159:GLY:O	6:E:179:LEU:HA	2.21	0.41
1:B:642:ILE:HD13	2:G:496:VAL:HG11	2.03	0.41
2:G:446:VAL:O	15:O:1:NAG:H5	2.21	0.41
3:H:29:MET:O	3:H:71:ARG:NH1	2.54	0.40
6:E:67:SER:N	6:E:70:THR:O	2.44	0.40
2:G:456:ARG:HH12	6:E:93:ASP:CG	2.23	0.40
4:L:31:ARG:HA	4:L:92:ASP:HA	2.03	0.40
6:E:23:CYS:HB2	6:E:35:TRP:CH2	2.57	0.40
6:E:38:GLN:O	6:E:84:ALA:HB1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:96:TRP:HH2	2:G:285:LEU:HG	1.86	0.40
6:E:82:ASP:O	6:E:104:LEU:HD23	2.22	0.40
15:O:4:MAN:H2	15:O:5:MAN:H2	1.65	0.40
2:G:213:ILE:O	2:G:215:ILE:HG13	2.22	0.40
5:D:114:ALA:HB3	5:D:146:PHE:CD1	2.57	0.40
6:E:132:THR:HA	6:E:179:LEU:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	122/153 (80%)	106 (87%)	15 (12%)	1 (1%)	16	50
2	G	441/481 (92%)	407 (92%)	32 (7%)	2 (0%)	24	59
3	H	226/238 (95%)	216 (96%)	10 (4%)	0	100	100
4	L	209/214 (98%)	199 (95%)	10 (5%)	0	100	100
5	D	227/232 (98%)	216 (95%)	10 (4%)	1 (0%)	30	64
6	E	208/214 (97%)	193 (93%)	13 (6%)	2 (1%)	12	45
All	All	1433/1532 (94%)	1337 (93%)	90 (6%)	6 (0%)	30	64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	599	SER
2	G	138	ILE
5	D	100(D)	SER
6	E	93	ASP
2	G	457	ASP
6	E	51	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	108/129 (84%)	103 (95%)	5 (5%)	24	48
2	G	401/428 (94%)	389 (97%)	12 (3%)	36	57
3	H	202/208 (97%)	198 (98%)	4 (2%)	48	65
4	L	175/178 (98%)	167 (95%)	8 (5%)	24	48
5	D	194/197 (98%)	191 (98%)	3 (2%)	57	70
6	E	173/177 (98%)	169 (98%)	4 (2%)	44	63
All	All	1253/1317 (95%)	1217 (97%)	36 (3%)	37	58

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	603	ILE
1	B	606	THR
1	B	607	ASN
1	B	619	LEU
1	B	627	THR
2	G	57	ASP
2	G	68	VAL
2	G	127	VAL
2	G	182	VAL
2	G	192	ARG
2	G	195	ASN
2	G	205	CYS
2	G	208	VAL
2	G	309	ILE
2	G	322	ILE
2	G	396	ILE
2	G	414	ILE
3	H	2	VAL
3	H	37	ILE
3	H	181	VAL
3	H	208	ASP
4	L	60	GLU

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Mol	Chain	Res	Type
4	L	94	ARG
4	L	122	SER
4	L	137	ILE
4	L	145	VAL
4	L	181	LEU
4	L	186	TRP
4	L	190	ARG
5	D	54	ARG
5	D	142	VAL
5	D	178	LEU
6	E	47	ILE
6	E	51	VAL
6	E	52	ASN
6	E	170	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	658	GLN
2	G	67	ASN
2	G	105	HIS
2	G	170	GLN
2	G	203	GLN
2	G	377	ASN
2	G	411	ASN
3	H	60	ASN
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](#)

113 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	7,1	14,14,15	0.28	0	17,19,21	0.76	0
7	FUC	A	2	7	10,10,11	0.73	0	14,14,16	0.82	0
8	NAG	C	1	8,1	14,14,15	0.34	0	17,19,21	1.38	2 (11%)
8	NAG	C	2	8	14,14,15	0.32	0	17,19,21	1.05	2 (11%)
8	BMA	C	3	8	11,11,12	0.26	0	15,15,17	0.63	0
8	FUC	C	4	8	10,10,11	0.67	0	14,14,16	0.79	0
9	NAG	F	1	9,2	14,14,15	0.32	0	17,19,21	0.95	1 (5%)
9	NAG	F	2	9	14,14,15	0.28	0	17,19,21	0.62	0
9	FUC	F	3	9	10,10,11	0.72	0	14,14,16	0.86	0
10	NAG	I	1	2,10	14,14,15	0.43	0	17,19,21	1.44	4 (23%)
10	NAG	I	2	10	14,14,15	0.33	0	17,19,21	0.92	0
10	BMA	I	3	10	11,11,12	0.25	0	15,15,17	0.69	0
11	NAG	J	1	2,11	14,14,15	0.39	0	17,19,21	0.81	1 (5%)
11	GAL	J	10	11	11,11,12	0.24	0	15,15,17	0.67	0
11	NAG	J	11	11	14,14,15	0.33	0	17,19,21	0.82	0
11	GAL	J	12	11	11,11,12	0.25	0	15,15,17	0.66	0
11	FUC	J	13	11	10,10,11	0.69	0	14,14,16	0.78	0
11	NAG	J	2	11	14,14,15	0.37	0	17,19,21	1.04	1 (5%)
11	BMA	J	3	11	11,11,12	0.45	0	15,15,17	1.27	2 (13%)
11	MAN	J	4	11	11,11,12	0.40	0	15,15,17	1.71	2 (13%)
11	NAG	J	5	11	14,14,15	0.47	0	17,19,21	1.30	1 (5%)
11	GAL	J	6	11	11,11,12	0.25	0	15,15,17	0.65	0
11	NAG	J	7	11	14,14,15	0.32	0	17,19,21	1.07	1 (5%)
11	MAN	J	8	11	11,11,12	0.50	0	15,15,17	1.79	2 (13%)
11	NAG	J	9	11	14,14,15	0.35	0	17,19,21	1.15	2 (11%)
12	NAG	K	1	2,12	14,14,15	0.46	0	17,19,21	1.37	2 (11%)
12	FUC	K	10	12	10,10,11	0.70	0	14,14,16	0.88	0
12	NAG	K	2	12	14,14,15	0.60	0	17,19,21	2.31	4 (23%)
12	BMA	K	3	12	11,11,12	0.35	0	15,15,17	1.42	3 (20%)
12	MAN	K	4	12	11,11,12	0.38	0	15,15,17	0.97	1 (6%)
12	NAG	K	5	12	14,14,15	0.35	0	17,19,21	0.99	1 (5%)
12	GAL	K	6	12	11,11,12	0.28	0	15,15,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	K	7	12	11,11,12	0.25	0	15,15,17	0.87	0
12	NAG	K	8	12	14,14,15	0.25	0	17,19,21	0.60	0
12	GAL	K	9	12	11,11,12	0.25	0	15,15,17	0.65	0
13	NAG	M	1	13,2	14,14,15	0.59	0	17,19,21	2.51	7 (41%)
13	NAG	M	2	13	14,14,15	0.71	1 (7%)	17,19,21	1.96	5 (29%)
13	BMA	M	3	13	11,11,12	0.52	0	15,15,17	1.36	3 (20%)
13	MAN	M	4	13	11,11,12	0.38	0	15,15,17	1.30	2 (13%)
13	NAG	M	5	13	14,14,15	0.34	0	17,19,21	0.82	1 (5%)
13	GAL	M	6	13	11,11,12	0.25	0	15,15,17	0.73	0
13	SIA	M	7	13	20,20,21	1.62	2 (10%)	21,28,31	1.55	3 (14%)
13	MAN	M	8	13	11,11,12	0.25	0	15,15,17	0.89	0
13	NAG	M	9	13	14,14,15	0.26	0	17,19,21	0.63	0
14	NAG	N	1	14,2	14,14,15	0.33	0	17,19,21	1.35	2 (11%)
14	NAG	N	2	14	14,14,15	0.25	0	17,19,21	0.74	0
15	NAG	O	1	2,15	14,14,15	0.38	0	17,19,21	0.84	0
15	NAG	O	2	15	14,14,15	0.31	0	17,19,21	1.27	4 (23%)
15	BMA	O	3	15	11,11,12	0.31	0	15,15,17	0.78	0
15	MAN	O	4	15	11,11,12	0.24	0	15,15,17	0.77	0
15	MAN	O	5	15	11,11,12	0.28	0	15,15,17	0.67	0
15	MAN	O	6	15	11,11,12	0.27	0	15,15,17	0.72	0
15	MAN	O	7	15	11,11,12	0.32	0	15,15,17	0.83	1 (6%)
16	NAG	P	1	2,16	14,14,15	0.47	0	17,19,21	1.24	3 (17%)
16	NAG	P	10	16	14,14,15	0.40	0	17,19,21	1.40	4 (23%)
16	GAL	P	11	16	11,11,12	0.28	0	15,15,17	0.92	0
16	SIA	P	12	16	20,20,21	1.61	1 (5%)	21,28,31	1.65	4 (19%)
16	NAG	P	13	16	14,14,15	0.45	0	17,19,21	1.09	1 (5%)
16	GAL	P	14	16	11,11,12	0.25	0	15,15,17	0.76	0
16	NAG	P	15	16	14,14,15	0.55	0	17,19,21	1.18	1 (5%)
16	FUC	P	16	16	10,10,11	0.62	0	14,14,16	0.87	0
16	NAG	P	2	16	14,14,15	0.31	0	17,19,21	1.07	3 (17%)
16	BMA	P	3	16	11,11,12	0.41	0	15,15,17	1.68	6 (40%)
16	MAN	P	4	16	11,11,12	0.35	0	15,15,17	1.42	3 (20%)
16	NAG	P	5	16	14,14,15	0.28	0	17,19,21	0.57	0
16	GAL	P	6	16	11,11,12	0.25	0	15,15,17	0.66	0
16	SIA	P	7	16	20,20,21	1.61	1 (5%)	21,28,31	1.56	3 (14%)
16	NAG	P	8	16	14,14,15	0.28	0	17,19,21	0.59	0
16	MAN	P	9	16	11,11,12	0.91	0	15,15,17	2.78	9 (60%)
14	NAG	Q	1	14,2	14,14,15	0.35	0	17,19,21	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAG	Q	2	14	14,14,15	0.30	0	17,19,21	0.68	0
17	NAG	R	1	2,17	14,14,15	0.47	0	17,19,21	1.75	5 (29%)
17	NAG	R	2	17	14,14,15	0.37	0	17,19,21	0.92	2 (11%)
17	BMA	R	3	17	11,11,12	0.29	0	15,15,17	0.88	0
17	MAN	R	4	17	11,11,12	0.27	0	15,15,17	0.97	0
17	NAG	R	5	17	14,14,15	0.31	0	17,19,21	0.44	0
17	MAN	R	6	17	11,11,12	0.26	0	15,15,17	0.76	0
17	NAG	R	7	17	14,14,15	0.28	0	17,19,21	0.67	0
18	NAG	S	1	2,18	14,14,15	0.31	0	17,19,21	0.74	0
18	MAN	S	10	18	11,11,12	0.27	0	15,15,17	0.66	0
18	NAG	S	2	18	14,14,15	0.26	0	17,19,21	1.35	3 (17%)
18	BMA	S	3	18	11,11,12	0.30	0	15,15,17	0.93	1 (6%)
18	MAN	S	4	18	11,11,12	0.34	0	15,15,17	1.30	2 (13%)
18	MAN	S	5	18	11,11,12	0.33	0	15,15,17	1.17	1 (6%)
18	MAN	S	6	18	11,11,12	0.22	0	15,15,17	0.84	0
18	MAN	S	7	18	11,11,12	0.24	0	15,15,17	1.13	2 (13%)
18	MAN	S	8	18	11,11,12	0.44	0	15,15,17	1.27	1 (6%)
18	MAN	S	9	18	11,11,12	0.22	0	15,15,17	0.71	0
14	NAG	T	1	14,2	14,14,15	0.36	0	17,19,21	0.63	0
14	NAG	T	2	14	14,14,15	0.32	0	17,19,21	0.56	0
19	NAG	U	1	2,19	14,14,15	0.53	0	17,19,21	2.18	4 (23%)
19	NAG	U	2	19	14,14,15	0.45	0	17,19,21	1.83	3 (17%)
19	BMA	U	3	19	11,11,12	0.39	0	15,15,17	1.05	1 (6%)
19	MAN	U	4	19	11,11,12	0.38	0	15,15,17	0.85	0
19	MAN	U	5	19	11,11,12	0.26	0	15,15,17	0.74	0
19	MAN	U	6	19	11,11,12	0.28	0	15,15,17	0.74	0
19	MAN	U	7	19	11,11,12	0.31	0	15,15,17	0.66	0
20	NAG	V	1	2,20	14,14,15	0.32	0	17,19,21	1.21	2 (11%)
20	NAG	V	2	20	14,14,15	0.64	0	17,19,21	1.79	5 (29%)
20	BMA	V	3	20	11,11,12	0.34	0	15,15,17	1.01	1 (6%)
20	MAN	V	4	20	11,11,12	0.28	0	15,15,17	0.64	0
20	MAN	V	5	20	11,11,12	0.27	0	15,15,17	0.62	0
21	NAG	W	1	21,2	14,14,15	0.37	0	17,19,21	1.00	0
21	NAG	W	2	21	14,14,15	0.28	0	17,19,21	0.82	0
21	BMA	W	3	21	11,11,12	0.44	0	15,15,17	1.38	2 (13%)
21	MAN	W	4	21	11,11,12	0.26	0	15,15,17	0.62	0
21	MAN	W	5	21	11,11,12	0.27	0	15,15,17	0.67	0
21	FUC	W	6	21	10,10,11	0.88	0	14,14,16	0.99	1 (7%)
22	NAG	X	1	2,22	14,14,15	0.29	0	17,19,21	1.14	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	NAG	X	2	22	14,14,15	0.60	0	17,19,21	2.17	6 (35%)
22	BMA	X	3	22	11,11,12	0.32	0	15,15,17	1.00	1 (6%)
22	MAN	X	4	22	11,11,12	0.24	0	15,15,17	0.58	0
22	MAN	X	5	22	11,11,12	0.25	0	15,15,17	0.64	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
7	NAG	A	1	7,1	-	1/6/23/26	0/1/1/1
7	FUC	A	2	7	-	-	0/1/1/1
8	NAG	C	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	C	2	8	-	2/6/23/26	0/1/1/1
8	BMA	C	3	8	-	0/2/19/22	0/1/1/1
8	FUC	C	4	8	-	-	0/1/1/1
9	NAG	F	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	F	2	9	-	2/6/23/26	0/1/1/1
9	FUC	F	3	9	-	-	0/1/1/1
10	NAG	I	1	2,10	-	1/6/23/26	0/1/1/1
10	NAG	I	2	10	-	2/6/23/26	0/1/1/1
10	BMA	I	3	10	-	0/2/19/22	0/1/1/1
11	NAG	J	1	2,11	-	0/6/23/26	0/1/1/1
11	GAL	J	10	11	-	0/2/19/22	0/1/1/1
11	NAG	J	11	11	-	2/6/23/26	0/1/1/1
11	GAL	J	12	11	-	0/2/19/22	0/1/1/1
11	FUC	J	13	11	-	-	0/1/1/1
11	NAG	J	2	11	-	1/6/23/26	0/1/1/1
11	BMA	J	3	11	-	2/2/19/22	0/1/1/1
11	MAN	J	4	11	-	0/2/19/22	0/1/1/1
11	NAG	J	5	11	-	0/6/23/26	0/1/1/1
11	GAL	J	6	11	-	0/2/19/22	0/1/1/1
11	NAG	J	7	11	-	0/6/23/26	0/1/1/1
11	MAN	J	8	11	-	0/2/19/22	0/1/1/1
11	NAG	J	9	11	-	2/6/23/26	0/1/1/1
12	NAG	K	1	2,12	-	2/6/23/26	0/1/1/1
12	FUC	K	10	12	-	-	0/1/1/1
12	NAG	K	2	12	-	5/6/23/26	0/1/1/1
12	BMA	K	3	12	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	K	4	12	-	0/2/19/22	0/1/1/1
12	NAG	K	5	12	-	0/6/23/26	0/1/1/1
12	GAL	K	6	12	-	0/2/19/22	0/1/1/1
12	MAN	K	7	12	-	2/2/19/22	0/1/1/1
12	NAG	K	8	12	-	2/6/23/26	0/1/1/1
12	GAL	K	9	12	-	0/2/19/22	0/1/1/1
13	NAG	M	1	13,2	-	2/6/23/26	0/1/1/1
13	NAG	M	2	13	-	2/6/23/26	0/1/1/1
13	BMA	M	3	13	-	2/2/19/22	0/1/1/1
13	MAN	M	4	13	-	2/2/19/22	0/1/1/1
13	NAG	M	5	13	-	2/6/23/26	0/1/1/1
13	GAL	M	6	13	-	2/2/19/22	0/1/1/1
13	SIA	M	7	13	-	3/18/34/38	0/1/1/1
13	MAN	M	8	13	-	0/2/19/22	0/1/1/1
13	NAG	M	9	13	-	2/6/23/26	0/1/1/1
14	NAG	N	1	14,2	-	0/6/23/26	0/1/1/1
14	NAG	N	2	14	-	2/6/23/26	0/1/1/1
15	NAG	O	1	2,15	-	2/6/23/26	0/1/1/1
15	NAG	O	2	15	-	2/6/23/26	0/1/1/1
15	BMA	O	3	15	-	1/2/19/22	0/1/1/1
15	MAN	O	4	15	-	0/2/19/22	0/1/1/1
15	MAN	O	5	15	-	1/2/19/22	0/1/1/1
15	MAN	O	6	15	-	2/2/19/22	0/1/1/1
15	MAN	O	7	15	-	2/2/19/22	0/1/1/1
16	NAG	P	1	2,16	-	2/6/23/26	0/1/1/1
16	NAG	P	10	16	-	4/6/23/26	0/1/1/1
16	GAL	P	11	16	-	0/2/19/22	0/1/1/1
16	SIA	P	12	16	-	1/18/34/38	0/1/1/1
16	NAG	P	13	16	-	1/6/23/26	0/1/1/1
16	GAL	P	14	16	-	0/2/19/22	0/1/1/1
16	NAG	P	15	16	-	1/6/23/26	0/1/1/1
16	FUC	P	16	16	-	-	0/1/1/1
16	NAG	P	2	16	-	1/6/23/26	0/1/1/1
16	BMA	P	3	16	-	2/2/19/22	0/1/1/1
16	MAN	P	4	16	-	2/2/19/22	0/1/1/1
16	NAG	P	5	16	-	2/6/23/26	0/1/1/1
16	GAL	P	6	16	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	SIA	P	7	16	-	3/18/34/38	0/1/1/1
16	NAG	P	8	16	-	0/6/23/26	0/1/1/1
16	MAN	P	9	16	-	0/2/19/22	0/1/1/1
14	NAG	Q	1	14,2	-	1/6/23/26	0/1/1/1
14	NAG	Q	2	14	-	0/6/23/26	0/1/1/1
17	NAG	R	1	2,17	-	0/6/23/26	0/1/1/1
17	NAG	R	2	17	-	2/6/23/26	0/1/1/1
17	BMA	R	3	17	-	0/2/19/22	0/1/1/1
17	MAN	R	4	17	-	0/2/19/22	0/1/1/1
17	NAG	R	5	17	-	2/6/23/26	0/1/1/1
17	MAN	R	6	17	-	2/2/19/22	0/1/1/1
17	NAG	R	7	17	-	4/6/23/26	0/1/1/1
18	NAG	S	1	2,18	-	0/6/23/26	0/1/1/1
18	MAN	S	10	18	-	0/2/19/22	0/1/1/1
18	NAG	S	2	18	-	2/6/23/26	0/1/1/1
18	BMA	S	3	18	-	0/2/19/22	0/1/1/1
18	MAN	S	4	18	-	0/2/19/22	0/1/1/1
18	MAN	S	5	18	-	1/2/19/22	0/1/1/1
18	MAN	S	6	18	-	0/2/19/22	0/1/1/1
18	MAN	S	7	18	-	0/2/19/22	0/1/1/1
18	MAN	S	8	18	-	2/2/19/22	0/1/1/1
18	MAN	S	9	18	-	0/2/19/22	0/1/1/1
14	NAG	T	1	14,2	-	0/6/23/26	0/1/1/1
14	NAG	T	2	14	-	2/6/23/26	0/1/1/1
19	NAG	U	1	2,19	-	0/6/23/26	0/1/1/1
19	NAG	U	2	19	-	2/6/23/26	0/1/1/1
19	BMA	U	3	19	-	0/2/19/22	0/1/1/1
19	MAN	U	4	19	-	1/2/19/22	0/1/1/1
19	MAN	U	5	19	-	1/2/19/22	0/1/1/1
19	MAN	U	6	19	-	0/2/19/22	0/1/1/1
19	MAN	U	7	19	-	1/2/19/22	0/1/1/1
20	NAG	V	1	2,20	-	2/6/23/26	0/1/1/1
20	NAG	V	2	20	-	2/6/23/26	0/1/1/1
20	BMA	V	3	20	-	0/2/19/22	0/1/1/1
20	MAN	V	4	20	-	0/2/19/22	0/1/1/1
20	MAN	V	5	20	-	0/2/19/22	0/1/1/1
21	NAG	W	1	21,2	-	0/6/23/26	0/1/1/1
21	NAG	W	2	21	-	1/6/23/26	0/1/1/1
21	BMA	W	3	21	-	0/2/19/22	0/1/1/1
21	MAN	W	4	21	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	MAN	W	5	21	-	0/2/19/22	0/1/1/1
21	FUC	W	6	21	-	-	0/1/1/1
22	NAG	X	1	2,22	-	2/6/23/26	0/1/1/1
22	NAG	X	2	22	-	2/6/23/26	0/1/1/1
22	BMA	X	3	22	-	0/2/19/22	0/1/1/1
22	MAN	X	4	22	-	2/2/19/22	0/1/1/1
22	MAN	X	5	22	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	7	SIA	C2-C1	5.69	1.59	1.52
16	P	12	SIA	C2-C1	5.63	1.59	1.52
16	P	7	SIA	C2-C1	5.62	1.59	1.52
13	M	7	SIA	O6-C2	2.01	1.47	1.43
13	M	2	NAG	C1-C2	2.00	1.55	1.52

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	2	NAG	C2-N2-C7	7.17	132.51	122.90
19	U	1	NAG	O4-C4-C5	6.24	124.69	109.32
13	M	1	NAG	O3-C3-C2	-5.92	97.10	109.40
22	X	2	NAG	O4-C4-C3	-5.54	97.31	110.38
11	J	8	MAN	O2-C2-C3	5.32	121.17	110.15
16	P	9	MAN	O4-C4-C5	5.25	122.26	109.32
16	P	7	SIA	O1A-C1-C2	-4.92	112.22	122.85
16	P	9	MAN	O2-C2-C3	4.90	120.30	110.15
16	P	12	SIA	O1A-C1-C2	-4.87	112.33	122.85
13	M	7	SIA	O1A-C1-C2	-4.65	112.80	122.85
22	X	2	NAG	O5-C1-C2	-4.44	104.42	111.29
11	J	4	MAN	C1-C2-C3	-4.38	103.26	109.64
19	U	2	NAG	O4-C4-C5	4.24	119.77	109.32
13	M	1	NAG	O4-C4-C5	-4.15	99.11	109.32
13	M	1	NAG	O4-C4-C3	-4.07	100.79	110.38
13	M	2	NAG	C4-C3-C2	3.99	116.87	111.02
18	S	8	MAN	C1-O5-C5	-3.95	106.89	112.19
20	V	2	NAG	O5-C1-C2	-3.94	105.20	111.29
13	M	2	NAG	O4-C4-C3	-3.94	101.09	110.38
12	K	1	NAG	C1-O5-C5	3.78	117.25	112.19
19	U	2	NAG	C1-O5-C5	3.73	117.19	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	U	1	NAG	C1-O5-C5	3.73	117.18	112.19
16	P	9	MAN	O5-C5-C6	-3.72	100.42	107.66
19	U	2	NAG	O4-C4-C3	3.59	118.84	110.38
14	N	1	NAG	O4-C4-C3	3.57	118.79	110.38
17	R	1	NAG	O4-C4-C3	-3.56	101.98	110.38
13	M	2	NAG	O5-C1-C2	-3.52	105.84	111.29
11	J	4	MAN	O4-C4-C5	3.52	118.00	109.32
17	R	1	NAG	O5-C1-C2	-3.38	106.06	111.29
13	M	1	NAG	O5-C1-C2	-3.38	106.07	111.29
16	P	9	MAN	O2-C2-C1	3.38	116.95	109.22
17	R	1	NAG	O5-C5-C6	-3.37	101.10	107.66
16	P	1	NAG	O4-C4-C5	-3.29	101.21	109.32
16	P	10	NAG	C1-O5-C5	3.28	116.58	112.19
20	V	2	NAG	O4-C4-C3	-3.25	102.72	110.38
12	K	1	NAG	O5-C1-C2	-3.23	106.30	111.29
12	K	2	NAG	C8-C7-N2	3.22	121.46	116.12
13	M	2	NAG	O4-C4-C5	-3.18	101.50	109.32
11	J	8	MAN	O3-C3-C2	3.17	116.53	110.05
16	P	13	NAG	C1-O5-C5	3.17	116.44	112.19
11	J	5	NAG	C8-C7-N2	-3.14	110.91	116.12
12	K	2	NAG	O5-C1-C2	-3.10	106.49	111.29
21	W	3	BMA	O2-C2-C3	-3.10	103.74	110.15
18	S	4	MAN	C1-C2-C3	3.09	114.14	109.64
18	S	4	MAN	O2-C2-C3	3.06	116.48	110.15
13	M	1	NAG	C1-O5-C5	-3.04	108.11	112.19
10	I	1	NAG	O5-C1-C2	-3.01	106.63	111.29
11	J	7	NAG	C1-O5-C5	2.98	116.18	112.19
20	V	2	NAG	O4-C4-C5	-2.96	102.03	109.32
11	J	9	NAG	C1-O5-C5	2.92	116.10	112.19
22	X	1	NAG	O4-C4-C3	-2.89	103.56	110.38
12	K	2	NAG	C1-C2-N2	2.88	114.97	110.43
8	C	1	NAG	O5-C5-C6	2.88	113.27	107.66
12	K	4	MAN	C1-O5-C5	-2.86	108.35	112.19
10	I	1	NAG	C2-N2-C7	-2.84	119.10	122.90
16	P	12	SIA	O6-C2-C3	-2.83	106.75	110.56
16	P	2	NAG	O4-C4-C5	-2.83	102.36	109.32
13	M	3	BMA	C1-O5-C5	-2.80	108.43	112.19
14	N	1	NAG	C4-C3-C2	-2.79	106.93	111.02
22	X	2	NAG	C1-C2-N2	2.78	114.81	110.43
16	P	4	MAN	O5-C1-C2	-2.77	104.18	110.79
19	U	1	NAG	C4-C3-C2	-2.75	106.98	111.02
16	P	9	MAN	C1-C2-C3	2.71	113.58	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	S	2	NAG	C1-C2-N2	2.70	114.69	110.43
16	P	15	NAG	O5-C1-C2	-2.70	107.11	111.29
13	M	4	MAN	C1-C2-C3	-2.70	105.71	109.64
20	V	1	NAG	C3-C4-C5	-2.69	105.36	110.23
16	P	3	BMA	C1-C2-C3	2.67	113.53	109.64
19	U	1	NAG	O5-C1-C2	-2.66	107.17	111.29
16	P	10	NAG	O4-C4-C5	2.61	115.75	109.32
22	X	3	BMA	C1-O5-C5	-2.59	108.71	112.19
13	M	1	NAG	C4-C3-C2	2.56	114.77	111.02
12	K	3	BMA	C1-C2-C3	2.55	113.35	109.64
16	P	4	MAN	C1-O5-C5	2.53	115.57	112.19
10	I	1	NAG	O4-C4-C5	-2.53	103.10	109.32
11	J	9	NAG	C2-N2-C7	-2.52	119.52	122.90
16	P	9	MAN	O4-C4-C3	-2.50	104.49	110.38
16	P	7	SIA	O1B-C1-O1A	2.49	129.74	124.08
16	P	3	BMA	O3-C3-C2	-2.49	104.97	110.05
20	V	3	BMA	C1-C2-C3	2.47	113.24	109.64
22	X	2	NAG	C2-N2-C7	2.47	126.21	122.90
15	O	7	MAN	C1-O5-C5	-2.46	108.89	112.19
20	V	1	NAG	O5-C1-C2	-2.46	107.48	111.29
13	M	5	NAG	O5-C1-C2	-2.44	107.51	111.29
12	K	5	NAG	O5-C1-C2	-2.44	107.51	111.29
19	U	3	BMA	C1-C2-C3	2.44	113.19	109.64
17	R	2	NAG	O5-C1-C2	-2.44	107.52	111.29
16	P	12	SIA	O1B-C1-O1A	2.43	129.59	124.08
20	V	2	NAG	C1-C2-N2	2.41	114.22	110.43
15	O	2	NAG	O5-C1-C2	-2.38	107.61	111.29
16	P	9	MAN	C3-C4-C5	-2.38	105.92	110.23
16	P	3	BMA	O4-C4-C3	2.37	115.96	110.38
13	M	7	SIA	O1B-C1-O1A	2.37	129.45	124.08
16	P	3	BMA	C2-C3-C4	-2.36	106.70	110.86
16	P	10	NAG	O5-C5-C6	-2.33	103.13	107.66
11	J	2	NAG	O5-C1-C2	-2.31	107.71	111.29
13	M	4	MAN	O2-C2-C3	-2.31	105.37	110.15
18	S	3	BMA	O3-C3-C2	-2.31	105.34	110.05
13	M	3	BMA	O3-C3-C4	-2.31	104.94	110.38
16	P	9	MAN	C1-O5-C5	2.29	115.26	112.19
12	K	3	BMA	O5-C5-C6	2.29	112.13	107.66
13	M	7	SIA	O6-C2-C3	-2.29	107.48	110.56
16	P	3	BMA	C3-C4-C5	-2.28	106.10	110.23
11	J	1	NAG	O5-C1-C2	-2.28	107.77	111.29
12	K	3	BMA	O3-C3-C4	-2.28	105.01	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	2	NAG	O4-C4-C5	-2.27	103.72	109.32
16	P	9	MAN	O5-C1-C2	-2.23	105.46	110.79
17	R	1	NAG	C1-C2-N2	2.23	113.94	110.43
16	P	3	BMA	O3-C3-C4	2.23	115.63	110.38
11	J	3	BMA	O3-C3-C2	-2.22	105.52	110.05
8	C	1	NAG	O4-C4-C5	-2.22	103.85	109.32
17	R	1	NAG	C4-C3-C2	2.20	114.25	111.02
11	J	3	BMA	C1-C2-C3	2.18	112.82	109.64
13	M	2	NAG	C1-O5-C5	-2.17	109.28	112.19
21	W	6	FUC	O2-C2-C1	2.17	114.18	109.22
21	W	3	BMA	O5-C1-C2	-2.16	105.62	110.79
22	X	2	NAG	C4-C3-C2	2.16	114.19	111.02
15	O	2	NAG	C1-C2-N2	2.15	113.83	110.43
18	S	2	NAG	O4-C4-C5	-2.15	104.04	109.32
18	S	7	MAN	C1-C2-C3	-2.14	106.53	109.64
16	P	1	NAG	O3-C3-C2	-2.13	104.97	109.40
20	V	2	NAG	C2-N2-C7	2.13	125.75	122.90
15	O	2	NAG	C2-N2-C7	2.13	125.75	122.90
9	F	1	NAG	O5-C1-C2	-2.12	108.02	111.29
16	P	10	NAG	C6-C5-C4	-2.11	107.84	113.02
18	S	5	MAN	O5-C1-C2	-2.10	105.79	110.79
8	C	2	NAG	C2-N2-C7	2.09	125.71	122.90
8	C	2	NAG	C1-O5-C5	2.09	114.98	112.19
18	S	2	NAG	C2-N2-C7	2.08	125.69	122.90
16	P	4	MAN	O4-C4-C5	-2.07	104.23	109.32
16	P	12	SIA	O1B-C1-C2	2.07	118.08	112.71
16	P	2	NAG	O5-C1-C2	-2.05	108.11	111.29
16	P	7	SIA	O1B-C1-C2	2.05	118.04	112.71
22	X	2	NAG	O4-C4-C5	-2.04	104.29	109.32
13	M	1	NAG	O3-C3-C4	-2.04	105.56	110.38
10	I	1	NAG	O4-C4-C3	-2.03	105.59	110.38
17	R	2	NAG	O4-C4-C3	-2.03	105.60	110.38
16	P	1	NAG	O5-C1-C2	-2.02	108.16	111.29
13	M	3	BMA	O5-C1-C2	-2.02	105.97	110.79
16	P	2	NAG	O4-C4-C3	-2.02	105.62	110.38
18	S	7	MAN	O3-C3-C4	2.01	115.11	110.38

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	P	7	SIA	O1A-C1-C2-O6

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Mol	Chain	Res	Type	Atoms
22	X	2	NAG	C1-C2-N2-C7
16	P	3	BMA	O5-C5-C6-O6
13	M	3	BMA	O5-C5-C6-O6
13	M	4	MAN	O5-C5-C6-O6
16	P	6	GAL	O5-C5-C6-O6
14	N	2	NAG	O5-C5-C6-O6
12	K	3	BMA	O5-C5-C6-O6
11	J	11	NAG	O5-C5-C6-O6
16	P	1	NAG	O5-C5-C6-O6
18	S	8	MAN	O5-C5-C6-O6
13	M	3	BMA	C4-C5-C6-O6
12	K	7	MAN	O5-C5-C6-O6
13	M	2	NAG	O5-C5-C6-O6
16	P	10	NAG	O5-C5-C6-O6
16	P	3	BMA	C4-C5-C6-O6
16	P	6	GAL	C4-C5-C6-O6
17	R	7	NAG	O5-C5-C6-O6
17	R	6	MAN	C4-C5-C6-O6
12	K	3	BMA	C4-C5-C6-O6
13	M	4	MAN	C4-C5-C6-O6
17	R	6	MAN	O5-C5-C6-O6
14	N	2	NAG	C4-C5-C6-O6
16	P	4	MAN	O5-C5-C6-O6
16	P	1	NAG	C4-C5-C6-O6
17	R	7	NAG	C4-C5-C6-O6
11	J	11	NAG	C4-C5-C6-O6
12	K	7	MAN	C4-C5-C6-O6
17	R	5	NAG	O5-C5-C6-O6
13	M	2	NAG	C4-C5-C6-O6
16	P	10	NAG	C4-C5-C6-O6
18	S	8	MAN	C4-C5-C6-O6
15	O	6	MAN	O5-C5-C6-O6
15	O	7	MAN	O5-C5-C6-O6
22	X	4	MAN	O5-C5-C6-O6
17	R	5	NAG	C4-C5-C6-O6
12	K	1	NAG	C8-C7-N2-C2
12	K	1	NAG	O7-C7-N2-C2
12	K	2	NAG	C8-C7-N2-C2
12	K	2	NAG	O7-C7-N2-C2
12	K	8	NAG	C8-C7-N2-C2
12	K	8	NAG	O7-C7-N2-C2
13	M	5	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
13	M	5	NAG	O7-C7-N2-C2
13	M	9	NAG	C8-C7-N2-C2
13	M	9	NAG	O7-C7-N2-C2
16	P	5	NAG	C8-C7-N2-C2
16	P	5	NAG	O7-C7-N2-C2
16	P	10	NAG	C8-C7-N2-C2
16	P	10	NAG	O7-C7-N2-C2
17	R	7	NAG	C8-C7-N2-C2
17	R	7	NAG	O7-C7-N2-C2
9	F	1	NAG	O5-C5-C6-O6
15	O	7	MAN	C4-C5-C6-O6
13	M	6	GAL	C4-C5-C6-O6
22	X	4	MAN	C4-C5-C6-O6
15	O	6	MAN	C4-C5-C6-O6
22	X	1	NAG	C4-C5-C6-O6
19	U	2	NAG	O5-C5-C6-O6
20	V	1	NAG	C4-C5-C6-O6
9	F	2	NAG	C4-C5-C6-O6
13	M	1	NAG	C4-C5-C6-O6
9	F	2	NAG	O5-C5-C6-O6
11	J	3	BMA	C4-C5-C6-O6
16	P	4	MAN	C4-C5-C6-O6
13	M	6	GAL	O5-C5-C6-O6
10	I	2	NAG	C4-C5-C6-O6
22	X	1	NAG	O5-C5-C6-O6
15	O	1	NAG	C4-C5-C6-O6
13	M	7	SIA	C6-C7-C8-O8
10	I	1	NAG	O5-C5-C6-O6
17	R	2	NAG	O5-C5-C6-O6
15	O	1	NAG	O5-C5-C6-O6
18	S	5	MAN	O5-C5-C6-O6
19	U	5	MAN	O5-C5-C6-O6
12	K	2	NAG	O5-C5-C6-O6
11	J	2	NAG	O5-C5-C6-O6
9	F	1	NAG	C4-C5-C6-O6
16	P	15	NAG	O5-C5-C6-O6
11	J	9	NAG	O5-C5-C6-O6
13	M	1	NAG	O5-C5-C6-O6
15	O	5	MAN	O5-C5-C6-O6
16	P	12	SIA	O1A-C1-C2-O6
11	J	9	NAG	C4-C5-C6-O6
19	U	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	I	2	NAG	O5-C5-C6-O6
20	V	1	NAG	O5-C5-C6-O6
15	O	2	NAG	C1-C2-N2-C7
16	P	7	SIA	O1A-C1-C2-C3
16	P	7	SIA	O1B-C1-C2-C3
14	T	2	NAG	C4-C5-C6-O6
15	O	3	BMA	C4-C5-C6-O6
8	C	2	NAG	C3-C2-N2-C7
15	O	2	NAG	C3-C2-N2-C7
18	S	2	NAG	C3-C2-N2-C7
20	V	2	NAG	C3-C2-N2-C7
16	P	13	NAG	O5-C5-C6-O6
21	W	2	NAG	O5-C5-C6-O6
13	M	7	SIA	O7-C7-C8-O8
19	U	4	MAN	O5-C5-C6-O6
11	J	3	BMA	O5-C5-C6-O6
7	A	1	NAG	C1-C2-N2-C7
8	C	2	NAG	C1-C2-N2-C7
12	K	2	NAG	C1-C2-N2-C7
18	S	2	NAG	C1-C2-N2-C7
20	V	2	NAG	C1-C2-N2-C7
14	Q	1	NAG	O5-C5-C6-O6
14	T	2	NAG	O5-C5-C6-O6
12	K	2	NAG	C3-C2-N2-C7
22	X	2	NAG	C3-C2-N2-C7
16	P	2	NAG	C4-C5-C6-O6
19	U	7	MAN	C4-C5-C6-O6
17	R	2	NAG	C4-C5-C6-O6
13	M	7	SIA	O7-C7-C8-C9

There are no ring outliers.

32 monomers are involved in 20 short contacts:

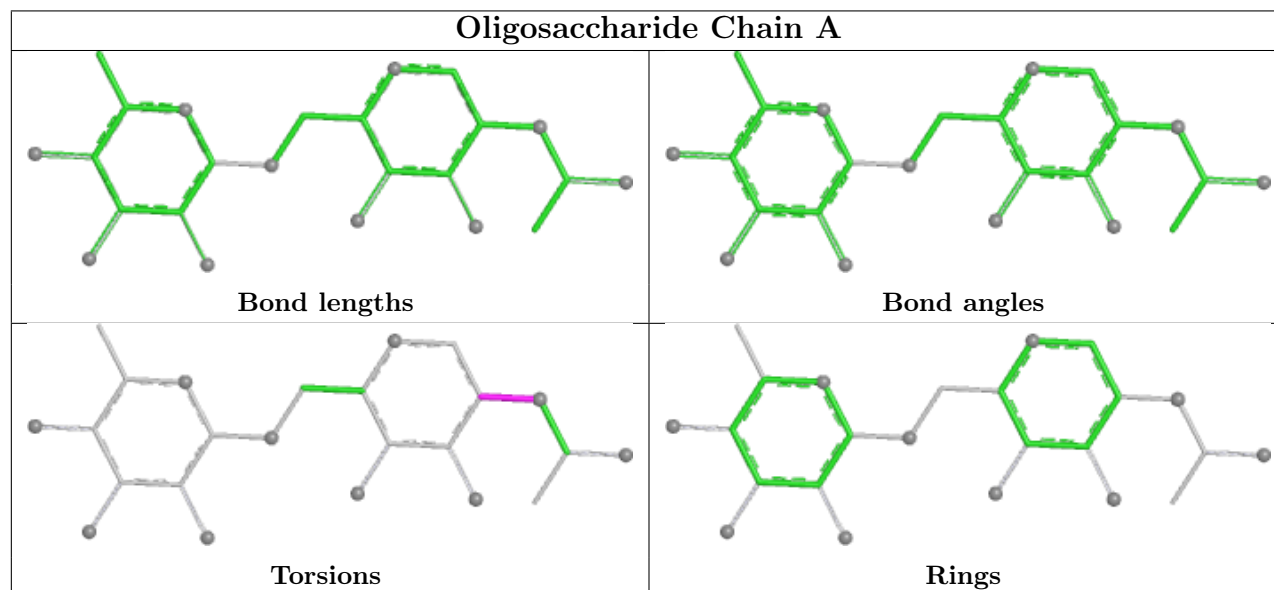
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	5	NAG	1	0
18	S	2	NAG	1	0
12	K	1	NAG	1	0
15	O	4	MAN	1	0
16	P	15	NAG	2	0
11	J	4	MAN	1	0
15	O	1	NAG	1	0
16	P	3	BMA	1	0

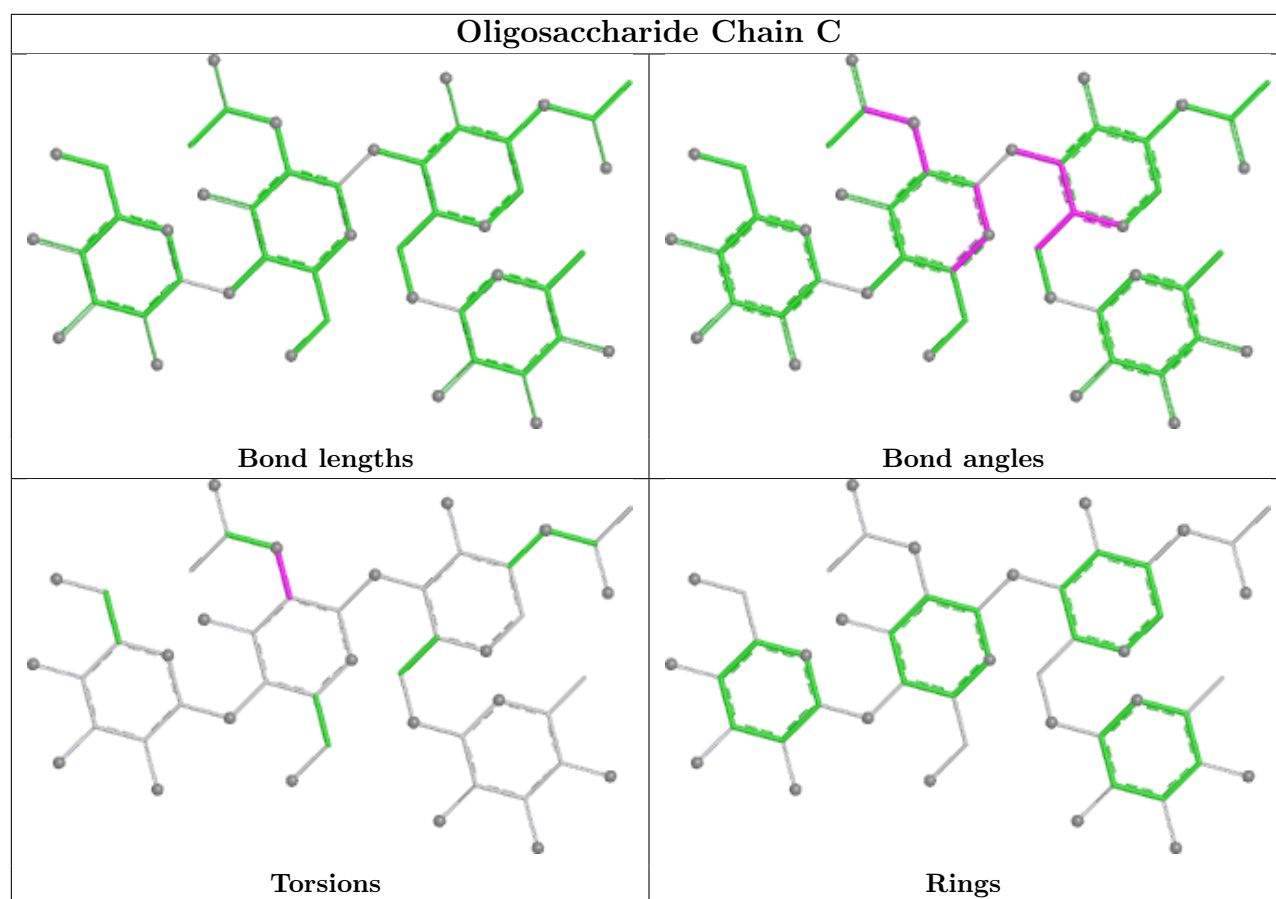
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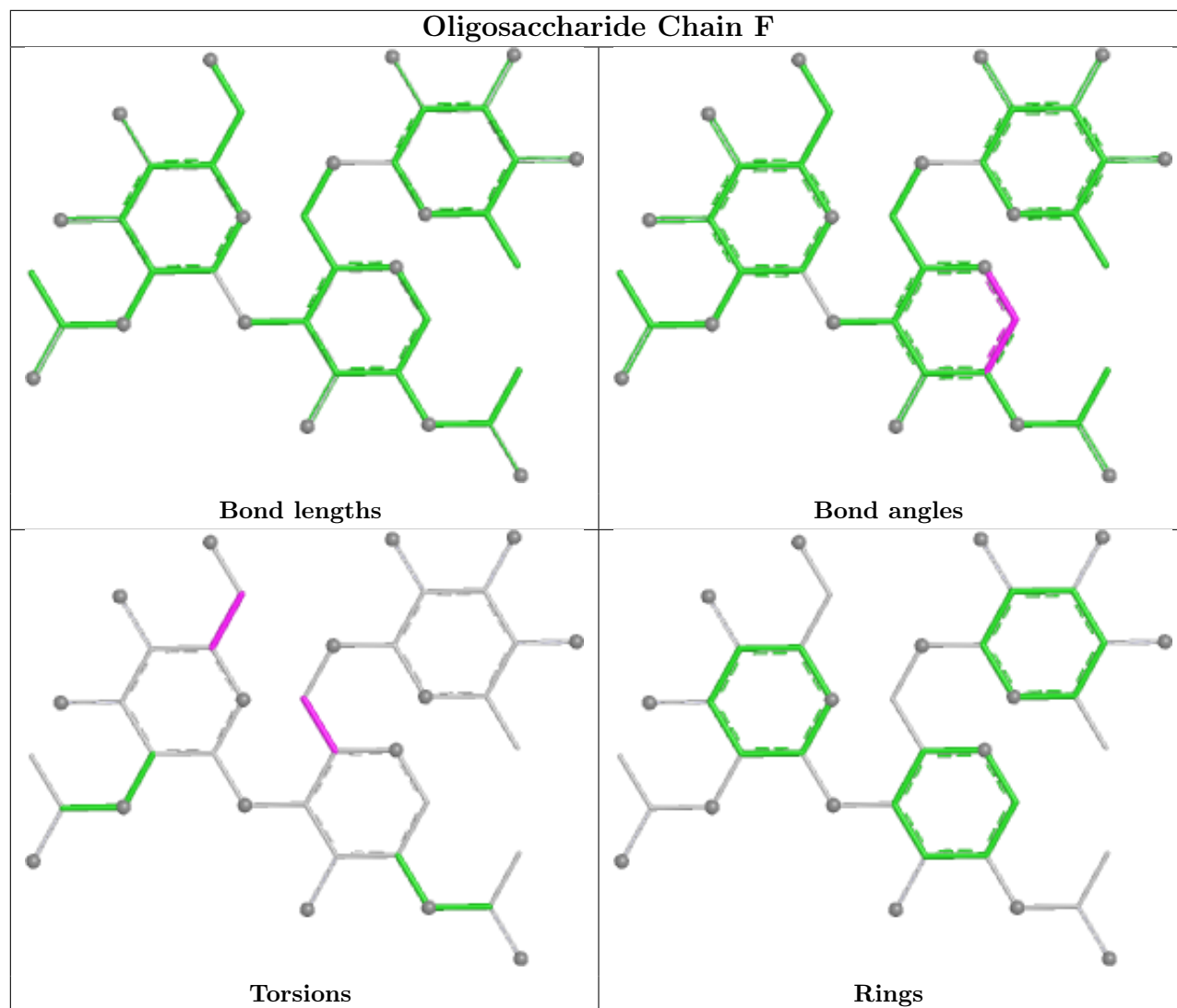
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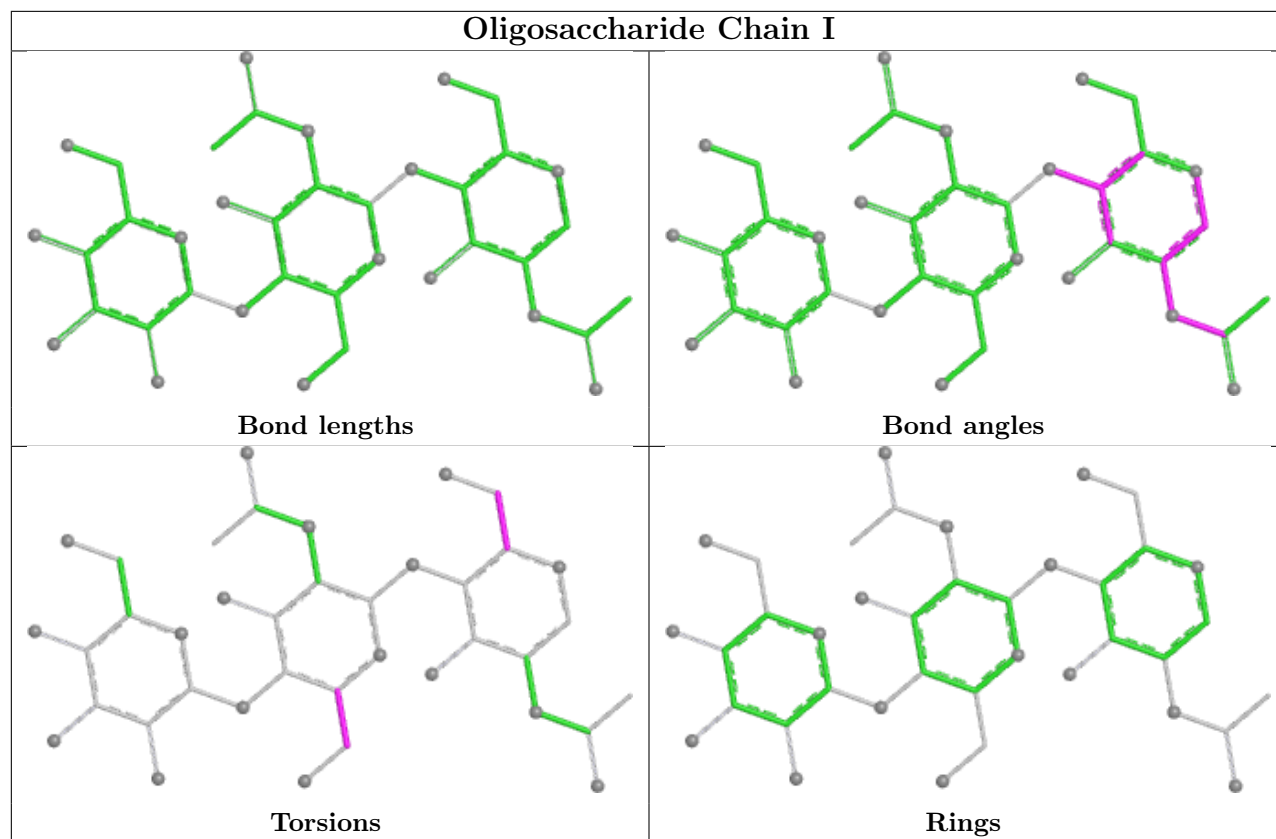
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	P	16	FUC	1	0
21	W	3	BMA	1	0
16	P	4	MAN	2	0
10	I	2	NAG	1	0
17	R	1	NAG	1	0
18	S	5	MAN	1	0
20	V	1	NAG	1	0
17	R	2	NAG	1	0
18	S	9	MAN	1	0
11	J	9	NAG	1	0
21	W	2	NAG	1	0
16	P	9	MAN	1	0
22	X	2	NAG	1	0
22	X	1	NAG	1	0
10	I	1	NAG	1	0
20	V	2	NAG	1	0
13	M	4	MAN	1	0
11	J	5	NAG	1	0
15	O	5	MAN	1	0
11	J	7	NAG	1	0
17	R	6	MAN	1	0
18	S	8	MAN	1	0
18	S	4	MAN	1	0
12	K	2	NAG	1	0

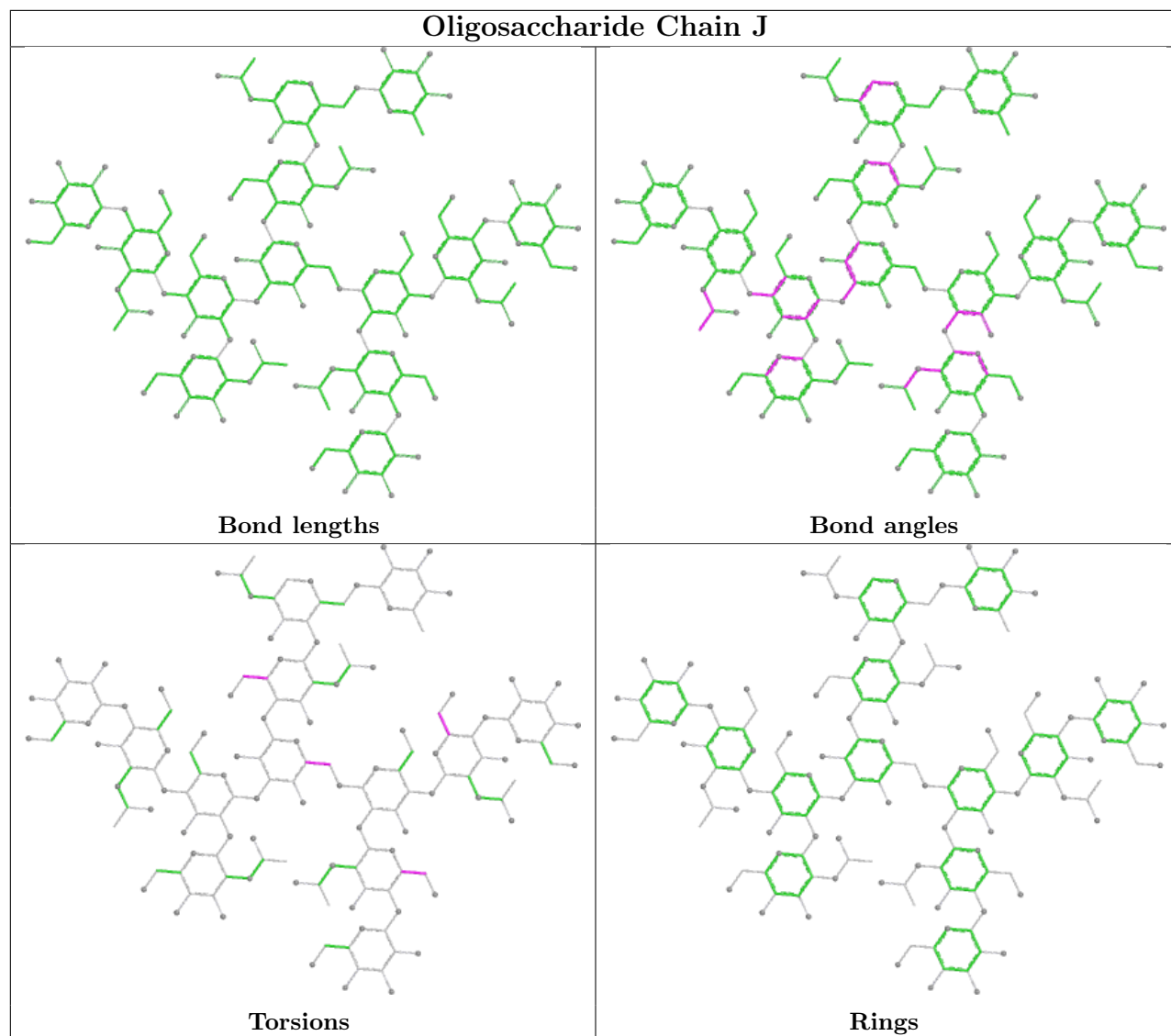
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

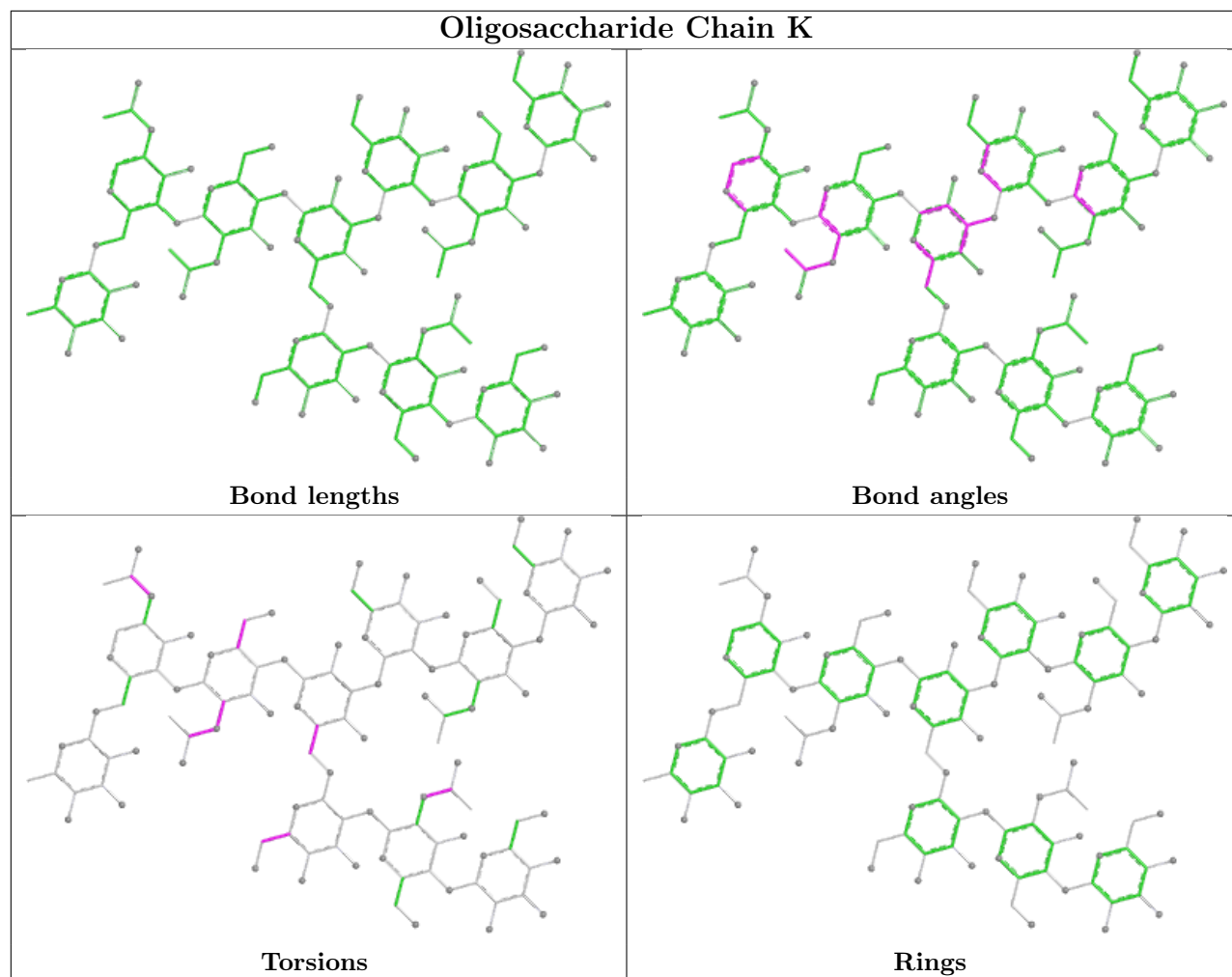


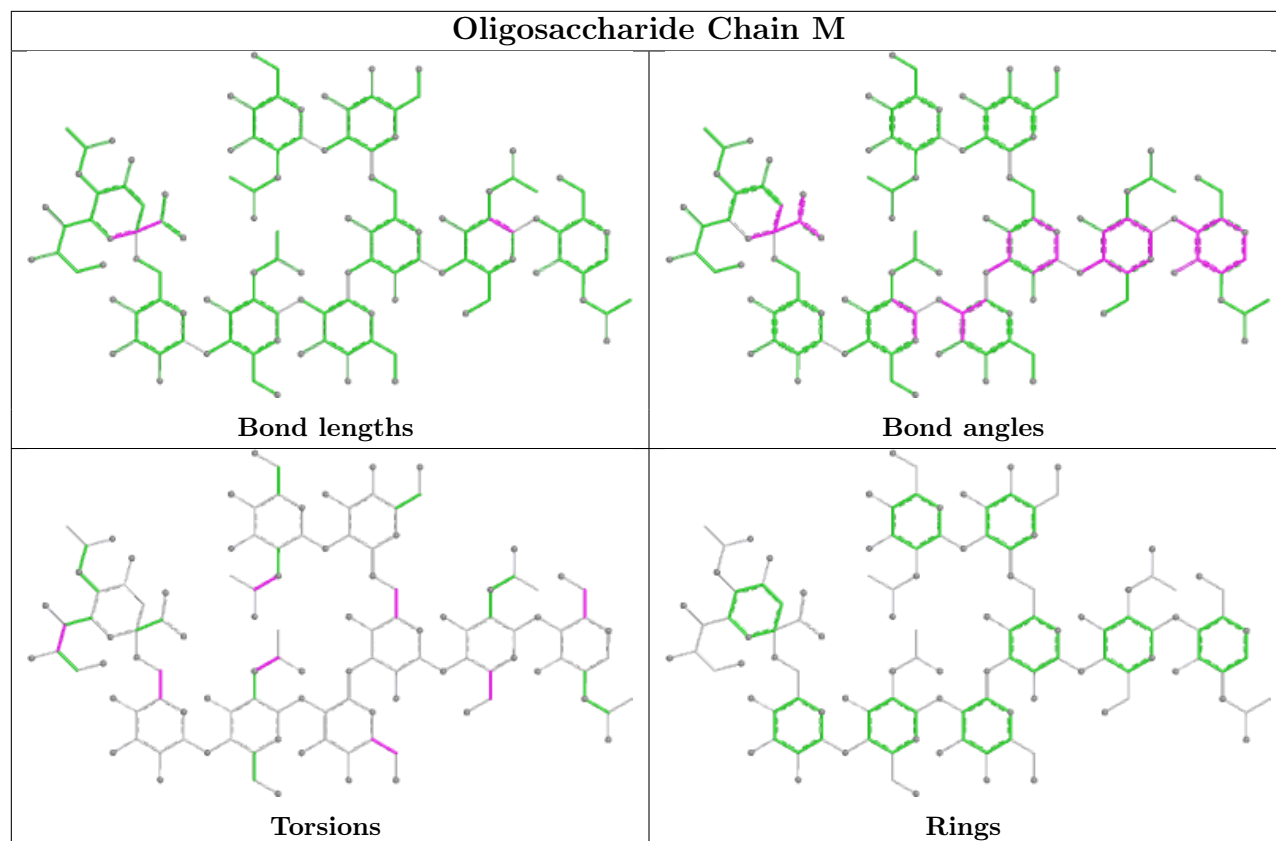


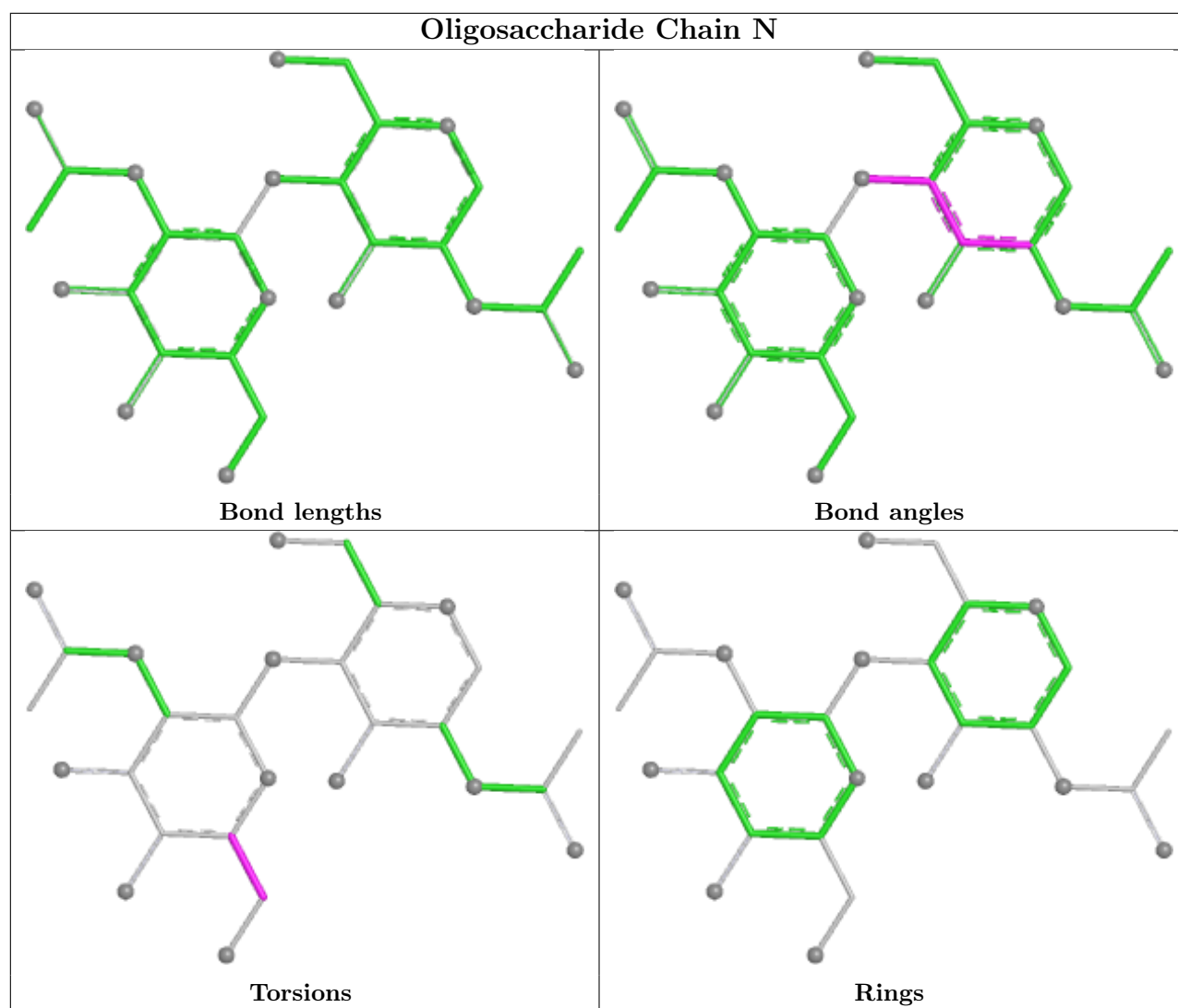


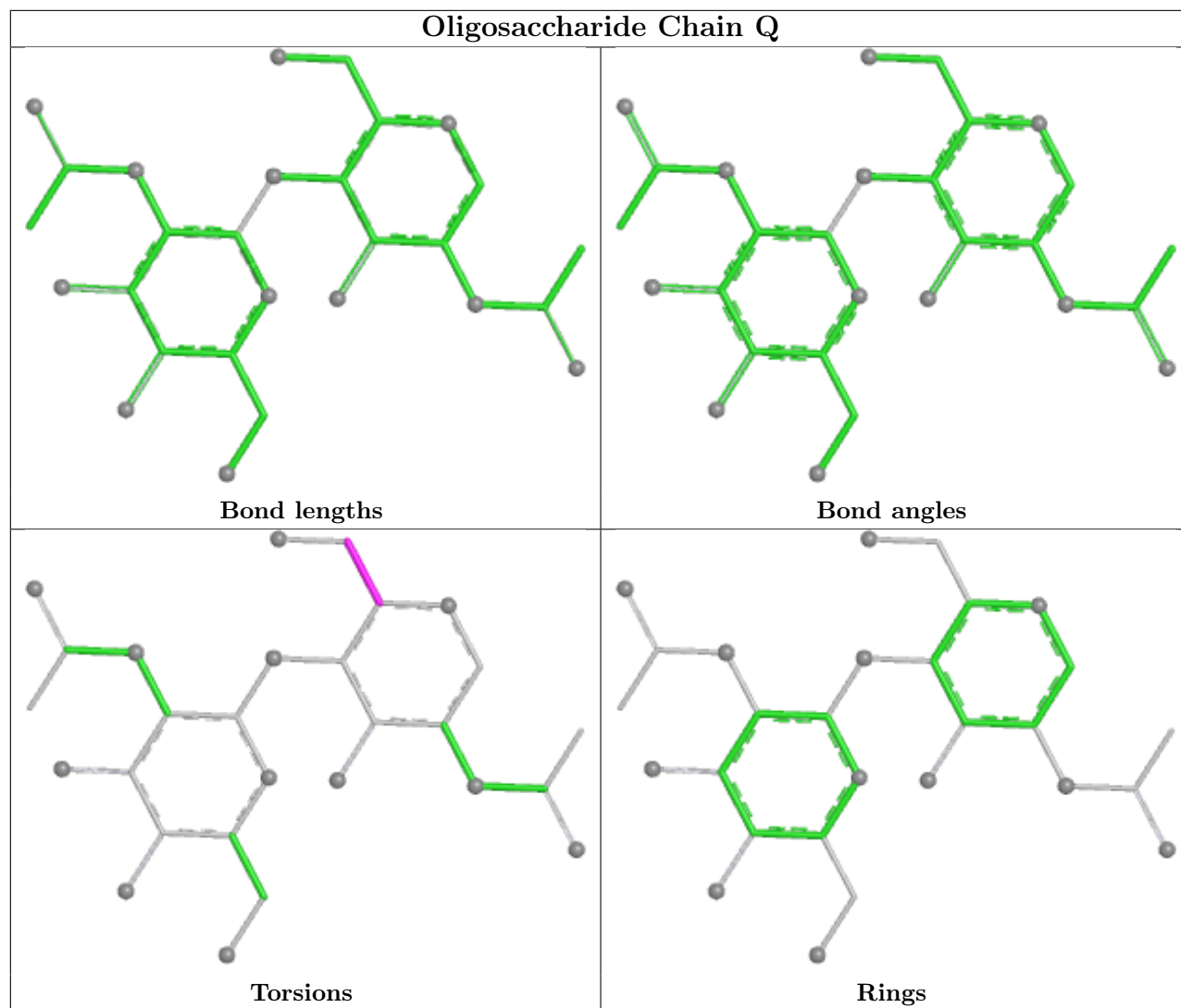


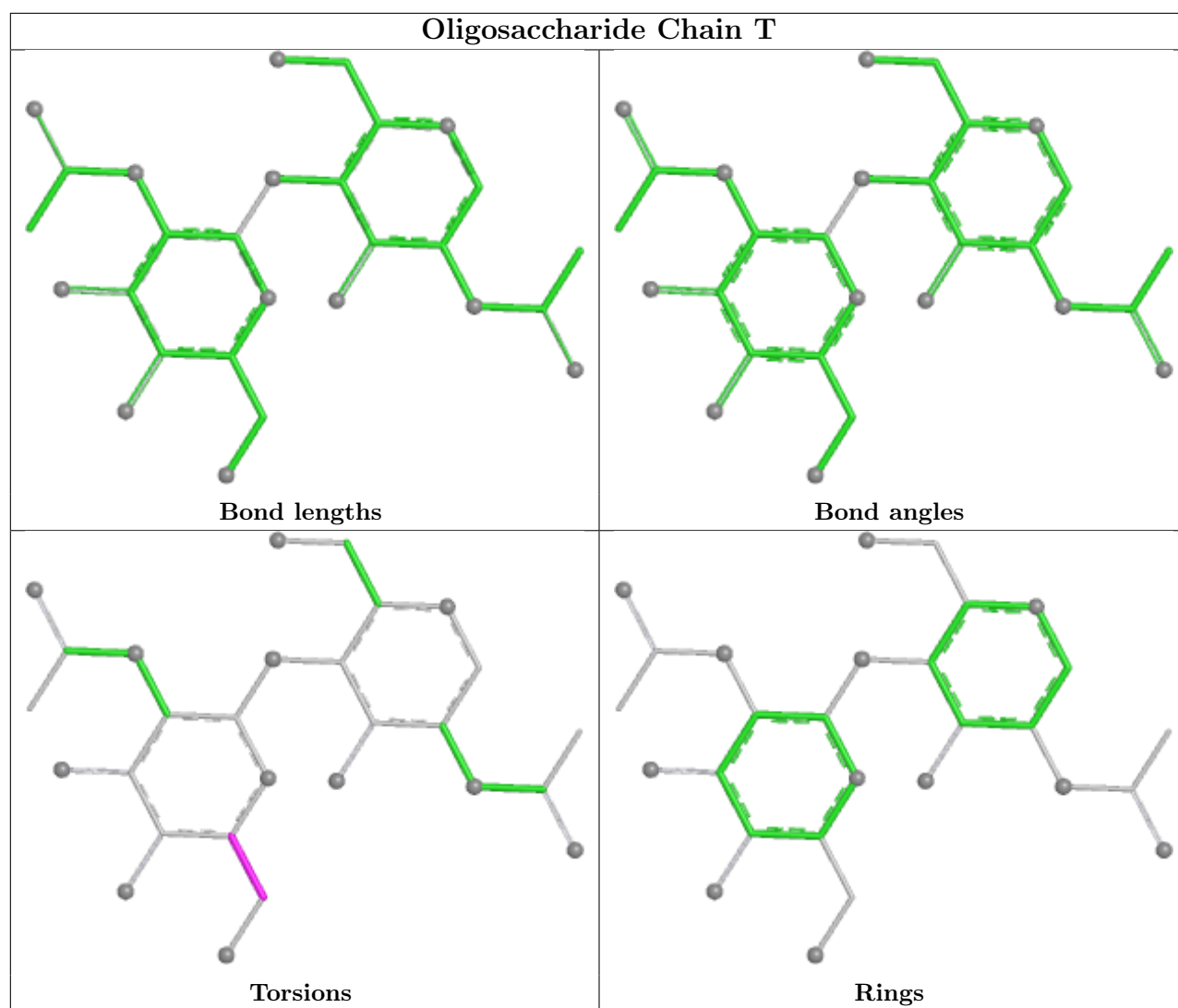


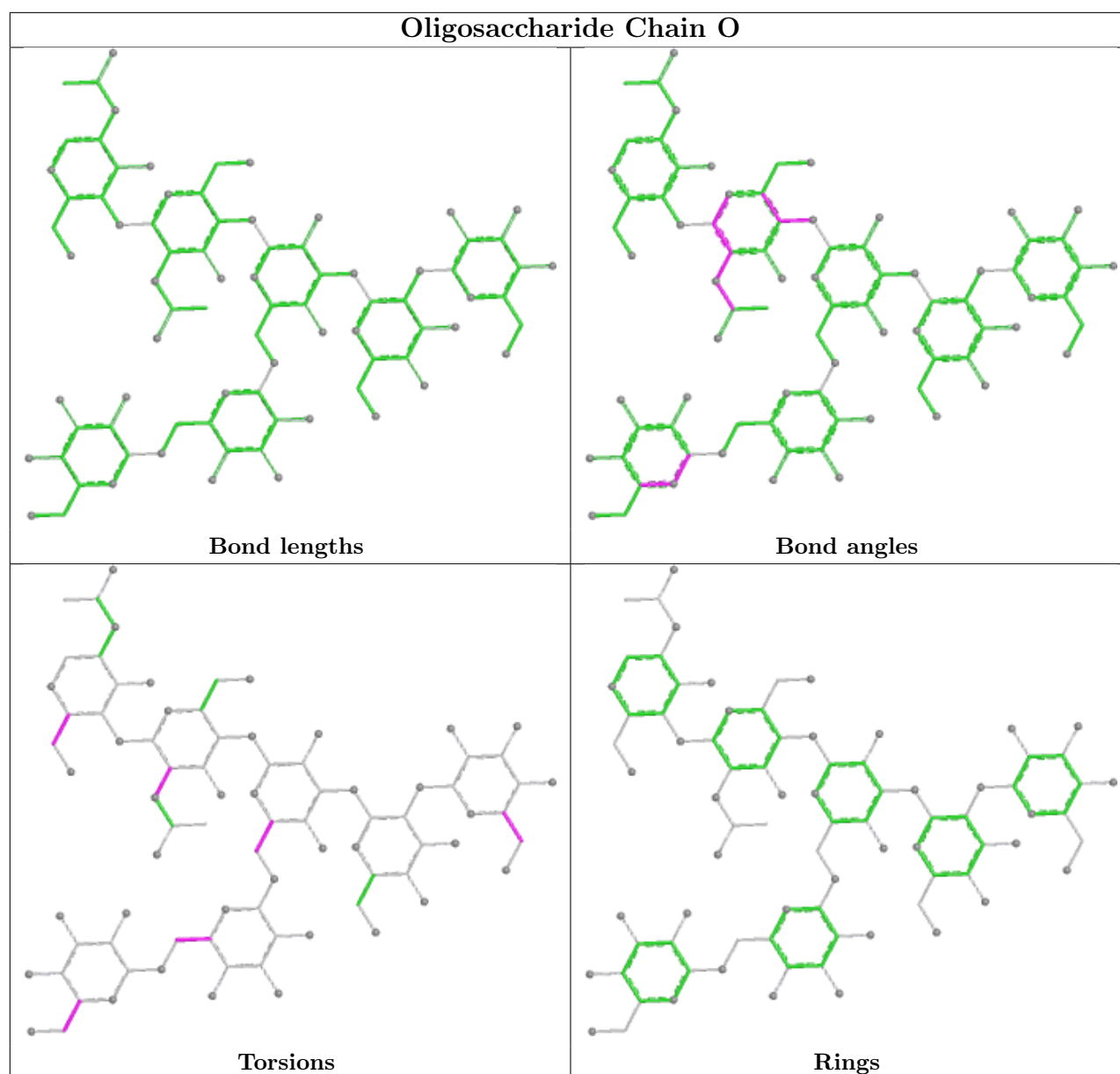


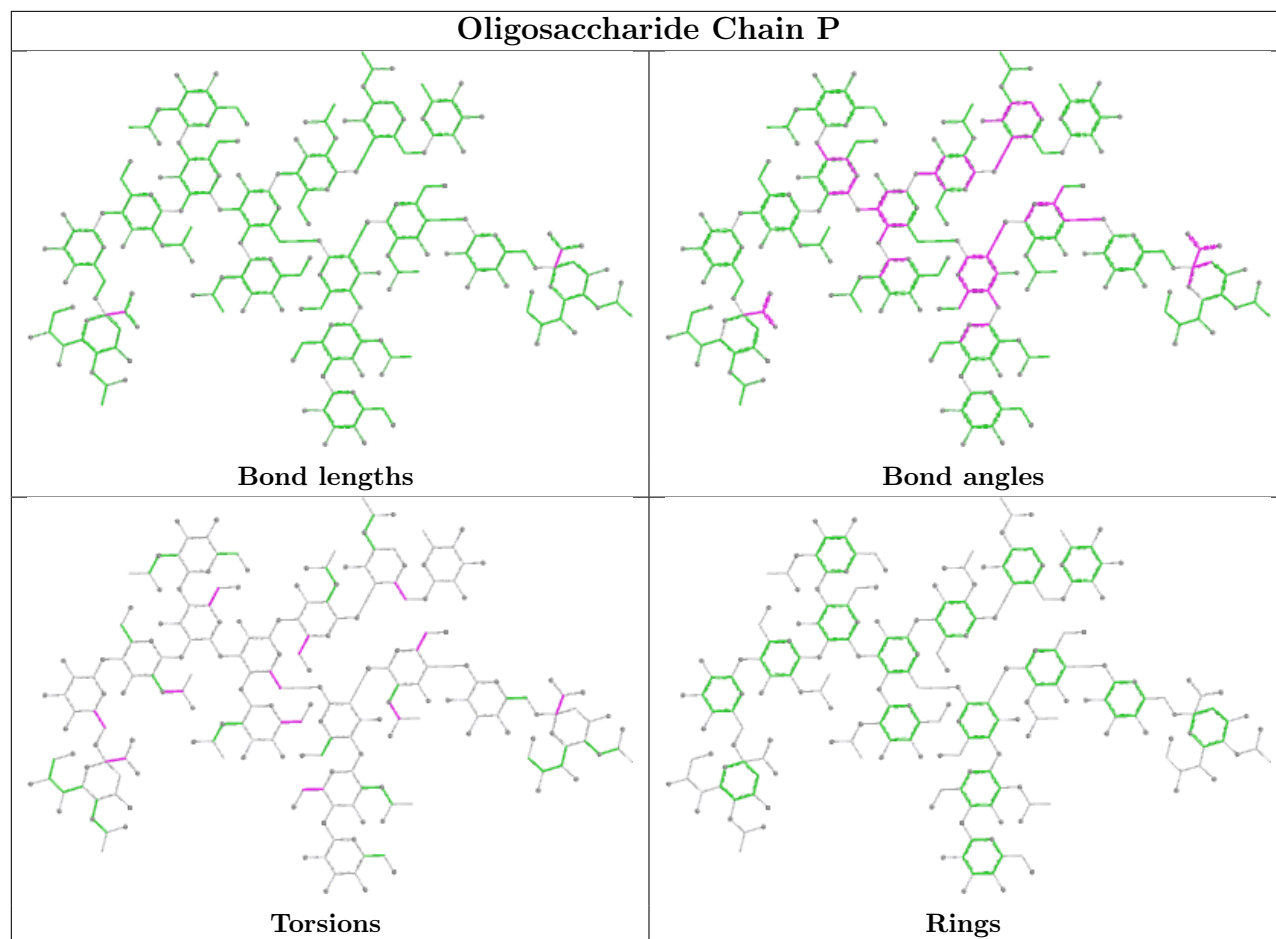


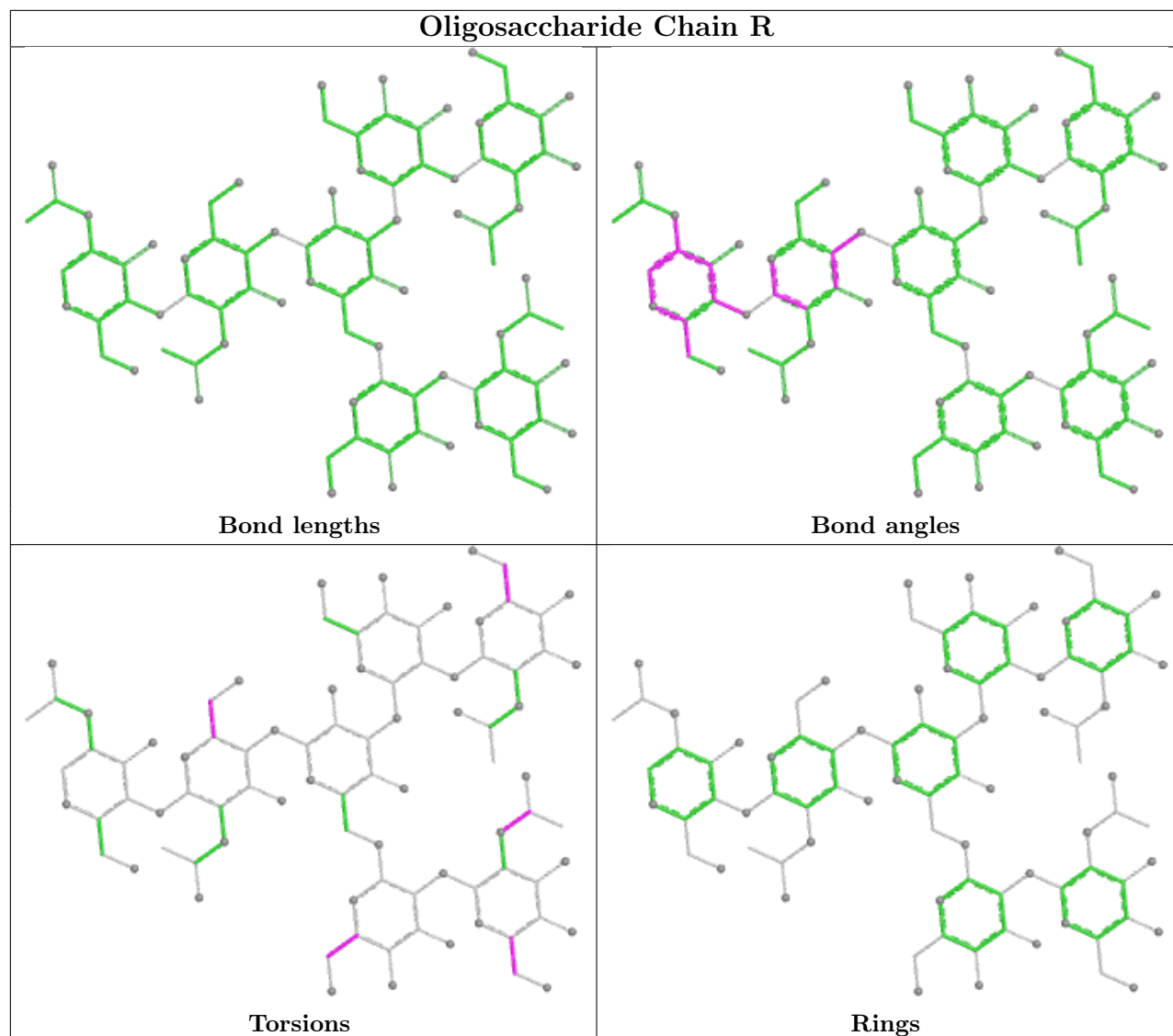


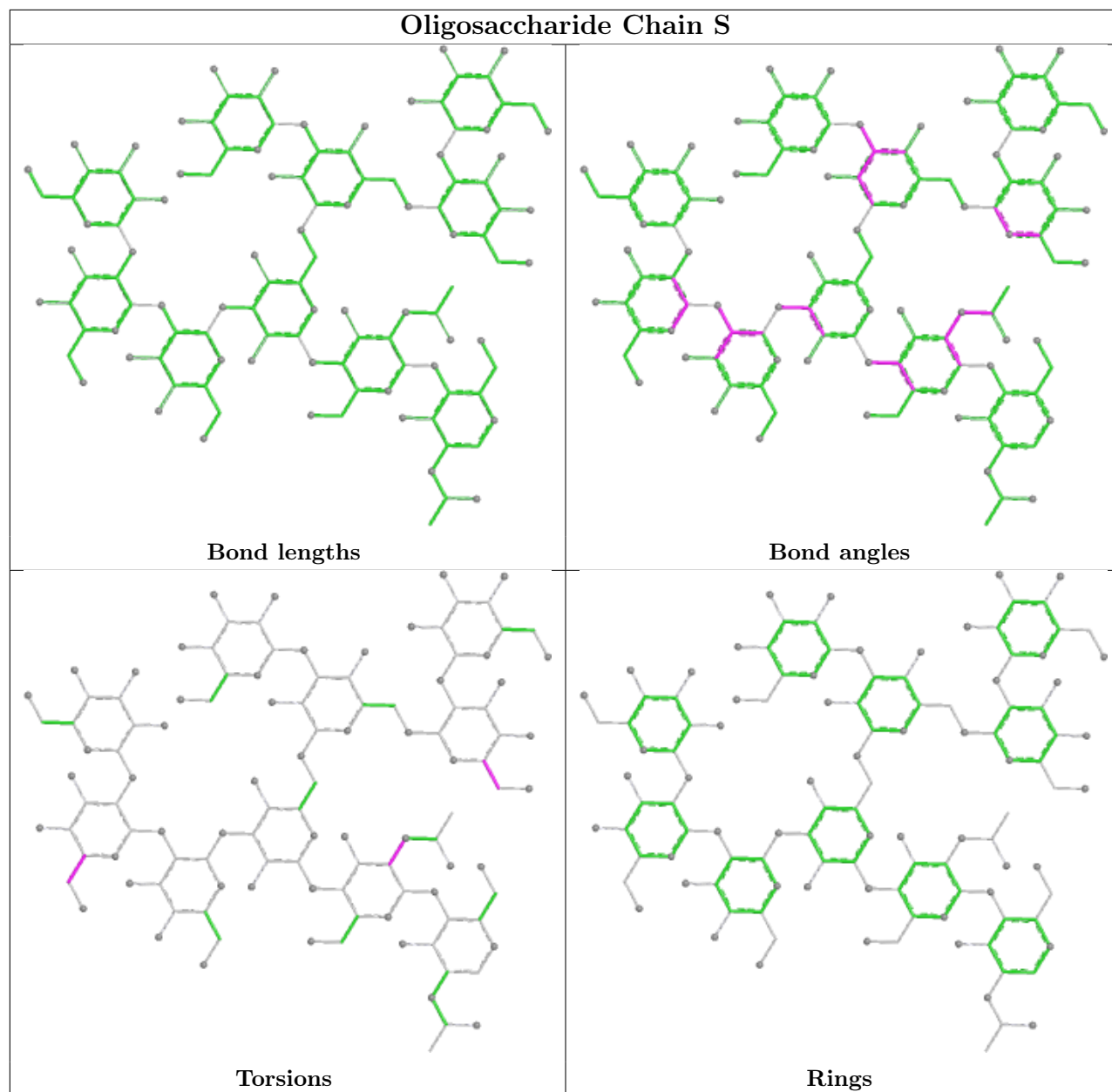


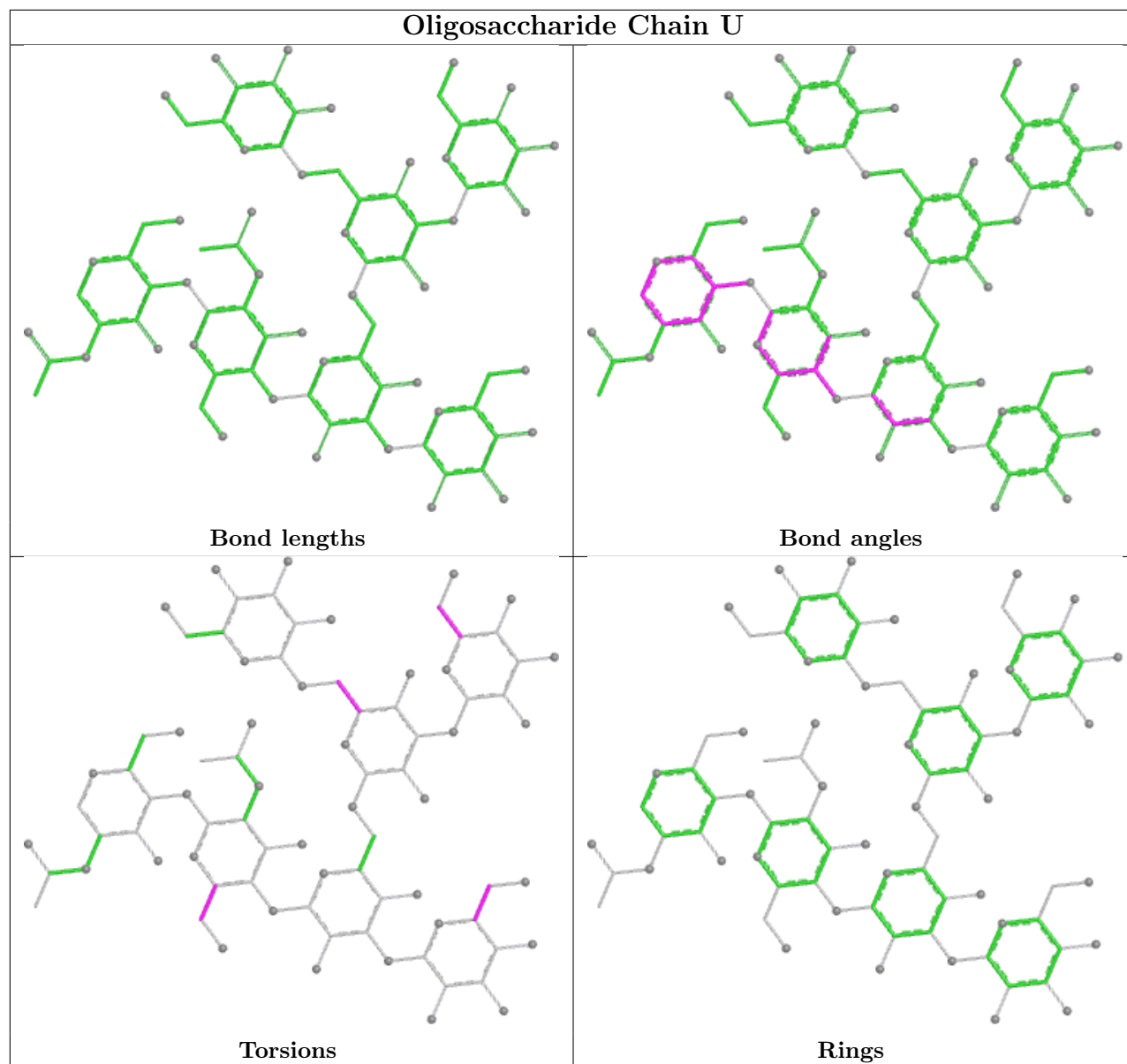


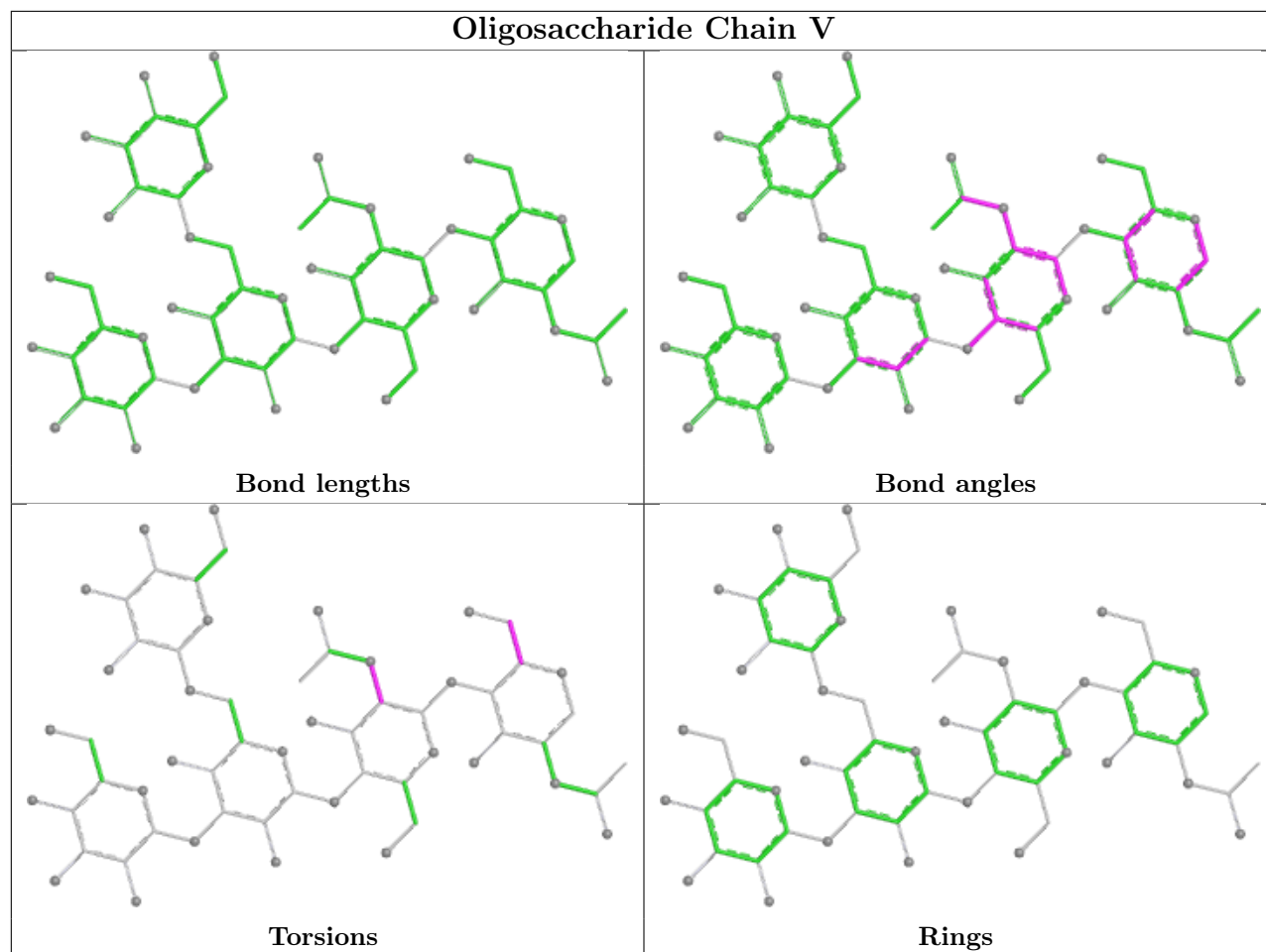


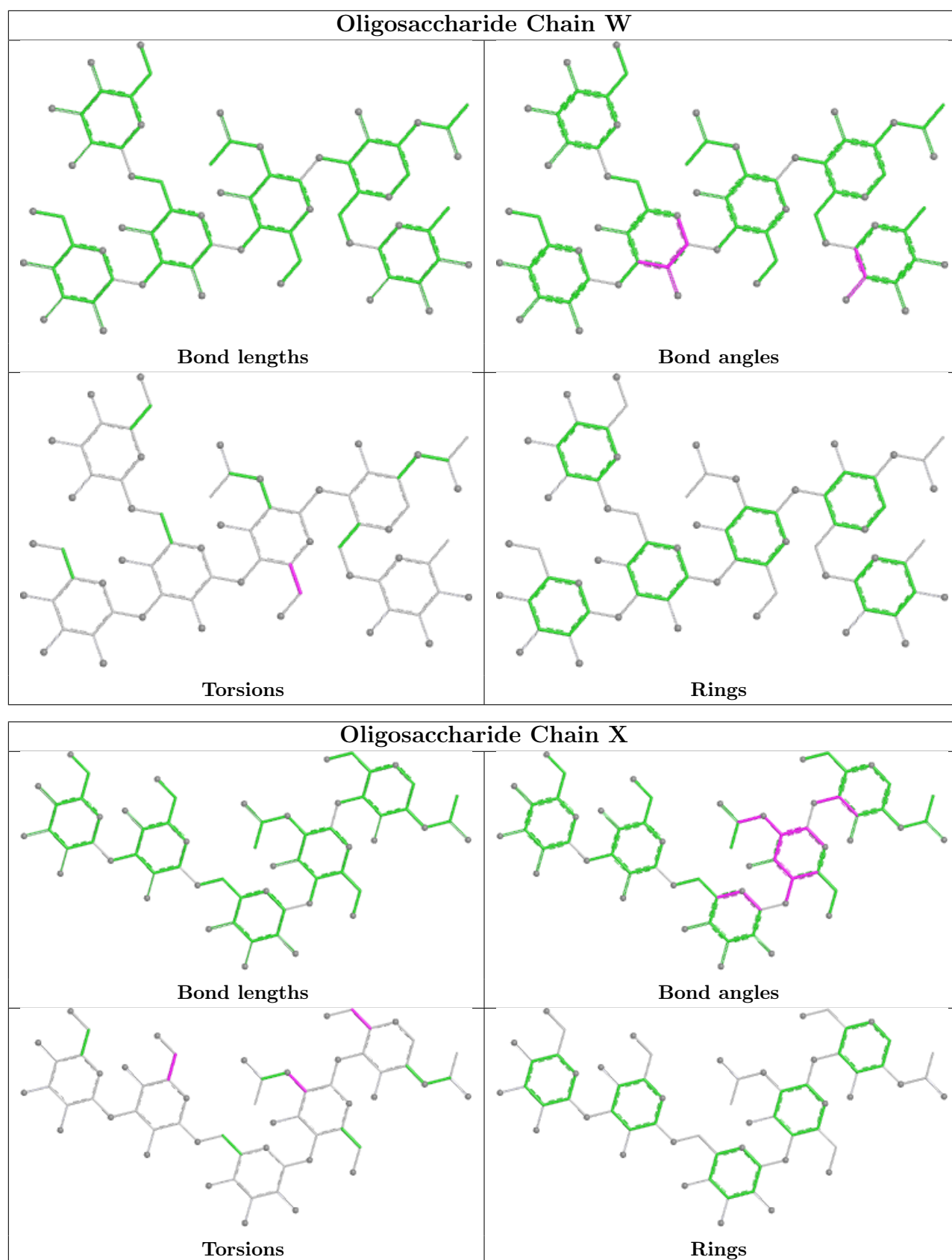












5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
23	NAG	G	3390	2	14,14,15	0.33	0	17,19,21	0.62	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
23	NAG	G	3390	2	-	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.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	G	3390	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	B	126/153 (82%)	0.86	17 (13%)	7	10	163, 268, 331, 391	0
2	G	449/481 (93%)	0.81	42 (9%)	14	16	45, 199, 352, 455	0
3	H	230/238 (96%)	0.83	18 (7%)	19	18	154, 314, 444, 501	0
4	L	211/214 (98%)	0.59	12 (5%)	29	24	147, 347, 430, 482	0
5	D	229/232 (98%)	0.54	12 (5%)	33	26	109, 244, 640, 874	0
6	E	210/214 (98%)	0.74	18 (8%)	16	17	157, 319, 909, 1023	0
All	All	1455/1532 (94%)	0.73	119 (8%)	17	18	45, 266, 651, 1023	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	599	SER	9.5
6	E	145	VAL	5.5
6	E	146	THR	5.1
1	B	593	LEU	5.1
5	D	100(G)	ARG	4.9
1	B	520	LEU	4.6
2	G	72	HIS	4.5
4	L	86	TYR	4.5
3	H	90	TYR	4.2
6	E	106	VAL	4.1
1	B	600	GLY	4.0
3	H	101	ASP	4.0
2	G	73	ALA	4.0
2	G	389	GLY	3.9
3	H	38	ARG	3.9
3	H	180	SER	3.8
6	E	107	LEU	3.7
3	H	181	VAL	3.7
2	G	235	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	545	LEU	3.7
6	E	92	ALA	3.7
2	G	463	SER	3.5
3	H	152	VAL	3.5
1	B	598	CYS	3.4
6	E	143	GLY	3.4
2	G	277	ILE	3.4
2	G	454	LEU	3.2
2	G	505	VAL	3.1
4	L	47	LEU	3.1
2	G	472	GLY	3.1
5	D	105	GLN	3.1
3	H	68	VAL	3.1
3	H	179	SER	3.1
5	D	100(D)	SER	3.1
5	D	97	PHE	3.0
4	L	37	GLN	3.0
2	G	69	TRP	3.0
6	E	98	PHE	3.0
2	G	40	TYR	2.9
6	E	194	CYS	2.9
2	G	468	PHE	2.8
6	E	142	PRO	2.8
3	H	4	LEU	2.8
6	E	135	CYS	2.8
1	B	531	GLY	2.8
2	G	217	TYR	2.7
1	B	587	LEU	2.7
2	G	38	VAL	2.7
5	D	35	HIS	2.7
3	H	198	VAL	2.7
5	D	126	PRO	2.7
3	H	216	CYS	2.7
2	G	81	PRO	2.6
4	L	212	CYS	2.6
2	G	351	LYS	2.6
2	G	473	GLY	2.6
6	E	151	ALA	2.6
5	D	30	THR	2.6
2	G	136	ASN	2.6
2	G	429	ARG	2.6
5	D	53	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
4	L	36	TYR	2.6
2	G	358	ILE	2.5
2	G	321(A)	ASP	2.5
2	G	66	HIS	2.5
1	B	523	LEU	2.5
2	G	167	ASP	2.5
2	G	416	LEU	2.5
1	B	656	ASN	2.5
2	G	188	ASN	2.5
1	B	578	ALA	2.4
2	G	58	ALA	2.4
5	D	100	SER	2.4
2	G	139	THR	2.4
2	G	225	ILE	2.4
1	B	575	GLN	2.3
4	L	38	HIS	2.3
2	G	236	THR	2.3
3	H	92	CYS	2.3
4	L	145	VAL	2.3
4	L	12	SER	2.3
6	E	193	SER	2.3
6	E	149	TRP	2.3
6	E	96	VAL	2.3
2	G	371	VAL	2.3
6	E	108	GLY	2.3
2	G	390	LEU	2.3
4	L	39	ARG	2.3
3	H	150	VAL	2.2
1	B	580	VAL	2.2
2	G	285	LEU	2.2
1	B	586	TYR	2.2
2	G	100	MET	2.2
1	B	602	LEU	2.2
2	G	347	LYS	2.2
2	G	380	GLY	2.2
2	G	352	HIS	2.2
6	E	3	ALA	2.1
4	L	155	PRO	2.1
2	G	465	THR	2.1
3	H	137	ALA	2.1
1	B	571	TRP	2.1
3	H	184	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	455	THR	2.1
2	G	137	ASN	2.1
3	H	30	ASN	2.1
5	D	33	HIS	2.1
2	G	33	ASN	2.1
2	G	292	VAL	2.1
5	D	45	LEU	2.1
4	L	210	THR	2.1
4	L	162	THR	2.1
6	E	144	ALA	2.0
2	G	323	ILE	2.0
3	H	103	TRP	2.0
1	B	546	SER	2.0
3	H	178	LEU	2.0
5	D	100(B)	ASP	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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	A	1	14/15	-	-	285,298,351,352	0
7	FUC	A	2	10/11	-	-	312,312,312,312	0
8	NAG	C	1	14/15	-	-	333,351,364,365	0
8	NAG	C	2	14/15	-	-	318,318,318,318	0
8	BMA	C	3	11/12	-	-	311,311,311,311	0
8	FUC	C	4	10/11	-	-	351,351,351,351	0
9	NAG	F	1	14/15	-	-	331,341,358,361	0
9	NAG	F	2	14/15	-	-	336,357,359,360	0
9	FUC	F	3	10/11	-	-	318,324,334,342	0
16	NAG	P	10	14/15	0.08	0.17	404,417,422,424	0
17	BMA	R	3	11/12	0.11	0.15	350,357,361,366	0
10	BMA	I	3	11/12	-	-	274,274,274,274	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	SIA	P	12	20/21	0.29	0.16	456,456,456,456	0
16	GAL	P	6	11/12	0.29	0.11	351,351,351,351	0
11	BMA	J	3	11/12	0.31	0.13	313,313,313,313	0
11	MAN	J	4	11/12	-	-	340,340,340,340	0
11	NAG	J	5	14/15	-	-	346,346,346,346	0
11	GAL	J	6	11/12	-	-	350,350,350,350	0
11	NAG	J	7	14/15	-	-	340,340,340,340	0
11	MAN	J	8	11/12	-	-	330,330,330,330	0
11	NAG	J	9	14/15	-	-	315,315,315,315	0
11	GAL	J	10	11/12	-	-	336,336,336,336	0
11	NAG	J	11	14/15	-	-	383,383,383,383	0
11	GAL	J	12	11/12	-	-	401,401,401,401	0
11	FUC	J	13	10/11	-	-	294,294,294,294	0
22	BMA	X	3	11/12	0.32	0.10	307,324,340,341	0
15	MAN	O	7	11/12	0.33	0.18	399,413,420,421	0
13	NAG	M	5	14/15	0.33	0.17	355,368,372,374	0
21	NAG	W	2	14/15	0.33	0.13	300,321,323,323	0
14	NAG	T	1	14/15	0.33	0.17	385,385,385,385	0
21	MAN	W	4	11/12	0.34	0.13	294,294,294,294	0
12	MAN	K	7	11/12	-	-	350,350,350,350	0
12	NAG	K	8	14/15	-	-	339,352,356,358	0
12	GAL	K	9	11/12	-	-	350,355,364,366	0
12	FUC	K	10	10/11	-	-	329,329,329,329	0
14	NAG	T	2	14/15	0.37	0.11	369,369,369,369	0
19	MAN	U	6	11/12	0.42	0.12	355,370,377,378	0
16	NAG	P	5	14/15	0.44	0.13	352,366,370,372	0
20	MAN	V	5	11/12	0.45	0.16	314,331,337,347	0
16	SIA	P	7	20/21	0.45	0.12	397,397,397,397	0
19	MAN	U	5	11/12	0.46	0.12	342,342,342,342	0
11	NAG	J	2	14/15	0.46	0.16	254,274,287,287	0
17	NAG	R	7	14/15	0.46	0.19	332,345,349,351	0
20	MAN	V	4	11/12	0.47	0.13	313,318,336,356	0
16	NAG	P	8	14/15	0.48	0.16	371,371,371,371	0
21	BMA	W	3	11/12	0.49	0.12	314,321,325,329	0
12	NAG	K	5	14/15	0.50	0.14	363,363,363,363	0
16	NAG	P	2	14/15	0.50	0.19	297,317,320,320	0
16	MAN	P	9	11/12	0.50	0.14	390,390,390,390	0
19	BMA	U	3	11/12	0.51	0.14	397,414,429,431	0
17	NAG	R	5	14/15	0.54	0.16	347,356,371,376	0
13	SIA	M	7	20/21	0.56	0.14	371,371,371,371	0
22	MAN	X	4	11/12	0.56	0.18	380,397,403,413	0
22	MAN	X	5	11/12	0.57	0.16	408,410,419,425	0

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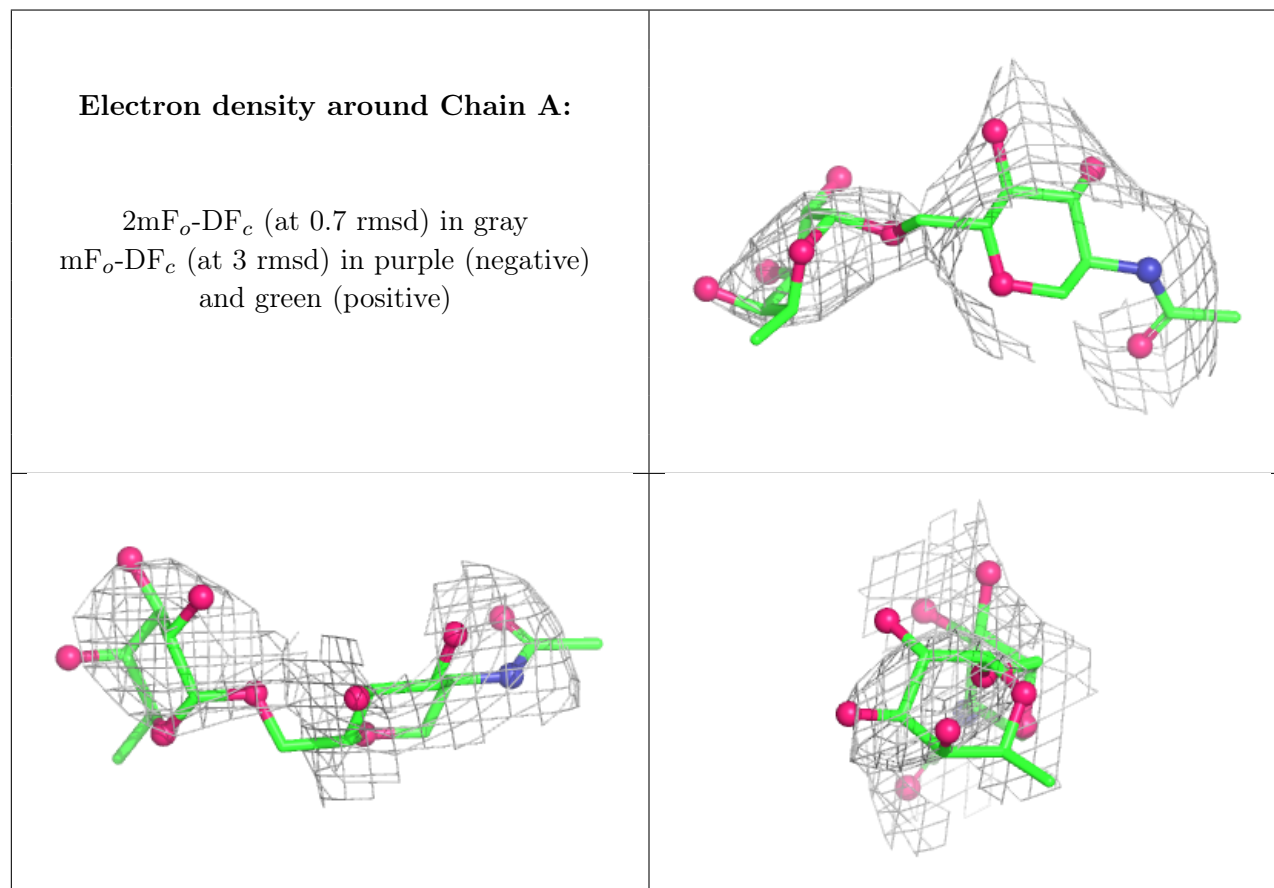
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	NAG	P	15	14/15	0.59	0.12	376,376,376,376	0
16	GAL	P	11	11/12	0.59	0.15	435,435,435,435	0
16	NAG	P	13	14/15	0.59	0.17	394,394,394,394	0
12	MAN	K	4	11/12	0.60	0.13	338,338,338,338	0
18	MAN	S	9	11/12	0.60	0.16	280,280,280,280	0
21	MAN	W	5	11/12	0.60	0.17	400,400,400,400	0
20	BMA	V	3	11/12	0.61	0.13	318,336,351,352	0
13	GAL	M	6	11/12	0.61	0.14	358,363,372,375	0
18	MAN	S	10	11/12	0.64	0.14	250,252,261,267	0
13	NAG	M	9	14/15	0.64	0.24	307,320,324,326	0
19	MAN	U	4	11/12	0.65	0.10	350,368,374,383	0
12	GAL	K	6	11/12	0.66	0.13	411,411,411,411	0
10	NAG	I	2	14/15	0.66	0.13	271,271,271,271	0
17	MAN	R	4	11/12	0.66	0.11	317,323,334,335	0
14	NAG	Q	2	14/15	0.70	0.12	283,298,308,317	0
15	MAN	O	5	11/12	0.70	0.20	311,311,311,311	0
21	NAG	W	1	14/15	0.71	0.14	296,306,324,327	0
17	NAG	R	1	14/15	0.71	0.21	258,258,258,258	0
19	MAN	U	7	11/12	0.72	0.14	370,375,393,413	0
14	NAG	N	2	14/15	0.72	0.13	270,272,275,276	0
16	GAL	P	14	11/12	0.72	0.13	367,367,367,367	0
12	NAG	K	2	14/15	0.73	0.20	277,290,302,308	0
12	BMA	K	3	11/12	0.74	0.12	330,330,330,330	0
16	FUC	P	16	10/11	0.74	0.27	309,309,309,309	0
22	NAG	X	2	14/15	0.74	0.14	241,258,278,284	0
18	MAN	S	6	11/12	0.76	0.15	203,208,213,213	0
16	MAN	P	4	11/12	0.76	0.14	393,393,393,393	0
13	MAN	M	4	11/12	0.76	0.14	337,337,337,337	0
15	MAN	O	6	11/12	0.76	0.13	318,335,341,351	0
22	NAG	X	1	14/15	0.77	0.19	215,226,243,248	0
18	MAN	S	8	11/12	0.78	0.11	261,274,297,307	0
17	MAN	R	6	11/12	0.79	0.14	360,369,374,374	0
16	BMA	P	3	11/12	0.79	0.11	355,362,366,371	0
15	BMA	O	3	11/12	0.79	0.20	287,304,319,321	0
21	FUC	W	6	10/11	0.80	0.18	308,313,323,331	0
13	MAN	M	8	11/12	0.80	0.14	283,291,296,297	0
20	NAG	V	2	14/15	0.80	0.20	326,343,363,369	0
18	MAN	S	7	11/12	0.81	0.12	208,225,231,240	0
19	NAG	U	2	14/15	0.81	0.31	431,431,431,431	0
17	NAG	R	2	14/15	0.82	0.17	338,352,362,366	0
18	MAN	S	5	11/12	0.84	0.08	180,183,196,204	0
11	NAG	J	1	14/15	0.84	0.15	211,224,277,278	0

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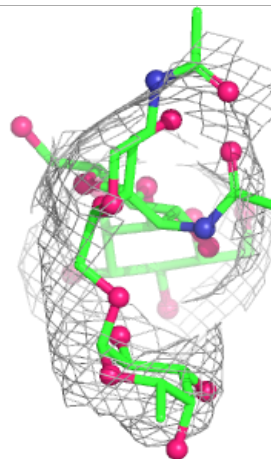
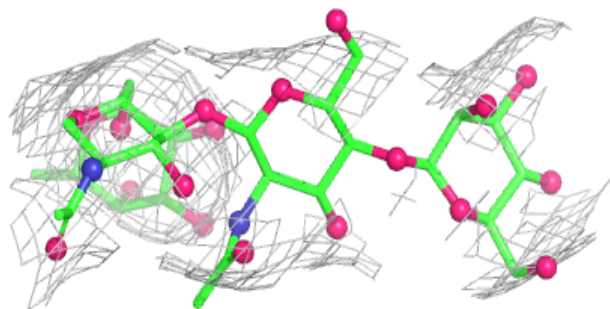
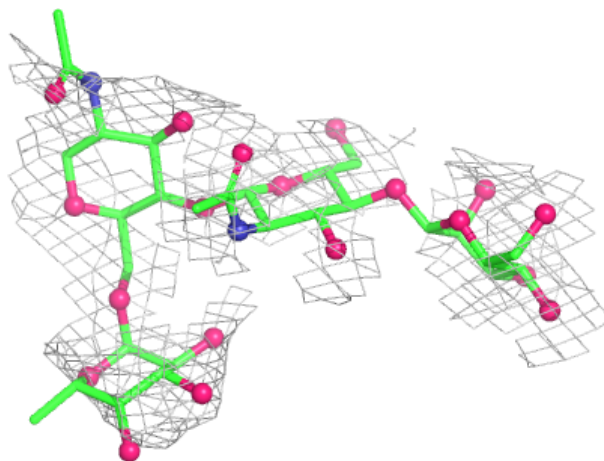
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	NAG	V	1	14/15	0.84	0.23	245,256,273,279	0
13	NAG	M	2	14/15	0.85	0.19	221,241,244,244	0
15	NAG	O	2	14/15	0.85	0.14	203,219,240,245	0
15	MAN	O	4	11/12	0.86	0.23	281,286,304,324	0
14	NAG	N	1	14/15	0.86	0.15	232,246,263,271	0
16	NAG	P	1	14/15	0.87	0.17	289,299,317,320	0
13	NAG	M	1	14/15	0.88	0.24	198,208,226,229	0
12	NAG	K	1	14/15	0.89	0.11	236,260,269,281	0
10	NAG	I	1	14/15	0.89	0.12	251,251,251,251	0
18	NAG	S	2	14/15	0.89	0.12	162,179,199,205	0
18	MAN	S	4	11/12	0.89	0.10	195,200,218,238	0
13	BMA	M	3	11/12	0.91	0.13	254,261,265,270	0
15	NAG	O	1	14/15	0.92	0.13	169,179,197,202	0
14	NAG	Q	1	14/15	0.92	0.10	204,220,246,255	0
19	NAG	U	1	14/15	0.94	0.28	290,299,323,342	0
18	NAG	S	1	14/15	0.96	0.15	200,211,228,234	0
18	BMA	S	3	11/12	0.97	0.06	136,153,169,170	0

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



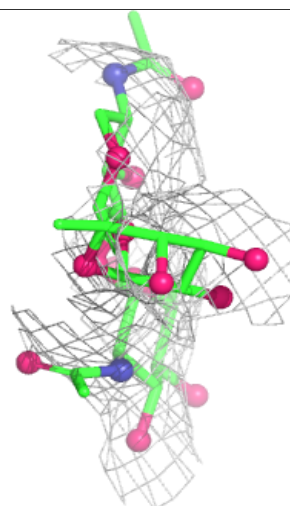
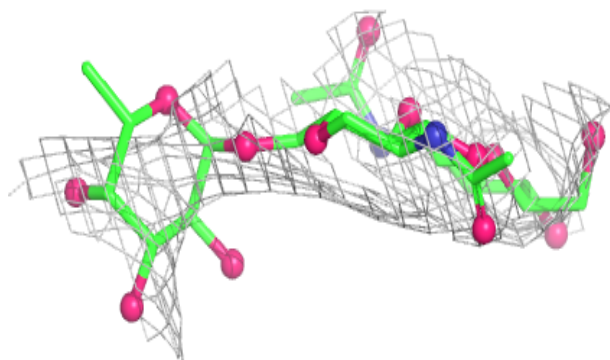
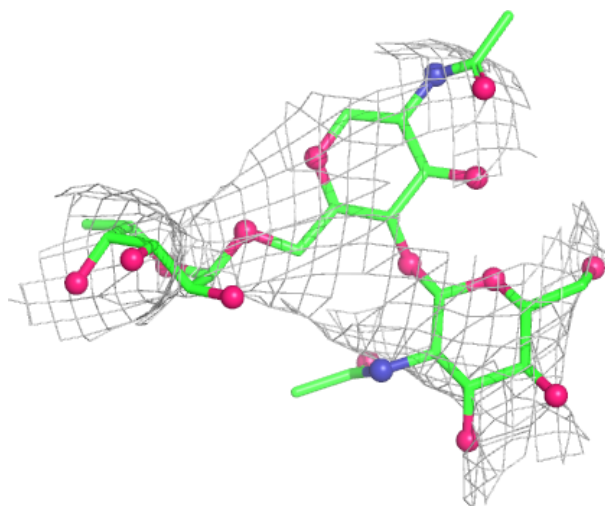
Electron density around Chain C:

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



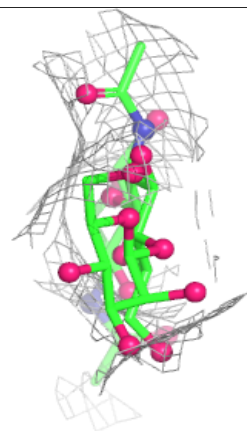
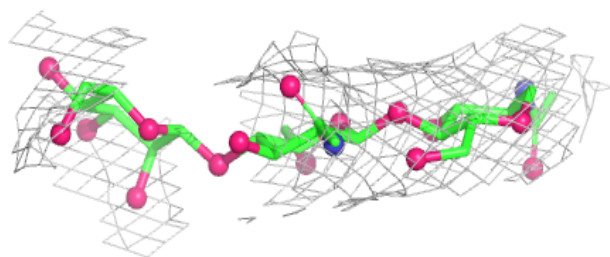
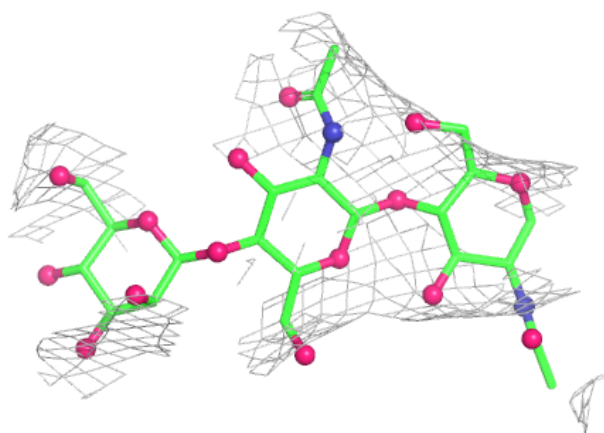
Electron density around Chain F:

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

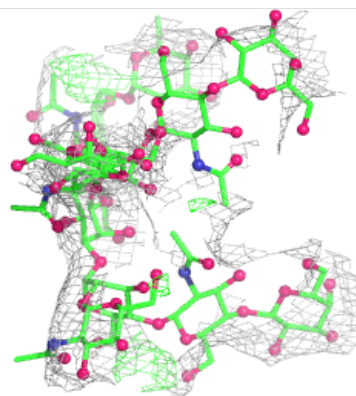
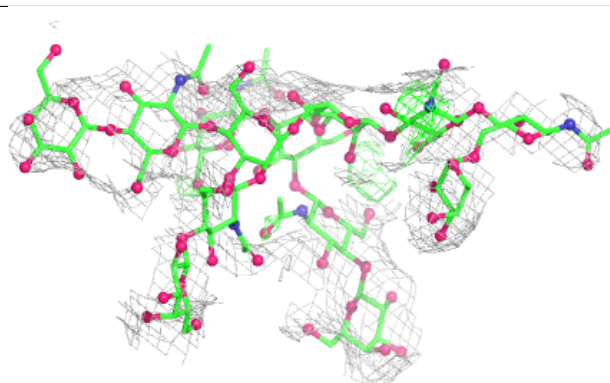
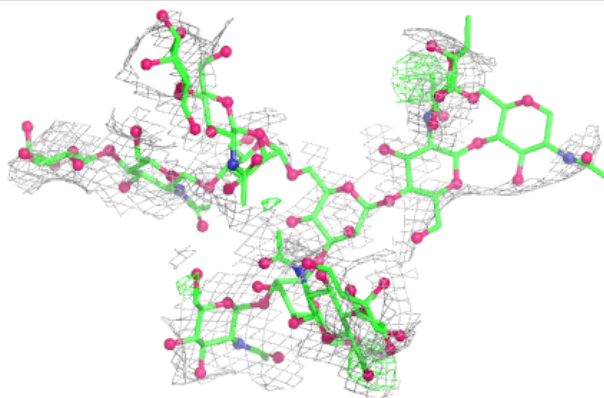


Electron density around Chain I:

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

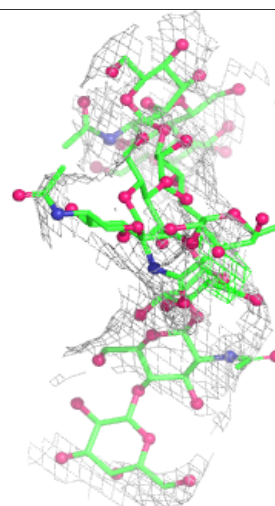
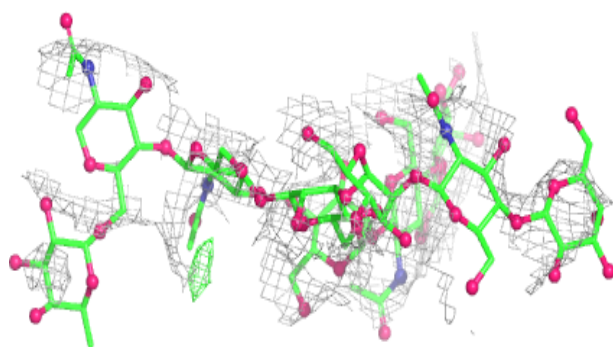
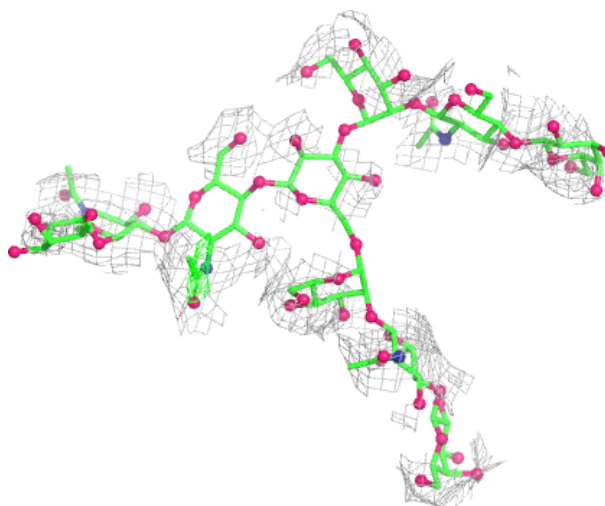
**Electron density around Chain J:**

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



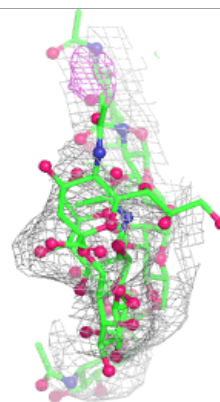
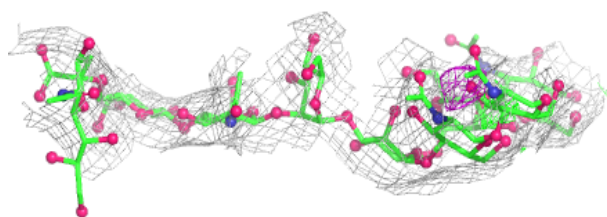
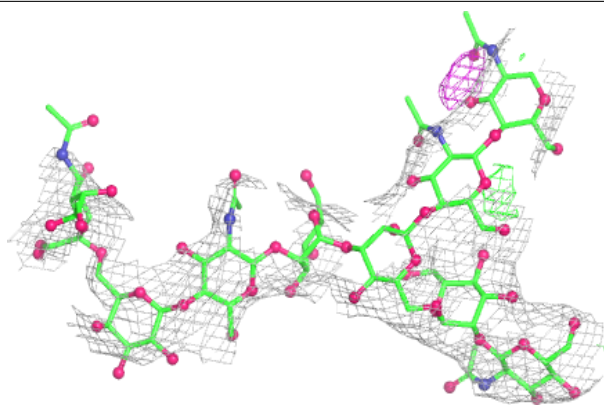
Electron density around Chain K:

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

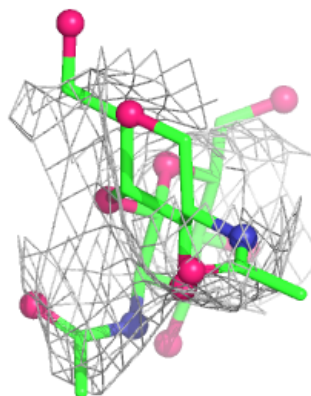
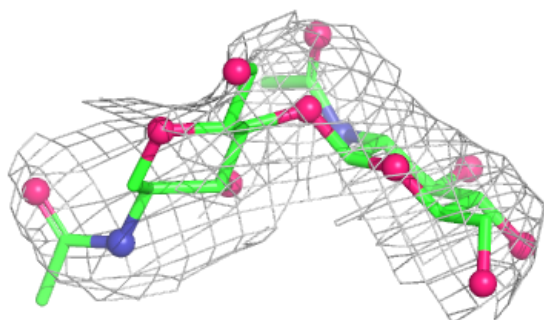
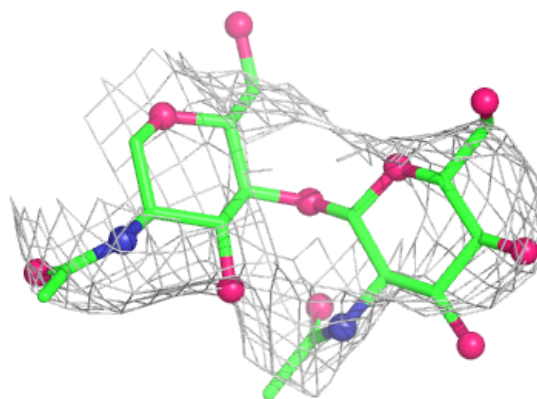


Electron density around Chain M:

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

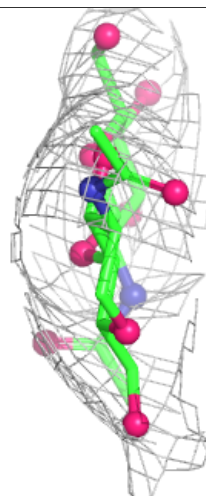
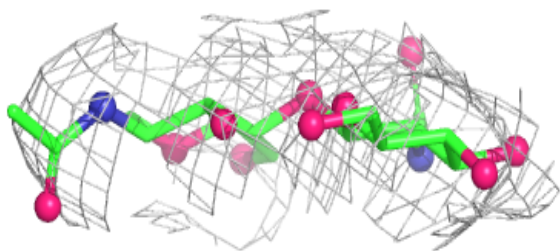
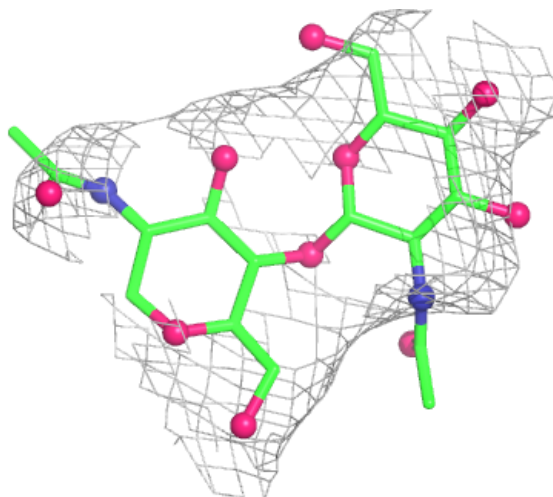
**Electron density around Chain N:**

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



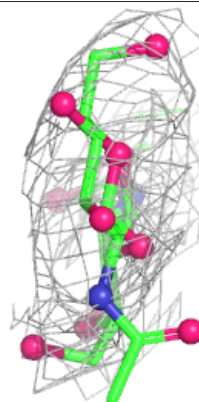
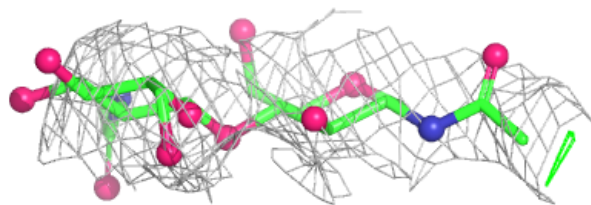
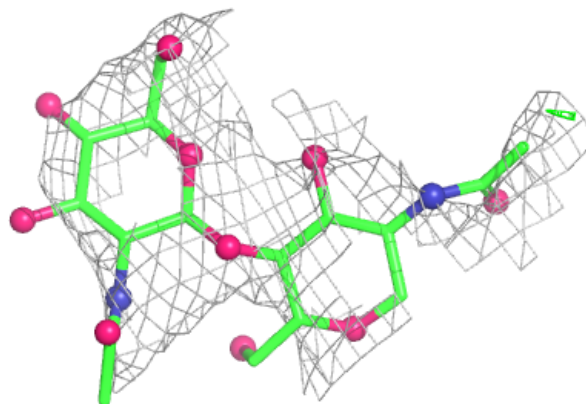
Electron density around Chain Q:

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



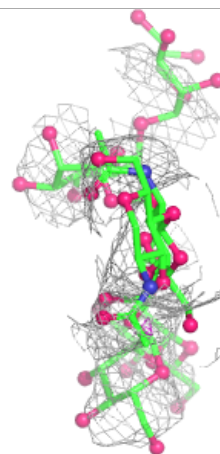
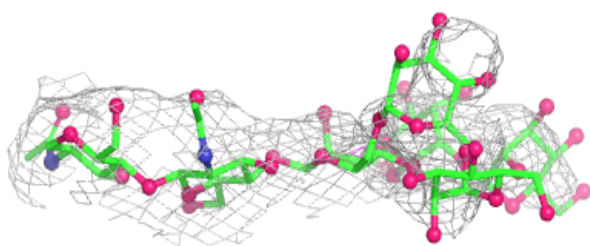
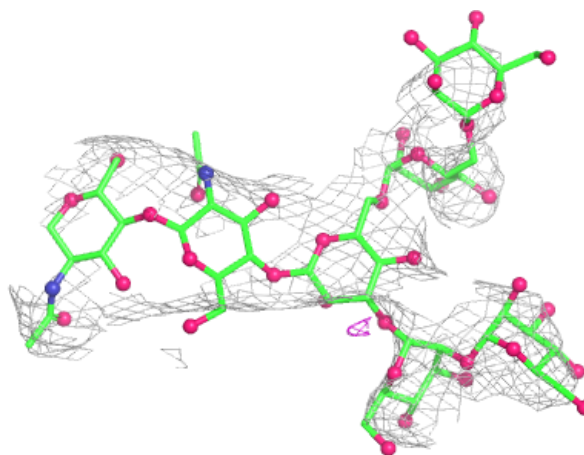
Electron density around Chain T:

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



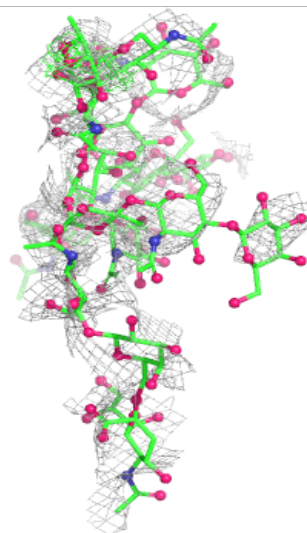
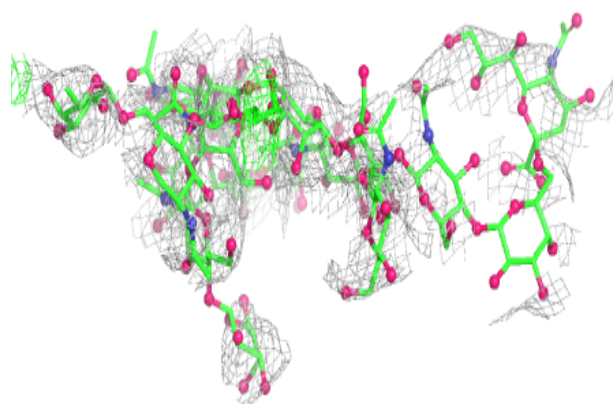
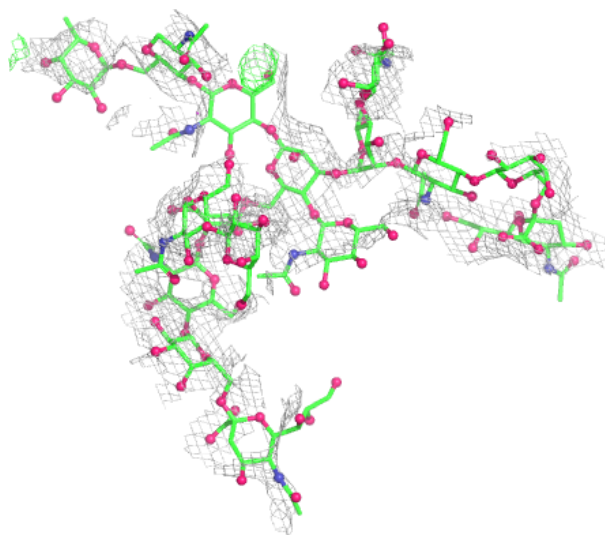
Electron density around Chain O:

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



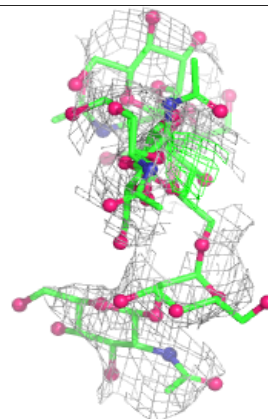
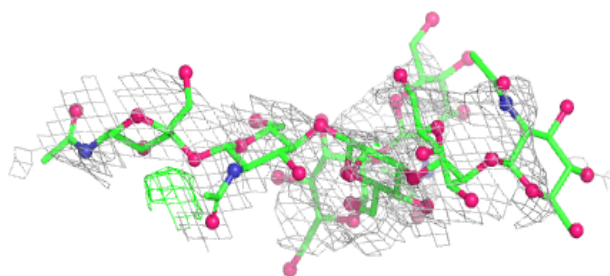
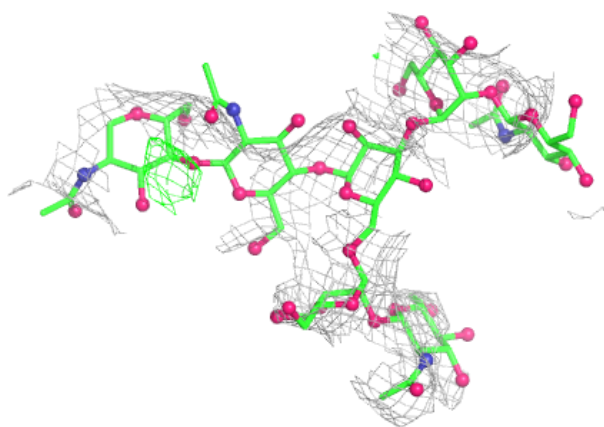
Electron density around Chain P:

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



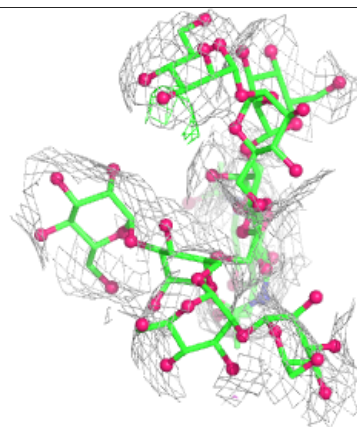
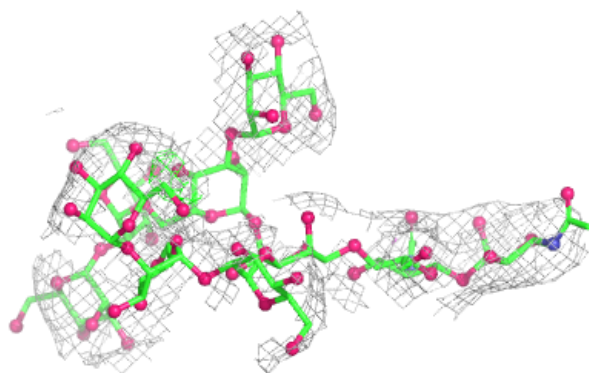
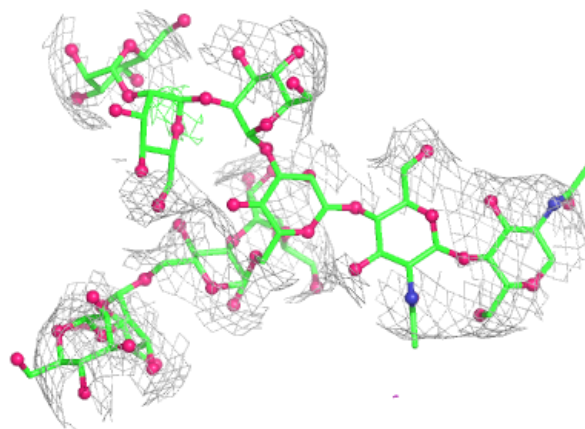
Electron density around Chain R:

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

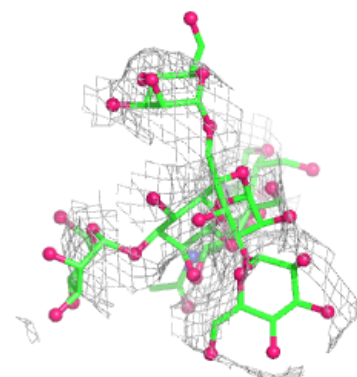
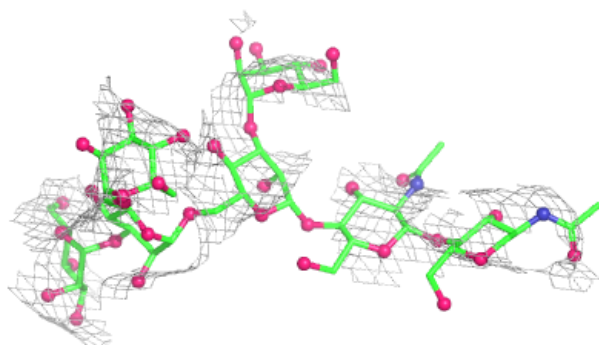
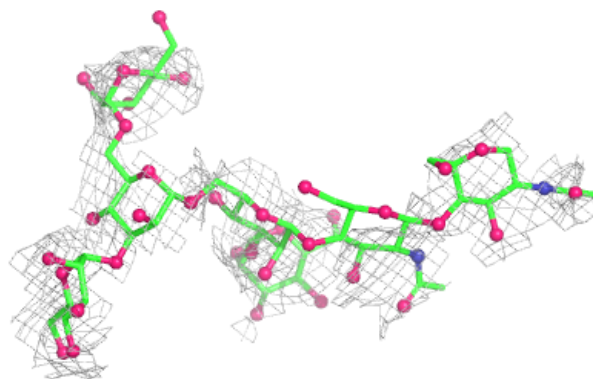


Electron density around Chain S:

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

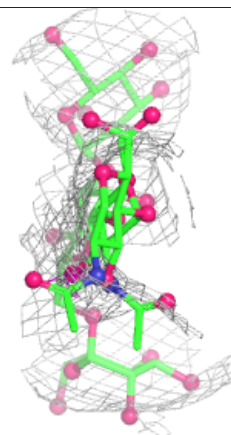
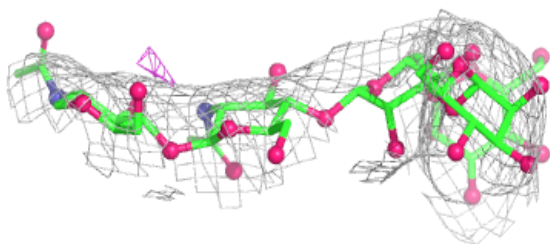
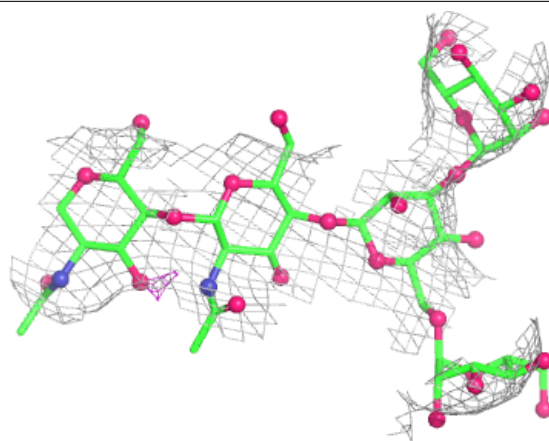
**Electron density around Chain U:**

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



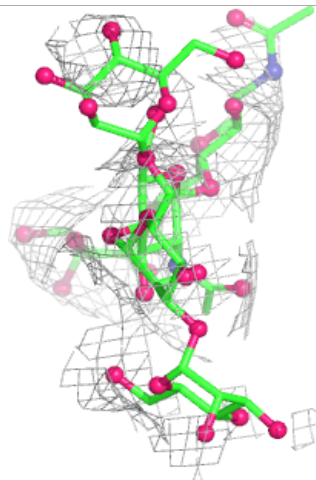
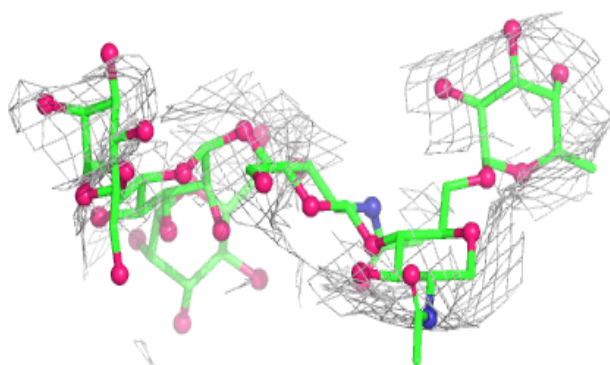
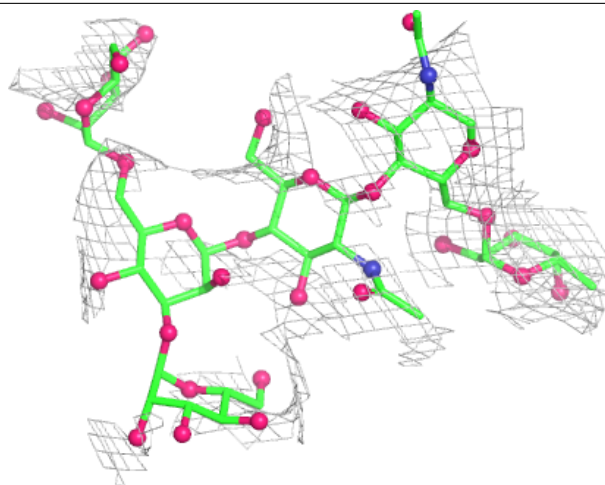
Electron density around Chain V:

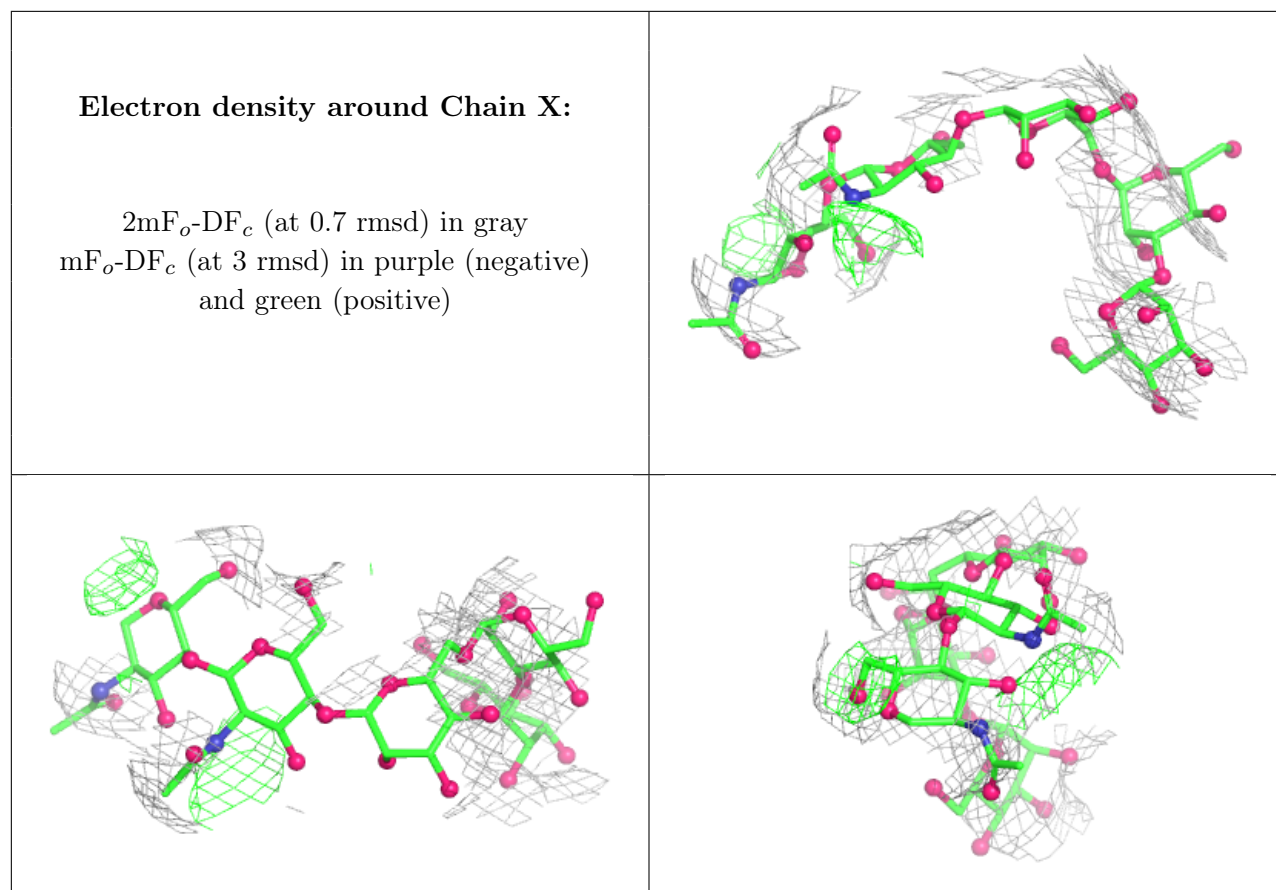
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain W:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	NAG	G	3390	14/15	0.58	0.15	288,306,313,318	0

6.5 Other polymers [i](#)

There are no such residues in this entry.