



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2024 – 08:56 am GMT

PDB ID : 5FYK  
Title : Crystal Structure at 3.7 Å Resolution of Fully Glycosylated HIV-1 Clade B JR-FL SOSIP.664 Prefusion Env Trimer in Complex with Broadly Neutralizing Antibodies PGT122, 35O22 and VRC01  
Authors : Stewart-Jones, G.B.E.; Zhou, T.; Thomas, P.V.; Kwong, P.D.  
Deposited on : 2016-03-08  
Resolution : 3.11 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

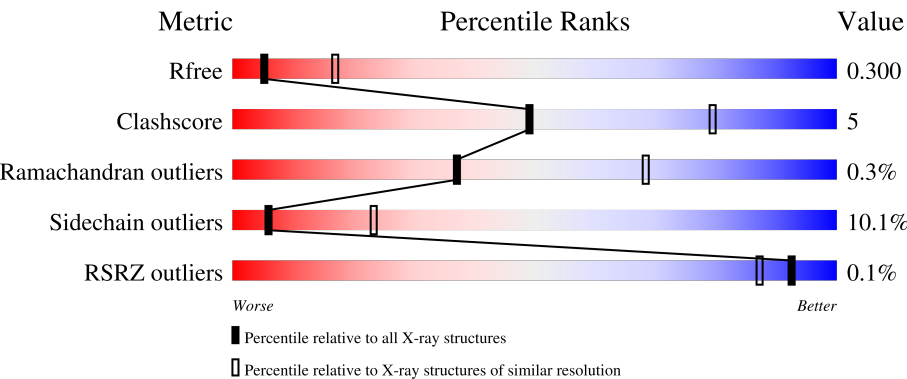
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 Å.

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






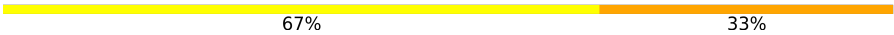
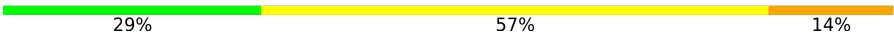
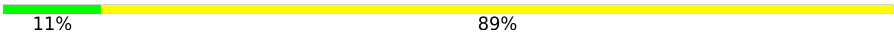
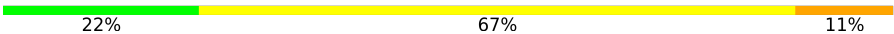
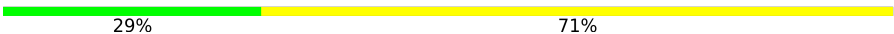
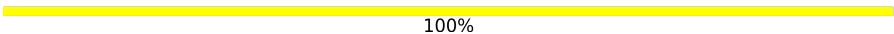
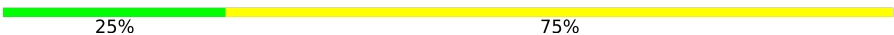
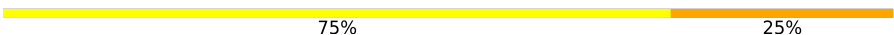
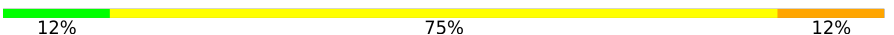
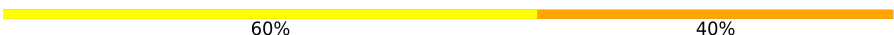
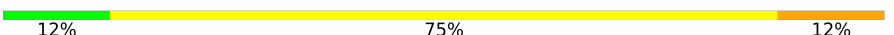





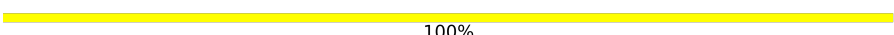



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	B	161	<div><div></div><div>61%27%6%6%</div></div>
2	D	243	<div><div></div><div>90%10%</div></div>
3	E	216	<div><div></div><div>81%15%..</div></div>
4	G	475	<div><div></div><div>69%23%.5%</div></div>
5	H	244	<div><div></div><div>82%12%7%</div></div>

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Mol	Chain	Length	Quality of chain
6	L	213	 81% 16% ..
7	U	240	 42% 7% 50%
7	V	240	 36% 59%
8	A	3	 67% 33%
9	C	7	 29% 57% 14%
10	F	9	 11% 89%
10	M	9	 22% 67% 11%
11	I	7	 29% 71%
12	J	7	 100%
13	K	4	 25% 75%
13	T	4	 75% 25%
14	N	8	 12% 75% 12%
15	O	5	 60% 40%
16	P	8	 12% 75% 12%
17	Q	10	 20% 70% 10%
18	R	7	 43% 57%
18	S	7	 43% 57%
19	W	8	 25% 75%
20	X	6	 17% 83%
21	Y	2	 100%
21	a	2	 50% 50%
22	Z	6	 33% 67%
23	b	6	 17% 83%

## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 14824 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 JR-FL, GP41 ENV ECTODOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	151	Total	C	N	O	S	0	0	0
			1195	753	206	228	8			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q6BC19
B	563	GLU	GLN	conflict	UNP Q6BC19
B	605	CYS	THR	engineered mutation	UNP Q6BC19
B	665	GLY	-	expression tag	UNP Q6BC19
B	666	GLY	-	expression tag	UNP Q6BC19
B	667	LEU	-	expression tag	UNP Q6BC19
B	668	GLU	-	expression tag	UNP Q6BC19
B	669	VAL	-	expression tag	UNP Q6BC19
B	670	LEU	-	expression tag	UNP Q6BC19
B	671	PHE	-	expression tag	UNP Q6BC19
B	672	GLN	-	expression tag	UNP Q6BC19

- Molecule 2 is a protein called 35O22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	243	Total	C	N	O	S	0	0	1
			1833	1165	307	353	8			

- Molecule 3 is a protein called 35O22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 4 is a protein called JR-FL, GP120 ENV ECTODOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	451	Total	C	N	O	S	0	0	0
			3571	2248	627	668	28			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	168	LYS	GLU	engineered mutation	UNP Q75760
G	430	ILE	VAL	conflict	UNP Q75760
G	459	CYS	GLY	engineered mutation	UNP Q75760
G	501	CYS	ALA	engineered mutation	UNP Q75760
G	507	GLY	-	expression tag	UNP Q75760
G	508	ARG	-	expression tag	UNP Q75760
G	509	ARG	-	expression tag	UNP Q75760
G	510	ARG	-	expression tag	UNP Q75760
G	511	ARG	-	expression tag	UNP Q75760
G	512	ARG	-	expression tag	UNP Q75760
G	513	ARG	-	expression tag	UNP Q75760

- Molecule 5 is a protein called PGT122.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			

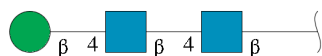
- Molecule 6 is a protein called PGT122.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	210	Total	C	N	O	S	0	0	0
			1589	998	267	320	4			

- Molecule 7 is a protein called VRC01.

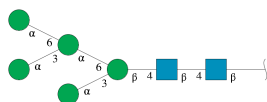
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	U	119	Total	C	N	O	S	0	0	0
			956	603	173	171	9			
7	V	98	Total	C	N	O	S	0	0	0
			758	479	130	147	2			

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



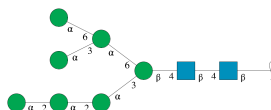
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	A	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



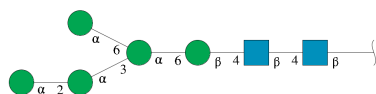
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	C	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



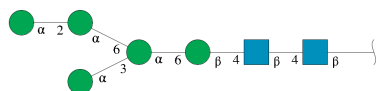
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	F	9	Total	C	N	O	0	0	0
			105	58	2	45			
10	M	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 11 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
11	I	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 12 is an oligosaccharide called 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.



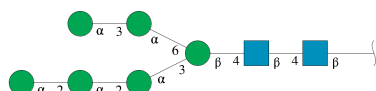
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	J	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 13 is an oligosaccharide called 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.



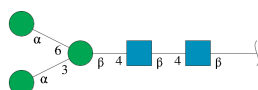
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
13	T	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



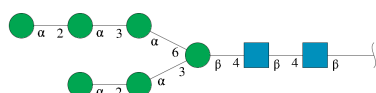
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	N	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 15 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.



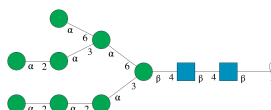
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	O	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



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

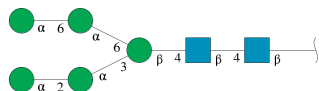
- Molecule 17 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

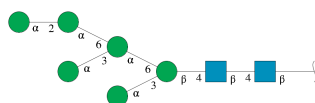


- Molecule 18 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



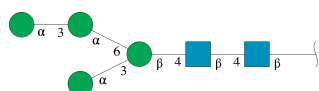
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	7	Total	C	N	O	0	0	0
			83	46	2	35			
18	S	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 19 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



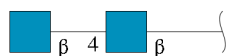
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	W	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 20 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 21 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



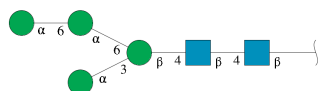
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			
21	a	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 23 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 24 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

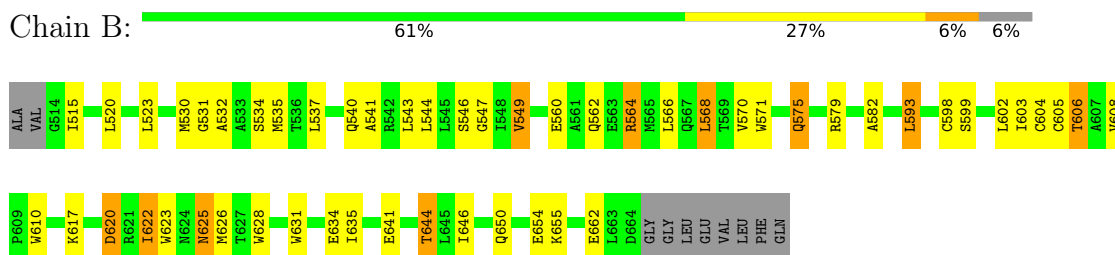


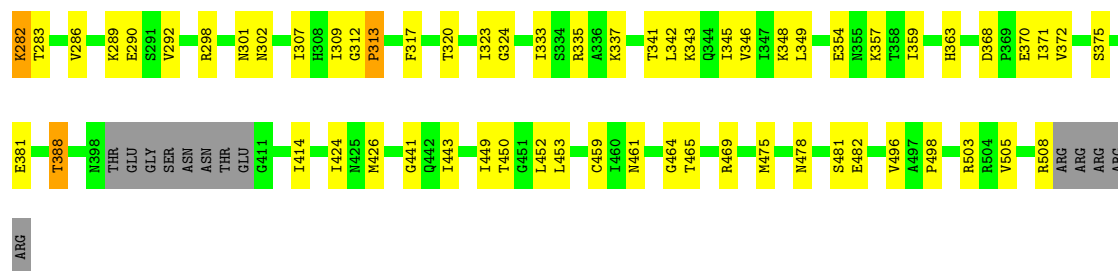
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	B	1	Total	C	N	O	0	0
			14	8	1	5		
24	B	1	Total	C	N	O	0	0
			14	8	1	5		
24	B	1	Total	C	N	O	0	0
			14	8	1	5		
24	G	1	Total	C	N	O	0	0
			14	8	1	5		
24	H	1	Total	C	N	O	0	0
			14	8	1	5		

### 3 Residue-property plots

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

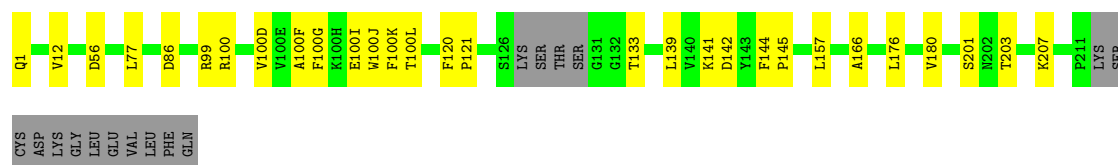
- Molecule 1: JR-FL, GP41 ENV ECTODOMAIN





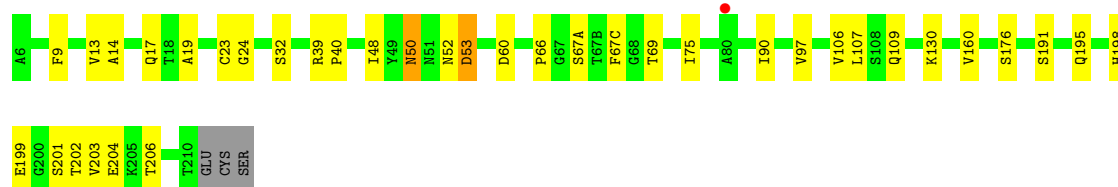
• Molecule 5: PGT122

Chain H: 82% 12% 7%



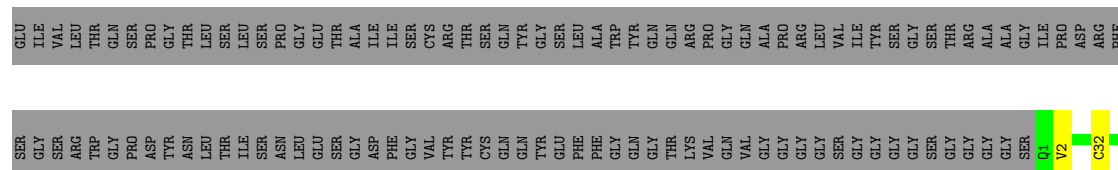
• Molecule 6: PGT122

Chain L: 81% 16% ..



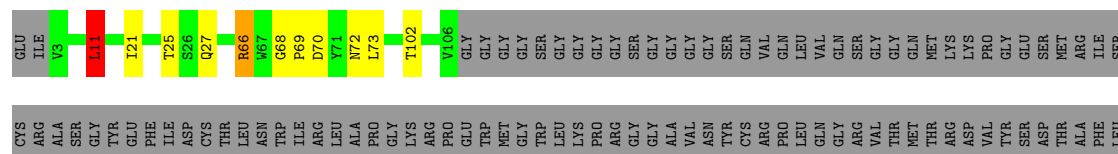
• Molecule 7: VRC01

Chain U: 42% 7% 50%



• Molecule 7: VRC01

Chain V: 36% 59%



GLU LEU ARG SER LEU THR VAL ASP ASP THR ALA VAL TYR PHE CYS THR ARG GLY LYS ASN CYS ASP TYR ASN TRP ASP PHE GLU HIS TRP GLY ARG GLY THR PRO VAL ILE VAL GLY GLY LEU VAL PRO ARG

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

Chain A:  67% 33%

MAG1  
MAG2  
BMA3

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

Chain C:  29% 57% 14%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7

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

Chain F:  11% 89%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9

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

Chain M:  22% 67% 11%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9

- Molecule 11: 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

Chain I:  29% 71%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7

- Molecule 12: 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-

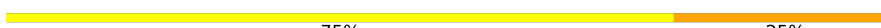
## D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

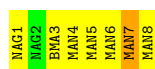
- Molecule 13: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  25% 75%

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

Chain T:  75% 25%

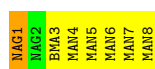
- Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  12% 75% 12%


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

Chain O:  60% 40%

- Molecule 16: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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 P:  12% 75% 12%

- Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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

Chain Q:  20% 70% 10%



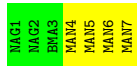
- Molecule 18: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  43% 57%



- Molecule 18: 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

Chain S:  43% 57%

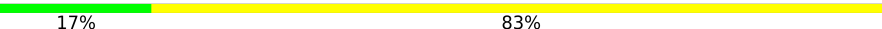


- Molecule 19: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  25% 75%



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

Chain X:  17% 83%



- Molecule 21: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



Chain Y:  100%

MAG1  
MAG2

- Molecule 21: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  50% 50%


MAG1  
MAG2

- Molecule 22: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  33% 67%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

- Molecule 23: 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 b:  17% 83%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.78Å 130.78Å 314.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.81 – 3.11 42.81 – 3.11	Depositor EDS
% Data completeness (in resolution range)	58.3 (42.81-3.11) 58.6 (42.81-3.11)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, $R_{free}$	0.246 , 0.303 0.248 , 0.300	Depositor DCC
$R_{free}$ test set	1583 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	93.3	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 142.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.146 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14824	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	162.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	B	0.29	0/1215	0.50	0/1647
2	D	0.25	0/1881	0.43	0/2562
3	E	0.26	0/1658	0.48	0/2266
4	G	0.29	0/3645	0.47	0/4946
5	H	0.24	0/1789	0.47	0/2443
6	L	0.26	0/1632	0.47	0/2236
7	U	0.22	0/981	0.40	0/1328
7	V	0.31	0/778	0.57	1/1058 (0.1%)
All	All	0.27	0/13579	0.47	1/18486 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	V	11	LEU	CB-CG-CD1	5.30	120.02	111.00

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	1195	0	1176	30	0
2	D	1833	0	1806	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1615	0	1541	21	0
4	G	3571	0	3513	60	0
5	H	1742	0	1715	11	0
6	L	1589	0	1530	18	0
7	U	956	0	928	6	0
7	V	758	0	719	4	0
8	A	39	0	34	1	0
9	C	83	0	70	2	0
10	F	105	0	88	0	0
10	M	105	0	88	1	0
11	I	83	0	70	0	0
12	J	83	0	70	0	0
13	K	50	0	43	1	0
13	T	50	0	43	1	0
14	N	94	0	79	1	0
15	O	61	0	52	2	0
16	P	94	0	79	2	0
17	Q	116	0	97	1	0
18	R	83	0	70	4	0
18	S	83	0	70	0	0
19	W	94	0	79	0	0
20	X	72	0	61	0	0
21	Y	28	0	25	2	0
21	a	28	0	25	0	0
22	Z	72	0	61	0	0
23	b	72	0	61	0	0
24	B	42	0	39	1	0
24	G	14	0	13	0	0
24	H	14	0	13	0	0
All	All	14824	0	14258	155	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 5.

All (155) 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)
3:E:50:GLU:HB2	3:E:53:GLU:HB2	1.60	0.83
6:L:106:VAL:HG13	6:L:109:GLN:HE21	1.49	0.76
1:B:546:SER:HA	1:B:549:VAL:HG22	1.72	0.71
1:B:617:LYS:HA	24:B:1668:NAG:H82	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:106:VAL:O	6:L:109:GLN:NE2	2.28	0.66
4:G:292:VAL:HG12	4:G:337:LYS:HE3	1.78	0.65
1:B:605:CYS:HA	4:G:37:THR:HG22	1.80	0.64
4:G:186:ASN:O	4:G:188:ASN:ND2	2.31	0.63
3:E:50:GLU:HB3	3:E:53:GLU:H	1.65	0.61
4:G:342:LEU:HA	4:G:345:ILE:HD12	1.82	0.60
15:O:1:NAG:H62	15:O:2:NAG:HN2	1.67	0.59
4:G:298:ARG:NH1	4:G:302:ASN:OD1	2.35	0.59
3:E:127:ALA:N	3:E:128:ASN:HA	2.17	0.59
18:R:3:BMA:H3	18:R:4:MAN:H5	1.84	0.59
1:B:540:GLN:O	1:B:544:LEU:HD21	2.03	0.58
5:H:100(D):VAL:N	5:H:100(I):GLU:OE1	2.36	0.58
4:G:153:GLU:HA	4:G:178:LYS:HB2	1.85	0.57
4:G:478:ASN:O	4:G:481:SER:OG	2.23	0.57
7:V:69:PRO:HD3	14:N:7:MAN:H62	1.87	0.56
3:E:189:ARG:O	3:E:190:SER:OG	2.24	0.56
6:L:13:VAL:HG21	6:L:19:ALA:HB2	1.88	0.56
4:G:164:SER:HB3	4:G:313:PRO:HA	1.87	0.56
4:G:251:ILE:HD12	4:G:482:GLU:HB3	1.87	0.55
3:E:150:ALA:HB1	3:E:188:HIS:NE2	2.21	0.54
4:G:357:LYS:HB3	21:Y:2:NAG:H3	1.88	0.54
3:E:50:GLU:CB	3:E:53:GLU:H	2.19	0.54
1:B:575:GLN:O	1:B:579:ARG:N	2.35	0.54
6:L:198:HIS:HB3	6:L:201:SER:H	1.72	0.54
5:H:120:PHE:CE1	5:H:141:LYS:HE3	2.43	0.53
6:L:14:ALA:HB3	6:L:17:GLN:HG3	1.89	0.53
4:G:324:GLY:HA2	6:L:67(C):PHE:CD1	2.43	0.53
4:G:335:ARG:HB3	4:G:414:ILE:HG13	1.90	0.53
1:B:537:LEU:O	1:B:541:ALA:N	2.41	0.53
4:G:123:THR:HG23	4:G:124:PRO:HD3	1.91	0.53
6:L:13:VAL:O	6:L:107:LEU:N	2.42	0.52
3:E:150:ALA:HB1	3:E:188:HIS:CD2	2.44	0.52
1:B:564:ARG:HG3	1:B:568:LEU:CD2	2.41	0.51
6:L:198:HIS:N	6:L:199:GLU:HA	2.26	0.51
7:U:62:PRO:HG2	7:U:63:LEU:HD12	1.93	0.51
5:H:166:ALA:HA	5:H:176:LEU:HB3	1.92	0.51
1:B:610:TRP:CD2	4:G:498:PRO:HB3	2.46	0.51
4:G:131:CYS:N	4:G:189:THR:O	2.44	0.50
1:B:571:TRP:HD1	4:G:73:ALA:HB3	1.76	0.50
3:E:50:GLU:OE1	3:E:52:ASN:ND2	2.45	0.49
7:U:82(A):ARG:NH2	13:T:4:MAN:O3	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:187:ASN:N	4:G:187:ASN:OD1	2.44	0.49
1:B:570:VAL:HG21	4:G:111:LEU:HD22	1.95	0.49
6:L:106:VAL:C	6:L:109:GLN:HE22	2.16	0.49
7:U:65:GLY:O	7:U:82(A):ARG:NH1	2.46	0.49
7:U:83:THR:HG22	7:U:84:VAL:H	1.78	0.49
8:A:1:NAG:H62	8:A:2:NAG:C7	4.32	0.49
1:B:650:GLN:O	1:B:654:GLU:HG2	2.13	0.48
7:U:68:THR:HB	7:U:81:GLU:HB3	1.94	0.48
4:G:164:SER:HA	4:G:312:GLY:HA3	1.95	0.48
3:E:167:GLN:N	3:E:171:LYS:O	2.35	0.48
4:G:102:GLU:O	4:G:106:GLU:CD	2.51	0.48
7:U:44:ARG:HG2	7:U:45:PRO:HD2	1.95	0.48
21:Y:1:NAG:H62	21:Y:2:NAG:C7	2.43	0.48
4:G:33:LYS:HE2	4:G:35:TRP:CZ2	2.49	0.48
3:E:50:GLU:N	3:E:51:ASP:HA	2.29	0.47
3:E:187:SER:O	3:E:189:ARG:NH1	2.47	0.47
4:G:346:VAL:HG13	4:G:359:ILE:HD12	1.97	0.47
6:L:39:ARG:HG3	6:L:40:PRO:HD2	1.97	0.47
3:E:27(C):CYS:HA	3:E:28:CYS:HA	1.77	0.47
7:V:11:LEU:HD11	7:V:21:ILE:CD1	2.45	0.47
1:B:631:TRP:O	1:B:635:ILE:HG12	2.15	0.47
1:B:622:ILE:HG22	1:B:623:TRP:CD1	2.50	0.47
4:G:424:ILE:HD12	4:G:426:MET:HG3	1.96	0.46
6:L:195:GLN:HG2	6:L:204:GLU:HB3	1.97	0.46
2:D:18:VAL:HG12	2:D:82(C):LEU:HD11	1.97	0.46
4:G:185:ASP:OD1	4:G:186:ASN:N	2.48	0.46
4:G:95:MET:HE1	4:G:273:ARG:HD3	1.98	0.46
6:L:106:VAL:C	6:L:109:GLN:NE2	2.69	0.46
1:B:631:TRP:CE2	1:B:635:ILE:HG13	2.50	0.46
4:G:131:CYS:HB2	4:G:191:TYR:CD1	2.51	0.46
2:D:47:TRP:CZ2	2:D:49:GLY:HA2	2.50	0.46
4:G:55:ALA:HB2	4:G:218:CYS:SG	2.55	0.45
7:V:11:LEU:HD11	7:V:21:ILE:HD11	1.98	0.45
4:G:357:LYS:HB2	4:G:465:THR:HG21	1.98	0.45
7:V:66:ARG:NH1	7:V:68:GLY:HA3	2.31	0.45
5:H:100(D):VAL:HG12	5:H:100(F):ALA:H	1.82	0.45
4:G:302:ASN:HB3	4:G:320:THR:HG22	1.98	0.45
4:G:464:GLY:HA3	4:G:465:THR:HA	1.62	0.45
1:B:608:VAL:O	4:G:36:VAL:HG12	2.17	0.44
4:G:270:VAL:HG12	4:G:289:LYS:H	1.81	0.44
13:K:1:NAG:H61	13:K:2:NAG:N2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:3:BMA:H3	15:O:4:MAN:H2	1.71	0.44
1:B:543:LEU:HD23	1:B:547:GLY:HA2	1.98	0.44
2:D:168:ALA:HB1	2:D:177:SER:H	1.83	0.44
1:B:531:GLY:O	1:B:534:SER:OG	2.16	0.44
1:B:532:ALA:O	1:B:535:MET:HG2	2.17	0.44
4:G:52:LEU:HD23	4:G:219:ALA:HA	1.99	0.44
4:G:67:ASN:N	4:G:67:ASN:OD1	2.51	0.44
1:B:593:LEU:HB3	1:B:599:SER:HA	2.00	0.44
3:E:54:ARG:NE	3:E:60:PRO:HA	2.33	0.44
3:E:190:SER:HA	3:E:208:PRO:HD3	1.99	0.44
4:G:323:ILE:HD13	16:P:1:NAG:H61	2.00	0.43
4:G:193:LEU:HA	4:G:193:LEU:HD23	1.77	0.43
4:G:208:ILE:HD11	4:G:210:PHE:CE1	2.53	0.43
5:H:100:ARG:NH2	17:Q:5:MAN:H5	2.32	0.43
1:B:530:MET:HE3	1:B:622:ILE:HG23	1.99	0.43
1:B:625:ASN:OD1	1:B:626:MET:N	2.51	0.43
4:G:80:ASN:HA	4:G:81:PRO:HD3	1.89	0.43
4:G:324:GLY:HA2	6:L:67(C):PHE:CG	2.53	0.43
4:G:301:ASN:OD1	4:G:441:GLY:HA2	2.18	0.43
4:G:95:MET:CE	4:G:273:ARG:HD3	2.48	0.43
4:G:368:ASP:O	4:G:372:VAL:HG22	2.18	0.43
5:H:100:ARG:HG2	5:H:100(K):PHE:CZ	2.54	0.43
5:H:201:SER:HG	5:H:203:THR:HG1	1.66	0.43
10:M:3:BMA:H61	10:M:7:MAN:H2	1.68	0.42
5:H:121:PRO:HD3	5:H:207:LYS:HG2	2.02	0.42
6:L:66:PRO:O	6:L:67(A):SER:N	2.52	0.42
2:D:51:ILE:HG13	2:D:57:LYS:HG2	2.01	0.42
4:G:38:VAL:HB	4:G:496:VAL:HG12	2.01	0.42
3:E:20:THR:HA	3:E:73:LEU:O	2.20	0.42
6:L:23:CYS:SG	6:L:24:GLY:N	2.93	0.42
2:D:100:GLY:HA2	9:C:7:MAN:H62	2.02	0.42
4:G:270:VAL:O	4:G:348:LYS:HE3	2.20	0.42
2:D:200:HIS:HB3	2:D:203:SER:HG	1.84	0.42
4:G:323:ILE:HD13	16:P:1:NAG:O5	2.19	0.42
1:B:564:ARG:HG3	1:B:568:LEU:HD21	2.02	0.41
5:H:157:LEU:HD21	5:H:180:VAL:HG11	2.03	0.41
3:E:55:ALA:HB3	3:E:58:ILE:HD13	2.02	0.41
6:L:50:ASN:OD1	6:L:50:ASN:N	2.53	0.41
1:B:641:GLU:O	1:B:644:THR:HG22	2.20	0.41
1:B:544:LEU:O	4:G:221:ALA:HB1	2.21	0.41
4:G:354:GLU:C	4:G:357:LYS:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:CYS:SG	4:G:38:VAL:HG22	2.61	0.41
4:G:67:ASN:HB2	4:G:208:ILE:HG22	2.02	0.41
4:G:67:ASN:HB2	4:G:208:ILE:HA	2.03	0.41
4:G:99:ASN:HA	4:G:102:GLU:HG2	2.02	0.41
4:G:363:HIS:HB3	4:G:388:THR:HG22	2.03	0.41
6:L:53:ASP:OD1	6:L:53:ASP:N	2.54	0.41
18:R:1:NAG:H61	18:R:2:NAG:N2	2.36	0.41
1:B:530:MET:HA	1:B:628:TRP:CD1	2.55	0.41
1:B:564:ARG:HG3	1:B:568:LEU:HD22	2.03	0.41
4:G:275:ASP:HB3	4:G:282:LYS:HG2	2.03	0.41
18:R:3:BMA:H3	18:R:4:MAN:C5	2.47	0.41
1:B:582:ALA:HB1	4:G:221:ALA:HB3	2.03	0.41
1:B:606:THR:HA	4:G:503:ARG:HD2	2.03	0.41
4:G:255:VAL:HG23	4:G:475:MET:SD	2.61	0.41
4:G:114:GLN:O	4:G:117:LYS:HB2	2.21	0.40
4:G:189:THR:O	4:G:189:THR:OG1	2.39	0.40
6:L:60:ASP:N	6:L:60:ASP:OD1	2.54	0.40
4:G:87:GLU:HG2	9:C:1:NAG:H82	2.03	0.40
5:H:144:PHE:HA	5:H:145:PRO:HA	1.88	0.40
1:B:620:ASP:N	1:B:620:ASP:OD1	2.51	0.40
2:D:100(D):TRP:HZ2	3:E:91:TYR:HB2	1.86	0.40
18:R:4:MAN:H2	18:R:5:MAN:H2	1.79	0.40
3:E:54:ARG:HB2	3:E:54:ARG:HH11	1.87	0.40
4:G:292:VAL:HG23	4:G:449:ILE:HB	2.02	0.40
5:H:100(D):VAL:O	5:H:100(I):GLU:HB2	2.22	0.40
3:E:63:SER:O	3:E:73:LEU:HD12	2.22	0.40
3:E:84:THR:O	3:E:104:VAL:HG22	2.22	0.40
3:E:207:ALA:HA	3:E:208:PRO:HD3	1.92	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	149/161 (92%)	135 (91%)	14 (9%)	0	100	100
2	D	241/243 (99%)	217 (90%)	24 (10%)	0	100	100
3	E	209/216 (97%)	188 (90%)	19 (9%)	2 (1%)	13	42
4	G	445/475 (94%)	397 (89%)	45 (10%)	3 (1%)	19	51
5	H	224/244 (92%)	202 (90%)	22 (10%)	0	100	100
6	L	208/213 (98%)	191 (92%)	17 (8%)	0	100	100
7	U	117/240 (49%)	105 (90%)	12 (10%)	0	100	100
7	V	96/240 (40%)	81 (84%)	15 (16%)	0	100	100
All	All	1689/2032 (83%)	1516 (90%)	168 (10%)	5 (0%)	37	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	187	SER
4	G	313	PRO
4	G	188	ASN
3	E	208	PRO
4	G	65	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	127/134 (95%)	104 (82%)	23 (18%)	1	6
2	D	205/206 (100%)	192 (94%)	13 (6%)	15	42
3	E	186/189 (98%)	171 (92%)	15 (8%)	9	33
4	G	406/427 (95%)	354 (87%)	52 (13%)	3	15
5	H	198/213 (93%)	186 (94%)	12 (6%)	15	43
6	L	178/181 (98%)	161 (90%)	17 (10%)	7	26
7	U	102/192 (53%)	92 (90%)	10 (10%)	6	25
7	V	81/192 (42%)	73 (90%)	8 (10%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1483/1734 (86%)	1333 (90%)	150 (10%)	6 23

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	515	ILE
1	B	520	LEU
1	B	523	LEU
1	B	549	VAL
1	B	560	GLU
1	B	562	GLN
1	B	564	ARG
1	B	566	LEU
1	B	568	LEU
1	B	575	GLN
1	B	593	LEU
1	B	598	CYS
1	B	602	LEU
1	B	603	ILE
1	B	606	THR
1	B	620	ASP
1	B	622	ILE
1	B	625	ASN
1	B	634	GLU
1	B	644	THR
1	B	646	ILE
1	B	655	LYS
1	B	662	GLU
2	D	40	THR
2	D	54	SER
2	D	58	ASN
2	D	63	PHE
2	D	66	ARG
2	D	100(C)	THR
2	D	102	LEU
2	D	108	LEU
2	D	138	LEU
2	D	163	VAL
2	D	182	VAL
2	D	194	TYR
2	D	217	ASP
3	E	45	THR

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Mol	Chain	Res	Type
3	E	50	GLU
3	E	51	ASP
3	E	54	ARG
3	E	63	SER
3	E	89	CYS
3	E	96	CYS
3	E	116	THR
3	E	134	CYS
3	E	138	ASP
3	E	153	SER
3	E	166	LYS
3	E	177	TYR
3	E	180	LEU
3	E	195	VAL
4	G	38	VAL
4	G	54	CYS
4	G	57	ASP
4	G	61	TYR
4	G	67	ASN
4	G	68	VAL
4	G	80	ASN
4	G	108	ILE
4	G	112	TRP
4	G	115	SER
4	G	123	THR
4	G	163	THR
4	G	166	ARG
4	G	169	VAL
4	G	172	GLU
4	G	179	LEU
4	G	187	ASN
4	G	189	THR
4	G	192	ARG
4	G	196	CYS
4	G	203	GLN
4	G	208	ILE
4	G	228	CYS
4	G	252	ARG
4	G	255	VAL
4	G	260	LEU
4	G	269	GLU
4	G	282	LYS

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Mol	Chain	Res	Type
4	G	283	THR
4	G	286	VAL
4	G	290	GLU
4	G	307	ILE
4	G	309	ILE
4	G	317	PHE
4	G	333	ILE
4	G	341	THR
4	G	343	LYS
4	G	349	LEU
4	G	370	GLU
4	G	371	ILE
4	G	375	SER
4	G	381	GLU
4	G	388	THR
4	G	443	ILE
4	G	450	THR
4	G	452	LEU
4	G	453	LEU
4	G	459	CYS
4	G	461	ASN
4	G	469	ARG
4	G	505	VAL
4	G	508	ARG
5	H	1	GLN
5	H	12	VAL
5	H	56	ASP
5	H	77	LEU
5	H	86	ASP
5	H	99	ARG
5	H	100(G)	PHE
5	H	100(J)	TRP
5	H	100(L)	THR
5	H	133	THR
5	H	139	LEU
5	H	142	ASP
6	L	9	PHE
6	L	32	SER
6	L	48	ILE
6	L	50	ASN
6	L	52	ASN
6	L	53	ASP

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Mol	Chain	Res	Type
6	L	69	THR
6	L	75	ILE
6	L	90	ILE
6	L	97	VAL
6	L	130	LYS
6	L	160	VAL
6	L	176	SER
6	L	191	SER
6	L	202	THR
6	L	203	VAL
6	L	206	THR
7	U	2	VAL
7	U	32	CYS
7	U	70	THR
7	U	71	ARG
7	U	76	ASP
7	U	82(A)	ARG
7	U	83	THR
7	U	85	ASP
7	U	93	THR
7	U	109	VAL
7	V	11	LEU
7	V	25	THR
7	V	27	GLN
7	V	66	ARG
7	V	70	ASP
7	V	72	ASN
7	V	73	LEU
7	V	102	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	G	188	ASN
6	L	109	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

125 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
8	NAG	A	1	8,1	14,14,15	0.39	0	17,19,21	0.47	0
8	NAG	A	2	8	14,14,15	0.42	0	17,19,21	1.16	3 (17%)
8	BMA	A	3	8	11,11,12	1.09	1 (9%)	15,15,17	1.33	3 (20%)
9	NAG	C	1	9,4	14,14,15	0.44	0	17,19,21	0.48	0
9	NAG	C	2	9	14,14,15	0.29	0	17,19,21	0.43	0
9	BMA	C	3	9	11,11,12	0.49	0	15,15,17	0.83	0
9	MAN	C	4	9	11,11,12	0.59	0	15,15,17	1.16	1 (6%)
9	MAN	C	5	9	11,11,12	0.79	0	15,15,17	0.94	1 (6%)
9	MAN	C	6	9	11,11,12	0.60	0	15,15,17	1.10	2 (13%)
9	MAN	C	7	9	11,11,12	0.94	1 (9%)	15,15,17	0.88	1 (6%)
10	NAG	F	1	4,10	14,14,15	0.44	0	17,19,21	0.53	0
10	NAG	F	2	10	14,14,15	0.39	0	17,19,21	0.81	1 (5%)
10	BMA	F	3	10	11,11,12	1.11	0	15,15,17	1.19	2 (13%)
10	MAN	F	4	10	11,11,12	0.63	0	15,15,17	1.06	2 (13%)
10	MAN	F	5	10	11,11,12	0.84	0	15,15,17	1.47	2 (13%)
10	MAN	F	6	10	11,11,12	0.66	0	15,15,17	0.96	2 (13%)
10	MAN	F	7	10	11,11,12	0.93	1 (9%)	15,15,17	1.31	3 (20%)
10	MAN	F	8	10	11,11,12	0.76	0	15,15,17	0.92	1 (6%)
10	MAN	F	9	10	11,11,12	0.61	0	15,15,17	0.96	2 (13%)
11	NAG	I	1	4,11	14,14,15	0.32	0	17,19,21	0.86	1 (5%)
11	NAG	I	2	11	14,14,15	0.27	0	17,19,21	0.64	0
11	BMA	I	3	11	11,11,12	0.67	0	15,15,17	0.81	0
11	MAN	I	4	11	11,11,12	0.90	0	15,15,17	1.63	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	MAN	I	5	11	11,11,12	0.83	0	15,15,17	0.93	1 (6%)
11	MAN	I	6	11	11,11,12	0.97	1 (9%)	15,15,17	1.58	2 (13%)
11	MAN	I	7	11	11,11,12	0.72	0	15,15,17	0.93	1 (6%)
12	NAG	J	1	12,4	14,14,15	0.88	1 (7%)	17,19,21	0.71	0
12	NAG	J	2	12	14,14,15	0.39	0	17,19,21	0.95	2 (11%)
12	BMA	J	3	12	11,11,12	0.50	0	15,15,17	0.98	1 (6%)
12	MAN	J	4	12	11,11,12	0.81	0	15,15,17	1.03	2 (13%)
12	MAN	J	5	12	11,11,12	0.60	0	15,15,17	1.05	2 (13%)
12	MAN	J	6	12	11,11,12	0.67	0	15,15,17	1.02	2 (13%)
12	MAN	J	7	12	11,11,12	0.70	0	15,15,17	1.18	2 (13%)
13	NAG	K	1	13,4	14,14,15	0.36	0	17,19,21	0.39	0
13	NAG	K	2	13	14,14,15	0.19	0	17,19,21	0.47	0
13	BMA	K	3	13	11,11,12	0.62	0	15,15,17	0.71	0
13	MAN	K	4	13	11,11,12	0.66	0	15,15,17	0.91	2 (13%)
10	NAG	M	1	4,10	14,14,15	0.23	0	17,19,21	0.59	0
10	NAG	M	2	10	14,14,15	0.34	0	17,19,21	0.52	0
10	BMA	M	3	10	11,11,12	0.63	0	15,15,17	0.73	0
10	MAN	M	4	10	11,11,12	0.63	0	15,15,17	1.19	1 (6%)
10	MAN	M	5	10	11,11,12	0.81	1 (9%)	15,15,17	1.42	1 (6%)
10	MAN	M	6	10	11,11,12	0.90	1 (9%)	15,15,17	0.99	1 (6%)
10	MAN	M	7	10	11,11,12	1.04	0	15,15,17	1.43	2 (13%)
10	MAN	M	8	10	11,11,12	0.72	0	15,15,17	1.02	2 (13%)
10	MAN	M	9	10	11,11,12	0.71	0	15,15,17	1.03	2 (13%)
14	NAG	N	1	4,14	14,14,15	0.60	1 (7%)	17,19,21	0.69	0
14	NAG	N	2	14	14,14,15	0.20	0	17,19,21	0.83	0
14	BMA	N	3	14	11,11,12	1.25	1 (9%)	15,15,17	1.83	3 (20%)
14	MAN	N	4	14	11,11,12	0.72	0	15,15,17	0.96	1 (6%)
14	MAN	N	5	14	11,11,12	0.90	1 (9%)	15,15,17	1.14	1 (6%)
14	MAN	N	6	14	11,11,12	0.72	0	15,15,17	0.93	2 (13%)
14	MAN	N	7	14	11,11,12	1.27	2 (18%)	15,15,17	1.19	2 (13%)
14	MAN	N	8	14	11,11,12	0.66	0	15,15,17	1.31	2 (13%)
15	NAG	O	1	15,4	14,14,15	0.40	0	17,19,21	0.50	0
15	NAG	O	2	15	14,14,15	0.23	0	17,19,21	0.53	0
15	BMA	O	3	15	11,11,12	1.44	1 (9%)	15,15,17	1.02	1 (6%)
15	MAN	O	4	15	11,11,12	0.77	1 (9%)	15,15,17	1.06	2 (13%)
15	MAN	O	5	15	11,11,12	0.83	1 (9%)	15,15,17	1.13	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	NAG	P	1	16,4	14,14,15	0.65	1 (7%)	17,19,21	0.84	1 (5%)
16	NAG	P	2	16	14,14,15	0.29	0	17,19,21	0.64	0
16	BMA	P	3	16	11,11,12	0.92	1 (9%)	15,15,17	1.11	1 (6%)
16	MAN	P	4	16	11,11,12	1.22	1 (9%)	15,15,17	1.12	0
16	MAN	P	5	16	11,11,12	1.77	4 (36%)	15,15,17	1.20	2 (13%)
16	MAN	P	6	16	11,11,12	0.76	0	15,15,17	1.01	1 (6%)
16	MAN	P	7	16	11,11,12	0.72	0	15,15,17	1.32	2 (13%)
16	MAN	P	8	16	11,11,12	0.89	0	15,15,17	1.01	1 (6%)
17	NAG	Q	1	4,17	14,14,15	0.32	0	17,19,21	0.48	0
17	MAN	Q	10	17	11,11,12	0.68	0	15,15,17	1.05	2 (13%)
17	NAG	Q	2	17	14,14,15	0.21	0	17,19,21	0.71	0
17	BMA	Q	3	17	11,11,12	0.93	1 (9%)	15,15,17	0.88	0
17	MAN	Q	4	17	11,11,12	0.73	1 (9%)	15,15,17	1.38	2 (13%)
17	MAN	Q	5	17	11,11,12	0.67	0	15,15,17	0.93	2 (13%)
17	MAN	Q	6	17	11,11,12	0.73	0	15,15,17	1.04	2 (13%)
17	MAN	Q	7	17	11,11,12	0.68	0	15,15,17	1.08	2 (13%)
17	MAN	Q	8	17	11,11,12	0.68	0	15,15,17	1.10	2 (13%)
17	MAN	Q	9	17	11,11,12	0.66	0	15,15,17	0.92	2 (13%)
18	NAG	R	1	18,4	14,14,15	0.75	1 (7%)	17,19,21	0.78	0
18	NAG	R	2	18	14,14,15	0.19	0	17,19,21	0.37	0
18	BMA	R	3	18	11,11,12	0.94	1 (9%)	15,15,17	1.19	1 (6%)
18	MAN	R	4	18	11,11,12	1.38	2 (18%)	15,15,17	1.88	2 (13%)
18	MAN	R	5	18	11,11,12	0.88	1 (9%)	15,15,17	1.08	2 (13%)
18	MAN	R	6	18	11,11,12	0.60	0	15,15,17	1.23	2 (13%)
18	MAN	R	7	18	11,11,12	0.72	0	15,15,17	1.13	2 (13%)
18	NAG	S	1	18,4	14,14,15	0.24	0	17,19,21	0.39	0
18	NAG	S	2	18	14,14,15	0.28	0	17,19,21	0.74	0
18	BMA	S	3	18	11,11,12	0.82	0	15,15,17	0.97	0
18	MAN	S	4	18	11,11,12	0.64	0	15,15,17	1.08	2 (13%)
18	MAN	S	5	18	11,11,12	0.75	0	15,15,17	1.06	2 (13%)
18	MAN	S	6	18	11,11,12	0.51	0	15,15,17	1.03	2 (13%)
18	MAN	S	7	18	11,11,12	0.69	0	15,15,17	1.00	2 (13%)
13	NAG	T	1	13,4	14,14,15	0.38	0	17,19,21	0.84	2 (11%)
13	NAG	T	2	13	14,14,15	0.47	0	17,19,21	0.79	1 (5%)
13	BMA	T	3	13	11,11,12	1.04	1 (9%)	15,15,17	1.03	1 (6%)
13	MAN	T	4	13	11,11,12	0.74	0	15,15,17	1.29	2 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	NAG	W	1	4,19	14,14,15	0.34	0	17,19,21	0.67	0
19	NAG	W	2	19	14,14,15	0.57	0	17,19,21	0.73	1 (5%)
19	BMA	W	3	19	11,11,12	0.68	0	15,15,17	0.85	0
19	MAN	W	4	19	11,11,12	0.89	0	15,15,17	1.20	2 (13%)
19	MAN	W	5	19	11,11,12	0.71	0	15,15,17	1.18	2 (13%)
19	MAN	W	6	19	11,11,12	0.73	0	15,15,17	0.96	2 (13%)
19	MAN	W	7	19	11,11,12	0.67	0	15,15,17	0.91	1 (6%)
19	MAN	W	8	19	11,11,12	0.78	1 (9%)	15,15,17	1.23	2 (13%)
20	NAG	X	1	20,4	14,14,15	0.39	0	17,19,21	0.53	0
20	NAG	X	2	20	14,14,15	0.43	0	17,19,21	1.41	2 (11%)
20	BMA	X	3	20	11,11,12	0.95	0	15,15,17	1.46	1 (6%)
20	MAN	X	4	20	11,11,12	0.66	0	15,15,17	1.17	2 (13%)
20	MAN	X	5	20	11,11,12	0.70	0	15,15,17	0.93	2 (13%)
20	MAN	X	6	20	11,11,12	0.84	0	15,15,17	0.94	1 (6%)
21	NAG	Y	1	4,21	14,14,15	0.26	0	17,19,21	0.44	0
21	NAG	Y	2	21	14,14,15	0.27	0	17,19,21	0.40	0
22	NAG	Z	1	22,4	14,14,15	0.29	0	17,19,21	0.43	0
22	NAG	Z	2	22	14,14,15	0.26	0	17,19,21	0.46	0
22	BMA	Z	3	22	11,11,12	0.97	1 (9%)	15,15,17	1.22	2 (13%)
22	MAN	Z	4	22	11,11,12	0.73	0	15,15,17	1.45	2 (13%)
22	MAN	Z	5	22	11,11,12	1.91	4 (36%)	15,15,17	1.17	2 (13%)
22	MAN	Z	6	22	11,11,12	0.70	0	15,15,17	1.10	2 (13%)
21	NAG	a	1	4,21	14,14,15	0.73	1 (7%)	17,19,21	0.71	0
21	NAG	a	2	21	14,14,15	0.38	0	17,19,21	0.60	0
23	NAG	b	1	23,7	14,14,15	0.44	0	17,19,21	0.59	0
23	NAG	b	2	23	14,14,15	0.53	0	17,19,21	1.29	2 (11%)
23	BMA	b	3	23	11,11,12	0.55	0	15,15,17	1.34	2 (13%)
23	MAN	b	4	23	11,11,12	0.97	1 (9%)	15,15,17	1.39	3 (20%)
23	MAN	b	5	23	11,11,12	1.00	1 (9%)	15,15,17	0.84	1 (6%)
23	MAN	b	6	23	11,11,12	0.90	1 (9%)	15,15,17	1.60	2 (13%)

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
8	NAG	A	1	8,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	2	8	-	0/6/23/26	0/1/1/1
8	BMA	A	3	8	-	2/2/19/22	0/1/1/1
9	NAG	C	1	9,4	-	2/6/23/26	0/1/1/1
9	NAG	C	2	9	-	0/6/23/26	0/1/1/1
9	BMA	C	3	9	-	2/2/19/22	0/1/1/1
9	MAN	C	4	9	-	2/2/19/22	0/1/1/1
9	MAN	C	5	9	-	0/2/19/22	0/1/1/1
9	MAN	C	6	9	-	2/2/19/22	0/1/1/1
9	MAN	C	7	9	-	2/2/19/22	0/1/1/1
10	NAG	F	1	4,10	-	2/6/23/26	0/1/1/1
10	NAG	F	2	10	-	2/6/23/26	0/1/1/1
10	BMA	F	3	10	-	1/2/19/22	0/1/1/1
10	MAN	F	4	10	-	0/2/19/22	0/1/1/1
10	MAN	F	5	10	-	0/2/19/22	0/1/1/1
10	MAN	F	6	10	-	0/2/19/22	0/1/1/1
10	MAN	F	7	10	-	2/2/19/22	0/1/1/1
10	MAN	F	8	10	-	0/2/19/22	0/1/1/1
10	MAN	F	9	10	-	0/2/19/22	0/1/1/1
11	NAG	I	1	4,11	-	2/6/23/26	0/1/1/1
11	NAG	I	2	11	-	1/6/23/26	0/1/1/1
11	BMA	I	3	11	-	2/2/19/22	0/1/1/1
11	MAN	I	4	11	-	2/2/19/22	0/1/1/1
11	MAN	I	5	11	-	0/2/19/22	0/1/1/1
11	MAN	I	6	11	-	1/2/19/22	0/1/1/1
11	MAN	I	7	11	-	1/2/19/22	0/1/1/1
12	NAG	J	1	12,4	-	2/6/23/26	0/1/1/1
12	NAG	J	2	12	-	1/6/23/26	0/1/1/1
12	BMA	J	3	12	-	0/2/19/22	0/1/1/1
12	MAN	J	4	12	-	2/2/19/22	0/1/1/1
12	MAN	J	5	12	-	1/2/19/22	0/1/1/1
12	MAN	J	6	12	-	0/2/19/22	0/1/1/1
12	MAN	J	7	12	-	0/2/19/22	0/1/1/1
13	NAG	K	1	13,4	-	0/6/23/26	0/1/1/1
13	NAG	K	2	13	-	1/6/23/26	0/1/1/1
13	BMA	K	3	13	-	0/2/19/22	0/1/1/1
13	MAN	K	4	13	-	2/2/19/22	0/1/1/1
10	NAG	M	1	4,10	-	0/6/23/26	0/1/1/1
10	NAG	M	2	10	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BMA	M	3	10	-	0/2/19/22	0/1/1/1
10	MAN	M	4	10	-	0/2/19/22	0/1/1/1
10	MAN	M	5	10	-	0/2/19/22	0/1/1/1
10	MAN	M	6	10	-	0/2/19/22	0/1/1/1
10	MAN	M	7	10	-	1/2/19/22	0/1/1/1
10	MAN	M	8	10	-	0/2/19/22	0/1/1/1
10	MAN	M	9	10	-	0/2/19/22	0/1/1/1
14	NAG	N	1	4,14	-	1/6/23/26	0/1/1/1
14	NAG	N	2	14	-	3/6/23/26	0/1/1/1
14	BMA	N	3	14	-	1/2/19/22	0/1/1/1
14	MAN	N	4	14	-	0/2/19/22	0/1/1/1
14	MAN	N	5	14	-	0/2/19/22	0/1/1/1
14	MAN	N	6	14	-	1/2/19/22	0/1/1/1
14	MAN	N	7	14	-	2/2/19/22	0/1/1/1
14	MAN	N	8	14	-	1/2/19/22	0/1/1/1
15	NAG	O	1	15,4	-	0/6/23/26	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	-	0/2/19/22	0/1/1/1
16	NAG	P	1	16,4	-	2/6/23/26	0/1/1/1
16	NAG	P	2	16	-	2/6/23/26	0/1/1/1
16	BMA	P	3	16	-	1/2/19/22	0/1/1/1
16	MAN	P	4	16	-	0/2/19/22	0/1/1/1
16	MAN	P	5	16	-	1/2/19/22	0/1/1/1
16	MAN	P	6	16	-	0/2/19/22	0/1/1/1
16	MAN	P	7	16	-	1/2/19/22	0/1/1/1
16	MAN	P	8	16	-	0/2/19/22	0/1/1/1
17	NAG	Q	1	4,17	-	2/6/23/26	0/1/1/1
17	MAN	Q	10	17	-	2/2/19/22	0/1/1/1
17	NAG	Q	2	17	-	3/6/23/26	0/1/1/1
17	BMA	Q	3	17	-	0/2/19/22	0/1/1/1
17	MAN	Q	4	17	-	2/2/19/22	0/1/1/1
17	MAN	Q	5	17	-	2/2/19/22	0/1/1/1
17	MAN	Q	6	17	-	0/2/19/22	0/1/1/1
17	MAN	Q	7	17	-	0/2/19/22	0/1/1/1
17	MAN	Q	8	17	-	0/2/19/22	0/1/1/1
17	MAN	Q	9	17	-	0/2/19/22	0/1/1/1
18	NAG	R	1	18,4	-	0/6/23/26	0/1/1/1
18	NAG	R	2	18	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BMA	R	3	18	-	2/2/19/22	0/1/1/1
18	MAN	R	4	18	-	0/2/19/22	0/1/1/1
18	MAN	R	5	18	-	0/2/19/22	0/1/1/1
18	MAN	R	6	18	-	0/2/19/22	0/1/1/1
18	MAN	R	7	18	-	0/2/19/22	0/1/1/1
18	NAG	S	1	18,4	-	0/6/23/26	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	-	0/2/19/22	0/1/1/1
18	MAN	S	6	18	-	1/2/19/22	0/1/1/1
18	MAN	S	7	18	-	0/2/19/22	0/1/1/1
13	NAG	T	1	13,4	-	0/6/23/26	0/1/1/1
13	NAG	T	2	13	-	2/6/23/26	0/1/1/1
13	BMA	T	3	13	-	0/2/19/22	0/1/1/1
13	MAN	T	4	13	-	0/2/19/22	0/1/1/1
19	NAG	W	1	4,19	-	3/6/23/26	0/1/1/1
19	NAG	W	2	19	-	2/6/23/26	0/1/1/1
19	BMA	W	3	19	-	2/2/19/22	0/1/1/1
19	MAN	W	4	19	-	1/2/19/22	0/1/1/1
19	MAN	W	5	19	-	0/2/19/22	0/1/1/1
19	MAN	W	6	19	-	0/2/19/22	0/1/1/1
19	MAN	W	7	19	-	0/2/19/22	0/1/1/1
19	MAN	W	8	19	-	0/2/19/22	0/1/1/1
20	NAG	X	1	20,4	-	2/6/23/26	0/1/1/1
20	NAG	X	2	20	-	1/6/23/26	0/1/1/1
20	BMA	X	3	20	-	1/2/19/22	0/1/1/1
20	MAN	X	4	20	-	0/2/19/22	0/1/1/1
20	MAN	X	5	20	-	0/2/19/22	0/1/1/1
20	MAN	X	6	20	-	0/2/19/22	0/1/1/1
21	NAG	Y	1	4,21	-	0/6/23/26	0/1/1/1
21	NAG	Y	2	21	-	0/6/23/26	0/1/1/1
22	NAG	Z	1	22,4	-	2/6/23/26	0/1/1/1
22	NAG	Z	2	22	-	2/6/23/26	0/1/1/1
22	BMA	Z	3	22	-	2/2/19/22	0/1/1/1
22	MAN	Z	4	22	-	0/2/19/22	0/1/1/1
22	MAN	Z	5	22	-	0/2/19/22	0/1/1/1
22	MAN	Z	6	22	-	0/2/19/22	0/1/1/1
21	NAG	a	1	4,21	-	0/6/23/26	0/1/1/1
21	NAG	a	2	21	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	NAG	b	1	23,7	-	0/6/23/26	0/1/1/1
23	NAG	b	2	23	-	0/6/23/26	0/1/1/1
23	BMA	b	3	23	-	0/2/19/22	0/1/1/1
23	MAN	b	4	23	-	2/2/19/22	0/1/1/1
23	MAN	b	5	23	-	0/2/19/22	0/1/1/1
23	MAN	b	6	23	-	0/2/19/22	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	5	MAN	C2-C3	3.84	1.58	1.52
22	Z	5	MAN	C2-C3	3.71	1.58	1.52
15	O	3	BMA	C1-C2	3.55	1.60	1.52
18	R	4	MAN	C1-C2	3.36	1.59	1.52
14	N	3	BMA	O5-C5	3.25	1.50	1.43
12	J	1	NAG	O5-C1	-3.19	1.38	1.43
22	Z	5	MAN	O2-C2	3.02	1.49	1.43
22	Z	5	MAN	O5-C1	-3.00	1.38	1.43
13	T	3	BMA	C1-C2	2.89	1.58	1.52
14	N	7	MAN	C2-C3	2.87	1.56	1.52
8	A	3	BMA	O5-C5	2.86	1.49	1.43
16	P	5	MAN	O2-C2	2.75	1.49	1.43
23	b	4	MAN	C1-C2	2.66	1.58	1.52
18	R	1	NAG	O5-C1	-2.65	1.39	1.43
18	R	4	MAN	O5-C1	2.56	1.47	1.43
11	I	6	MAN	C1-C2	2.49	1.57	1.52
9	C	7	MAN	O5-C1	-2.48	1.39	1.43
21	a	1	NAG	O5-C1	-2.44	1.39	1.43
17	Q	3	BMA	O5-C1	-2.40	1.39	1.43
22	Z	5	MAN	C4-C3	2.40	1.58	1.52
10	M	5	MAN	C1-C2	2.37	1.57	1.52
16	P	4	MAN	C2-C3	2.37	1.56	1.52
10	M	6	MAN	C1-C2	2.35	1.57	1.52
16	P	3	BMA	C1-C2	2.35	1.57	1.52
10	F	7	MAN	C1-C2	2.33	1.57	1.52
15	O	5	MAN	C1-C2	2.29	1.57	1.52
16	P	5	MAN	O5-C1	-2.24	1.40	1.43
16	P	1	NAG	O5-C1	-2.23	1.40	1.43
23	b	5	MAN	C1-C2	2.22	1.57	1.52
18	R	5	MAN	C1-C2	2.21	1.57	1.52
14	N	5	MAN	O5-C1	-2.16	1.40	1.43
18	R	3	BMA	C4-C3	2.15	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	4	MAN	C1-C2	2.15	1.57	1.52
15	O	4	MAN	C1-C2	2.14	1.57	1.52
19	W	8	MAN	C1-C2	2.11	1.57	1.52
14	N	7	MAN	O3-C3	2.04	1.47	1.43
23	b	6	MAN	O5-C5	2.03	1.47	1.43
14	N	1	NAG	O5-C1	-2.03	1.40	1.43
16	P	5	MAN	C4-C3	2.03	1.57	1.52
22	Z	3	BMA	C1-C2	2.02	1.56	1.52

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	4	MAN	C1-O5-C5	5.94	120.25	112.19
23	b	6	MAN	C1-O5-C5	5.29	119.36	112.19
11	I	6	MAN	C1-O5-C5	5.07	119.06	112.19
10	F	5	MAN	C1-O5-C5	4.91	118.84	112.19
14	N	3	BMA	C1-O5-C5	4.53	118.33	112.19
10	M	5	MAN	C1-O5-C5	4.50	118.30	112.19
20	X	3	BMA	C1-O5-C5	4.49	118.28	112.19
20	X	2	NAG	C1-O5-C5	4.22	117.91	112.19
13	T	4	MAN	C1-O5-C5	4.02	117.64	112.19
10	M	7	MAN	C1-O5-C5	4.02	117.64	112.19
14	N	8	MAN	C1-O5-C5	3.96	117.56	112.19
17	Q	4	MAN	C1-O5-C5	3.93	117.52	112.19
11	I	4	MAN	O3-C3-C2	3.90	117.46	109.99
8	A	3	BMA	C1-O5-C5	3.86	117.42	112.19
23	b	3	BMA	C1-O5-C5	3.83	117.38	112.19
18	R	6	MAN	C1-O5-C5	3.74	117.26	112.19
11	I	4	MAN	C1-O5-C5	3.69	117.19	112.19
14	N	3	BMA	O3-C3-C2	3.68	117.04	109.99
22	Z	4	MAN	C1-O5-C5	3.67	117.17	112.19
10	M	4	MAN	C1-O5-C5	3.64	117.13	112.19
23	b	2	NAG	C1-O5-C5	3.60	117.07	112.19
14	N	5	MAN	O2-C2-C3	-3.59	102.95	110.14
19	W	8	MAN	C1-O5-C5	3.45	116.87	112.19
16	P	7	MAN	C1-O5-C5	3.45	116.87	112.19
20	X	4	MAN	C1-O5-C5	3.45	116.86	112.19
14	N	7	MAN	O3-C3-C2	3.37	116.45	109.99
9	C	4	MAN	C1-O5-C5	3.37	116.75	112.19
23	b	4	MAN	C1-O5-C5	3.30	116.66	112.19
22	Z	4	MAN	O3-C3-C2	3.26	116.24	109.99
16	P	7	MAN	O2-C2-C3	-3.22	103.68	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	J	7	MAN	C1-O5-C5	3.19	116.51	112.19
9	C	6	MAN	C1-O5-C5	3.13	116.44	112.19
10	M	7	MAN	O3-C3-C2	3.06	115.85	109.99
19	W	5	MAN	C1-O5-C5	3.03	116.30	112.19
18	R	7	MAN	C1-O5-C5	3.01	116.27	112.19
18	S	4	MAN	C1-O5-C5	2.96	116.20	112.19
19	W	4	MAN	C1-O5-C5	2.95	116.19	112.19
18	R	4	MAN	C1-C2-C3	2.95	113.29	109.67
12	J	5	MAN	C1-O5-C5	2.86	116.06	112.19
10	F	4	MAN	C1-O5-C5	2.85	116.06	112.19
10	F	3	BMA	O3-C3-C4	2.83	116.88	110.35
22	Z	5	MAN	O2-C2-C1	2.81	114.90	109.15
17	Q	7	MAN	C1-O5-C5	2.79	115.97	112.19
17	Q	6	MAN	C1-O5-C5	2.78	115.96	112.19
10	F	7	MAN	C1-C2-C3	2.78	113.08	109.67
20	X	2	NAG	O4-C4-C5	2.77	116.18	109.30
10	M	8	MAN	C1-O5-C5	2.77	115.94	112.19
17	Q	10	MAN	C1-O5-C5	2.76	115.93	112.19
18	R	5	MAN	C1-O5-C5	2.76	115.93	112.19
16	P	3	BMA	C1-C2-C3	2.74	113.04	109.67
10	F	7	MAN	C1-O5-C5	2.70	115.86	112.19
18	S	5	MAN	C1-O5-C5	2.70	115.85	112.19
19	W	4	MAN	O3-C3-C2	2.67	115.11	109.99
18	S	6	MAN	C1-O5-C5	2.64	115.76	112.19
16	P	5	MAN	O2-C2-C1	2.62	114.52	109.15
22	Z	6	MAN	C1-O5-C5	2.61	115.73	112.19
18	R	3	BMA	C1-C2-C3	-2.57	106.50	109.67
8	A	2	NAG	C1-O5-C5	2.57	115.67	112.19
14	N	3	BMA	C3-C4-C5	-2.53	105.72	110.24
19	W	5	MAN	O2-C2-C3	-2.53	105.07	110.14
12	J	3	BMA	C1-O5-C5	2.51	115.59	112.19
11	I	4	MAN	C1-C2-C3	-2.51	106.58	109.67
12	J	6	MAN	C1-O5-C5	2.49	115.57	112.19
15	O	5	MAN	C1-O5-C5	2.49	115.57	112.19
22	Z	3	BMA	C1-C2-C3	-2.49	106.61	109.67
17	Q	8	MAN	C1-O5-C5	2.48	115.56	112.19
12	J	2	NAG	C3-C4-C5	2.48	114.66	110.24
14	N	7	MAN	C1-O5-C5	2.47	115.54	112.19
13	T	3	BMA	O2-C2-C3	-2.47	105.20	110.14
12	J	4	MAN	C1-O5-C5	2.45	115.51	112.19
8	A	2	NAG	O4-C4-C5	2.44	115.36	109.30
14	N	4	MAN	O2-C2-C3	-2.44	105.26	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	8	MAN	O2-C2-C3	-2.43	105.27	110.14
22	Z	3	BMA	O2-C2-C3	-2.41	105.31	110.14
15	O	4	MAN	C1-O5-C5	2.38	115.41	112.19
20	X	6	MAN	O2-C2-C3	-2.36	105.41	110.14
18	S	4	MAN	O2-C2-C3	-2.36	105.41	110.14
22	Z	5	MAN	C2-C3-C4	2.35	114.97	110.89
12	J	5	MAN	O2-C2-C3	-2.34	105.45	110.14
15	O	4	MAN	O2-C2-C3	-2.34	105.45	110.14
11	I	6	MAN	O2-C2-C3	-2.33	105.46	110.14
17	Q	10	MAN	O2-C2-C3	-2.33	105.47	110.14
12	J	7	MAN	O2-C2-C3	-2.33	105.47	110.14
10	F	9	MAN	C1-O5-C5	2.33	115.34	112.19
17	Q	4	MAN	O2-C2-C3	-2.32	105.49	110.14
8	A	2	NAG	O4-C4-C3	2.32	115.71	110.35
9	C	6	MAN	O2-C2-C3	-2.32	105.50	110.14
10	F	8	MAN	O2-C2-C3	-2.31	105.50	110.14
11	I	5	MAN	C1-O5-C5	2.30	115.31	112.19
22	Z	6	MAN	O2-C2-C3	-2.28	105.56	110.14
19	W	7	MAN	O2-C2-C3	-2.28	105.57	110.14
16	P	6	MAN	O2-C2-C3	-2.28	105.57	110.14
14	N	8	MAN	O2-C2-C3	-2.28	105.58	110.14
18	R	6	MAN	O2-C2-C3	-2.27	105.58	110.14
18	S	7	MAN	O2-C2-C3	-2.27	105.58	110.14
19	W	6	MAN	O2-C2-C3	-2.26	105.61	110.14
10	F	3	BMA	C1-O5-C5	2.26	115.25	112.19
17	Q	9	MAN	O2-C2-C3	-2.26	105.62	110.14
18	R	7	MAN	O2-C2-C3	-2.24	105.64	110.14
18	S	7	MAN	C1-O5-C5	2.24	115.23	112.19
10	F	4	MAN	O2-C2-C3	-2.24	105.65	110.14
10	F	9	MAN	O2-C2-C3	-2.24	105.66	110.14
10	M	9	MAN	O2-C2-C3	-2.24	105.66	110.14
15	O	5	MAN	O2-C2-C3	-2.23	105.67	110.14
12	J	4	MAN	O2-C2-C3	-2.23	105.68	110.14
20	X	5	MAN	O2-C2-C3	-2.22	105.68	110.14
13	K	4	MAN	O2-C2-C3	-2.22	105.69	110.14
23	b	6	MAN	O2-C2-C3	-2.22	105.70	110.14
11	I	1	NAG	O5-C1-C2	-2.21	107.80	111.29
12	J	6	MAN	O2-C2-C3	-2.21	105.71	110.14
10	M	9	MAN	C1-O5-C5	2.21	115.18	112.19
11	I	7	MAN	O2-C2-C3	-2.20	105.73	110.14
19	W	8	MAN	O2-C2-C3	-2.18	105.77	110.14
23	b	2	NAG	O4-C4-C5	2.18	114.71	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	5	MAN	C2-C3-C4	2.18	114.67	110.89
10	F	6	MAN	C1-O5-C5	2.18	115.14	112.19
10	F	6	MAN	O2-C2-C3	-2.17	105.78	110.14
18	R	5	MAN	O2-C2-C3	-2.16	105.80	110.14
17	Q	7	MAN	O2-C2-C3	-2.16	105.81	110.14
9	C	5	MAN	O2-C2-C3	-2.16	105.81	110.14
17	Q	5	MAN	C1-O5-C5	2.16	115.12	112.19
17	Q	6	MAN	O2-C2-C3	-2.16	105.82	110.14
9	C	7	MAN	O2-C2-C3	-2.15	105.83	110.14
13	T	1	NAG	O4-C4-C5	-2.15	103.96	109.30
23	b	5	MAN	O2-C2-C3	-2.15	105.84	110.14
10	M	6	MAN	O2-C2-C3	-2.14	105.85	110.14
14	N	6	MAN	O2-C2-C3	-2.14	105.86	110.14
16	P	1	NAG	O4-C4-C3	-2.13	105.42	110.35
13	T	4	MAN	O2-C2-C3	-2.12	105.90	110.14
23	b	4	MAN	C1-C2-C3	2.11	112.26	109.67
23	b	4	MAN	O2-C2-C3	-2.09	105.95	110.14
13	T	1	NAG	O4-C4-C3	2.09	115.18	110.35
10	M	8	MAN	O2-C2-C3	-2.09	105.96	110.14
20	X	4	MAN	O2-C2-C3	-2.08	105.96	110.14
19	W	6	MAN	C1-O5-C5	2.08	115.01	112.19
8	A	3	BMA	O5-C1-C2	-2.08	107.56	110.77
17	Q	5	MAN	O2-C2-C3	-2.08	105.98	110.14
18	S	6	MAN	O2-C2-C3	-2.08	105.98	110.14
18	S	5	MAN	O2-C2-C3	-2.07	105.99	110.14
10	F	7	MAN	O2-C2-C3	-2.06	106.00	110.14
13	K	4	MAN	C1-O5-C5	2.06	114.98	112.19
8	A	3	BMA	O2-C2-C3	-2.06	106.02	110.14
16	P	8	MAN	O2-C2-C3	-2.05	106.04	110.14
14	N	6	MAN	C1-O5-C5	2.04	114.96	112.19
19	W	2	NAG	O4-C4-C3	-2.04	105.64	110.35
10	F	2	NAG	O4-C4-C3	2.04	115.06	110.35
20	X	5	MAN	C1-O5-C5	2.03	114.94	112.19
12	J	2	NAG	O4-C4-C5	-2.03	104.27	109.30
10	F	5	MAN	O2-C2-C3	-2.02	106.08	110.14
15	O	3	BMA	O2-C2-C3	-2.02	106.09	110.14
17	Q	9	MAN	C1-O5-C5	2.02	114.93	112.19
13	T	2	NAG	C1-O5-C5	2.02	114.92	112.19
23	b	3	BMA	C1-C2-C3	2.02	112.14	109.67

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	I	1	NAG	C8-C7-N2-C2
11	I	1	NAG	O7-C7-N2-C2
16	P	2	NAG	O5-C5-C6-O6
10	M	2	NAG	O5-C5-C6-O6
9	C	3	BMA	O5-C5-C6-O6
10	F	1	NAG	C4-C5-C6-O6
13	K	4	MAN	C4-C5-C6-O6
11	I	4	MAN	O5-C5-C6-O6
17	Q	4	MAN	O5-C5-C6-O6
17	Q	5	MAN	O5-C5-C6-O6
10	M	2	NAG	C4-C5-C6-O6
12	J	4	MAN	O5-C5-C6-O6
15	O	2	NAG	O5-C5-C6-O6
23	b	4	MAN	C4-C5-C6-O6
18	R	3	BMA	O5-C5-C6-O6
9	C	3	BMA	C4-C5-C6-O6
16	P	2	NAG	C4-C5-C6-O6
22	Z	3	BMA	C4-C5-C6-O6
9	C	7	MAN	O5-C5-C6-O6
10	F	2	NAG	O5-C5-C6-O6
14	N	2	NAG	O5-C5-C6-O6
22	Z	2	NAG	O5-C5-C6-O6
20	X	1	NAG	O5-C5-C6-O6
13	K	4	MAN	O5-C5-C6-O6
16	P	1	NAG	O5-C5-C6-O6
22	Z	3	BMA	O5-C5-C6-O6
23	b	4	MAN	O5-C5-C6-O6
11	I	2	NAG	C1-C2-N2-C7
11	I	3	BMA	O5-C5-C6-O6
17	Q	4	MAN	C4-C5-C6-O6
15	O	2	NAG	C4-C5-C6-O6
10	F	1	NAG	O5-C5-C6-O6
13	T	2	NAG	C4-C5-C6-O6
9	C	7	MAN	C4-C5-C6-O6
10	F	2	NAG	C4-C5-C6-O6
14	N	2	NAG	C4-C5-C6-O6
17	Q	5	MAN	C4-C5-C6-O6
18	R	3	BMA	C4-C5-C6-O6
11	I	4	MAN	C4-C5-C6-O6
16	P	1	NAG	C4-C5-C6-O6
22	Z	1	NAG	O5-C5-C6-O6
22	Z	2	NAG	C4-C5-C6-O6
20	X	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	A	3	BMA	O5-C5-C6-O6
18	S	6	MAN	O5-C5-C6-O6
17	Q	2	NAG	O5-C5-C6-O6
13	T	2	NAG	O5-C5-C6-O6
9	C	6	MAN	O5-C5-C6-O6
18	S	2	NAG	O5-C5-C6-O6
19	W	1	NAG	O5-C5-C6-O6
12	J	1	NAG	C4-C5-C6-O6
12	J	1	NAG	O5-C5-C6-O6
19	W	1	NAG	C4-C5-C6-O6
12	J	4	MAN	C4-C5-C6-O6
16	P	3	BMA	O5-C5-C6-O6
14	N	7	MAN	O5-C5-C6-O6
19	W	2	NAG	O5-C5-C6-O6
22	Z	1	NAG	C4-C5-C6-O6
14	N	7	MAN	C4-C5-C6-O6
11	I	3	BMA	C4-C5-C6-O6
9	C	4	MAN	C4-C5-C6-O6
19	W	4	MAN	O5-C5-C6-O6
10	F	3	BMA	O5-C5-C6-O6
12	J	5	MAN	O5-C5-C6-O6
20	X	3	BMA	O5-C5-C6-O6
14	N	6	MAN	O5-C5-C6-O6
11	I	6	MAN	O5-C5-C6-O6
11	I	7	MAN	O5-C5-C6-O6
12	J	2	NAG	O5-C5-C6-O6
15	O	3	BMA	O5-C5-C6-O6
16	P	5	MAN	O5-C5-C6-O6
14	N	8	MAN	O5-C5-C6-O6
14	N	3	BMA	O5-C5-C6-O6
17	Q	2	NAG	C4-C5-C6-O6
17	Q	10	MAN	C4-C5-C6-O6
9	C	6	MAN	C4-C5-C6-O6
8	A	3	BMA	C4-C5-C6-O6
19	W	3	BMA	C4-C5-C6-O6
9	C	4	MAN	O5-C5-C6-O6
10	F	7	MAN	O5-C5-C6-O6
10	M	7	MAN	O5-C5-C6-O6
17	Q	1	NAG	C4-C5-C6-O6
14	N	1	NAG	C3-C2-N2-C7
14	N	2	NAG	C3-C2-N2-C7
17	Q	2	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
19	W	1	NAG	C3-C2-N2-C7
20	X	2	NAG	C3-C2-N2-C7
10	F	7	MAN	C4-C5-C6-O6
19	W	3	BMA	O5-C5-C6-O6
17	Q	1	NAG	O5-C5-C6-O6
18	S	2	NAG	C4-C5-C6-O6
17	Q	10	MAN	O5-C5-C6-O6
19	W	2	NAG	C4-C5-C6-O6
9	C	1	NAG	C4-C5-C6-O6
9	C	1	NAG	O5-C5-C6-O6
13	K	2	NAG	O5-C5-C6-O6
16	P	7	MAN	O5-C5-C6-O6

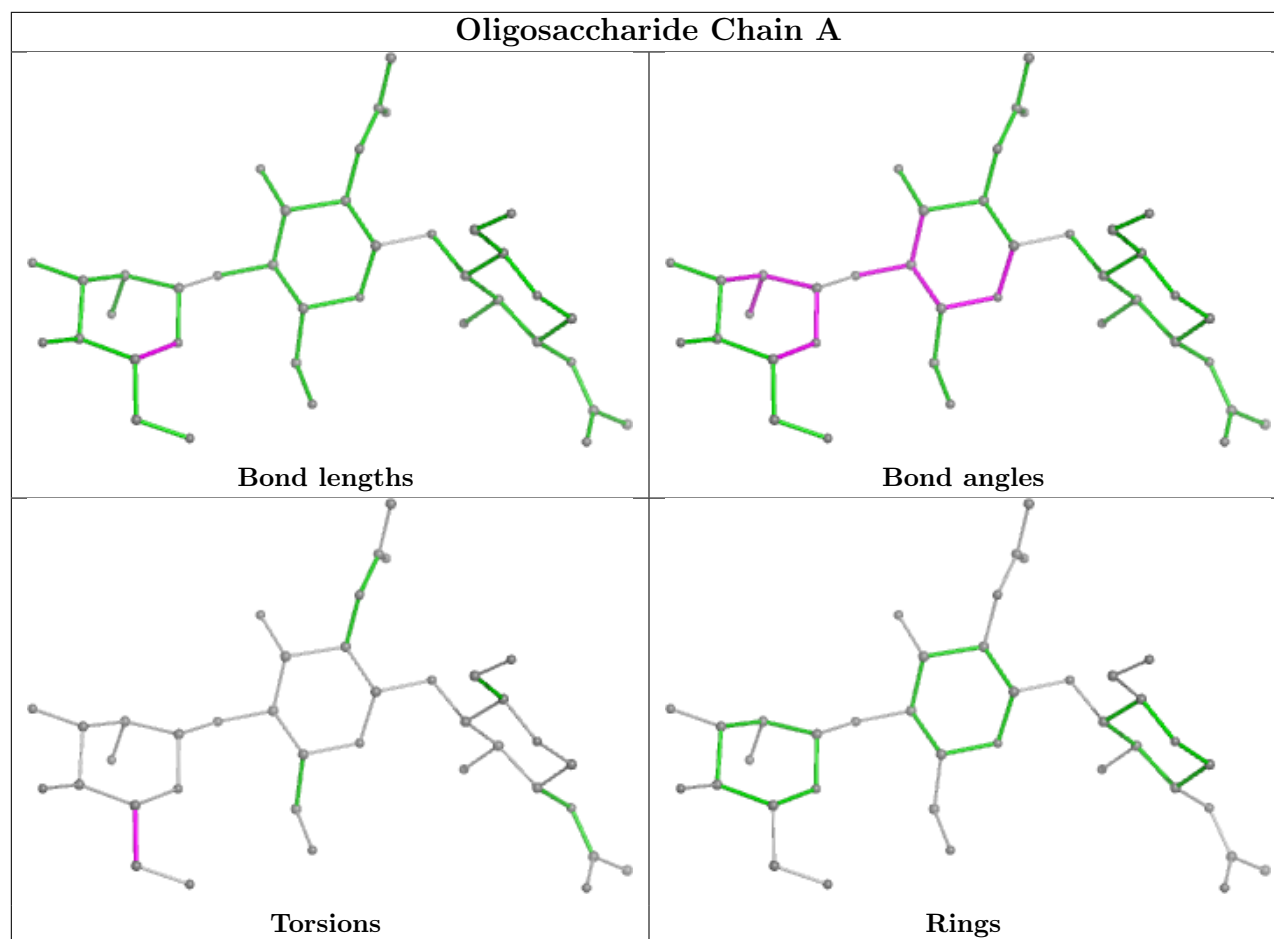
There are no ring outliers.

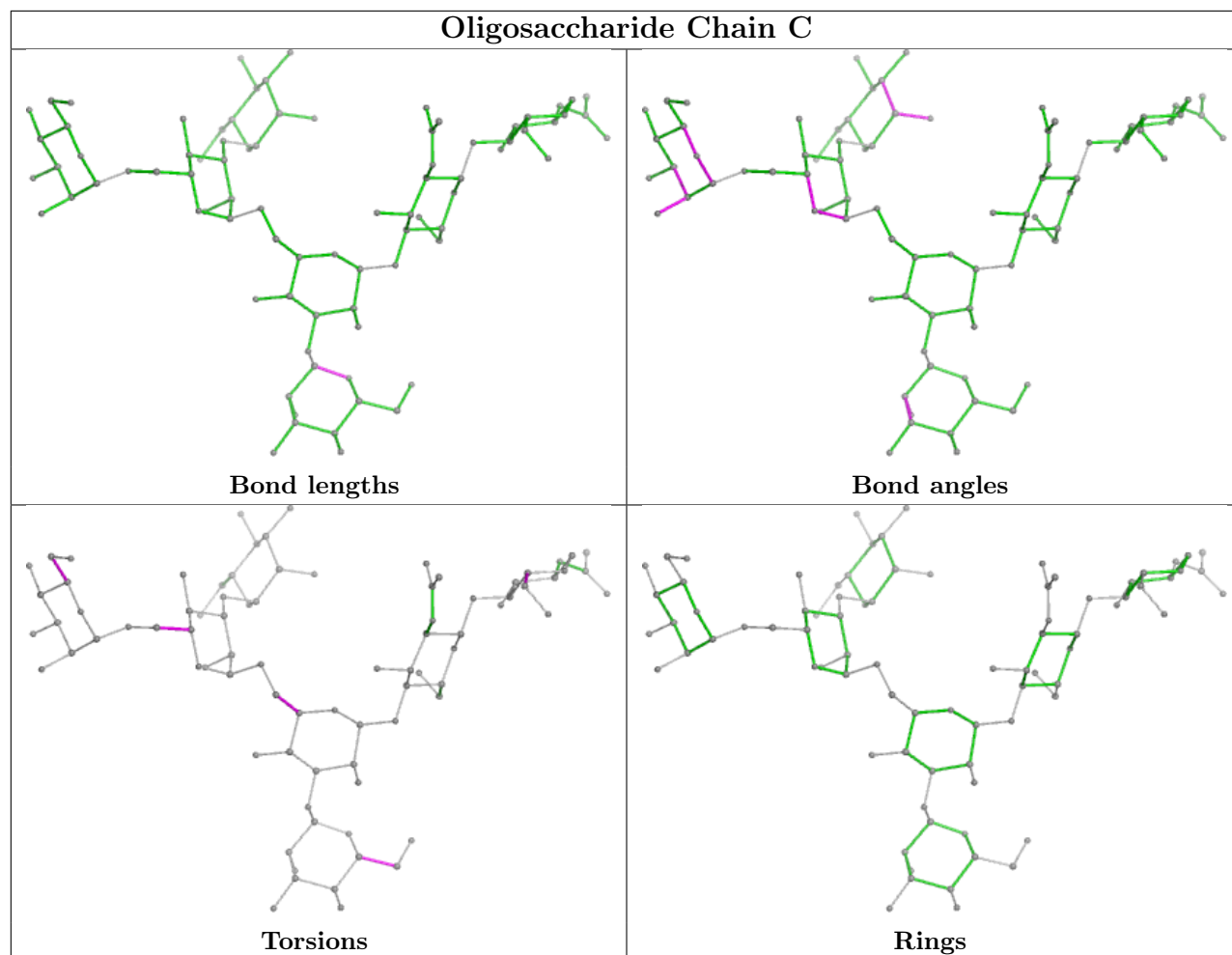
23 monomers are involved in 18 short contacts:

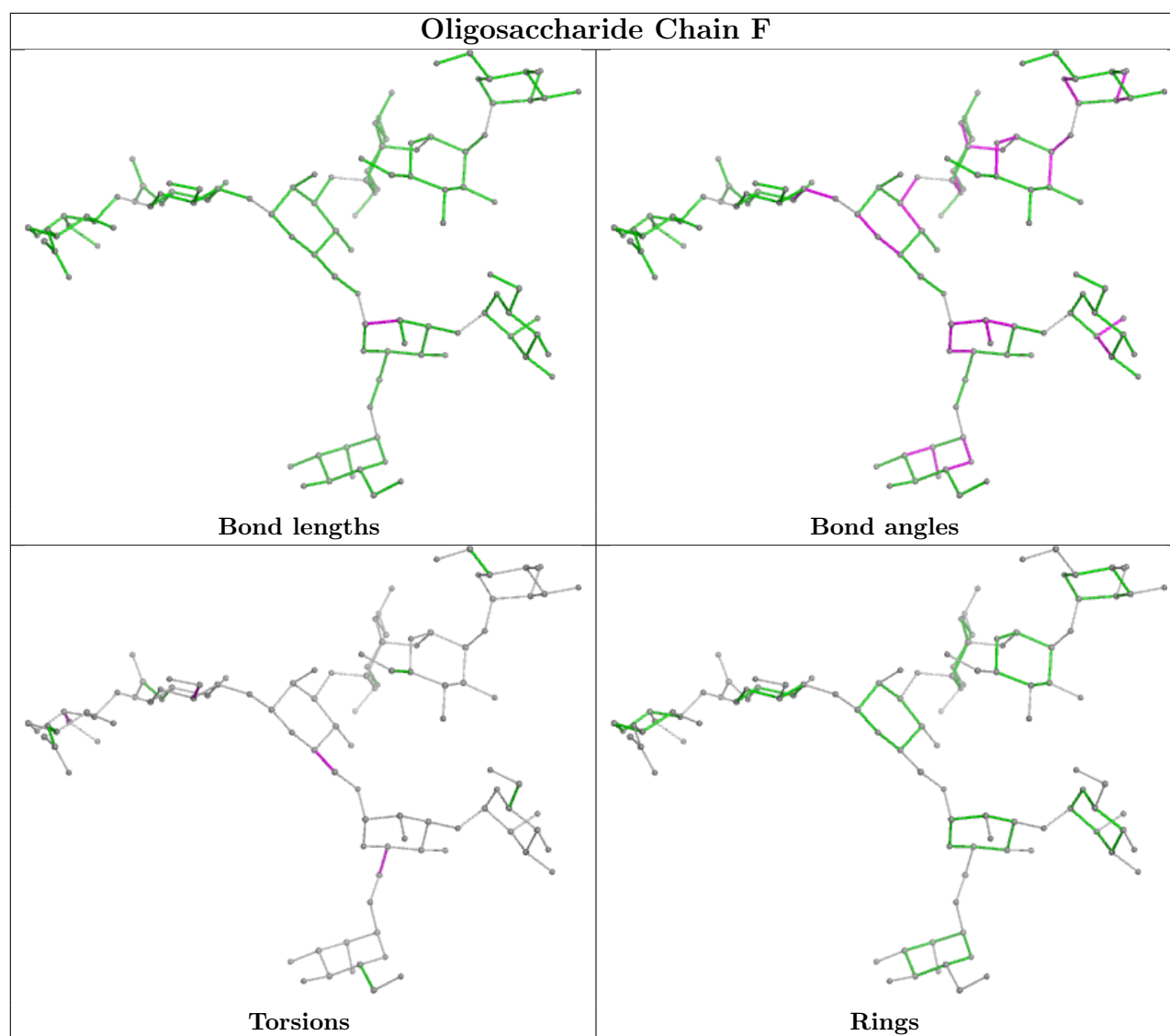
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	M	7	MAN	1	0
18	R	3	BMA	2	0
14	N	7	MAN	1	0
13	K	2	NAG	1	0
17	Q	5	MAN	1	0
18	R	4	MAN	3	0
9	C	1	NAG	1	0
8	A	2	NAG	1	0
15	O	1	NAG	1	0
13	T	4	MAN	1	0
10	M	3	BMA	1	0
21	Y	2	NAG	2	0
18	R	5	MAN	1	0
15	O	4	MAN	1	0
15	O	3	BMA	1	0
15	O	2	NAG	1	0
18	R	2	NAG	1	0
18	R	1	NAG	1	0
9	C	7	MAN	1	0
21	Y	1	NAG	1	0
8	A	1	NAG	1	0
16	P	1	NAG	2	0
13	K	1	NAG	1	0

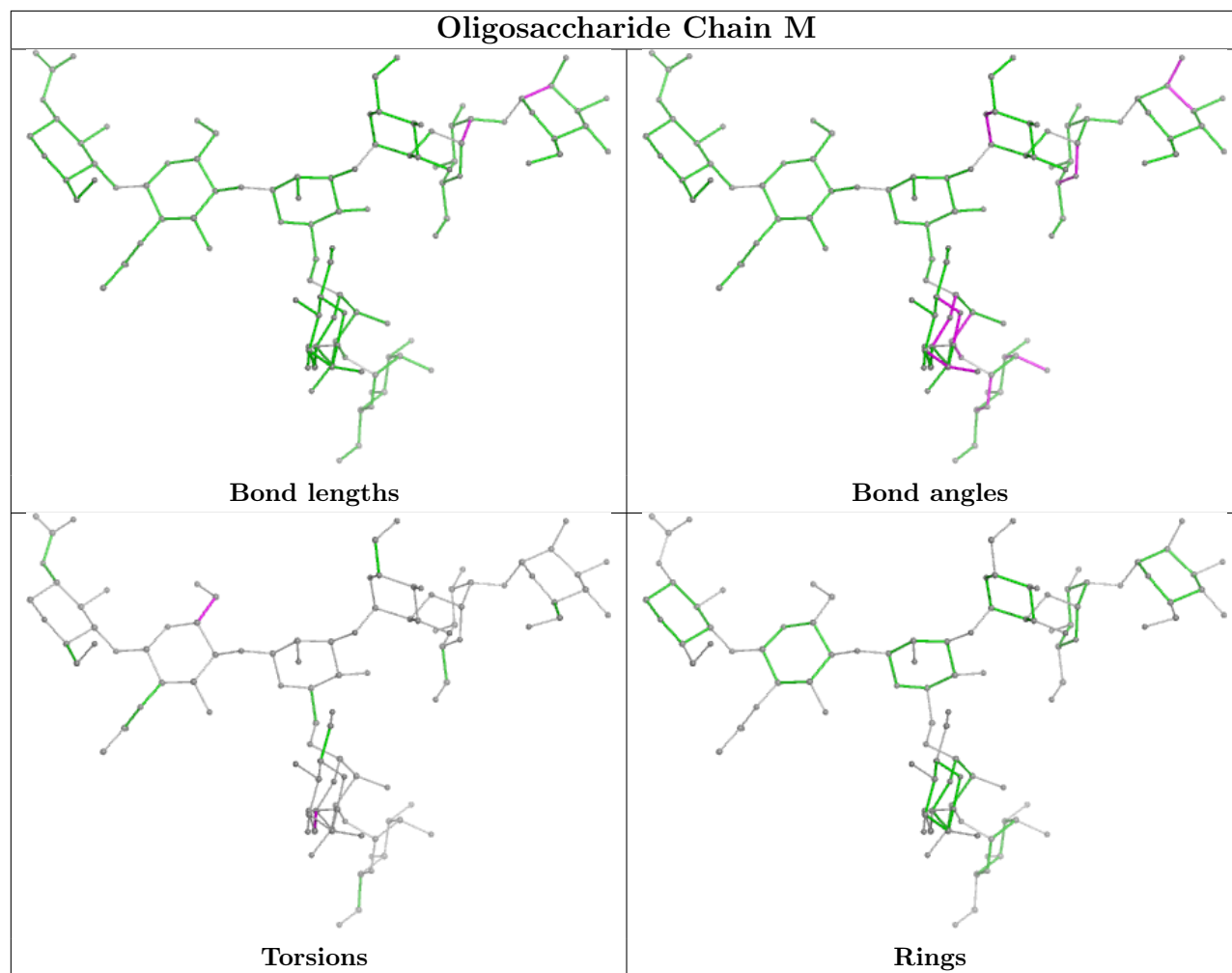
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

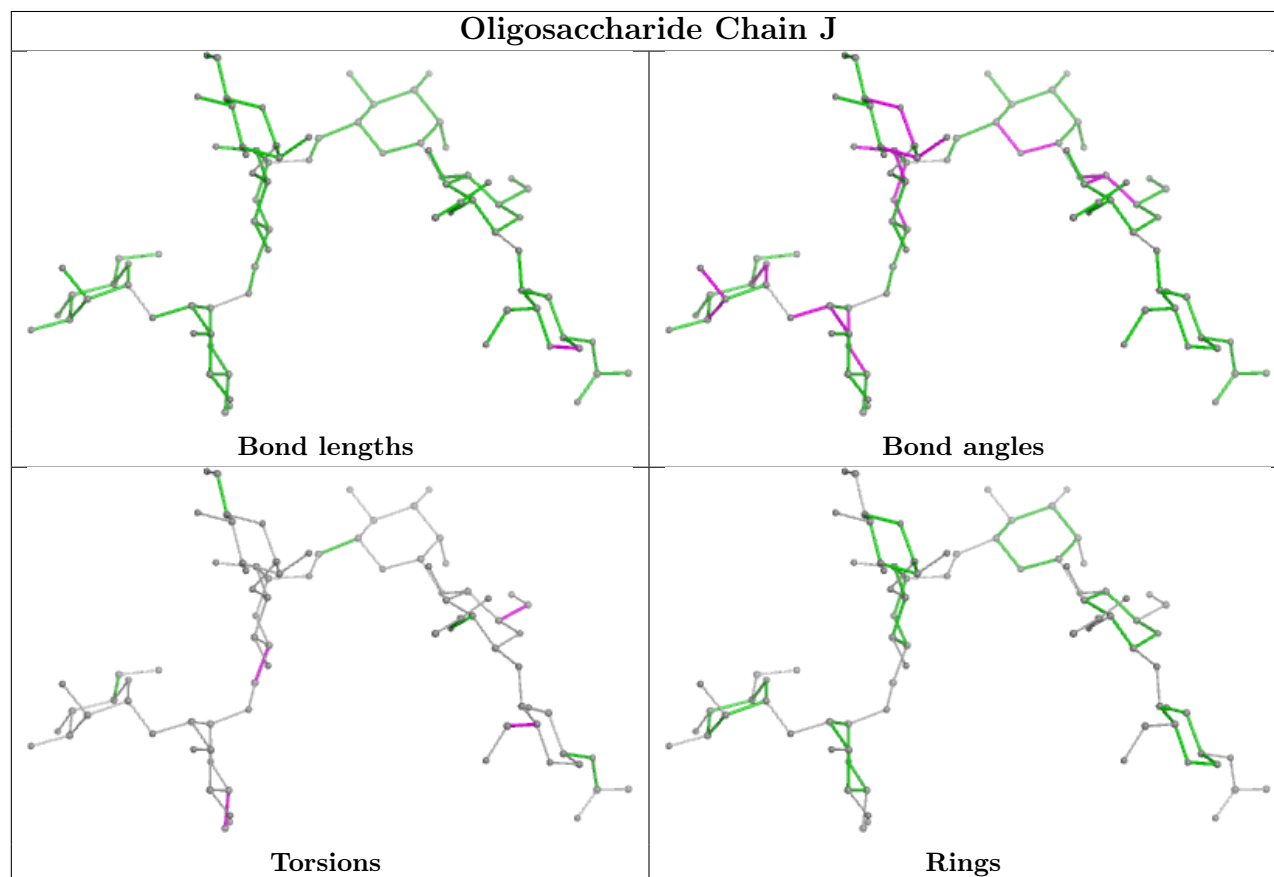
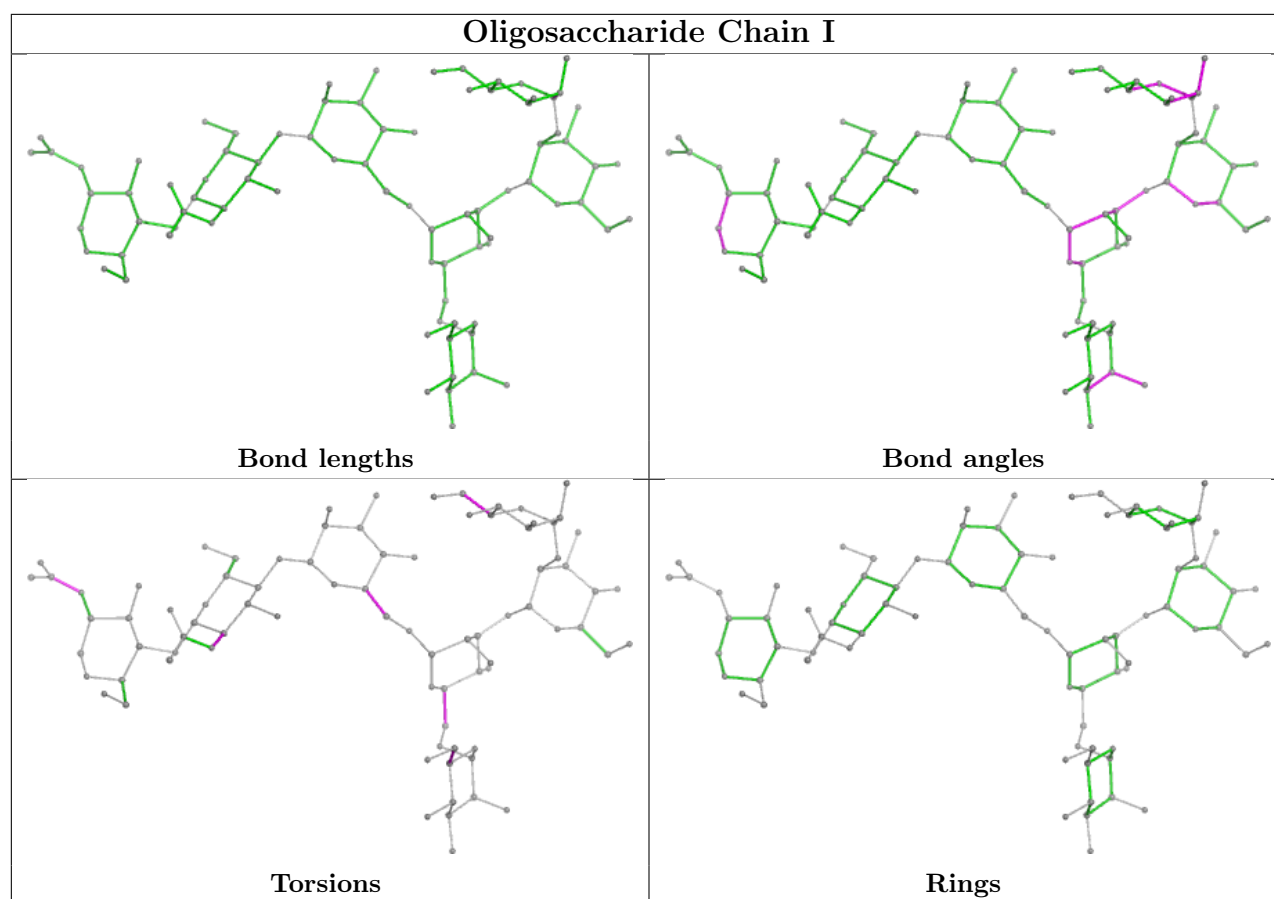


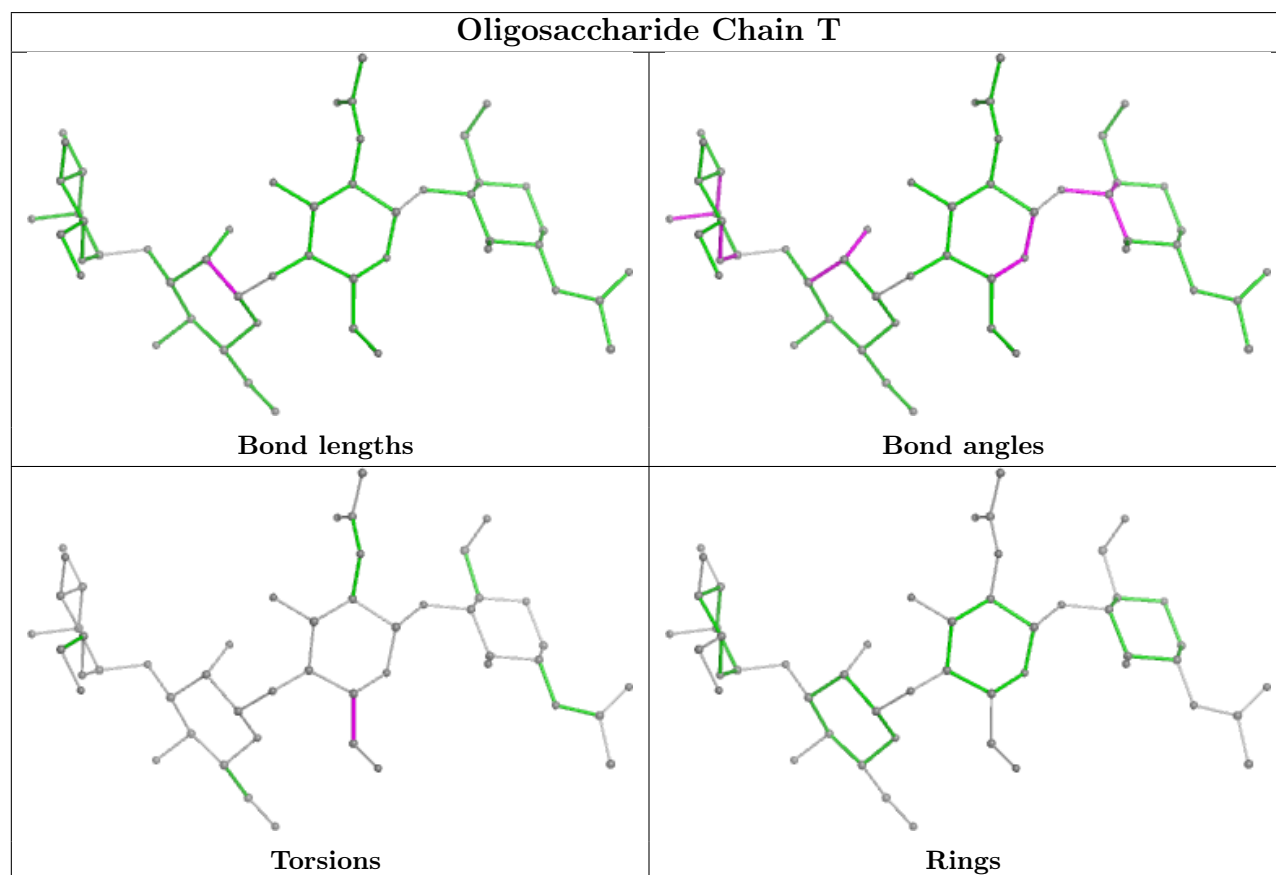
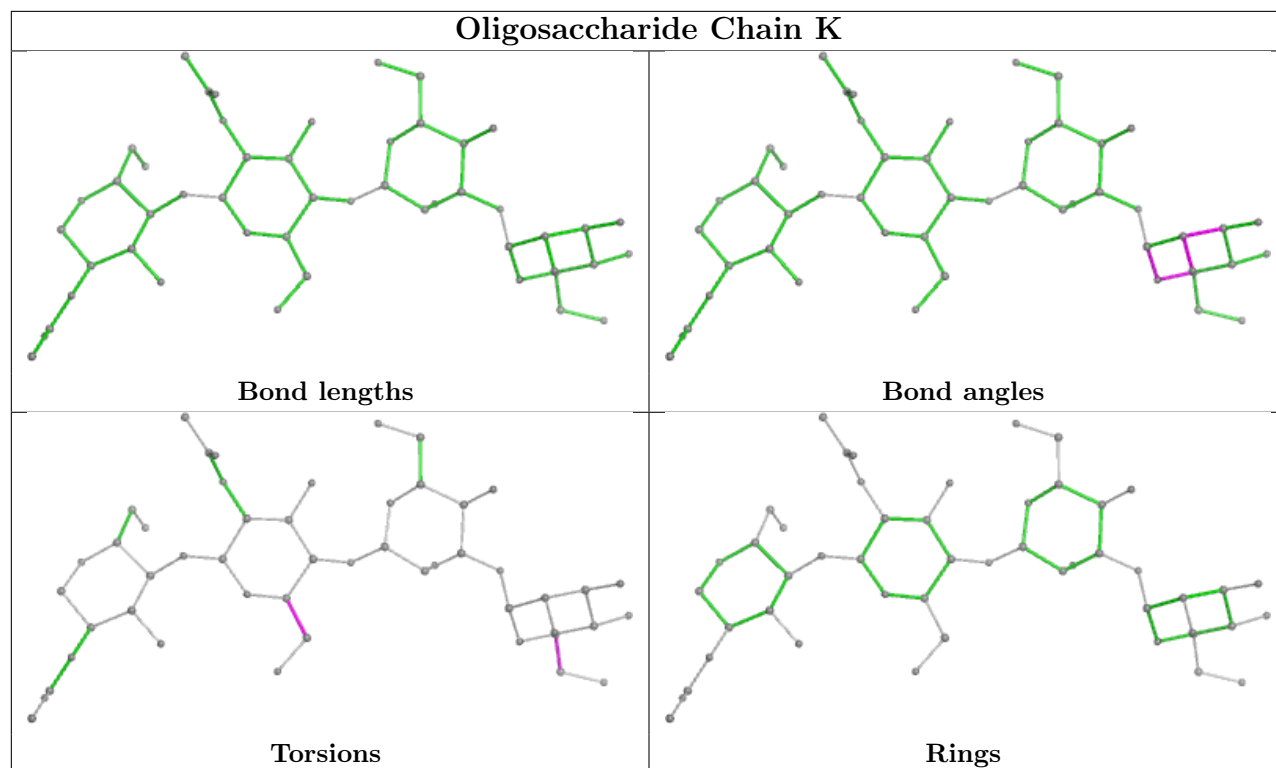


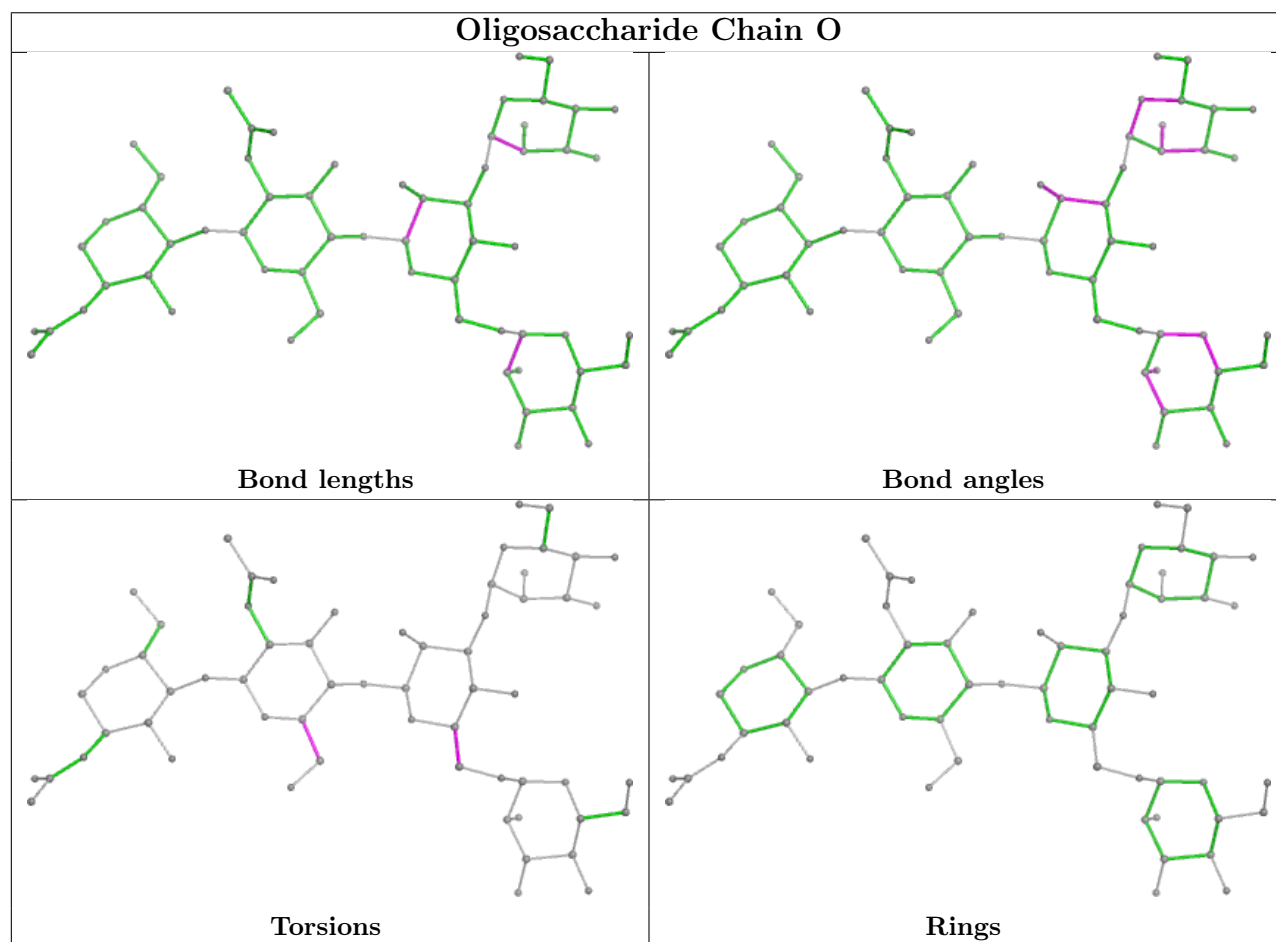
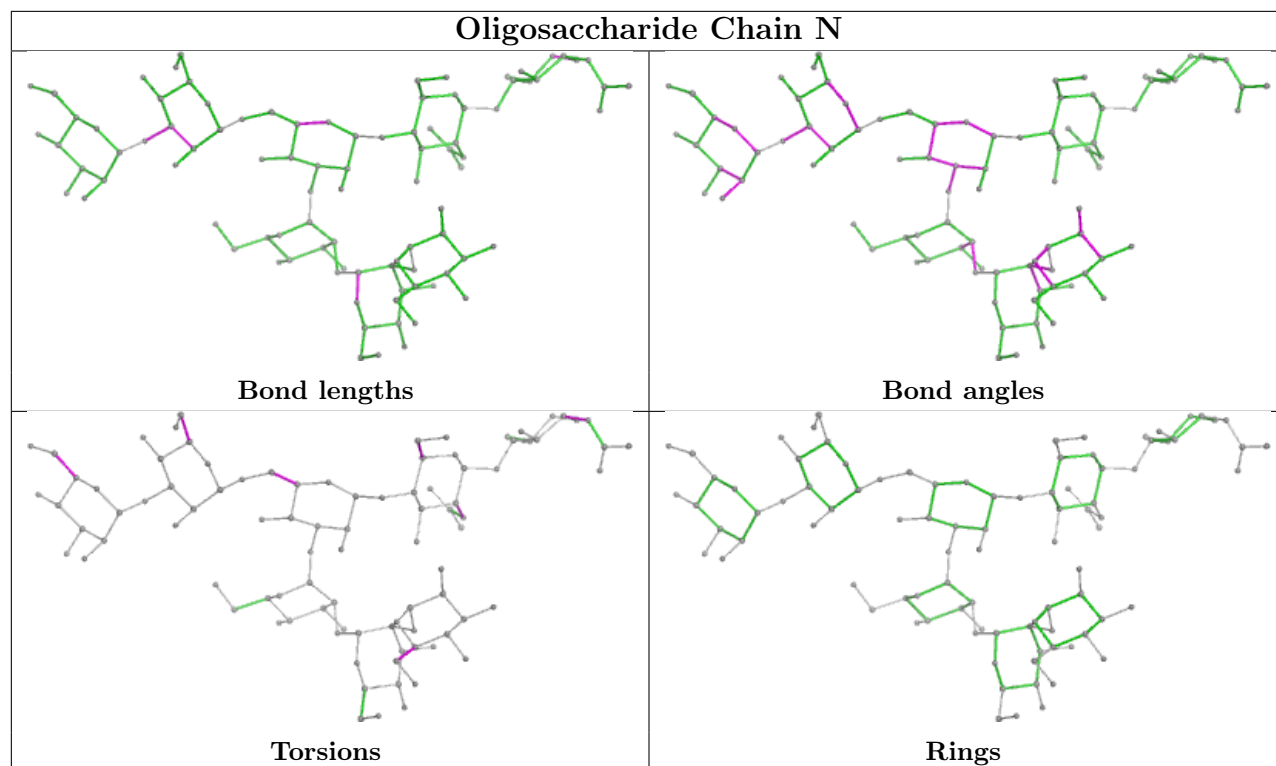


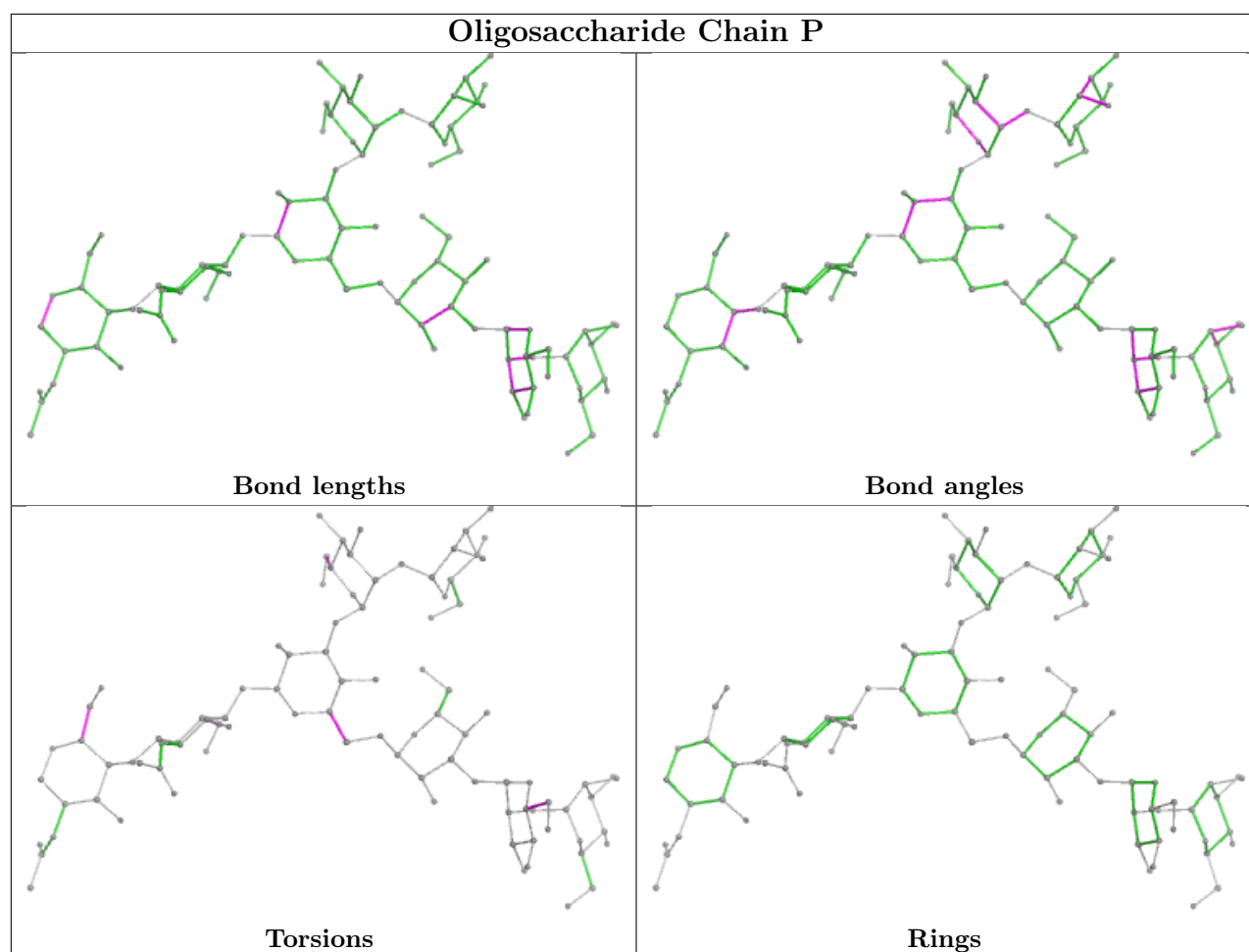


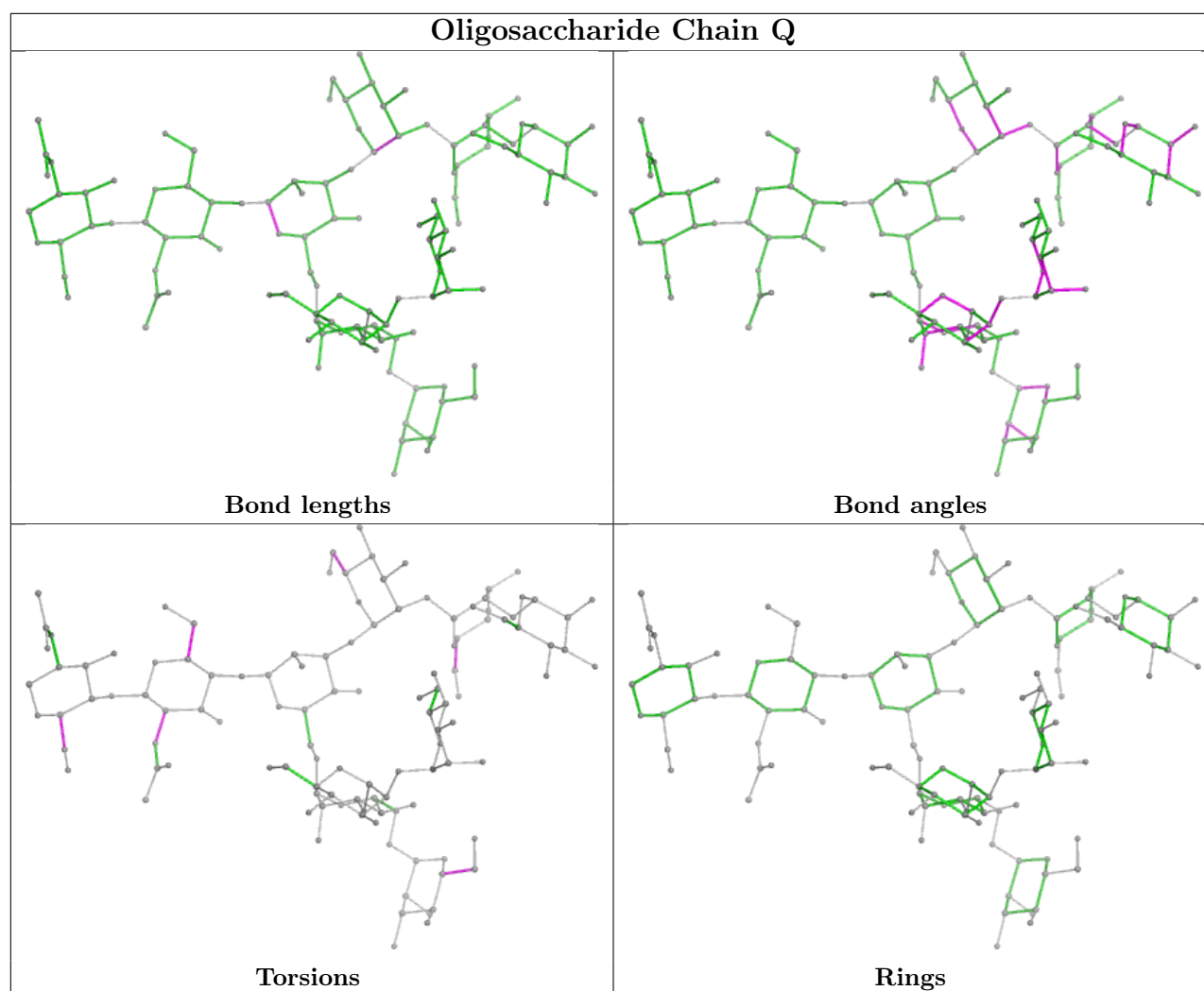


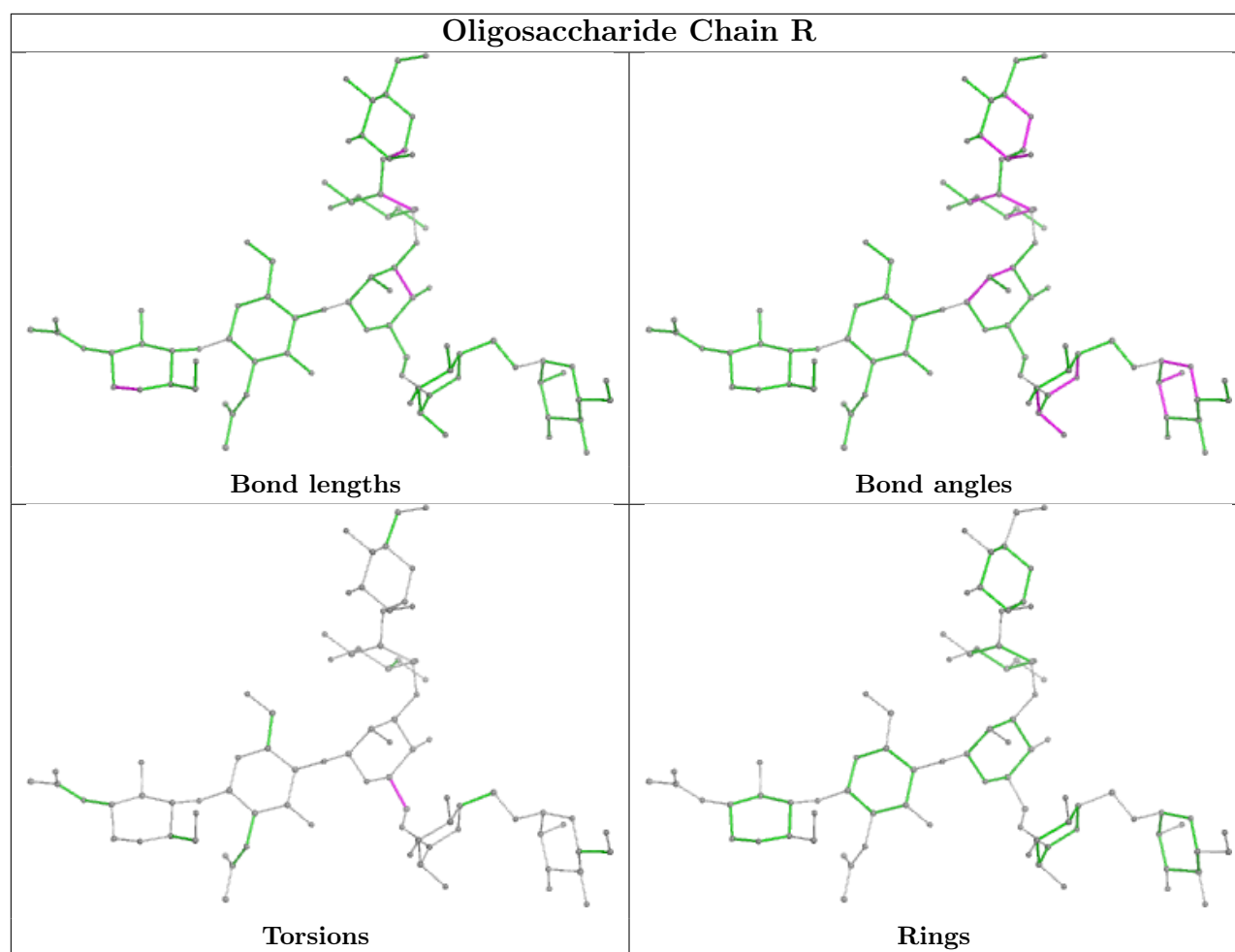


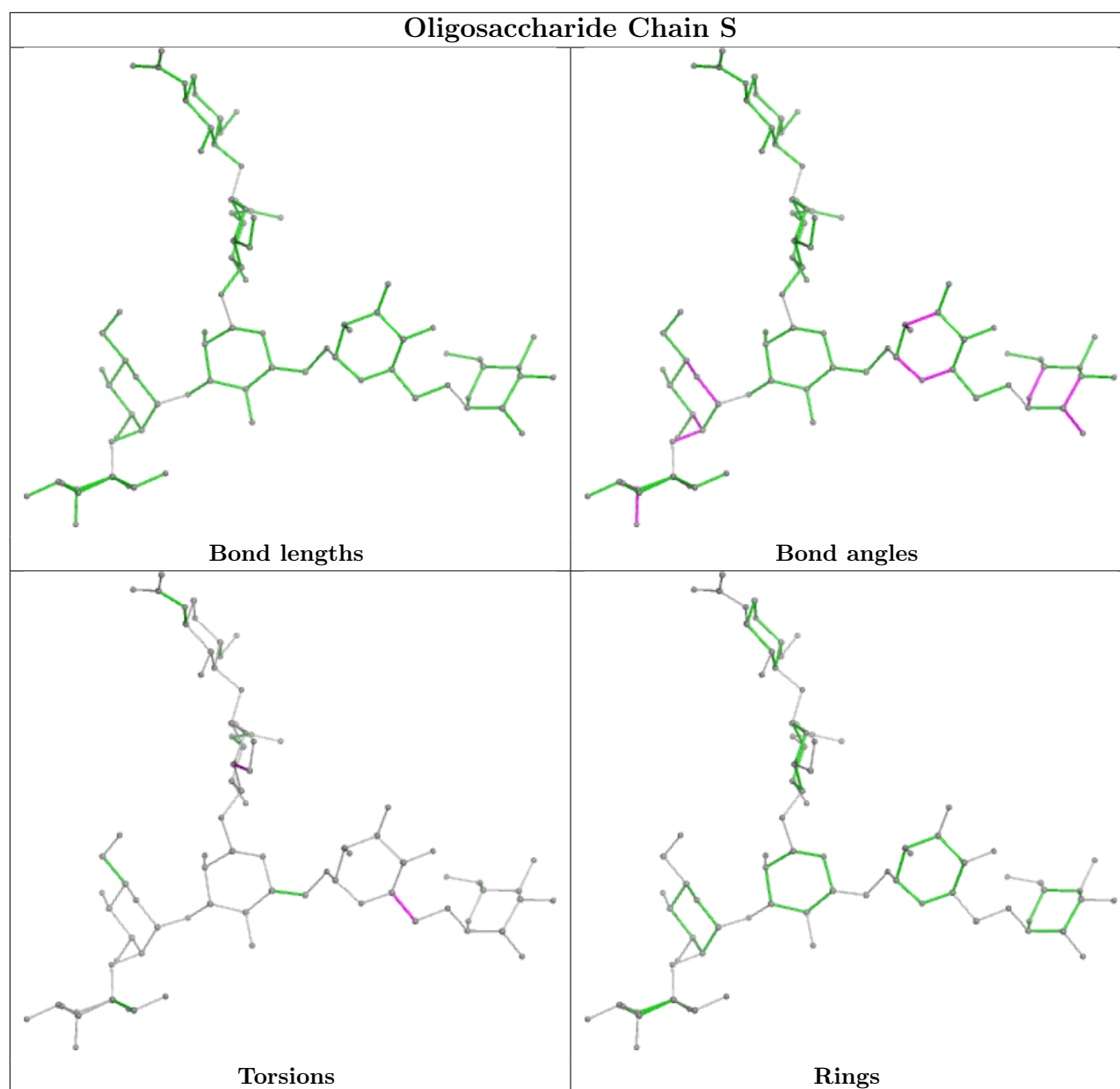


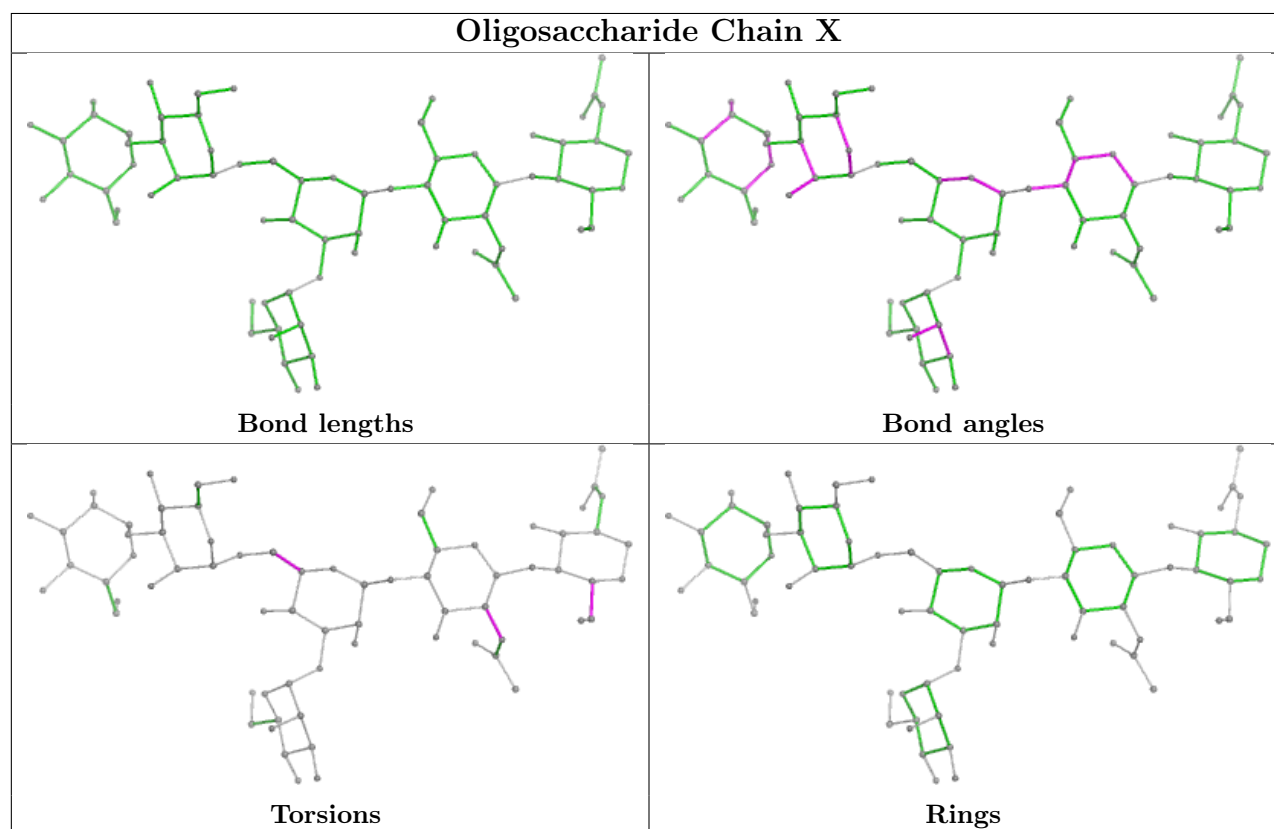
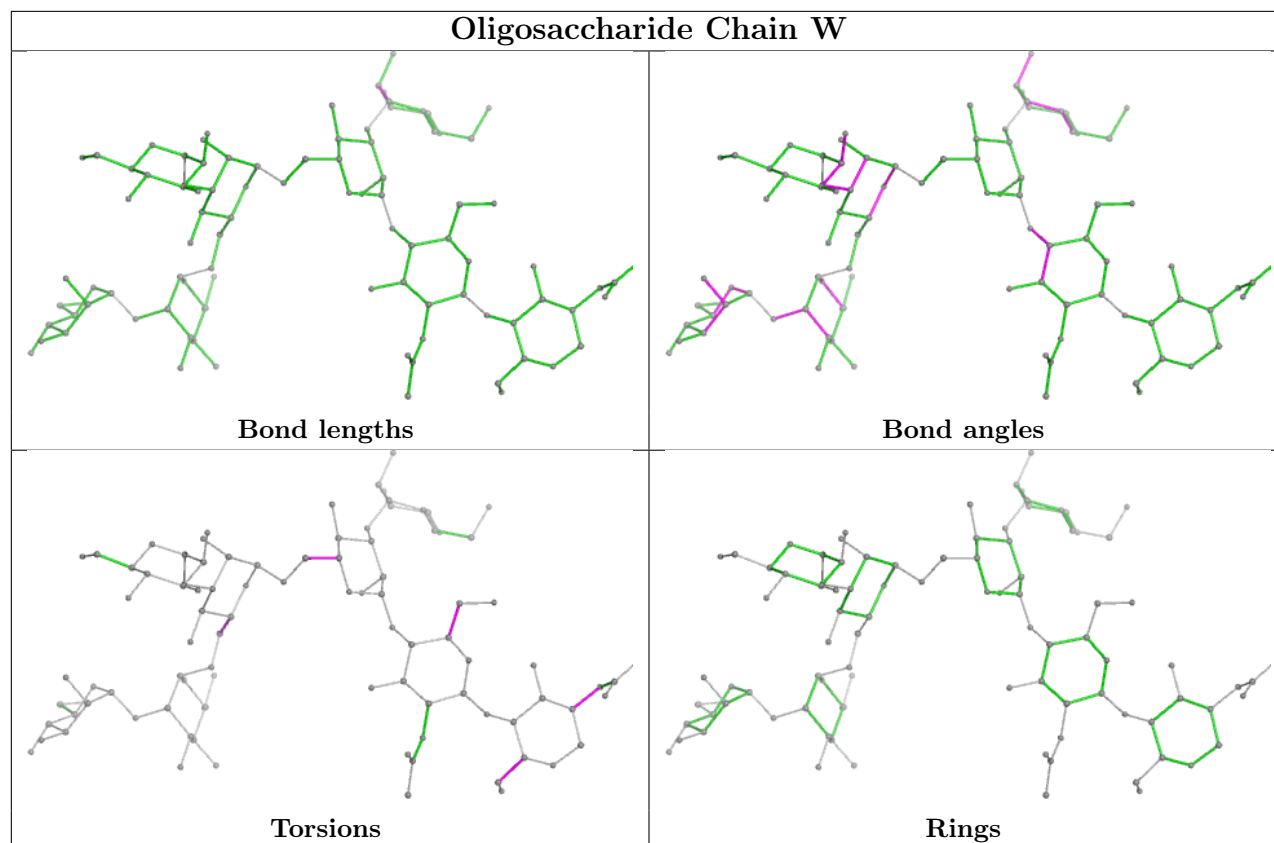




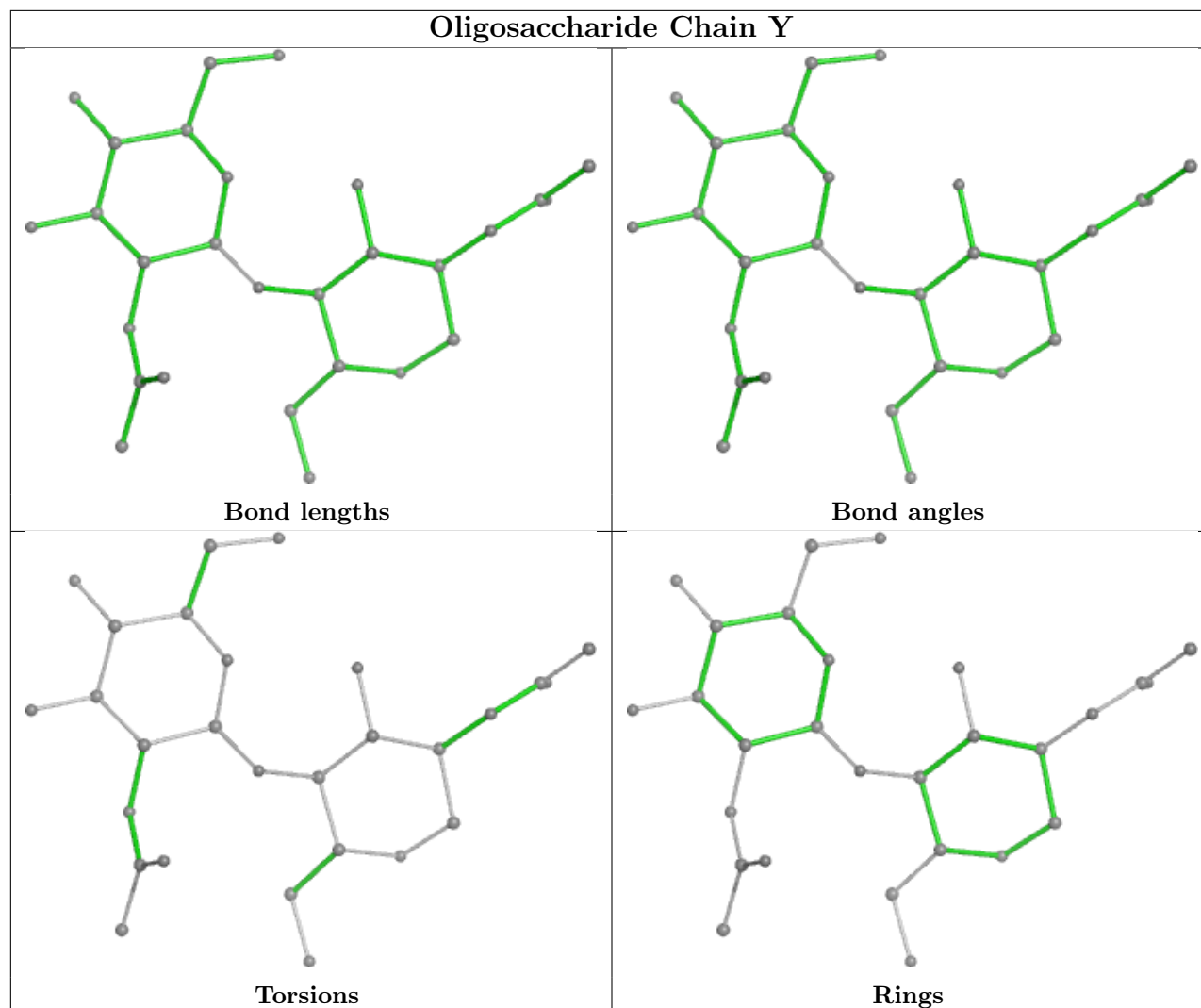


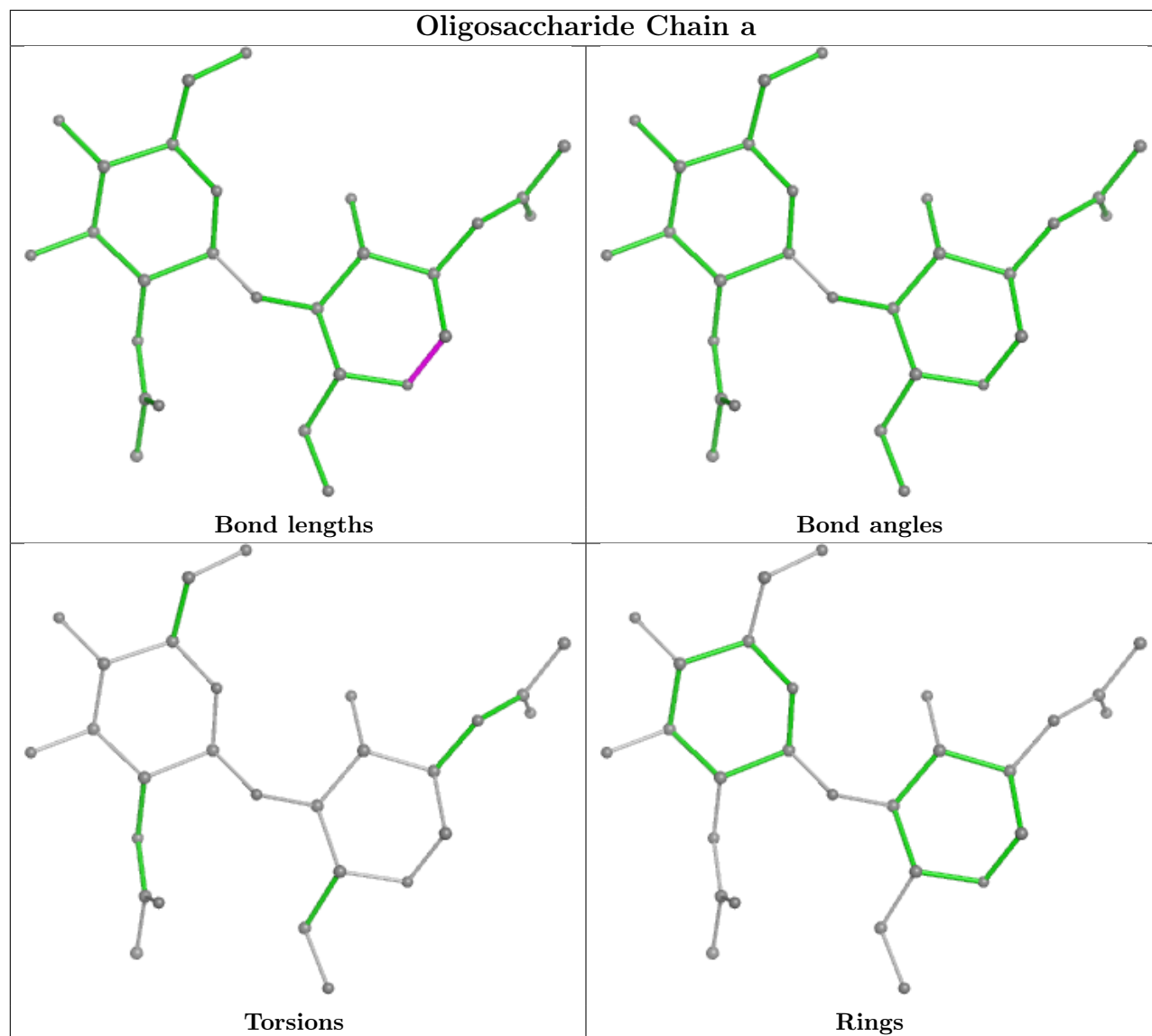


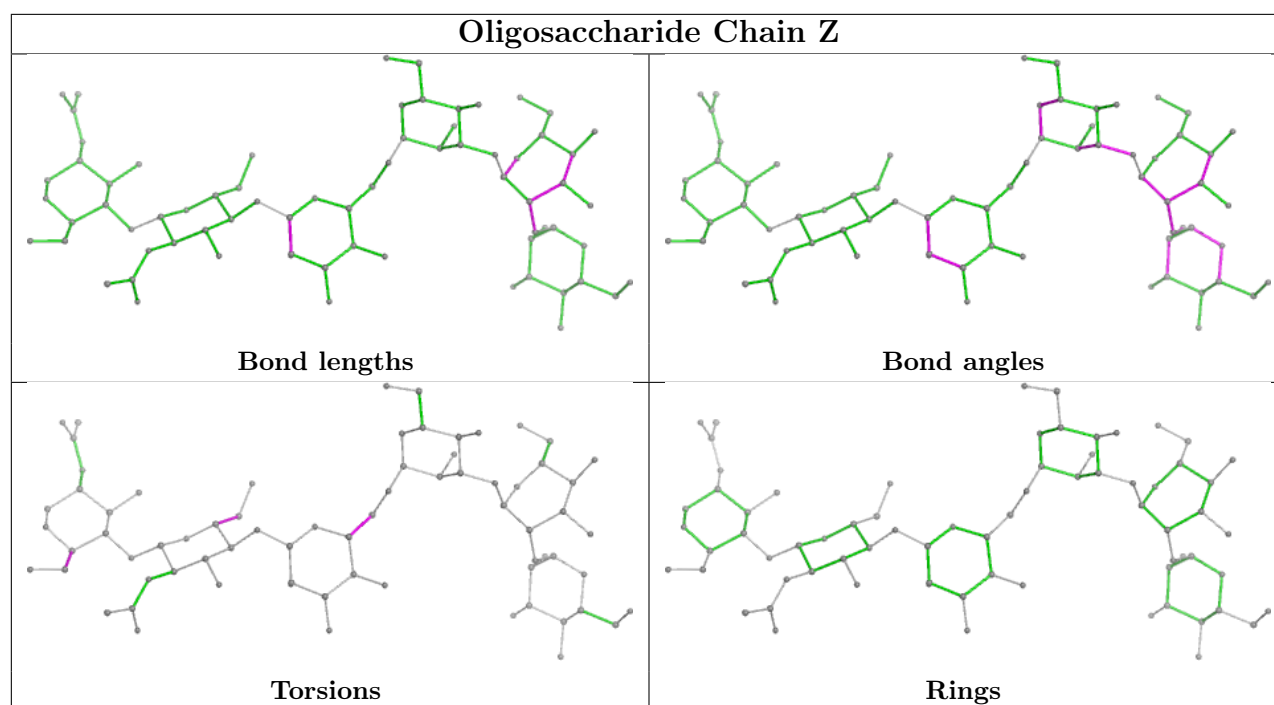


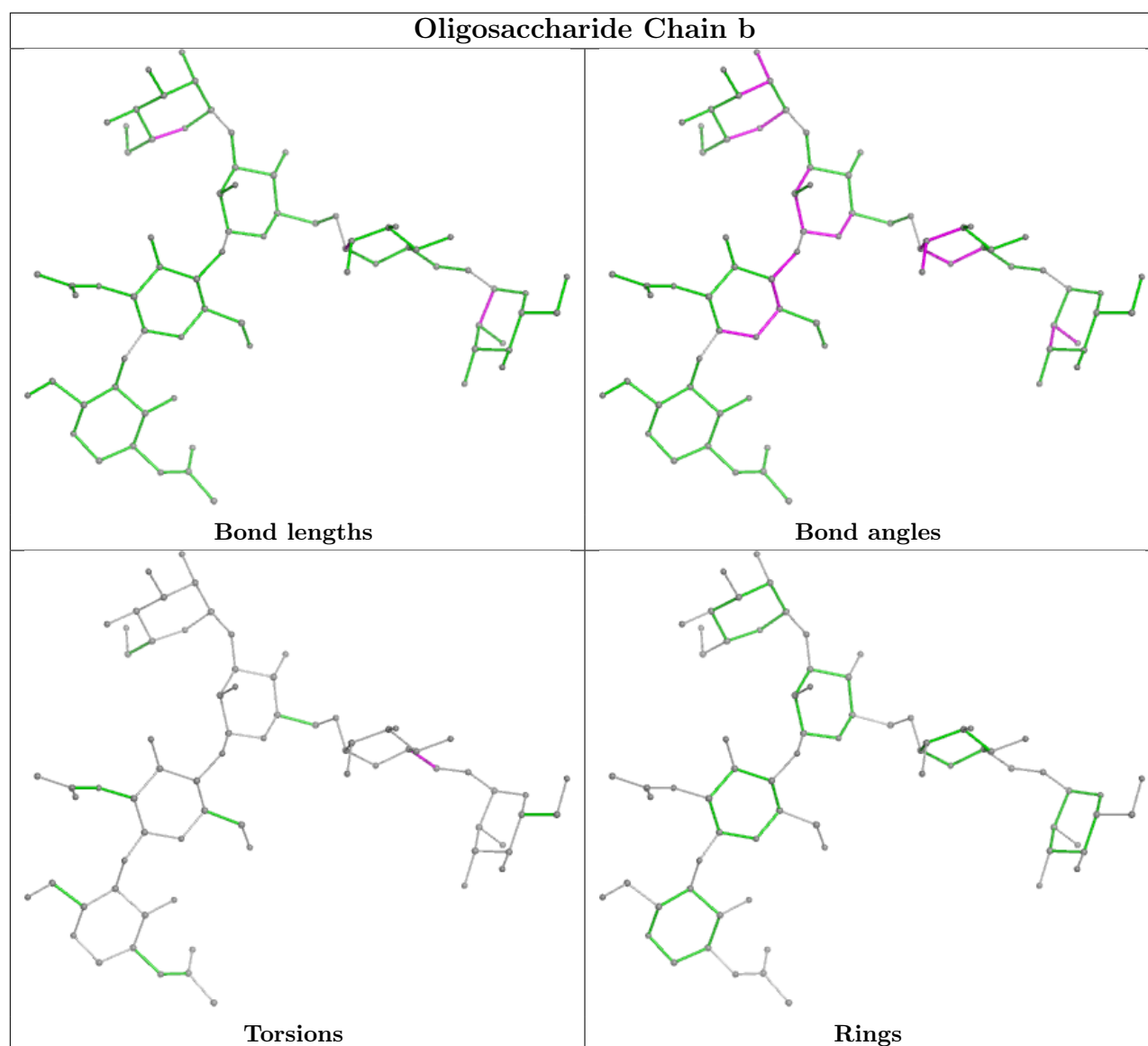












## 5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
24	NAG	H	1212	5	14,14,15	0.27	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	NAG	B	1670	1	14,14,15	0.40	0	17,19,21	0.43	0
24	NAG	B	1669	1	14,14,15	0.35	0	17,19,21	0.49	0
24	NAG	G	1509	4	14,14,15	0.39	0	17,19,21	0.43	0
24	NAG	B	1668	1	14,14,15	0.43	0	17,19,21	0.63	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	NAG	H	1212	5	-	0/6/23/26	0/1/1/1
24	NAG	B	1670	1	-	1/6/23/26	0/1/1/1
24	NAG	B	1669	1	-	2/6/23/26	0/1/1/1
24	NAG	G	1509	4	-	1/6/23/26	0/1/1/1
24	NAG	B	1668	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	1668	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	1669	NAG	O5-C5-C6-O6
24	B	1669	NAG	C4-C5-C6-O6
24	G	1509	NAG	O5-C5-C6-O6
24	B	1670	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	1668	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	95:SER	C	95(A):GLY	N	3.44

## 6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	B	151/161 (93%)	-1.33	0	100 100	39, 104, 220, 254	0
2	D	243/243 (100%)	-0.88	0	100 100	133, 213, 281, 315	0
3	E	213/216 (98%)	-0.90	0	100 100	131, 210, 284, 309	0
4	G	451/475 (94%)	-1.38	0	100 100	43, 110, 187, 295	0
5	H	228/244 (93%)	-1.03	0	100 100	105, 156, 197, 247	0
6	L	210/213 (98%)	-1.07	1 (0%)	87 75	85, 136, 179, 212	0
7	U	119/240 (49%)	-1.18	0	100 100	130, 167, 232, 248	0
7	V	98/240 (40%)	-1.15	0	100 100	136, 204, 240, 342	0
All	All	1713/2032 (84%)	-1.13	1 (0%)	92 87	39, 154, 264, 342	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	L	80	ALA	2.1

### 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](#)

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### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	NAG	B	1670	14/15	0.94	0.06	170,182,187,189	0
24	NAG	H	1212	14/15	0.96	0.04	121,132,140,149	0
24	NAG	G	1509	14/15	0.97	0.04	135,144,144,146	0
24	NAG	B	1668	14/15	0.97	0.04	147,156,161,162	0
24	NAG	B	1669	14/15	0.99	0.07	123,136,154,157	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.