



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:00 AM BST

PDB ID : 5FYJ  
Title : Crystal Structure at 3.4 Å Resolution of Fully Glycosylated HIV-1 Clade G X1193.c1 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

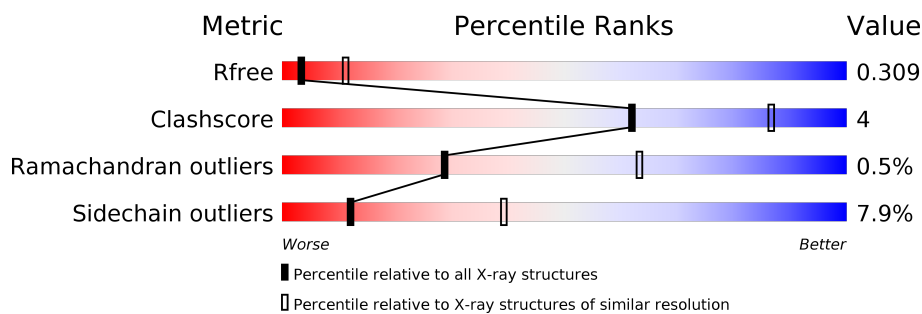
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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.




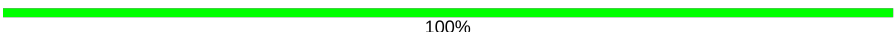

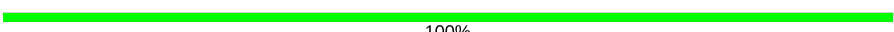
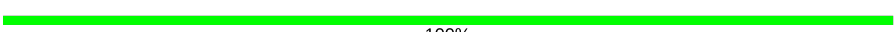
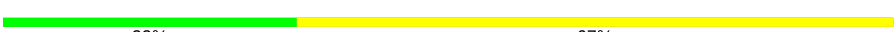
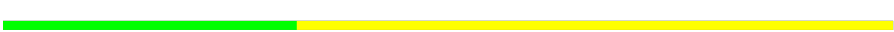







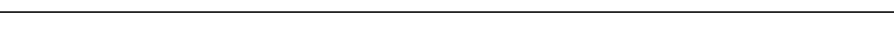
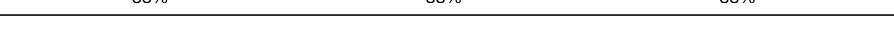
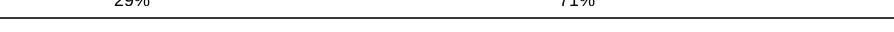

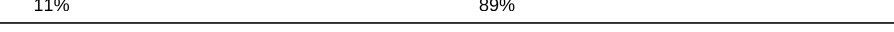



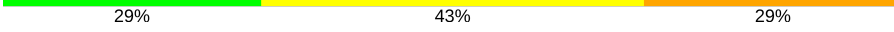

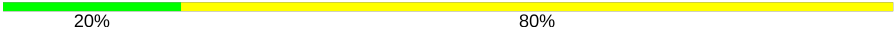
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	B	161	83% 12% .
2	D	243	85% 14% .
3	E	216	81% 17% .
4	G	484	78% 19% ..
5	H	244	82% 10% . 7%
6	L	213	79% 17% ..
7	U	240	41% 8% 50%

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Mol	Chain	Length	Quality of chain
7	V	240	
8	A	2	
8	C	2	
8	I	2	
8	d	2	
9	F	3	
9	O	3	
9	Z	3	
10	J	8	
11	K	11	
11	R	11	
12	M	10	
12	N	10	
12	X	10	
13	P	6	
14	Q	7	
15	S	9	
16	T	9	
17	W	6	
17	e	6	
17	f	6	
18	Y	7	
19	a	9	
20	b	10	
21	c	7	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	BMA	P	3	-	-	X	-
13	MAN	P	4	-	-	X	-

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 15476 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 GP41 ENV ECTODOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	154	Total	C	N	O	S	0	0	0
			1220	770	215	230	5			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP C6ZIG9
B	605	CYS	THR	engineered mutation	UNP C6ZIG9
B	666	GLY	-	expression tag	UNP C6ZIG9
B	667	GLY	-	expression tag	UNP C6ZIG9
B	668	GLY	-	expression tag	UNP C6ZIG9
B	669	LEU	-	expression tag	UNP C6ZIG9
B	670	VAL	-	expression tag	UNP C6ZIG9
B	671	PRO	-	expression tag	UNP C6ZIG9
B	672	ARG	-	expression tag	UNP C6ZIG9

- 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 GP120 ENV ECTODOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	479	Total	C	N	O	S	0	0	0
			3769	2351	674	716	28			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	29	ALA	-	expression tag	UNP C6ZIG9
G	30	LEU	-	expression tag	UNP C6ZIG9
G	31	ALA	-	expression tag	UNP C6ZIG9
G	32	GLY	-	expression tag	UNP C6ZIG9
G	459	CYS	GLY	engineered mutation	UNP C6ZIG9
G	501	CYS	ALA	engineered mutation	UNP C6ZIG9
G	509	ARG	-	expression tag	UNP C6ZIG9
G	510	ARG	-	expression tag	UNP C6ZIG9
G	511	ARG	-	expression tag	UNP C6ZIG9
G	512	ARG	-	expression tag	UNP C6ZIG9
G	513	ARG	-	expression tag	UNP C6ZIG9

- 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			

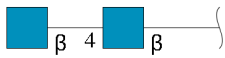
- Molecule 6 is a protein called PGT122.

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.

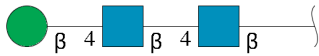
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	U	119	Total	C	N	O	S	0	0	0
			956	603	173	171	9			
7	V	98	Total	C	N	O	S	0	0	0
			758	479	130	147	2			

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



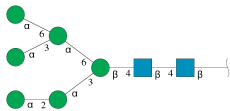
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	d	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 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
9	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
9	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
9	Z	3	Total	C	N	O	0	0	0
			39	22	2	15			

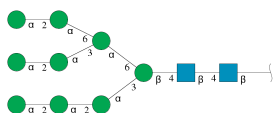
- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

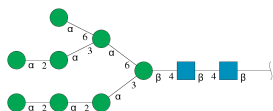
- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra

nose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-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.



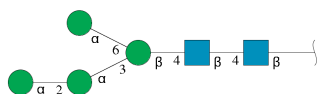
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	K	11	Total	C	N	O	0	0	0
			127	70	2	55			
11	R	11	Total	C	N	O	0	0	0
			127	70	2	55			

- Molecule 12 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.



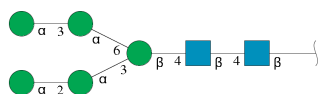
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	M	10	Total	C	N	O	0	0	0
			116	64	2	50			
12	N	10	Total	C	N	O	0	0	0
			116	64	2	50			
12	X	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 13 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.



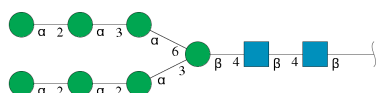
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	P	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



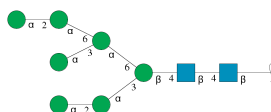
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	Q	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 15 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



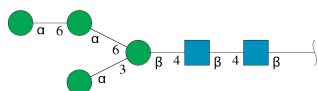
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	S	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 16 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-(1-2)-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.



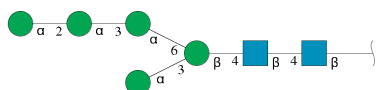
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	T	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 17 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.



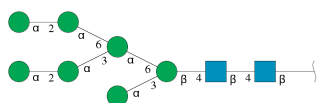
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	W	6	Total	C	N	O	0	0	0
			72	40	2	30			
17	e	6	Total	C	N	O	0	0	0
			72	40	2	30			
17	f	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



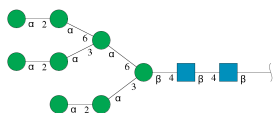
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	Y	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 19 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-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.



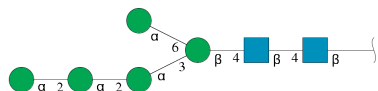
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	a	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 20 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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.



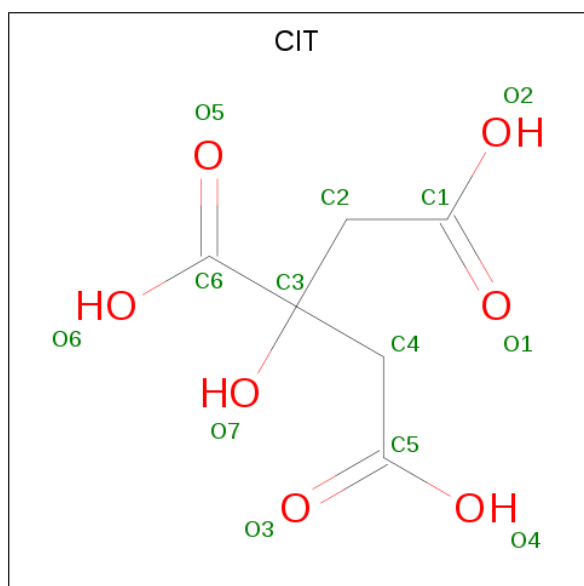
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
20	b	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 21 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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
21	c	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 22 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



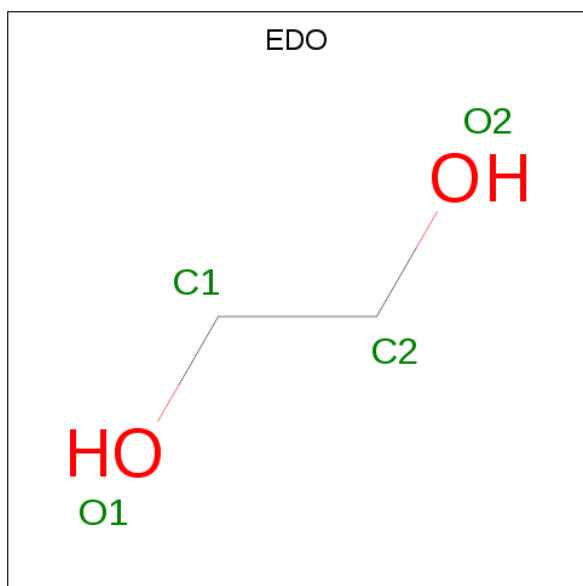
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			13	6	7		
22	G	1	Total	C	O	0	0
			13	6	7		

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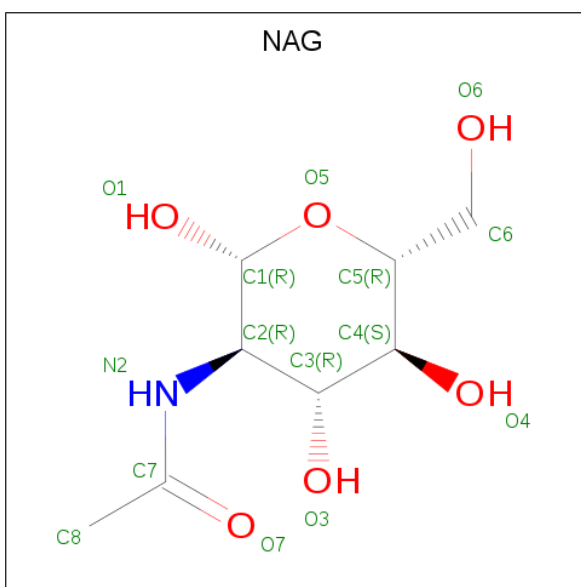
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	G	1	Total	C	O	0	0
			13	6	7		

- Molecule 23 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	D	1	Total	C	O	0	0
			4	2	2		
23	G	1	Total	C	O	0	0
			4	2	2		

- 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	G	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	G	1	Total	C	N	O	0	0
			14	8	1	5		


- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	B	4	Total	O	0	0
			4	4		
25	D	2	Total	O	0	0
			2	2		
25	E	1	Total	O	0	0
			1	1		
25	G	3	Total	O	0	0
			3	3		
25	H	1	Total	O	0	0
			1	1		
25	L	1	Total	O	0	0
			1	1		

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


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

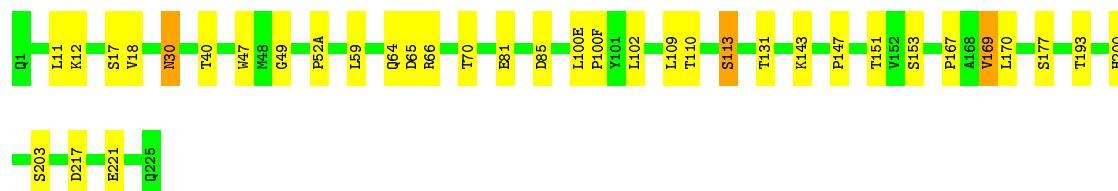
- Molecule 1: GP41 ENV ECTODOMAIN

Chain B: 




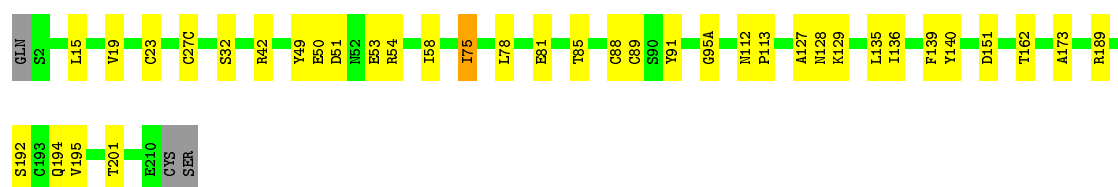
- Molecule 2: 35O22

Chain D: 




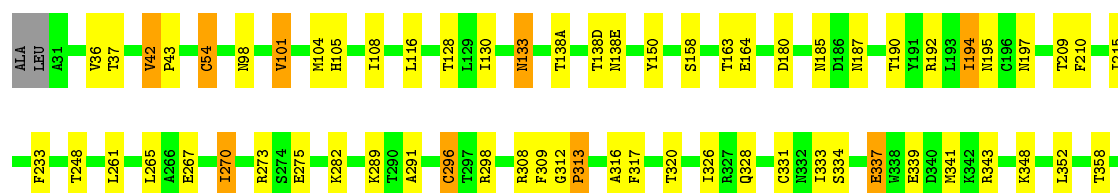
- Molecule 3: 35O22

Chain E: 



- Molecule 4: GP120 ENV ECTODOMAIN

Chain G: 





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

Chain A:  100%



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

Chain C:  50% 50%



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

Chain I:  100%



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

Chain d:  100%



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

Chain F:  33% 67%



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

Chain O:  33% 67%

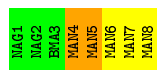


- Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

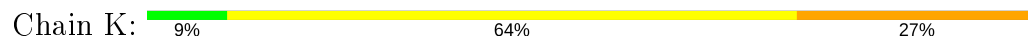
Chain Z:  67% 33%



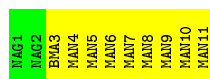
- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: 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-(1-2)-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 11: 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-(1-2)-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 12: 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



- Molecule 12: 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 N:  20% 60% 20%



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

Chain X:  20% 80%



- Molecule 13: 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 P:  33% 33% 33%



- Molecule 14: 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 Q:  29% 71%



- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-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:  33% 67%



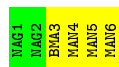
- Molecule 16: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  11% 89%



- Molecule 17: 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 W: 33% 67%



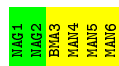
- Molecule 17: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 17% 83%



- Molecule 17: 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 f: 33% 67%



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

Chain Y: 29% 43% 29%



- Molecule 19: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-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 a: 22% 78%



- Molecule 20: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-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

-(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 b:  20% 80%

MAN1	MAN2	MAN3	MAN4	MAN5	MAN6	MAN7	MAN8	MAN9	MAN10
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● Molecule 21: alpha-D-mannopyranose-(1-2)-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 c:  29% 71%

MAN1	MAN2	MAN3	MAN4	MAN5	MAN6	MAN7
------	------	------	------	------	------	------

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.16Å 127.16Å 313.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.65 – 3.11 44.65 – 3.11	Depositor EDS
% Data completeness (in resolution range)	83.3 (44.65-3.11) 83.3 (44.65-3.11)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.63 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, $R_{free}$	0.214 , 0.273 0.274 , 0.309	Depositor DCC
$R_{free}$ test set	2003 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.9	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 69.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.114 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	15476	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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: MAN, BMA, CIT, NAG, EDO

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	0.38	1/1242 (0.1%)	0.46	0/1689
2	D	0.27	0/1881	0.44	0/2562
3	E	0.23	0/1659	0.44	0/2269
4	G	0.26	0/3843	0.47	0/5213
5	H	0.22	0/1789	0.43	0/2443
6	L	0.23	0/1632	0.44	0/2236
7	U	0.24	0/981	0.44	0/1328
7	V	0.23	0/778	0.44	0/1058
All	All	0.26	1/13805 (0.0%)	0.45	0/18798

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	644	ASN	C-N	8.99	1.54	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1220	0	1202	7	0
2	D	1833	0	1806	15	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1615	0	1542	17	0
4	G	3769	0	3705	44	0
5	H	1742	0	1715	11	0
6	L	1589	0	1530	15	0
7	U	956	0	928	8	0
7	V	758	0	719	5	0
8	A	28	0	25	0	0
8	C	28	0	25	1	0
8	I	28	0	25	0	0
8	d	28	0	25	0	0
9	F	39	0	34	0	0
9	O	39	0	34	0	0
9	Z	39	0	34	0	0
10	J	94	0	79	1	0
11	K	127	0	106	2	0
11	R	127	0	106	2	0
12	M	116	0	97	0	1
12	N	116	0	97	4	0
12	X	116	0	97	0	0
13	P	72	0	61	6	0
14	Q	83	0	70	0	0
15	S	105	0	88	0	0
16	T	105	0	88	0	0
17	W	72	0	61	0	0
17	e	72	0	61	0	0
17	f	72	0	61	0	0
18	Y	83	0	70	4	0
19	a	105	0	88	0	0
20	b	116	0	97	0	0
21	c	83	0	70	0	0
22	B	13	0	5	1	0
22	G	26	0	10	2	0
23	D	4	0	6	0	0
23	G	4	0	6	0	0
24	G	42	0	39	1	0
25	B	4	0	0	0	0
25	D	2	0	0	0	0
25	E	1	0	0	0	0
25	G	3	0	0	0	0
25	H	1	0	0	1	0
25	L	1	0	0	0	0
All	All	15476	0	14812	133	2

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 4.

All (133) 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)
18:Y:4:MAN:H3	18:Y:5:MAN:H5	1.19	1.13
13:P:3:BMA:H3	13:P:4:MAN:H5	1.44	0.96
4:G:459:CYS:HB2	7:U:61:ARG:HG2	1.47	0.93
18:Y:4:MAN:H3	18:Y:5:MAN:C5	2.02	0.89
12:N:3:BMA:H3	12:N:4:MAN:H3	1.56	0.86
6:L:109:GLN:OE1	6:L:171:ASN:ND2	2.13	0.80
4:G:105:HIS:HE2	22:G:1513:CIT:H22	1.47	0.79
13:P:3:BMA:H3	13:P:4:MAN:C5	2.16	0.76
4:G:233:PHE:O	4:G:273:ARG:NH1	2.19	0.75
18:Y:4:MAN:C3	18:Y:5:MAN:H5	2.11	0.74
13:P:3:BMA:C3	13:P:4:MAN:H5	2.18	0.72
12:N:3:BMA:C3	12:N:4:MAN:H3	2.24	0.68
7:V:66:ARG:NE	7:V:67:TRP:O	2.30	0.65
8:C:1:NAG:H4	8:C:2:NAG:N2	2.10	0.64
4:G:428:GLN:NE2	7:U:53:ARG:O	2.26	0.63
2:D:30:ASN:HA	2:D:52(A):PRO:HB2	1.82	0.62
3:E:127:ALA:HB3	3:E:129:LYS:N	2.17	0.59
3:E:54:ARG:NH1	3:E:58:ILE:O	2.35	0.59
22:B:1666:CIT:O7	22:B:1666:CIT:O3	2.17	0.58
12:N:3:BMA:O4	12:N:4:MAN:H5	2.03	0.58
7:V:61:ARG:HB3	7:V:75:ILE:HG13	1.85	0.58
4:G:308:ARG:HG2	4:G:316:ALA:HB2	1.85	0.57
4:G:333:ILE:HD13	4:G:390:LEU:HD21	1.86	0.57
4:G:105:HIS:NE2	22:G:1513:CIT:H22	2.16	0.57
4:G:343:ARG:HB2	4:G:397:PHE:CE1	2.39	0.57
5:H:83:THR:N	5:H:86:ASP:OD2	2.24	0.56
2:D:143:LYS:HD2	2:D:177:SER:HB3	1.88	0.55
12:N:3:BMA:H3	12:N:4:MAN:C3	2.18	0.55
4:G:194:ILE:HG13	4:G:423:ILE:HD11	1.87	0.55
4:G:334:SER:HB3	4:G:337:GLU:HB3	1.88	0.55
5:H:59:TYR:HB2	5:H:64:LYS:HG3	1.89	0.55
3:E:151:ASP:HB2	3:E:189:ARG:HB2	1.90	0.54
4:G:506:VAL:HG22	4:G:508:ARG:H	1.73	0.54
1:B:611:ASN:HB3	1:B:614:TRP:CD2	2.43	0.53
3:E:50:GLU:HB2	3:E:53:GLU:HB2	1.90	0.53
4:G:358:THR:O	4:G:465:THR:OG1	2.18	0.53
6:L:37:GLN:HB3	6:L:47:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:377:ASN:HB3	4:G:382:PHE:CD1	2.43	0.53
4:G:379:ARG:NH1	11:R:3:BMA:H3	2.24	0.53
4:G:133:ASN:HB3	24:G:1331:NAG:O5	2.09	0.53
4:G:373:THR:HG21	4:G:384:TYR:HB3	1.90	0.52
13:P:3:BMA:H3	13:P:4:MAN:H3	1.91	0.52
4:G:36:VAL:HG13	4:G:496:VAL:HG13	1.92	0.52
4:G:265:LEU:HD11	4:G:291:ALA:HB2	1.92	0.51
3:E:49:TYR:O	3:E:91:TYR:OH	2.21	0.51
4:G:298:ARG:NH2	4:G:441:GLY:O	2.43	0.51
4:G:180:ASP:HA	4:G:194:ILE:HD11	1.91	0.51
4:G:379:ARG:HH11	4:G:379:ARG:HG2	1.76	0.51
13:P:3:BMA:C3	13:P:4:MAN:C5	2.85	0.51
2:D:11:LEU:HD13	2:D:147:PRO:HG3	1.92	0.51
2:D:12:LYS:NZ	2:D:17:SER:O	2.43	0.51
1:B:610:TRP:CG	4:G:498:PRO:HB3	2.46	0.50
5:H:70:SER:HB2	5:H:79:SER:HB2	1.93	0.50
4:G:502:ARG:HB3	4:G:506:VAL:HG13	1.93	0.50
7:V:46:LEU:HD11	7:V:49:TYR:HB3	1.94	0.50
3:E:19:VAL:HG13	3:E:75:ILE:HG23	1.93	0.49
1:B:550:GLN:N	1:B:550:GLN:OE1	2.45	0.49
4:G:507:GLY:O	4:G:510:ARG:NH2	2.44	0.49
4:G:270:ILE:HG22	4:G:289:LYS:H	1.76	0.49
4:G:163:THR:OG1	4:G:164:GLU:N	2.45	0.49
4:G:392:ASN:O	4:G:393:THR:OG1	2.22	0.48
4:G:37:THR:OG1	4:G:499:THR:HB	2.14	0.48
2:D:47:TRP:CZ3	3:E:95(A):GLY:HA3	2.49	0.47
3:E:49:TYR:CD2	3:E:50:GLU:HG3	2.49	0.47
3:E:194:GLN:HG2	3:E:201:THR:HG22	1.96	0.47
3:E:127:ALA:HB3	3:E:129:LYS:H	1.76	0.47
5:H:48:ILE:HG23	5:H:63:LEU:HD11	1.97	0.46
18:Y:4:MAN:H2	18:Y:5:MAN:H3	1.96	0.46
3:E:136:ILE:HG21	3:E:195:VAL:HG21	1.97	0.46
4:G:312:GLY:HA2	4:G:313:PRO:C	2.36	0.46
5:H:188:GLY:HA3	5:H:190:GLN:N	2.31	0.46
4:G:130:ILE:HG13	4:G:158:SER:HB3	1.97	0.46
4:G:42:VAL:HA	4:G:43:PRO:HD3	1.77	0.45
1:B:535:ILE:HG23	1:B:536:THR:HG23	1.98	0.45
4:G:379:ARG:HH12	11:R:3:BMA:H3	1.81	0.45
6:L:21:ILE:HD11	6:L:73:LEU:HD23	1.99	0.45
6:L:53:ASP:N	6:L:53:ASP:OD1	2.49	0.45
7:U:60:CYS:SG	7:U:62:PRO:HD2	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:67:VAL:HG23	7:U:80:LEU:HD11	1.98	0.45
5:H:100(H):LYS:HA	5:H:100(J):TRP:CZ3	2.52	0.44
4:G:464:THR:HA	4:G:464(A):ASN:HA	1.67	0.44
4:G:296:CYS:SG	4:G:376:PHE:HZ	2.40	0.44
7:U:80:LEU:HD12	7:U:81:GLU:N	2.33	0.44
11:K:5:MAN:C2	11:K:6:MAN:H5	2.47	0.44
6:L:55:PRO:HD2	6:L:58:ILE:HD13	1.99	0.44
6:L:18:THR:HG23	6:L:76:THR:HA	1.99	0.43
4:G:98:ASN:O	4:G:101:VAL:HG13	2.19	0.43
4:G:275:GLU:HB3	4:G:282:LYS:HD3	1.99	0.43
5:H:84:ALA:N	25:H:2001:HOH:O	2.41	0.43
6:L:54:ARG:HA	6:L:55:PRO:HD3	1.84	0.43
2:D:102:LEU:HA	2:D:102:LEU:HD12	1.90	0.43
5:H:135:ALA:HB2	5:H:181:THR:HG22	1.99	0.43
6:L:151:ALA:HA	6:L:192:TYR:CE1	2.53	0.43
2:D:59:LEU:HD23	2:D:64:GLN:HA	1.99	0.43
11:K:7:MAN:O5	11:K:10:MAN:C1	2.67	0.43
7:V:65:SER:OG	7:V:66:ARG:N	2.51	0.43
2:D:169:VAL:HG22	3:E:162:THR:HG22	1.99	0.43
4:G:185:ASN:OD1	4:G:185:ASN:N	2.35	0.43
1:B:558:ALA:HB1	1:B:559:PRO:HD2	2.01	0.43
2:D:217:ASP:N	2:D:221:GLU:OE2	2.51	0.43
2:D:18:VAL:O	2:D:81:GLU:HA	2.19	0.42
1:B:571:TRP:CD2	4:G:54:CYS:HB3	2.54	0.42
6:L:46:LEU:HD23	6:L:47:ILE:N	2.35	0.42
4:G:138(D):THR:OG1	4:G:138(E):ASN:HA	2.20	0.42
6:L:152:ASP:O	6:L:153:SER:OG	2.24	0.42
13:P:3:BMA:H3	13:P:4:MAN:C3	2.49	0.42
4:G:343:ARG:HB2	4:G:397:PHE:CZ	2.55	0.42
2:D:100(E):LEU:HA	2:D:100(F):PRO:HD3	1.89	0.42
2:D:47:TRP:CH2	3:E:95(A):GLY:HA3	2.55	0.41
6:L:109:GLN:HE22	6:L:172:LYS:HG3	1.85	0.41
4:G:104:MET:O	4:G:108:ILE:HG12	2.20	0.41
7:U:52:LYS:HA	7:U:52(A):PRO:HD3	1.84	0.41
2:D:11:LEU:HD12	2:D:110:THR:O	2.21	0.41
6:L:137:ILE:HG21	6:L:196:VAL:HG21	2.03	0.41
3:E:139:PHE:CE2	3:E:173:ALA:HA	2.56	0.41
5:H:100(H):LYS:HA	5:H:100(J):TRP:CE3	2.56	0.41
7:V:36:TYR:O	7:V:86:TYR:HA	2.21	0.41
3:E:112:ASN:HA	3:E:113:PRO:HD3	1.84	0.41
2:D:47:TRP:CZ2	2:D:49:GLY:HA2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:36:TRP:HB3	5:H:48:ILE:HD12	2.01	0.41
6:L:110:PRO:O	6:L:111:LYS:HG3	2.21	0.41
4:G:362:LYS:HG3	4:G:363:SER:H	1.86	0.41
5:H:144:PHE:HA	5:H:145:PRO:HA	1.85	0.41
6:L:109:GLN:HB3	6:L:110:PRO:C	2.42	0.41
2:D:200:HIS:ND1	2:D:203:SER:OG	2.29	0.40
1:B:522:PHE:HZ	4:G:491:ILE:HG12	1.86	0.40
3:E:15:LEU:HA	3:E:78:LEU:HB2	2.03	0.40
7:U:21:SER:HB3	7:U:79:PHE:CE1	2.56	0.40
3:E:127:ALA:N	3:E:128:ASN:HA	2.36	0.40
4:G:195:ASN:C	4:G:197:ASN:N	2.75	0.40
10:J:4:MAN:H2	10:J:5:MAN:H2	1.82	0.40
7:U:48:MET:HE3	7:U:63:LEU:HD22	2.04	0.40
6:L:198:HIS:O	6:L:201:SER:HB3	2.20	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:ASP:OD1	2:D:113:SER:OG[2_555]	2.14	0.06
12:M:5:MAN:O6	12:M:8:MAN:O3[2_655]	2.18	0.02

## 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	152/161 (94%)	141 (93%)	11 (7%)	0	100	100
2	D	241/243 (99%)	213 (88%)	26 (11%)	2 (1%)	19	53
3	E	211/216 (98%)	187 (89%)	24 (11%)	0	100	100
4	G	477/484 (99%)	434 (91%)	40 (8%)	3 (1%)	25	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	H	224/244 (92%)	210 (94%)	14 (6%)	0	100	100
6	L	208/213 (98%)	185 (89%)	21 (10%)	2 (1%)	15	48
7	U	117/240 (49%)	108 (92%)	8 (7%)	1 (1%)	17	51
7	V	96/240 (40%)	87 (91%)	8 (8%)	1 (1%)	15	48
All	All	1726/2041 (85%)	1565 (91%)	152 (9%)	9 (0%)	29	63

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	393	THR
2	D	85	ASP
4	G	509	ARG
2	D	167	PRO
6	L	152	ASP
7	V	66	ARG
7	U	108	PRO
6	L	110	PRO
4	G	313	PRO

### 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	131/135 (97%)	122 (93%)	9 (7%)	15	44
2	D	205/206 (100%)	193 (94%)	12 (6%)	19	50
3	E	186/189 (98%)	173 (93%)	13 (7%)	15	44
4	G	428/432 (99%)	385 (90%)	43 (10%)	7	28
5	H	198/213 (93%)	185 (93%)	13 (7%)	16	46
6	L	178/181 (98%)	157 (88%)	21 (12%)	5	21
7	U	102/192 (53%)	95 (93%)	7 (7%)	15	44
7	V	81/192 (42%)	80 (99%)	1 (1%)	71	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1509/1740 (87%)	1390 (92%)	119 (8%)	12	39

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	539	VAL
1	B	540	GLN
1	B	542	ARG
1	B	564	HIS
1	B	565	LEU
1	B	566	LEU
1	B	620	SER
1	B	661	LEU
1	B	663	LEU
2	D	30	ASN
2	D	40	THR
2	D	66	ARG
2	D	70	THR
2	D	109	LEU
2	D	113	SER
2	D	131	THR
2	D	151	THR
2	D	153	SER
2	D	169	VAL
2	D	170	LEU
2	D	193	THR
3	E	23	CYS
3	E	27(C)	CYS
3	E	32	SER
3	E	42	ARG
3	E	51	ASP
3	E	75	ILE
3	E	81	GLU
3	E	85	THR
3	E	88	CYS
3	E	89	CYS
3	E	135	LEU
3	E	140	TYR
3	E	192	SER
4	G	42	VAL
4	G	54	CYS
4	G	101	VAL

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Mol	Chain	Res	Type
4	G	116	LEU
4	G	128	THR
4	G	133	ASN
4	G	138(A)	THR
4	G	150	TYR
4	G	187	ASN
4	G	190	THR
4	G	192	ARG
4	G	194	ILE
4	G	209	THR
4	G	210	PHE
4	G	215	ILE
4	G	248	THR
4	G	261	LEU
4	G	267	GLU
4	G	270	ILE
4	G	296	CYS
4	G	309	PHE
4	G	317	PHE
4	G	320	THR
4	G	326	ILE
4	G	328	GLN
4	G	331	CYS
4	G	337	GLU
4	G	339	GLU
4	G	341	MET
4	G	348	LYS
4	G	352	LEU
4	G	364	SER
4	G	388	SER
4	G	392	ASN
4	G	418	CYS
4	G	419	LYS
4	G	421	LYS
4	G	444	THR
4	G	448	ARG
4	G	466	GLU
4	G	488	VAL
4	G	503	ARG
4	G	509	ARG
5	H	3	HIS
5	H	6	GLU

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Mol	Chain	Res	Type
5	H	63	LEU
5	H	70	SER
5	H	78	VAL
5	H	92	CYS
5	H	95	THR
5	H	99	ARG
5	H	100(J)	TRP
5	H	100(L)	THR
5	H	149	THR
5	H	151	SER
5	H	176	LEU
6	L	9	PHE
6	L	31	ARG
6	L	48	ILE
6	L	52	ASN
6	L	53	ASP
6	L	63	SER
6	L	67(B)	THR
6	L	88	CYS
6	L	93	SER
6	L	94	ARG
6	L	116	VAL
6	L	117	THR
6	L	134	VAL
6	L	146	THR
6	L	147	VAL
6	L	161	GLU
6	L	162	THR
6	L	166	SER
6	L	171	ASN
6	L	180	SER
6	L	196	VAL
7	U	20	ILE
7	U	32	CYS
7	U	70	THR
7	U	71	ARG
7	U	81	GLU
7	U	93	THR
7	U	99	ASP
7	V	11	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

159 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	1,8	14,14,15	0.47	0	17,19,21	0.69	0
8	NAG	A	2	8	14,14,15	0.41	0	17,19,21	0.37	0
8	NAG	C	1	1,8	14,14,15	0.74	1 (7%)	17,19,21	0.99	1 (5%)
8	NAG	C	2	8	14,14,15	0.59	0	17,19,21	0.50	0
9	NAG	F	1	1,9	14,14,15	0.24	0	17,19,21	0.43	0
9	NAG	F	2	9	14,14,15	0.28	0	17,19,21	1.09	2 (11%)
9	BMA	F	3	9	11,11,12	0.46	0	15,15,17	1.07	1 (6%)
8	NAG	I	1	1,8	14,14,15	0.47	0	17,19,21	0.45	0
8	NAG	I	2	8	14,14,15	0.62	0	17,19,21	0.44	0
10	NAG	J	1	10,4	14,14,15	0.35	0	17,19,21	0.70	0
10	NAG	J	2	10	14,14,15	0.36	0	17,19,21	0.43	0
10	BMA	J	3	10	11,11,12	0.69	0	15,15,17	0.85	0
10	MAN	J	4	10	11,11,12	0.86	1 (9%)	15,15,17	1.33	2 (13%)
10	MAN	J	5	10	11,11,12	0.77	0	15,15,17	0.94	1 (6%)
10	MAN	J	6	10	11,11,12	1.05	1 (9%)	15,15,17	1.34	2 (13%)
10	MAN	J	7	10	11,11,12	0.99	1 (9%)	15,15,17	0.88	1 (6%)
10	MAN	J	8	10	11,11,12	0.67	0	15,15,17	1.04	1 (6%)
11	NAG	K	1	11,4	14,14,15	0.29	0	17,19,21	0.45	0
11	MAN	K	10	11	11,11,12	0.80	0	15,15,17	0.99	1 (6%)
11	MAN	K	11	11	11,11,12	0.65	0	15,15,17	0.95	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	K	2	11	14,14,15	0.41	0	17,19,21	0.89	1 (5%)
11	BMA	K	3	11	11,11,12	0.81	0	15,15,17	1.28	1 (6%)
11	MAN	K	4	11	11,11,12	0.68	0	15,15,17	0.93	1 (6%)
11	MAN	K	5	11	11,11,12	0.78	1 (9%)	15,15,17	1.42	2 (13%)
11	MAN	K	6	11	11,11,12	0.24	0	15,15,17	0.57	0
11	MAN	K	7	11	11,11,12	0.79	0	15,15,17	1.32	2 (13%)
11	MAN	K	8	11	11,11,12	0.66	0	15,15,17	1.18	2 (13%)
11	MAN	K	9	11	11,11,12	0.64	0	15,15,17	0.94	2 (13%)
12	NAG	M	1	12,4	14,14,15	0.30	0	17,19,21	0.67	1 (5%)
12	MAN	M	10	12	11,11,12	0.67	0	15,15,17	1.06	2 (13%)
12	NAG	M	2	12	14,14,15	0.35	0	17,19,21	0.46	0
12	BMA	M	3	12	11,11,12	0.88	1 (9%)	15,15,17	1.06	0
12	MAN	M	4	12	11,11,12	0.96	0	15,15,17	1.13	1 (6%)
12	MAN	M	5	12	11,11,12	0.86	0	15,15,17	1.32	2 (13%)
12	MAN	M	6	12	11,11,12	0.71	0	15,15,17	1.02	2 (13%)
12	MAN	M	7	12	11,11,12	0.84	0	15,15,17	1.18	3 (20%)
12	MAN	M	8	12	11,11,12	0.56	0	15,15,17	1.08	1 (6%)
12	MAN	M	9	12	11,11,12	0.67	0	15,15,17	1.02	2 (13%)
12	NAG	N	1	12,4	14,14,15	0.21	0	17,19,21	0.55	0
12	MAN	N	10	12	11,11,12	0.79	1 (9%)	15,15,17	1.03	2 (13%)
12	NAG	N	2	12	14,14,15	0.25	0	17,19,21	0.43	0
12	BMA	N	3	12	11,11,12	0.94	1 (9%)	15,15,17	1.19	1 (6%)
12	MAN	N	4	12	11,11,12	0.71	0	15,15,17	1.23	1 (6%)
12	MAN	N	5	12	11,11,12	0.62	0	15,15,17	1.30	2 (13%)
12	MAN	N	6	12	11,11,12	0.69	0	15,15,17	1.04	2 (13%)
12	MAN	N	7	12	11,11,12	0.69	0	15,15,17	1.16	2 (13%)
12	MAN	N	8	12	11,11,12	0.58	0	15,15,17	1.11	2 (13%)
12	MAN	N	9	12	11,11,12	0.74	0	15,15,17	0.90	1 (6%)
9	NAG	O	1	9,4	14,14,15	1.40	1 (7%)	17,19,21	0.87	1 (5%)
9	NAG	O	2	9	14,14,15	0.26	0	17,19,21	0.53	0
9	BMA	O	3	9	11,11,12	0.90	1 (9%)	15,15,17	0.84	0
13	NAG	P	1	13,4	14,14,15	0.27	0	17,19,21	0.50	0
13	NAG	P	2	13	14,14,15	0.45	0	17,19,21	0.38	0
13	BMA	P	3	13	11,11,12	0.44	0	15,15,17	1.24	1 (6%)
13	MAN	P	4	13	11,11,12	0.31	0	15,15,17	0.99	1 (6%)
13	MAN	P	5	13	11,11,12	0.81	0	15,15,17	0.79	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	MAN	P	6	13	11,11,12	0.76	1 (9%)	15,15,17	1.19	2 (13%)
14	NAG	Q	1	4,14	14,14,15	0.39	0	17,19,21	0.54	0
14	NAG	Q	2	14	14,14,15	0.45	0	17,19,21	0.70	0
14	BMA	Q	3	14	11,11,12	1.00	0	15,15,17	1.03	1 (6%)
14	MAN	Q	4	14	11,11,12	0.73	0	15,15,17	1.08	1 (6%)
14	MAN	Q	5	14	11,11,12	0.79	0	15,15,17	0.89	1 (6%)
14	MAN	Q	6	14	11,11,12	0.69	0	15,15,17	0.99	2 (13%)
14	MAN	Q	7	14	11,11,12	0.72	0	15,15,17	0.95	1 (6%)
11	NAG	R	1	11,4	14,14,15	0.42	0	17,19,21	0.44	0
11	MAN	R	10	11	11,11,12	0.63	0	15,15,17	1.07	2 (13%)
11	MAN	R	11	11	11,11,12	0.68	0	15,15,17	0.92	2 (13%)
11	NAG	R	2	11	14,14,15	0.30	0	17,19,21	0.38	0
11	BMA	R	3	11	11,11,12	0.66	0	15,15,17	0.86	0
11	MAN	R	4	11	11,11,12	0.80	0	15,15,17	1.26	2 (13%)
11	MAN	R	5	11	11,11,12	0.68	0	15,15,17	1.40	3 (20%)
11	MAN	R	6	11	11,11,12	0.88	1 (9%)	15,15,17	0.89	1 (6%)
11	MAN	R	7	11	11,11,12	0.69	0	15,15,17	1.08	2 (13%)
11	MAN	R	8	11	11,11,12	0.69	0	15,15,17	1.28	3 (20%)
11	MAN	R	9	11	11,11,12	0.78	0	15,15,17	0.91	1 (6%)
15	NAG	S	1	15,4	14,14,15	0.57	0	17,19,21	0.61	0
15	NAG	S	2	15	14,14,15	0.26	0	17,19,21	0.69	0
15	BMA	S	3	15	11,11,12	0.74	0	15,15,17	0.80	0
15	MAN	S	4	15	11,11,12	0.64	0	15,15,17	0.95	1 (6%)
15	MAN	S	5	15	11,11,12	0.63	0	15,15,17	1.38	2 (13%)
15	MAN	S	6	15	11,11,12	0.52	0	15,15,17	1.11	2 (13%)
15	MAN	S	7	15	11,11,12	1.00	0	15,15,17	1.06	2 (13%)
15	MAN	S	8	15	11,11,12	0.67	0	15,15,17	1.44	2 (13%)
15	MAN	S	9	15	11,11,12	0.61	0	15,15,17	1.18	2 (13%)
16	NAG	T	1	4,16	14,14,15	0.28	0	17,19,21	0.52	0
16	NAG	T	2	16	14,14,15	0.56	0	17,19,21	1.22	2 (11%)
16	BMA	T	3	16	11,11,12	0.63	0	15,15,17	1.45	2 (13%)
16	MAN	T	4	16	11,11,12	1.20	2 (18%)	15,15,17	1.54	3 (20%)
16	MAN	T	5	16	11,11,12	0.73	0	15,15,17	1.25	3 (20%)
16	MAN	T	6	16	11,11,12	0.67	0	15,15,17	0.90	1 (6%)
16	MAN	T	7	16	11,11,12	0.68	0	15,15,17	1.03	2 (13%)
16	MAN	T	8	16	11,11,12	1.39	3 (27%)	15,15,17	1.34	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	MAN	T	9	16	11,11,12	0.75	1 (9%)	15,15,17	1.05	2 (13%)
17	NAG	W	1	4,17	14,14,15	0.49	0	17,19,21	0.65	0
17	NAG	W	2	17	14,14,15	0.39	0	17,19,21	0.65	0
17	BMA	W	3	17	11,11,12	1.07	1 (9%)	15,15,17	1.14	1 (6%)
17	MAN	W	4	17	11,11,12	0.86	1 (9%)	15,15,17	1.33	2 (13%)
17	MAN	W	5	17	11,11,12	0.76	0	15,15,17	0.93	1 (6%)
17	MAN	W	6	17	11,11,12	0.78	1 (9%)	15,15,17	1.29	2 (13%)
12	NAG	X	1	12,4	14,14,15	0.49	0	17,19,21	0.44	0
12	MAN	X	10	12	11,11,12	0.78	0	15,15,17	0.90	1 (6%)
12	NAG	X	2	12	14,14,15	0.27	0	17,19,21	0.71	0
12	BMA	X	3	12	11,11,12	1.18	2 (18%)	15,15,17	1.42	2 (13%)
12	MAN	X	4	12	11,11,12	0.82	1 (9%)	15,15,17	1.44	2 (13%)
12	MAN	X	5	12	11,11,12	0.86	0	15,15,17	1.37	3 (20%)
12	MAN	X	6	12	11,11,12	1.06	1 (9%)	15,15,17	1.66	4 (26%)
12	MAN	X	7	12	11,11,12	0.65	0	15,15,17	1.11	2 (13%)
12	MAN	X	8	12	11,11,12	0.84	1 (9%)	15,15,17	1.18	1 (6%)
12	MAN	X	9	12	11,11,12	0.79	0	15,15,17	1.03	2 (13%)
18	NAG	Y	1	18,4	14,14,15	0.30	0	17,19,21	0.45	0
18	NAG	Y	2	18	14,14,15	0.20	0	17,19,21	0.42	0
18	BMA	Y	3	18	11,11,12	0.92	0	15,15,17	0.90	1 (6%)
18	MAN	Y	4	18	11,11,12	0.73	0	15,15,17	1.09	2 (13%)
18	MAN	Y	5	18	11,11,12	1.09	1 (9%)	15,15,17	1.69	2 (13%)
18	MAN	Y	6	18	11,11,12	0.67	0	15,15,17	1.21	2 (13%)
18	MAN	Y	7	18	11,11,12	0.64	0	15,15,17	1.01	2 (13%)
9	NAG	Z	1	9,4	14,14,15	0.27	0	17,19,21	0.45	0
9	NAG	Z	2	9	14,14,15	0.23	0	17,19,21	0.44	0
9	BMA	Z	3	9	11,11,12	0.58	0	15,15,17	0.99	1 (6%)
19	NAG	a	1	19,4	14,14,15	0.36	0	17,19,21	0.65	0
19	NAG	a	2	19	14,14,15	0.31	0	17,19,21	0.48	0
19	BMA	a	3	19	11,11,12	1.07	2 (18%)	15,15,17	1.22	1 (6%)
19	MAN	a	4	19	11,11,12	0.91	0	15,15,17	0.86	1 (6%)
19	MAN	a	5	19	11,11,12	0.62	0	15,15,17	1.17	2 (13%)
19	MAN	a	6	19	11,11,12	0.65	0	15,15,17	0.99	2 (13%)
19	MAN	a	7	19	11,11,12	0.68	0	15,15,17	1.24	2 (13%)
19	MAN	a	8	19	11,11,12	0.66	0	15,15,17	0.93	2 (13%)
19	MAN	a	9	19	11,11,12	0.89	1 (9%)	15,15,17	1.22	2 (13%)
20	NAG	b	1	20,4	14,14,15	0.33	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	MAN	b	10	20	11,11,12	0.72	1 (9%)	15,15,17	1.14	2 (13%)
20	NAG	b	2	20	14,14,15	0.21	0	17,19,21	0.51	0
20	BMA	b	3	20	11,11,12	0.69	0	15,15,17	1.01	1 (6%)
20	MAN	b	4	20	11,11,12	0.88	0	15,15,17	1.65	3 (20%)
20	MAN	b	5	20	11,11,12	0.76	0	15,15,17	0.90	1 (6%)
20	MAN	b	6	20	11,11,12	0.76	0	15,15,17	1.29	2 (13%)
20	MAN	b	7	20	11,11,12	0.74	0	15,15,17	0.95	1 (6%)
20	MAN	b	8	20	11,11,12	0.73	0	15,15,17	1.05	2 (13%)
20	MAN	b	9	20	11,11,12	1.11	2 (18%)	15,15,17	1.32	2 (13%)
21	NAG	c	1	4,21	14,14,15	0.29	0	17,19,21	0.47	0
21	NAG	c	2	21	14,14,15	0.26	0	17,19,21	0.65	0
21	BMA	c	3	21	11,11,12	0.74	0	15,15,17	1.51	4 (26%)
21	MAN	c	4	21	11,11,12	1.84	4 (36%)	15,15,17	1.39	2 (13%)
21	MAN	c	5	21	11,11,12	0.98	1 (9%)	15,15,17	0.87	0
21	MAN	c	6	21	11,11,12	0.73	1 (9%)	15,15,17	1.22	2 (13%)
21	MAN	c	7	21	11,11,12	0.70	0	15,15,17	1.05	2 (13%)
8	NAG	d	1	8,4	14,14,15	0.22	0	17,19,21	0.39	0
8	NAG	d	2	8	14,14,15	0.43	0	17,19,21	0.35	0
17	NAG	e	1	5,17	14,14,15	0.55	0	17,19,21	0.66	0
17	NAG	e	2	17	14,14,15	0.41	0	17,19,21	0.69	1 (5%)
17	BMA	e	3	17	11,11,12	1.07	1 (9%)	15,15,17	0.92	0
17	MAN	e	4	17	11,11,12	0.76	0	15,15,17	0.89	1 (6%)
17	MAN	e	5	17	11,11,12	0.96	1 (9%)	15,15,17	1.39	3 (20%)
17	MAN	e	6	17	11,11,12	0.75	0	15,15,17	1.05	2 (13%)
17	NAG	f	1	17,7	14,14,15	0.39	0	17,19,21	0.55	0
17	NAG	f	2	17	14,14,15	0.40	0	17,19,21	0.51	0
17	BMA	f	3	17	11,11,12	0.95	1 (9%)	15,15,17	0.86	1 (6%)
17	MAN	f	4	17	11,11,12	0.91	1 (9%)	15,15,17	1.33	2 (13%)
17	MAN	f	5	17	11,11,12	0.75	1 (9%)	15,15,17	1.10	2 (13%)
17	MAN	f	6	17	11,11,12	0.68	0	15,15,17	1.11	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	1,8	-	2/6/23/26	0/1/1/1
8	NAG	A	2	8	-	0/6/23/26	0/1/1/1
8	NAG	C	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	C	2	8	-	1/6/23/26	0/1/1/1
9	NAG	F	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	F	2	9	-	0/6/23/26	0/1/1/1
9	BMA	F	3	9	-	0/2/19/22	0/1/1/1
8	NAG	I	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	I	2	8	-	0/6/23/26	0/1/1/1
10	NAG	J	1	10,4	-	1/6/23/26	0/1/1/1
10	NAG	J	2	10	-	2/6/23/26	0/1/1/1
10	BMA	J	3	10	-	1/2/19/22	0/1/1/1
10	MAN	J	4	10	-	0/2/19/22	0/1/1/1
10	MAN	J	5	10	-	1/2/19/22	0/1/1/1
10	MAN	J	6	10	-	1/2/19/22	0/1/1/1
10	MAN	J	7	10	-	0/2/19/22	0/1/1/1
10	MAN	J	8	10	-	0/2/19/22	0/1/1/1
11	NAG	K	1	11,4	-	0/6/23/26	0/1/1/1
11	MAN	K	10	11	-	1/2/19/22	0/1/1/1
11	MAN	K	11	11	-	0/2/19/22	0/1/1/1
11	NAG	K	2	11	-	0/6/23/26	0/1/1/1
11	BMA	K	3	11	-	2/2/19/22	0/1/1/1
11	MAN	K	4	11	-	0/2/19/22	0/1/1/1
11	MAN	K	5	11	-	0/2/19/22	0/1/1/1
11	MAN	K	6	11	-	0/2/19/22	0/1/1/1
11	MAN	K	7	11	-	2/2/19/22	0/1/1/1
11	MAN	K	8	11	-	1/2/19/22	0/1/1/1
11	MAN	K	9	11	-	0/2/19/22	0/1/1/1
12	NAG	M	1	12,4	-	2/6/23/26	0/1/1/1
12	MAN	M	10	12	-	0/2/19/22	0/1/1/1
12	NAG	M	2	12	-	0/6/23/26	0/1/1/1
12	BMA	M	3	12	-	2/2/19/22	0/1/1/1
12	MAN	M	4	12	-	0/2/19/22	0/1/1/1
12	MAN	M	5	12	-	1/2/19/22	0/1/1/1
12	MAN	M	6	12	-	1/2/19/22	0/1/1/1
12	MAN	M	7	12	-	0/2/19/22	0/1/1/1
12	MAN	M	8	12	-	0/2/19/22	0/1/1/1
12	MAN	M	9	12	-	1/2/19/22	0/1/1/1
12	NAG	N	1	12,4	-	1/6/23/26	0/1/1/1
12	MAN	N	10	12	-	1/2/19/22	0/1/1/1
12	NAG	N	2	12	-	1/6/23/26	0/1/1/1
12	BMA	N	3	12	-	1/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	MAN	S	7	15	-	1/2/19/22	0/1/1/1
15	MAN	S	8	15	-	0/2/19/22	0/1/1/1
15	MAN	S	9	15	-	1/2/19/22	0/1/1/1
16	NAG	T	1	4,16	-	0/6/23/26	0/1/1/1
16	NAG	T	2	16	-	0/6/23/26	0/1/1/1
16	BMA	T	3	16	-	0/2/19/22	0/1/1/1
16	MAN	T	4	16	-	0/2/19/22	0/1/1/1
16	MAN	T	5	16	-	2/2/19/22	0/1/1/1
16	MAN	T	6	16	-	1/2/19/22	0/1/1/1
16	MAN	T	7	16	-	0/2/19/22	0/1/1/1
16	MAN	T	8	16	-	0/2/19/22	0/1/1/1
16	MAN	T	9	16	-	0/2/19/22	0/1/1/1
17	NAG	W	1	4,17	-	1/6/23/26	0/1/1/1
17	NAG	W	2	17	-	0/6/23/26	0/1/1/1
17	BMA	W	3	17	-	1/2/19/22	0/1/1/1
17	MAN	W	4	17	-	1/2/19/22	0/1/1/1
17	MAN	W	5	17	-	1/2/19/22	0/1/1/1
17	MAN	W	6	17	-	1/2/19/22	0/1/1/1
12	NAG	X	1	12,4	-	2/6/23/26	0/1/1/1
12	MAN	X	10	12	-	0/2/19/22	0/1/1/1
12	NAG	X	2	12	-	3/6/23/26	0/1/1/1
12	BMA	X	3	12	-	0/2/19/22	0/1/1/1
12	MAN	X	4	12	-	0/2/19/22	0/1/1/1
12	MAN	X	5	12	-	0/2/19/22	0/1/1/1
12	MAN	X	6	12	-	0/2/19/22	0/1/1/1
12	MAN	X	7	12	-	2/2/19/22	0/1/1/1
12	MAN	X	8	12	-	1/2/19/22	0/1/1/1
12	MAN	X	9	12	-	0/2/19/22	0/1/1/1
18	NAG	Y	1	18,4	-	2/6/23/26	0/1/1/1
18	NAG	Y	2	18	-	1/6/23/26	0/1/1/1
18	BMA	Y	3	18	-	2/2/19/22	0/1/1/1
18	MAN	Y	4	18	-	0/2/19/22	0/1/1/1
18	MAN	Y	5	18	-	1/2/19/22	0/1/1/1
18	MAN	Y	6	18	-	0/2/19/22	0/1/1/1
18	MAN	Y	7	18	-	0/2/19/22	0/1/1/1
9	NAG	Z	1	9,4	-	0/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	2/6/23/26	0/1/1/1
9	BMA	Z	3	9	-	1/2/19/22	0/1/1/1
19	NAG	a	1	19,4	-	1/6/23/26	0/1/1/1
19	NAG	a	2	19	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BMA	a	3	19	-	2/2/19/22	0/1/1/1
19	MAN	a	4	19	-	2/2/19/22	0/1/1/1
19	MAN	a	5	19	-	1/2/19/22	0/1/1/1
19	MAN	a	6	19	-	0/2/19/22	0/1/1/1
19	MAN	a	7	19	-	0/2/19/22	0/1/1/1
19	MAN	a	8	19	-	1/2/19/22	0/1/1/1
19	MAN	a	9	19	-	0/2/19/22	0/1/1/1
20	NAG	b	1	20,4	-	2/6/23/26	0/1/1/1
20	MAN	b	10	20	-	0/2/19/22	0/1/1/1
20	NAG	b	2	20	-	1/6/23/26	0/1/1/1
20	BMA	b	3	20	-	1/2/19/22	0/1/1/1
20	MAN	b	4	20	-	2/2/19/22	0/1/1/1
20	MAN	b	5	20	-	0/2/19/22	0/1/1/1
20	MAN	b	6	20	-	1/2/19/22	0/1/1/1
20	MAN	b	7	20	-	0/2/19/22	0/1/1/1
20	MAN	b	8	20	-	0/2/19/22	0/1/1/1
20	MAN	b	9	20	-	1/2/19/22	0/1/1/1
21	NAG	c	1	4,21	-	2/6/23/26	0/1/1/1
21	NAG	c	2	21	-	1/6/23/26	0/1/1/1
21	BMA	c	3	21	-	2/2/19/22	0/1/1/1
21	MAN	c	4	21	-	2/2/19/22	0/1/1/1
21	MAN	c	5	21	-	0/2/19/22	0/1/1/1
21	MAN	c	6	21	-	0/2/19/22	0/1/1/1
21	MAN	c	7	21	-	0/2/19/22	0/1/1/1
8	NAG	d	1	8,4	-	1/6/23/26	0/1/1/1
8	NAG	d	2	8	-	0/6/23/26	0/1/1/1
17	NAG	e	1	5,17	-	1/6/23/26	0/1/1/1
17	NAG	e	2	17	-	2/6/23/26	0/1/1/1
17	BMA	e	3	17	-	2/2/19/22	0/1/1/1
17	MAN	e	4	17	-	1/2/19/22	0/1/1/1
17	MAN	e	5	17	-	0/2/19/22	0/1/1/1
17	MAN	e	6	17	-	0/2/19/22	0/1/1/1
17	NAG	f	1	17,7	-	0/6/23/26	0/1/1/1
17	NAG	f	2	17	-	2/6/23/26	0/1/1/1
17	BMA	f	3	17	-	2/2/19/22	0/1/1/1
17	MAN	f	4	17	-	0/2/19/22	0/1/1/1
17	MAN	f	5	17	-	0/2/19/22	0/1/1/1
17	MAN	f	6	17	-	1/2/19/22	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	O	1	NAG	O5-C1	-4.99	1.35	1.43
21	c	4	MAN	C2-C3	4.28	1.58	1.52
18	Y	5	MAN	O2-C2	-3.42	1.36	1.43
12	X	6	MAN	C1-C2	3.14	1.59	1.52
16	T	4	MAN	C1-C2	2.97	1.59	1.52
17	e	5	MAN	C1-C2	2.87	1.58	1.52
20	b	9	MAN	C1-C2	2.76	1.58	1.52
16	T	8	MAN	C2-C3	2.71	1.56	1.52
19	a	9	MAN	C1-C2	2.70	1.58	1.52
17	f	4	MAN	C1-C2	2.56	1.58	1.52
21	c	4	MAN	O2-C2	2.56	1.48	1.43
12	X	3	BMA	C2-C3	2.56	1.56	1.52
17	W	4	MAN	C1-C2	2.55	1.58	1.52
12	N	3	BMA	C1-C2	2.53	1.58	1.52
10	J	7	MAN	O5-C1	-2.52	1.39	1.43
12	X	3	BMA	C1-C2	2.50	1.57	1.52
9	O	3	BMA	C1-C2	2.47	1.57	1.52
19	a	3	BMA	C1-C2	2.42	1.57	1.52
17	W	6	MAN	C1-C2	2.42	1.57	1.52
17	f	3	BMA	C1-C2	2.40	1.57	1.52
10	J	4	MAN	O5-C1	-2.31	1.40	1.43
12	X	4	MAN	C1-C2	2.29	1.57	1.52
16	T	8	MAN	C1-C2	2.27	1.57	1.52
16	T	8	MAN	O2-C2	2.27	1.48	1.43
12	X	8	MAN	C1-C2	2.27	1.57	1.52
21	c	4	MAN	C1-C2	2.26	1.57	1.52
12	M	3	BMA	C1-C2	2.25	1.57	1.52
8	C	1	NAG	C1-C2	2.25	1.55	1.52
21	c	5	MAN	O5-C1	-2.24	1.40	1.43
20	b	9	MAN	C2-C3	2.22	1.55	1.52
21	c	6	MAN	C1-C2	2.18	1.57	1.52
17	W	3	BMA	O3-C3	2.15	1.48	1.43
19	a	3	BMA	C2-C3	2.12	1.55	1.52
16	T	4	MAN	C2-C3	2.09	1.55	1.52
21	c	4	MAN	O5-C1	-2.08	1.40	1.43
11	R	6	MAN	O5-C1	-2.07	1.40	1.43
11	K	5	MAN	C1-C2	2.07	1.56	1.52
17	f	5	MAN	C1-C2	2.07	1.56	1.52
12	N	10	MAN	C1-C2	2.06	1.56	1.52
20	b	10	MAN	C1-C2	2.05	1.56	1.52
17	e	3	BMA	O3-C3	2.02	1.47	1.43
10	J	6	MAN	C1-C2	2.01	1.56	1.52
16	T	9	MAN	C1-C2	2.01	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	6	MAN	C1-C2	2.01	1.56	1.52

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	4	MAN	C1-O5-C5	4.77	118.66	112.19
18	Y	5	MAN	O2-C2-C3	-4.71	100.71	110.14
16	T	3	BMA	C1-O5-C5	4.64	118.47	112.19
12	X	6	MAN	C1-O5-C5	4.61	118.44	112.19
15	S	8	MAN	C1-O5-C5	4.27	117.98	112.19
12	X	4	MAN	C1-O5-C5	4.24	117.93	112.19
11	K	5	MAN	C1-O5-C5	4.03	117.65	112.19
20	b	6	MAN	C1-O5-C5	3.97	117.57	112.19
16	T	4	MAN	C1-C2-C3	3.92	114.49	109.67
11	R	5	MAN	O2-C2-C3	-3.88	102.37	110.14
11	K	3	BMA	C1-O5-C5	3.84	117.39	112.19
12	M	4	MAN	O2-C2-C3	-3.69	102.75	110.14
18	Y	5	MAN	O2-C2-C1	3.68	116.68	109.15
12	N	4	MAN	O2-C2-C1	3.67	116.66	109.15
15	S	5	MAN	C1-O5-C5	3.59	117.06	112.19
10	J	4	MAN	O2-C2-C3	-3.59	102.95	110.14
18	Y	6	MAN	C1-O5-C5	3.56	117.01	112.19
17	W	6	MAN	C1-O5-C5	3.55	117.00	112.19
17	e	5	MAN	C1-O5-C5	3.47	116.90	112.19
19	a	7	MAN	C1-O5-C5	3.43	116.84	112.19
12	N	5	MAN	C1-O5-C5	3.42	116.83	112.19
15	S	9	MAN	C1-O5-C5	3.41	116.81	112.19
21	c	3	BMA	C1-C2-C3	3.38	113.83	109.67
17	f	4	MAN	C1-O5-C5	3.38	116.77	112.19
11	K	7	MAN	O3-C3-C2	3.35	116.40	109.99
13	P	6	MAN	C1-O5-C5	3.33	116.70	112.19
11	R	4	MAN	O2-C2-C3	-3.32	103.48	110.14
11	K	8	MAN	C1-O5-C5	3.27	116.62	112.19
21	c	6	MAN	C1-O5-C5	3.26	116.60	112.19
9	F	3	BMA	C1-O5-C5	3.25	116.60	112.19
17	W	3	BMA	O3-C3-C2	3.23	116.18	109.99
17	W	4	MAN	C1-O5-C5	3.21	116.53	112.19
10	J	6	MAN	C1-C2-C3	3.21	113.61	109.67
12	X	5	MAN	C1-C2-C3	-3.19	105.74	109.67
9	F	2	NAG	C1-O5-C5	3.14	116.44	112.19
12	X	8	MAN	C1-O5-C5	3.14	116.44	112.19
12	M	5	MAN	O2-C2-C3	-3.13	103.86	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	2	NAG	C1-O5-C5	3.13	116.43	112.19
13	P	3	BMA	C1-C2-C3	3.12	113.50	109.67
12	M	8	MAN	C1-O5-C5	3.09	116.38	112.19
16	T	8	MAN	O2-C2-C1	3.09	115.47	109.15
17	f	6	MAN	C1-O5-C5	3.09	116.37	112.19
16	T	4	MAN	C1-O5-C5	3.06	116.34	112.19
12	X	3	BMA	C1-C2-C3	3.06	113.42	109.67
15	S	6	MAN	C1-O5-C5	3.05	116.32	112.19
12	M	5	MAN	C1-O5-C5	2.97	116.21	112.19
19	a	9	MAN	C1-O5-C5	2.96	116.20	112.19
12	N	7	MAN	C1-O5-C5	2.95	116.19	112.19
16	T	5	MAN	O2-C2-C3	-2.92	104.29	110.14
12	X	7	MAN	C1-O5-C5	2.90	116.13	112.19
12	N	8	MAN	O2-C2-C3	-2.89	104.35	110.14
20	b	9	MAN	C1-C2-C3	2.89	113.22	109.67
20	b	10	MAN	C1-O5-C5	2.88	116.09	112.19
19	a	3	BMA	C1-O5-C5	2.86	116.07	112.19
19	a	5	MAN	C1-O5-C5	2.86	116.06	112.19
14	Q	4	MAN	O2-C2-C3	-2.85	104.42	110.14
12	X	5	MAN	O3-C3-C2	2.84	115.44	109.99
12	X	4	MAN	O2-C2-C3	-2.84	104.45	110.14
18	Y	4	MAN	C1-O5-C5	2.81	116.00	112.19
12	M	10	MAN	C1-O5-C5	2.79	115.97	112.19
20	b	3	BMA	C1-O5-C5	2.75	115.92	112.19
21	c	4	MAN	C1-C2-C3	2.75	113.04	109.67
18	Y	7	MAN	C1-O5-C5	2.74	115.91	112.19
17	f	5	MAN	C1-O5-C5	2.73	115.90	112.19
11	R	4	MAN	C1-O5-C5	2.73	115.89	112.19
16	T	5	MAN	C1-O5-C5	2.72	115.88	112.19
21	c	7	MAN	C1-O5-C5	2.70	115.85	112.19
12	N	6	MAN	C1-O5-C5	2.69	115.84	112.19
16	T	7	MAN	C1-O5-C5	2.67	115.81	112.19
12	X	5	MAN	C1-O5-C5	2.67	115.81	112.19
9	F	2	NAG	O4-C4-C5	2.65	115.89	109.30
20	b	8	MAN	C1-O5-C5	2.63	115.76	112.19
11	R	8	MAN	C1-O5-C5	2.62	115.74	112.19
11	R	8	MAN	O2-C2-C3	-2.57	104.99	110.14
13	P	4	MAN	C1-O5-C5	2.56	115.67	112.19
19	a	6	MAN	C1-O5-C5	2.56	115.65	112.19
12	N	8	MAN	C1-O5-C5	2.55	115.65	112.19
20	b	9	MAN	C1-O5-C5	2.55	115.65	112.19
11	R	7	MAN	C1-O5-C5	2.55	115.64	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	X	7	MAN	O2-C2-C3	-2.55	105.04	110.14
11	R	8	MAN	C1-C2-C3	-2.54	106.55	109.67
11	K	8	MAN	O2-C2-C3	-2.53	105.08	110.14
16	T	9	MAN	C1-O5-C5	2.51	115.60	112.19
19	a	7	MAN	O2-C2-C3	-2.51	105.11	110.14
21	c	4	MAN	O2-C2-C1	2.51	114.29	109.15
15	S	4	MAN	C1-O5-C5	2.50	115.58	112.19
19	a	5	MAN	O2-C2-C3	-2.49	105.14	110.14
11	K	7	MAN	C1-C2-C3	2.48	112.72	109.67
20	b	7	MAN	O2-C2-C3	-2.47	105.19	110.14
11	R	5	MAN	C1-O5-C5	2.47	115.54	112.19
12	N	5	MAN	O2-C2-C3	-2.46	105.20	110.14
16	T	2	NAG	O4-C4-C5	2.45	115.39	109.30
10	J	6	MAN	O2-C2-C3	-2.45	105.24	110.14
11	K	10	MAN	O2-C2-C3	-2.44	105.25	110.14
11	K	4	MAN	C1-O5-C5	2.43	115.49	112.19
17	e	6	MAN	C1-O5-C5	2.43	115.49	112.19
12	M	9	MAN	C1-O5-C5	2.41	115.46	112.19
11	R	10	MAN	O2-C2-C3	-2.40	105.33	110.14
21	c	3	BMA	C1-O5-C5	2.38	115.42	112.19
8	C	1	NAG	C1-O5-C5	2.38	115.42	112.19
16	T	7	MAN	O2-C2-C3	-2.38	105.38	110.14
21	c	6	MAN	O2-C2-C3	-2.37	105.39	110.14
12	M	7	MAN	O2-C2-C3	-2.36	105.42	110.14
12	X	6	MAN	O5-C1-C2	2.35	114.41	110.77
11	R	10	MAN	C1-O5-C5	2.35	115.38	112.19
17	f	3	BMA	O2-C2-C3	-2.35	105.44	110.14
12	N	7	MAN	O2-C2-C3	-2.33	105.46	110.14
9	Z	3	BMA	C1-O5-C5	2.32	115.33	112.19
12	M	6	MAN	C1-O5-C5	2.32	115.33	112.19
11	K	5	MAN	C1-C2-C3	2.32	112.51	109.67
12	X	9	MAN	C1-O5-C5	2.31	115.33	112.19
17	e	2	NAG	C1-O5-C5	2.31	115.32	112.19
11	K	11	MAN	O2-C2-C3	-2.30	105.53	110.14
20	b	8	MAN	O2-C2-C3	-2.30	105.53	110.14
10	J	7	MAN	O2-C2-C3	-2.29	105.54	110.14
11	K	2	NAG	C1-O5-C5	2.29	115.30	112.19
17	e	6	MAN	O2-C2-C3	-2.29	105.55	110.14
15	S	7	MAN	O2-C2-C3	-2.29	105.56	110.14
11	R	11	MAN	O2-C2-C3	-2.29	105.56	110.14
17	f	4	MAN	O2-C2-C3	-2.28	105.56	110.14
18	Y	4	MAN	O2-C2-C3	-2.28	105.57	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	X	3	BMA	C1-O5-C5	2.28	115.28	112.19
15	S	7	MAN	C1-C2-C3	2.28	112.47	109.67
14	Q	6	MAN	C1-O5-C5	2.28	115.28	112.19
11	K	9	MAN	C1-O5-C5	2.27	115.27	112.19
12	M	9	MAN	O2-C2-C3	-2.27	105.59	110.14
10	J	8	MAN	C1-O5-C5	2.26	115.25	112.19
16	T	8	MAN	C1-C2-C3	2.26	112.44	109.67
16	T	4	MAN	O2-C2-C3	-2.26	105.62	110.14
12	M	6	MAN	O2-C2-C3	-2.25	105.62	110.14
19	a	8	MAN	O2-C2-C3	-2.25	105.63	110.14
20	b	4	MAN	O2-C2-C3	-2.25	105.64	110.14
17	W	4	MAN	O2-C2-C3	-2.24	105.66	110.14
16	T	9	MAN	O2-C2-C3	-2.23	105.67	110.14
20	b	4	MAN	C3-C4-C5	2.22	114.20	110.24
12	X	10	MAN	O2-C2-C3	-2.22	105.69	110.14
21	c	7	MAN	O2-C2-C3	-2.22	105.70	110.14
16	T	3	BMA	O3-C3-C2	2.21	114.23	109.99
17	f	5	MAN	O2-C2-C3	-2.21	105.71	110.14
12	M	10	MAN	O2-C2-C3	-2.20	105.72	110.14
19	a	9	MAN	O2-C2-C3	-2.20	105.72	110.14
10	J	5	MAN	O2-C2-C3	-2.19	105.74	110.14
17	f	6	MAN	O2-C2-C3	-2.19	105.76	110.14
13	P	6	MAN	O2-C2-C3	-2.19	105.76	110.14
16	T	6	MAN	O2-C2-C3	-2.18	105.76	110.14
12	N	10	MAN	O2-C2-C3	-2.18	105.77	110.14
14	Q	6	MAN	O2-C2-C3	-2.18	105.77	110.14
12	X	6	MAN	C1-C2-C3	2.18	112.34	109.67
19	a	6	MAN	O2-C2-C3	-2.18	105.78	110.14
17	e	4	MAN	O2-C2-C3	-2.17	105.79	110.14
12	N	10	MAN	C1-O5-C5	2.17	115.13	112.19
15	S	5	MAN	O2-C2-C3	-2.17	105.79	110.14
17	e	5	MAN	O2-C2-C3	-2.17	105.79	110.14
18	Y	6	MAN	O2-C2-C3	-2.17	105.80	110.14
12	N	9	MAN	O2-C2-C3	-2.17	105.80	110.14
16	T	5	MAN	O2-C2-C1	2.16	113.58	109.15
11	R	6	MAN	O2-C2-C3	-2.15	105.82	110.14
11	K	11	MAN	C1-O5-C5	2.14	115.10	112.19
12	M	7	MAN	C1-O5-C5	2.14	115.09	112.19
17	W	6	MAN	O2-C2-C3	-2.14	105.86	110.14
19	a	8	MAN	C1-O5-C5	2.13	115.08	112.19
14	Q	3	BMA	O3-C3-C4	2.13	115.26	110.35
11	K	9	MAN	O2-C2-C3	-2.12	105.89	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	X	9	MAN	O2-C2-C3	-2.12	105.89	110.14
17	W	5	MAN	O2-C2-C3	-2.12	105.89	110.14
14	Q	7	MAN	O2-C2-C3	-2.12	105.89	110.14
11	R	7	MAN	O2-C2-C3	-2.12	105.90	110.14
12	M	1	NAG	C1-O5-C5	2.12	115.06	112.19
18	Y	7	MAN	O2-C2-C3	-2.11	105.91	110.14
17	e	5	MAN	C1-C2-C3	2.11	112.26	109.67
15	S	9	MAN	O2-C2-C3	-2.10	105.92	110.14
21	c	3	BMA	C2-C3-C4	2.10	114.53	110.89
20	b	10	MAN	O2-C2-C3	-2.10	105.94	110.14
9	O	1	NAG	C3-C4-C5	2.09	113.98	110.24
21	c	3	BMA	O2-C2-C3	-2.09	105.95	110.14
20	b	6	MAN	O2-C2-C3	-2.08	105.97	110.14
12	X	6	MAN	O2-C2-C3	-2.08	105.98	110.14
11	R	9	MAN	O2-C2-C3	-2.08	105.98	110.14
19	a	4	MAN	O2-C2-C3	-2.07	105.99	110.14
20	b	5	MAN	C1-O5-C5	2.07	115.00	112.19
14	Q	5	MAN	O2-C2-C3	-2.06	106.00	110.14
15	S	6	MAN	O2-C2-C3	-2.06	106.01	110.14
12	M	7	MAN	C1-C2-C3	2.06	112.19	109.67
13	P	5	MAN	O2-C2-C3	-2.05	106.03	110.14
12	N	3	BMA	C1-O5-C5	2.05	114.97	112.19
11	R	11	MAN	C1-O5-C5	2.05	114.97	112.19
12	N	6	MAN	O2-C2-C3	-2.05	106.04	110.14
10	J	4	MAN	O2-C2-C1	2.04	113.32	109.15
11	R	5	MAN	C1-C2-C3	-2.02	107.19	109.67
15	S	8	MAN	O2-C2-C3	-2.01	106.12	110.14
18	Y	3	BMA	O3-C3-C2	2.01	113.84	109.99
16	T	8	MAN	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (121) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	S	3	BMA	C4-C5-C6-O6
11	K	7	MAN	O5-C5-C6-O6
21	c	4	MAN	O5-C5-C6-O6
11	K	3	BMA	O5-C5-C6-O6
20	b	1	NAG	O5-C5-C6-O6
9	Z	2	NAG	O5-C5-C6-O6
16	T	5	MAN	O5-C5-C6-O6
13	P	6	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
13	P	2	NAG	O5-C5-C6-O6
20	b	4	MAN	O5-C5-C6-O6
8	A	1	NAG	O5-C5-C6-O6
21	c	1	NAG	O5-C5-C6-O6
18	Y	3	BMA	C4-C5-C6-O6
15	S	3	BMA	O5-C5-C6-O6
14	Q	1	NAG	O5-C5-C6-O6
12	N	7	MAN	O5-C5-C6-O6
11	K	3	BMA	C4-C5-C6-O6
9	O	3	BMA	C4-C5-C6-O6
13	P	3	BMA	C4-C5-C6-O6
19	a	3	BMA	C4-C5-C6-O6
12	M	3	BMA	C4-C5-C6-O6
21	c	1	NAG	C4-C5-C6-O6
8	A	1	NAG	C4-C5-C6-O6
17	e	3	BMA	C4-C5-C6-O6
14	Q	1	NAG	C4-C5-C6-O6
11	K	7	MAN	C4-C5-C6-O6
12	N	7	MAN	C4-C5-C6-O6
20	b	1	NAG	C4-C5-C6-O6
20	b	4	MAN	C4-C5-C6-O6
19	a	3	BMA	O5-C5-C6-O6
12	M	1	NAG	O5-C5-C6-O6
9	O	3	BMA	O5-C5-C6-O6
17	e	2	NAG	O5-C5-C6-O6
14	Q	3	BMA	O5-C5-C6-O6
13	P	3	BMA	O5-C5-C6-O6
12	M	3	BMA	O5-C5-C6-O6
19	a	5	MAN	O5-C5-C6-O6
21	c	4	MAN	C4-C5-C6-O6
19	a	4	MAN	C4-C5-C6-O6
12	M	1	NAG	C4-C5-C6-O6
17	e	3	BMA	O5-C5-C6-O6
9	Z	2	NAG	C4-C5-C6-O6
18	Y	1	NAG	O5-C5-C6-O6
16	T	5	MAN	C4-C5-C6-O6
13	P	2	NAG	C4-C5-C6-O6
15	S	5	MAN	O5-C5-C6-O6
18	Y	3	BMA	O5-C5-C6-O6
14	Q	2	NAG	O5-C5-C6-O6
15	S	2	NAG	O5-C5-C6-O6
17	W	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
21	c	3	BMA	C4-C5-C6-O6
17	W	4	MAN	O5-C5-C6-O6
8	d	1	NAG	O5-C5-C6-O6
20	b	2	NAG	O5-C5-C6-O6
17	W	1	NAG	O5-C5-C6-O6
12	N	10	MAN	O5-C5-C6-O6
9	Z	3	BMA	O5-C5-C6-O6
11	K	8	MAN	O5-C5-C6-O6
15	S	7	MAN	O5-C5-C6-O6
20	b	6	MAN	O5-C5-C6-O6
8	C	2	NAG	O5-C5-C6-O6
12	N	3	BMA	O5-C5-C6-O6
12	M	5	MAN	O5-C5-C6-O6
18	Y	5	MAN	O5-C5-C6-O6
10	J	5	MAN	O5-C5-C6-O6
19	a	8	MAN	O5-C5-C6-O6
11	K	10	MAN	O5-C5-C6-O6
12	M	9	MAN	O5-C5-C6-O6
17	W	3	BMA	O5-C5-C6-O6
18	Y	2	NAG	O5-C5-C6-O6
20	b	3	BMA	O5-C5-C6-O6
12	N	2	NAG	O5-C5-C6-O6
12	N	9	MAN	O5-C5-C6-O6
13	P	5	MAN	O5-C5-C6-O6
16	T	6	MAN	O5-C5-C6-O6
19	a	4	MAN	O5-C5-C6-O6
15	S	9	MAN	O5-C5-C6-O6
12	N	1	NAG	O5-C5-C6-O6
17	f	6	MAN	O5-C5-C6-O6
17	e	1	NAG	O5-C5-C6-O6
12	M	6	MAN	O5-C5-C6-O6
12	X	8	MAN	O5-C5-C6-O6
10	J	3	BMA	O5-C5-C6-O6
17	W	6	MAN	O5-C5-C6-O6
20	b	9	MAN	O5-C5-C6-O6
12	X	7	MAN	C4-C5-C6-O6
17	f	3	BMA	C4-C5-C6-O6
11	R	1	NAG	O5-C5-C6-O6
11	R	1	NAG	C4-C5-C6-O6
17	e	2	NAG	C4-C5-C6-O6
17	f	2	NAG	C4-C5-C6-O6
12	X	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
17	f	3	BMA	O5-C5-C6-O6
13	P	6	MAN	C4-C5-C6-O6
21	c	3	BMA	O5-C5-C6-O6
9	O	1	NAG	C4-C5-C6-O6
12	X	2	NAG	C4-C5-C6-O6
12	X	7	MAN	O5-C5-C6-O6
14	Q	6	MAN	O5-C5-C6-O6
12	X	1	NAG	O5-C5-C6-O6
21	c	2	NAG	O5-C5-C6-O6
19	a	2	NAG	C4-C5-C6-O6
18	Y	1	NAG	C4-C5-C6-O6
15	S	2	NAG	C3-C2-N2-C7
9	O	2	NAG	C3-C2-N2-C7
12	X	2	NAG	C3-C2-N2-C7
19	a	1	NAG	C3-C2-N2-C7
10	J	1	NAG	C3-C2-N2-C7
14	Q	3	BMA	C4-C5-C6-O6
15	S	2	NAG	C4-C5-C6-O6
17	f	2	NAG	O5-C5-C6-O6
9	O	1	NAG	O5-C5-C6-O6
11	R	5	MAN	O5-C5-C6-O6
10	J	2	NAG	O5-C5-C6-O6
10	J	6	MAN	O5-C5-C6-O6
17	e	4	MAN	C4-C5-C6-O6
12	X	2	NAG	O5-C5-C6-O6
10	J	2	NAG	C4-C5-C6-O6
8	C	1	NAG	C3-C2-N2-C7
14	Q	2	NAG	C4-C5-C6-O6
14	Q	4	MAN	C4-C5-C6-O6

There are no ring outliers.

17 monomers are involved in 21 short contacts:

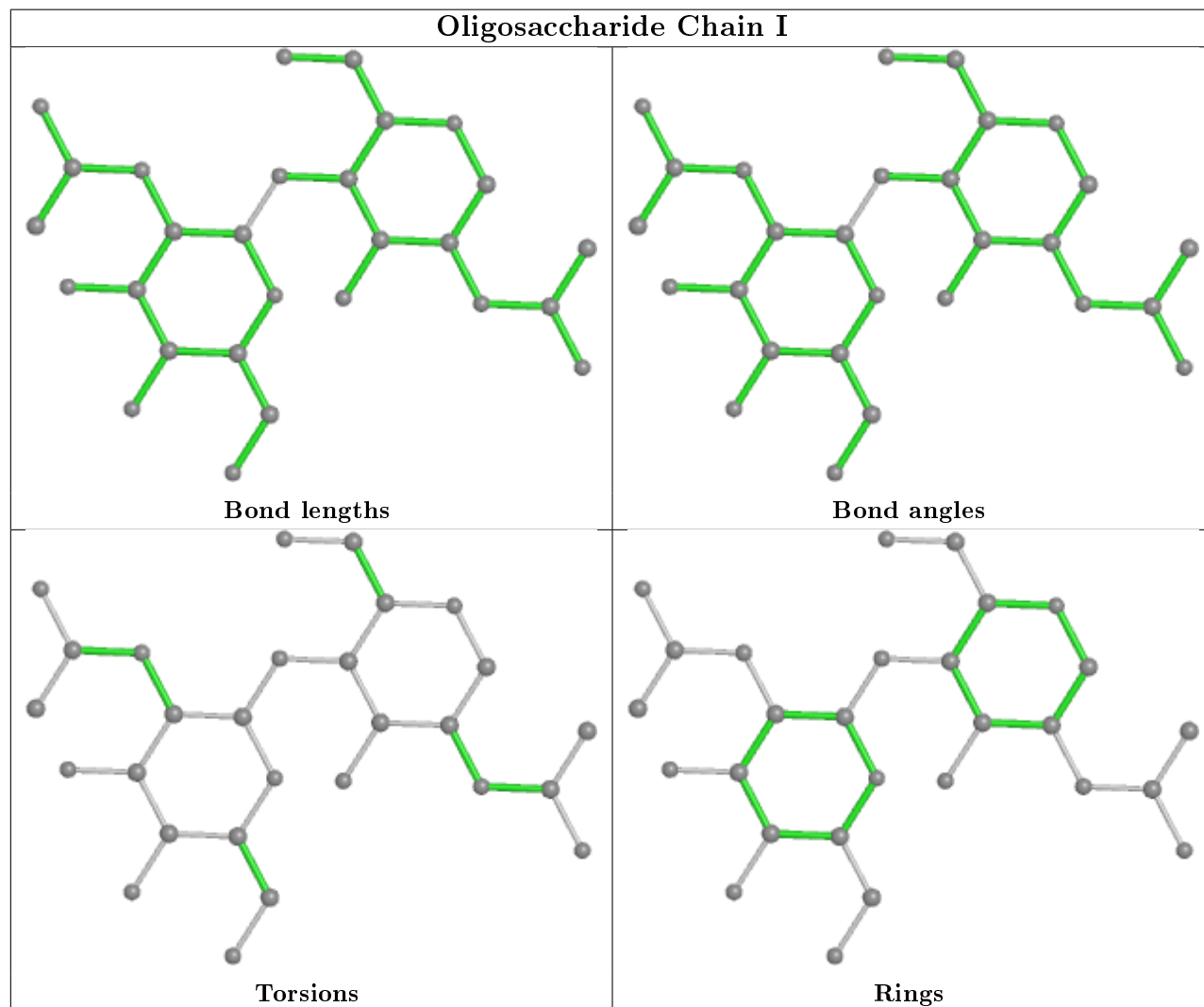
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	7	MAN	1	0
18	Y	4	MAN	4	0
11	K	6	MAN	1	0
12	N	4	MAN	4	0
10	J	4	MAN	1	0
8	C	1	NAG	1	0
13	P	3	BMA	6	0
18	Y	5	MAN	4	0

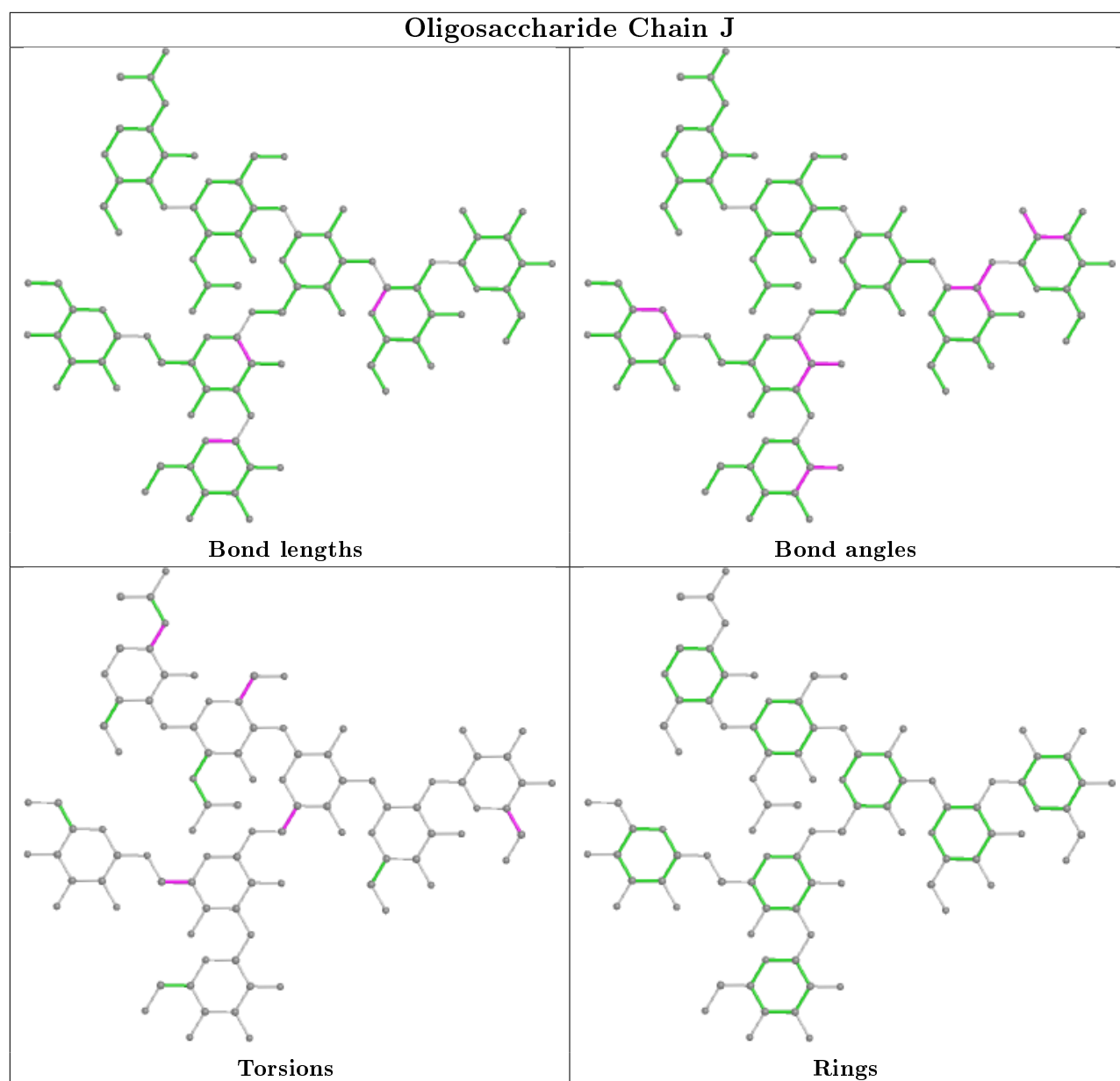
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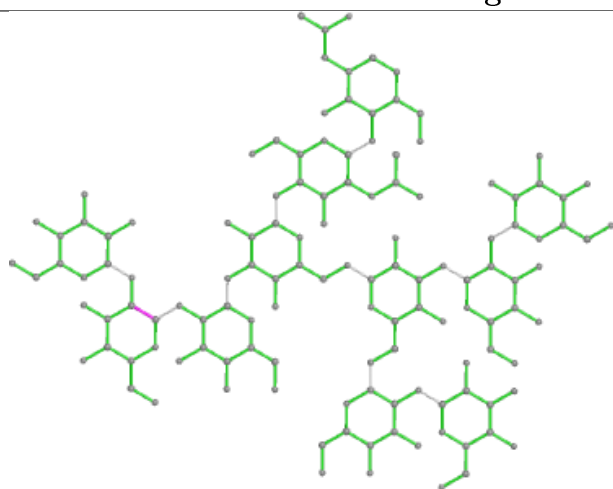
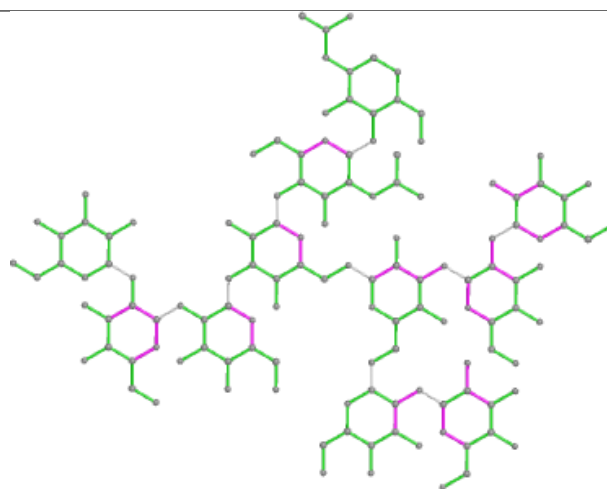
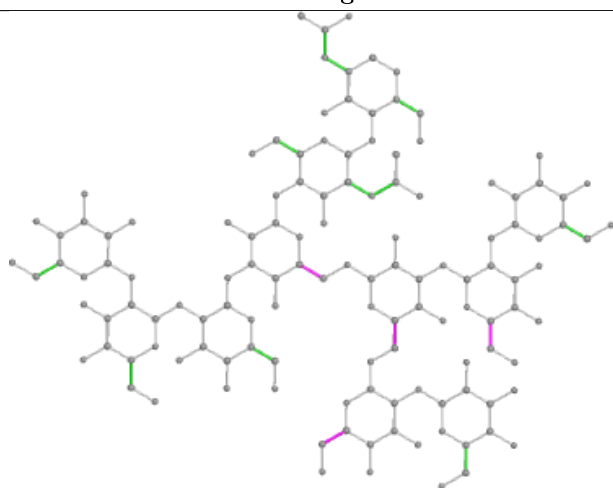
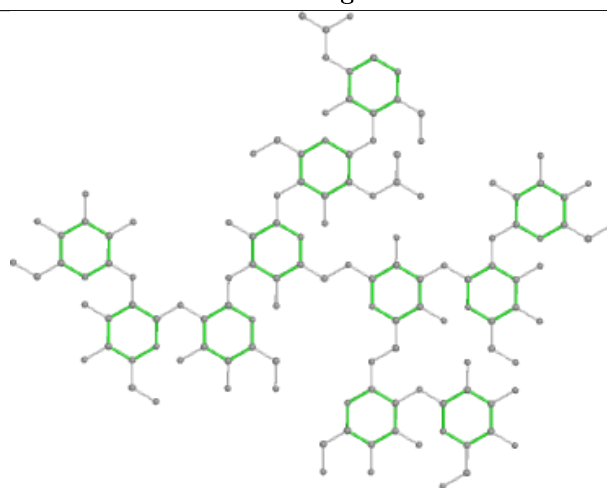
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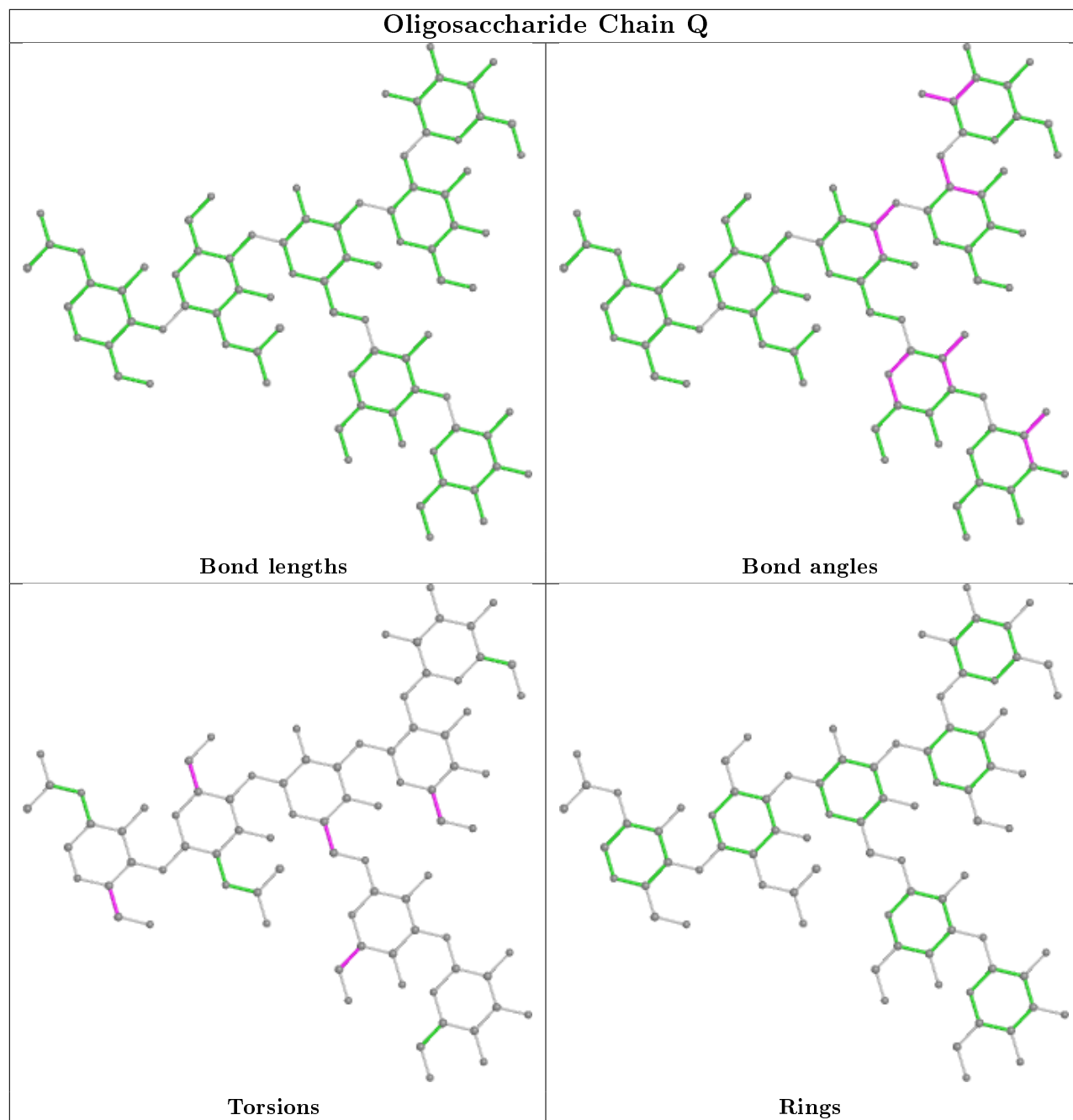
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	J	5	MAN	1	0
11	R	3	BMA	2	0
12	M	8	MAN	0	1
11	K	10	MAN	1	0
8	C	2	NAG	1	0
12	N	3	BMA	4	0
12	M	5	MAN	0	1
13	P	4	MAN	6	0
11	K	5	MAN	1	0

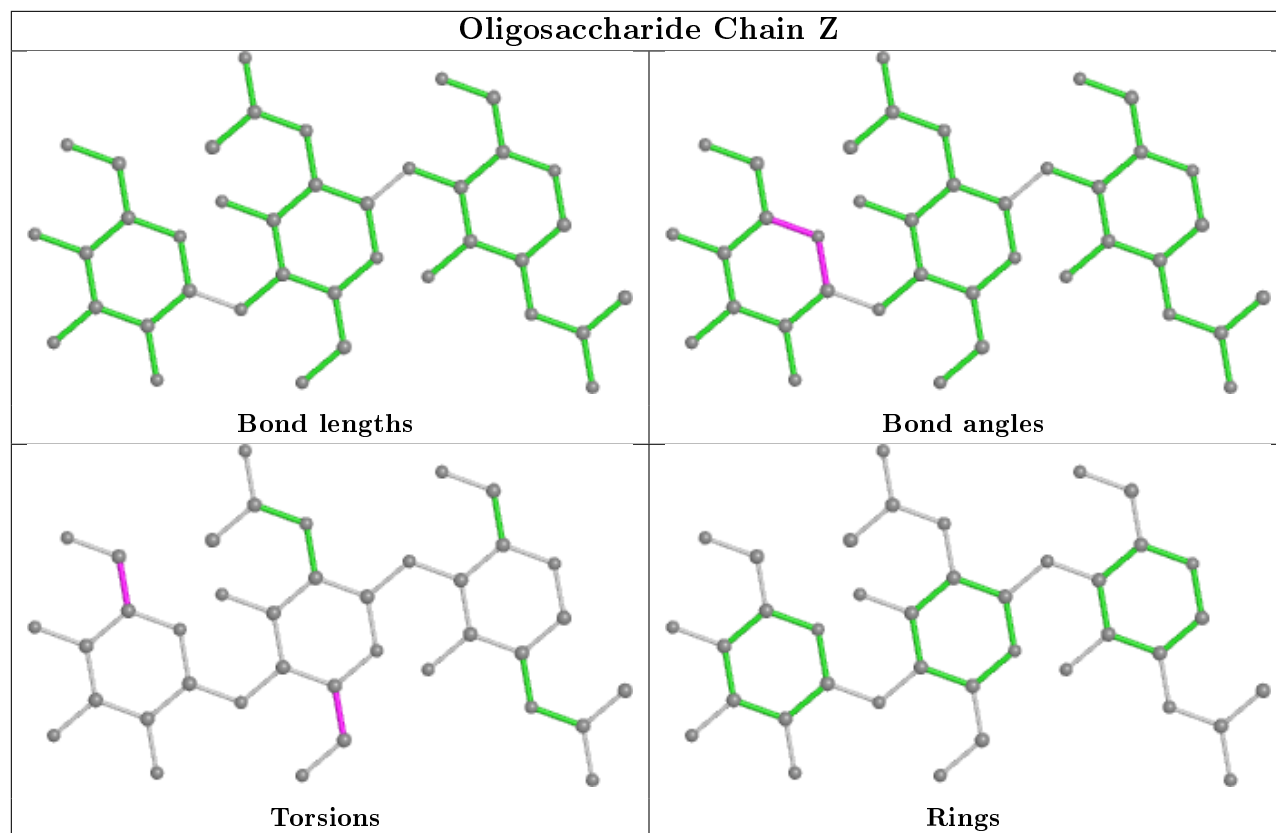
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

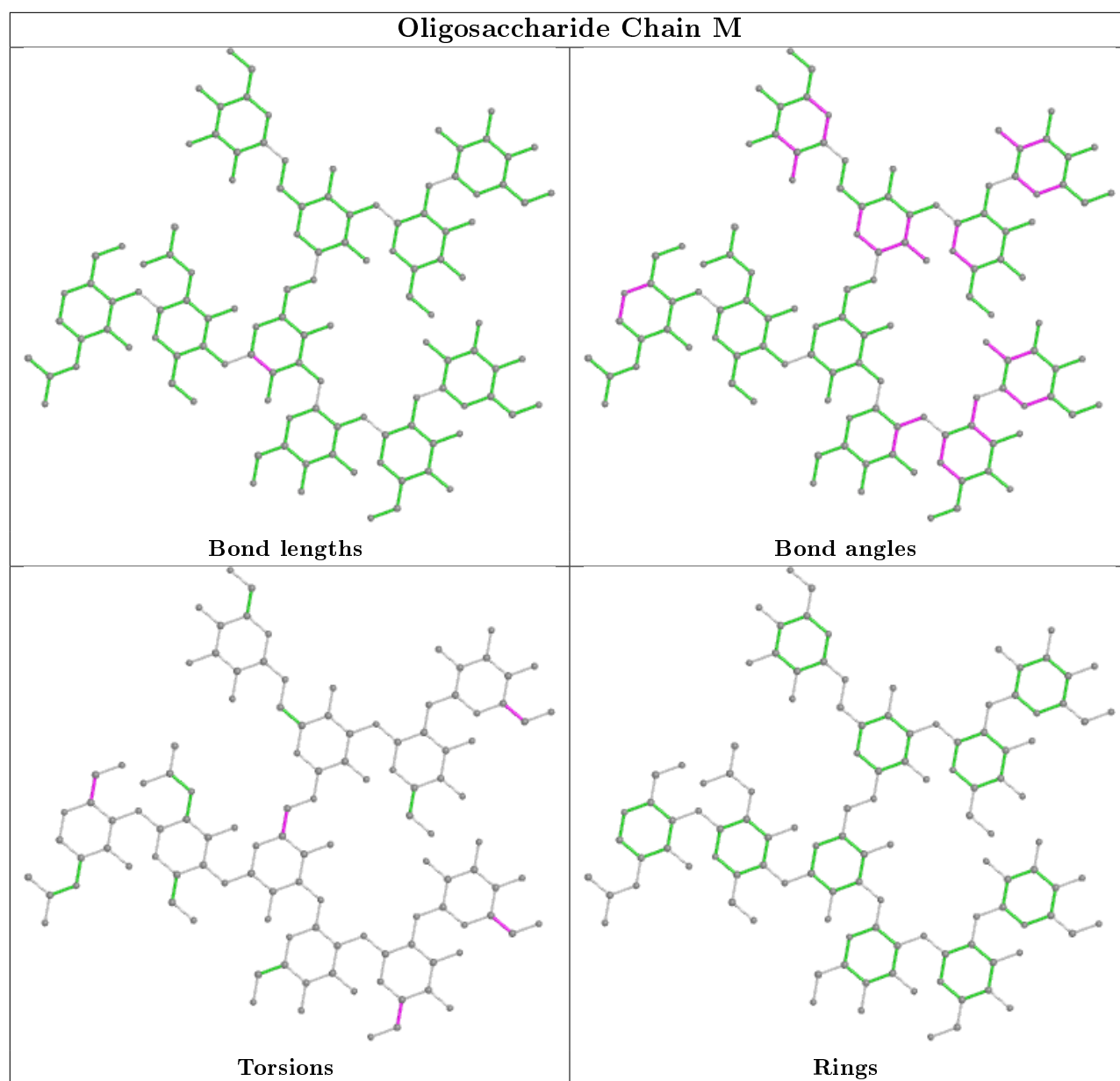


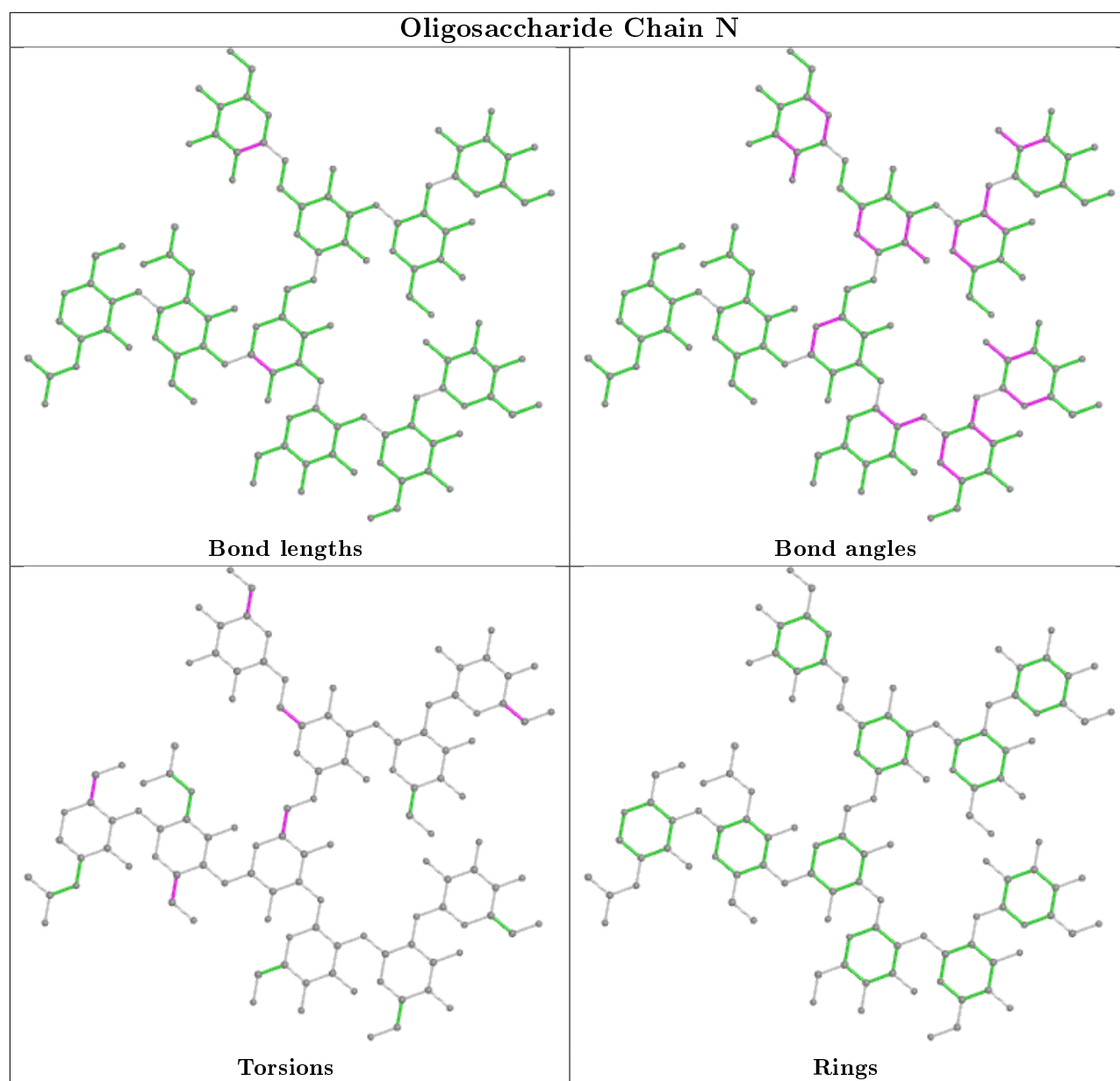


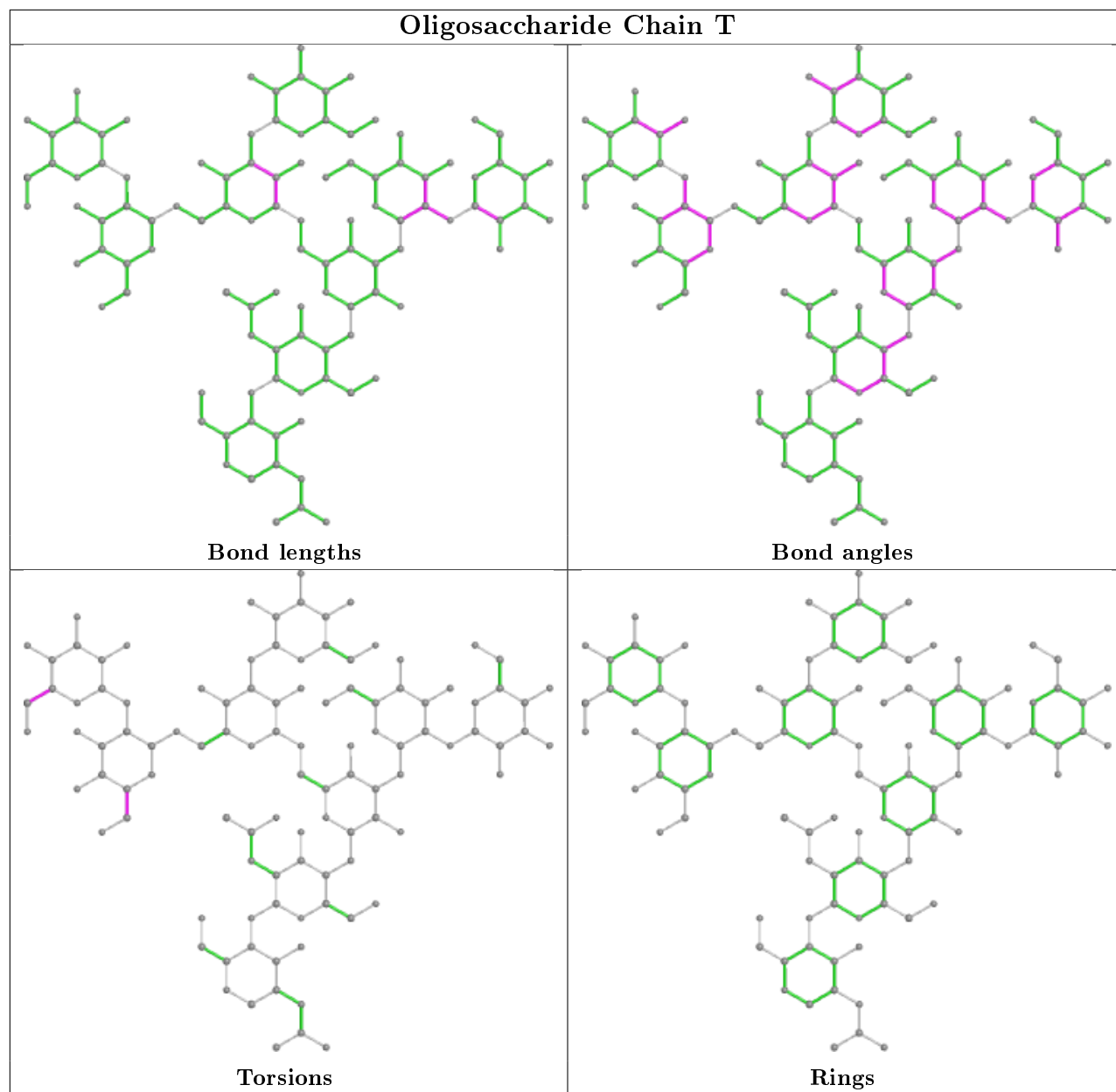
**Oligosaccharide Chain K****Bond lengths****Bond angles****Torsions****Rings**

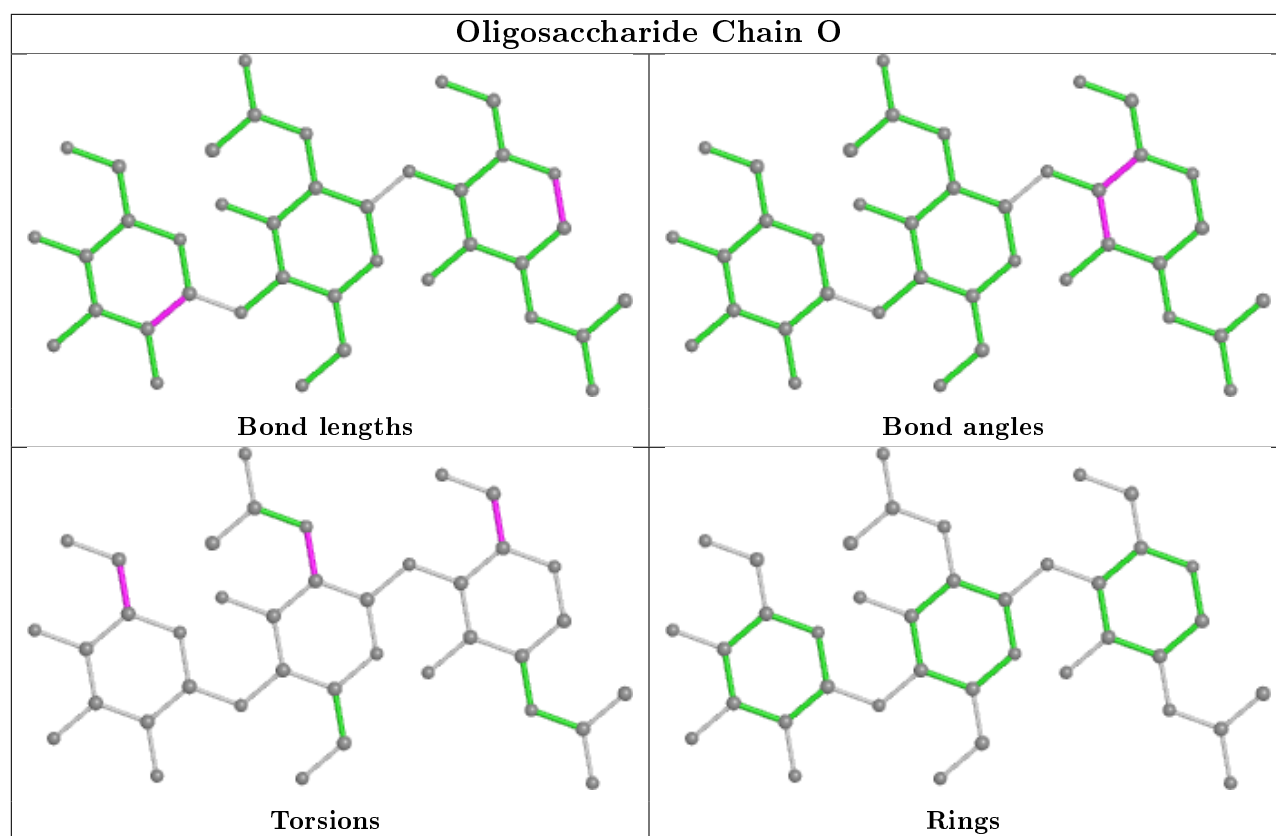


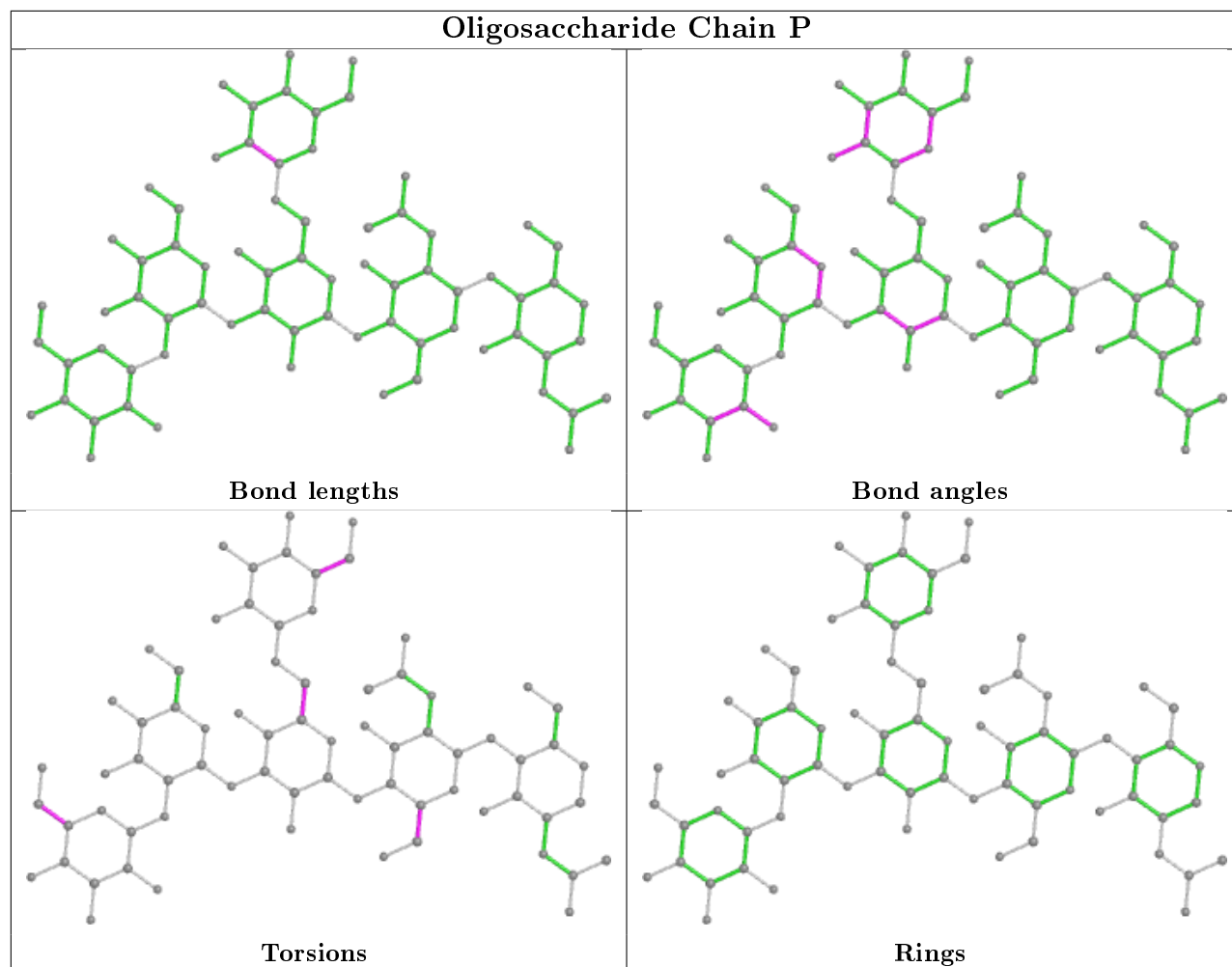


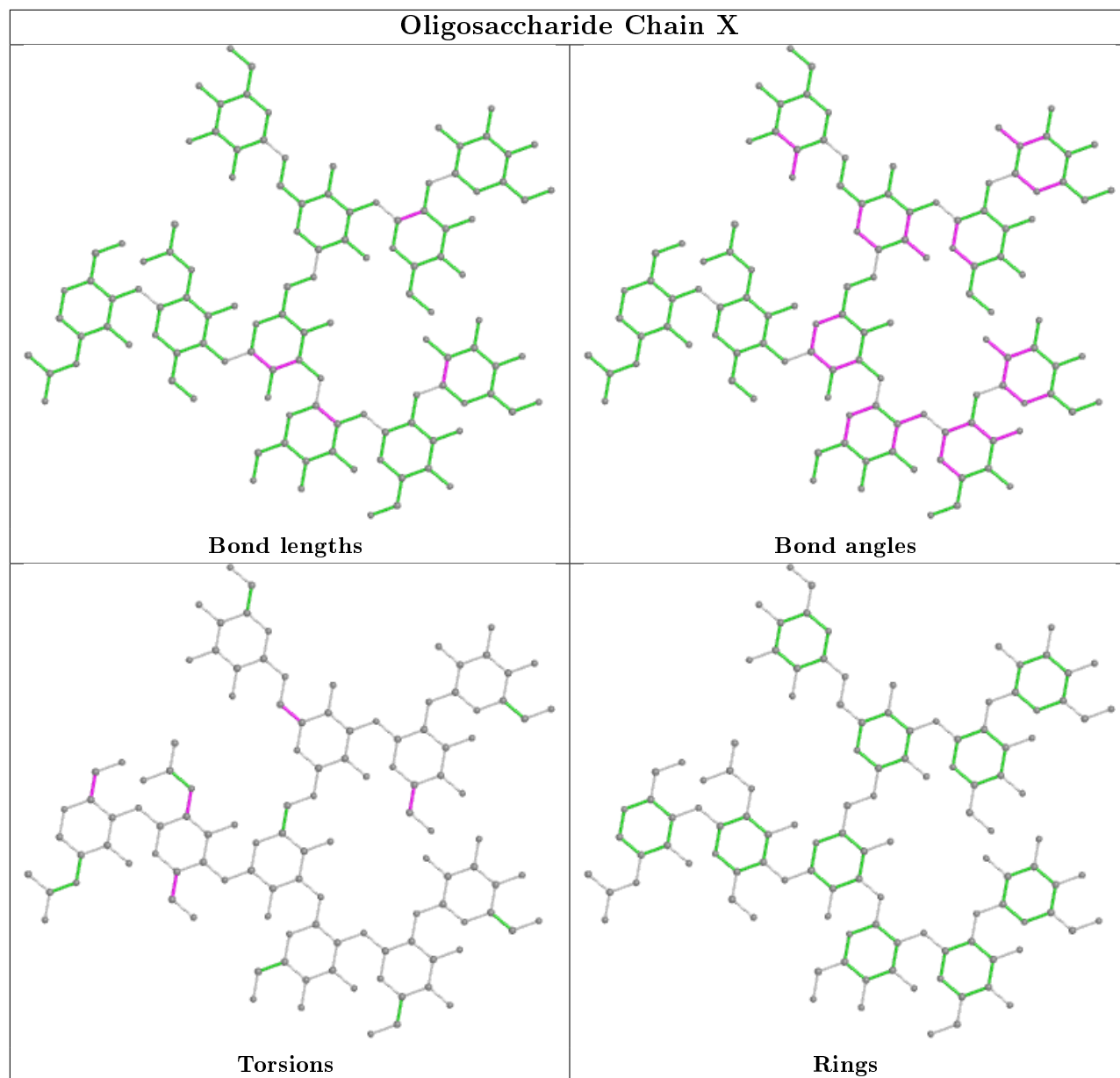


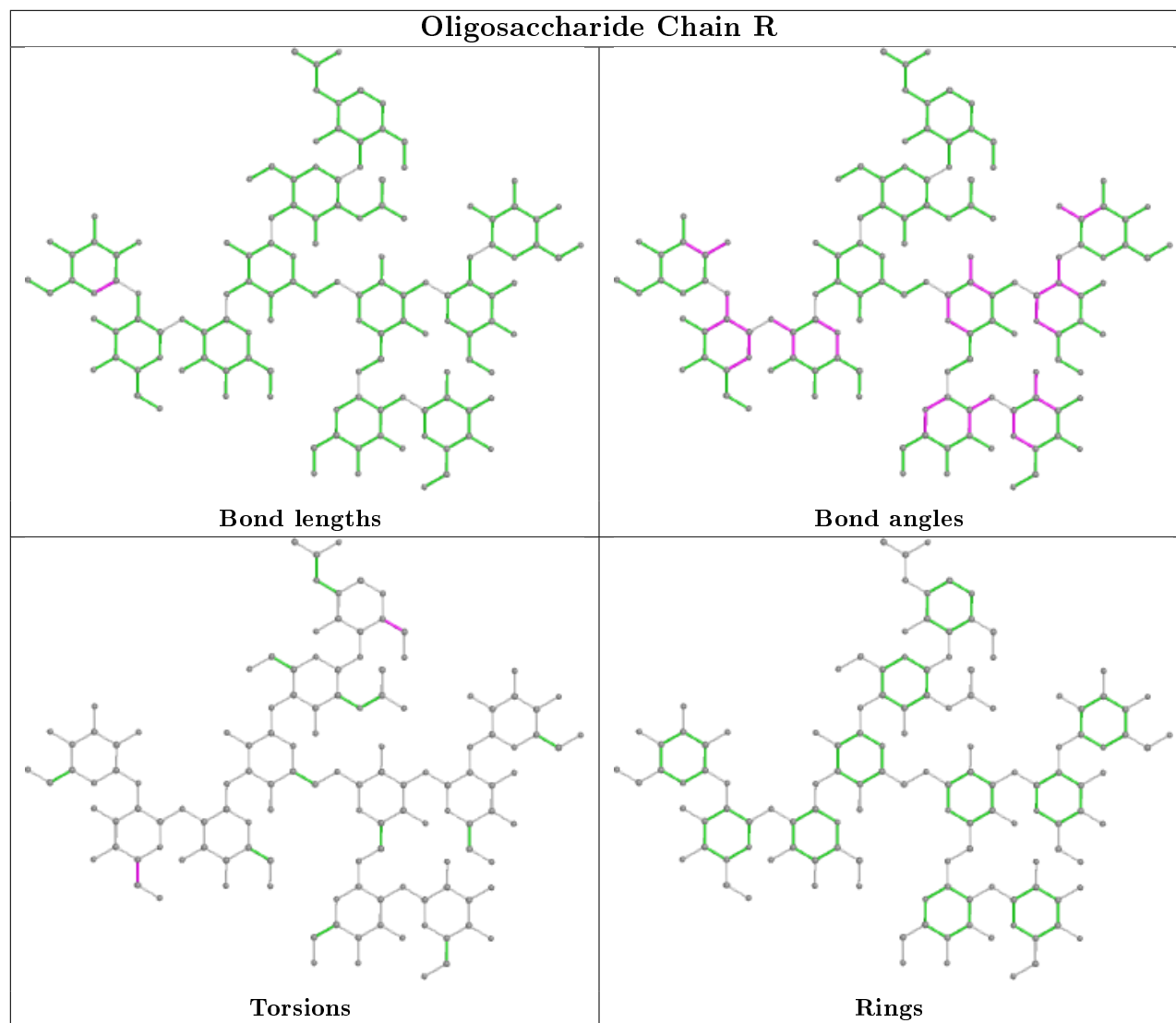


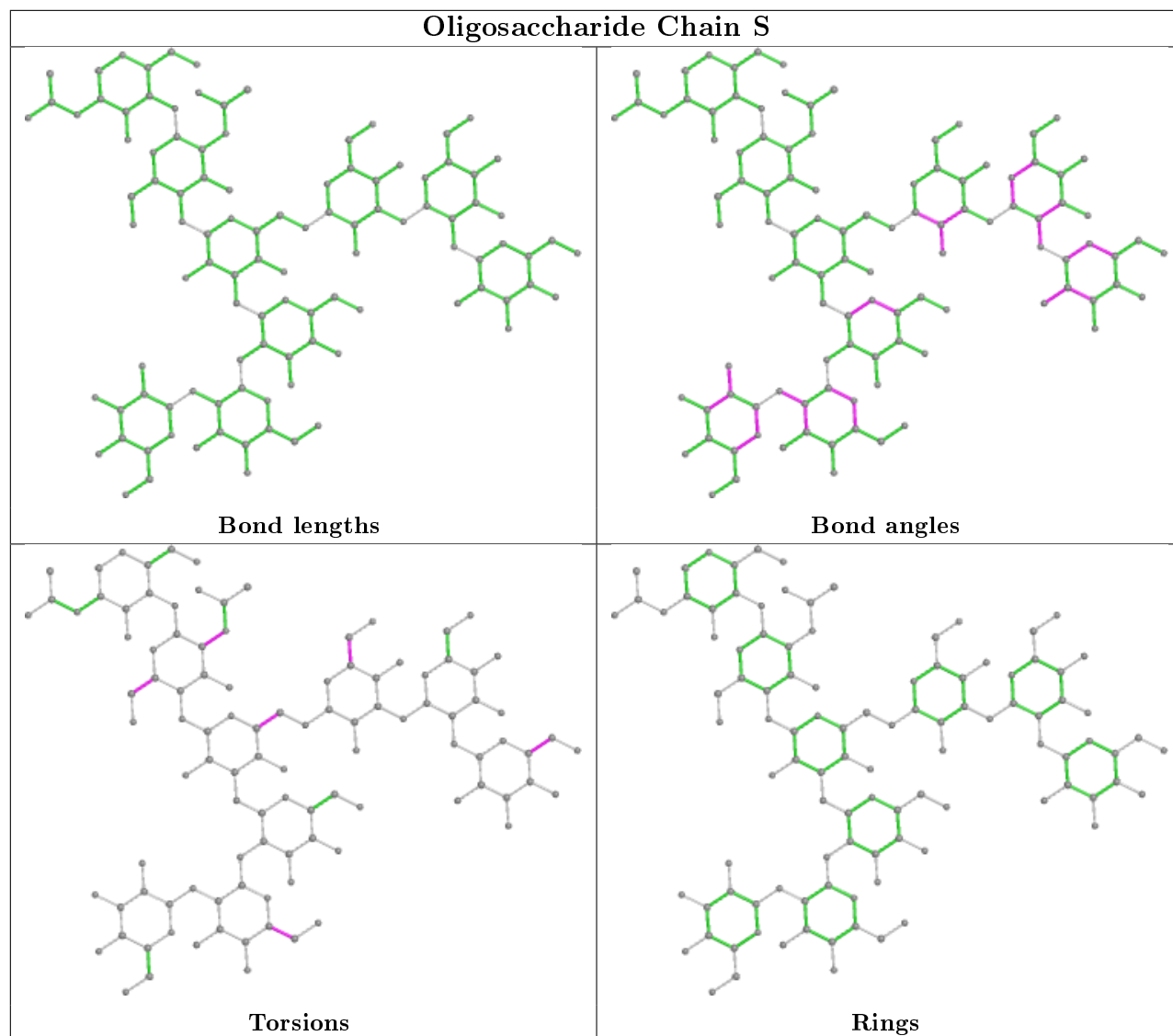


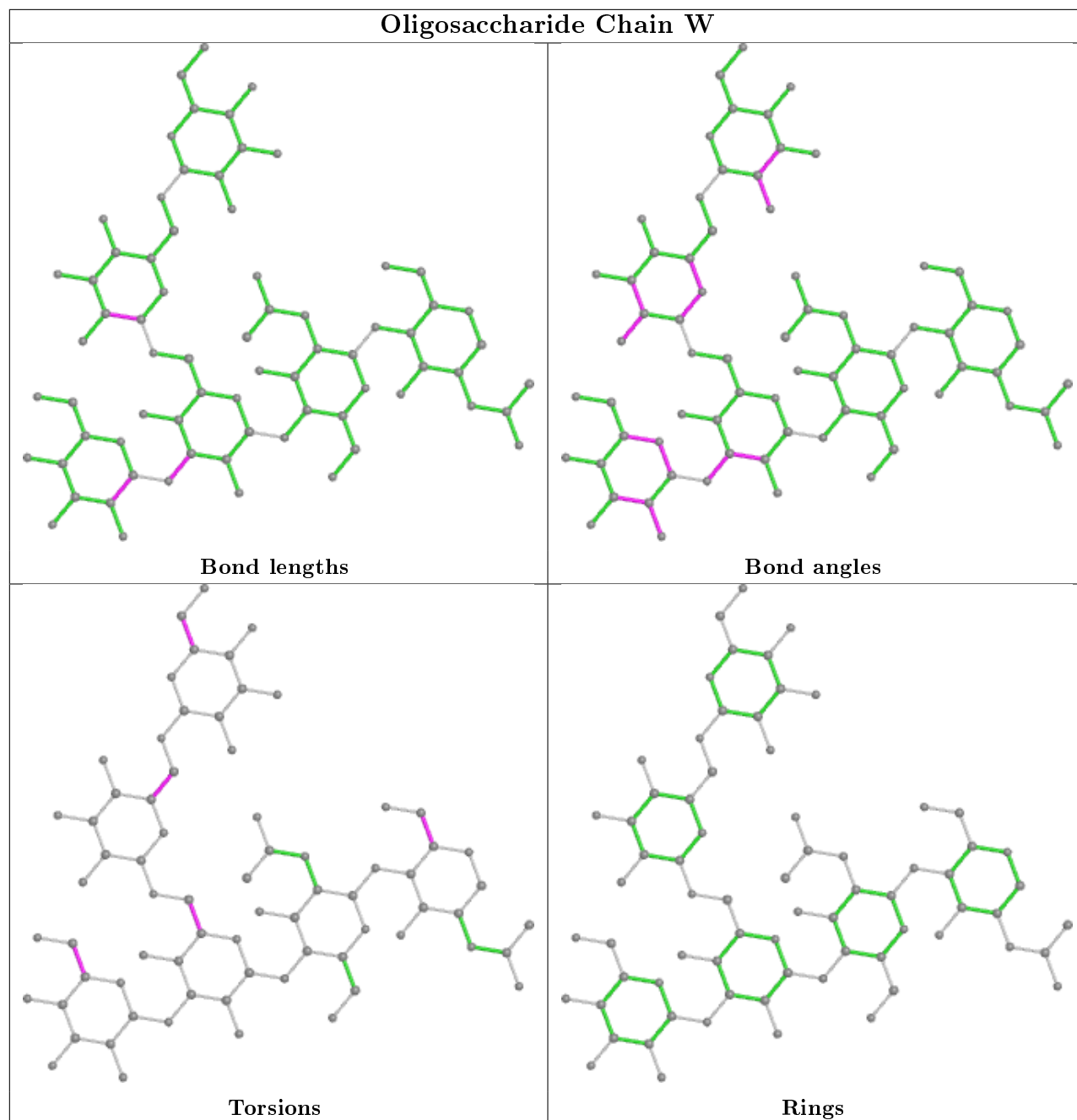


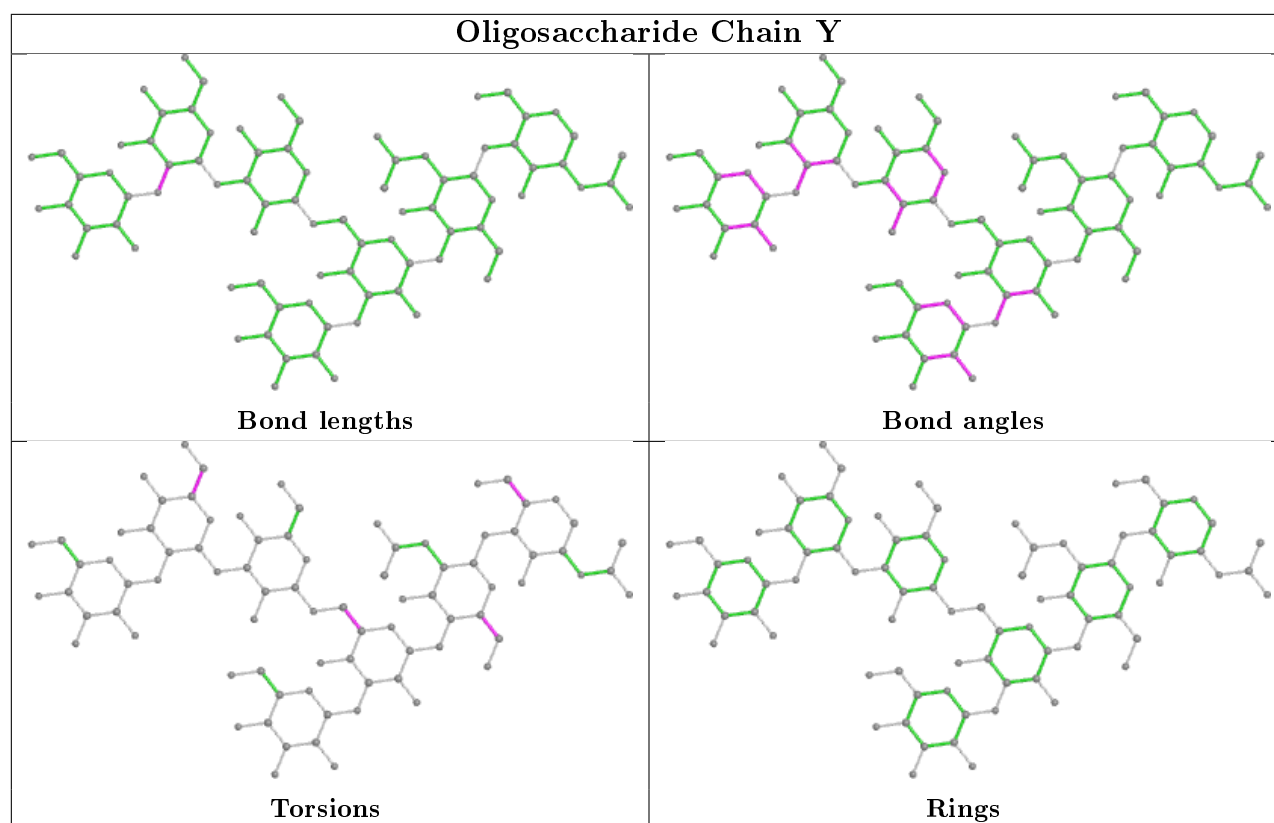












## 5.6 Ligand geometry [i](#)

8 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	$\# Z  > 2$
22	CIT	G	1511	-	3,12,12	1.26	0	3,17,17	1.19	0
23	EDO	G	1512	-	3,3,3	0.47	0	2,2,2	0.31	0
24	NAG	G	3921	4	14,14,15	0.34	0	17,19,21	0.51	0
24	NAG	G	1331	4	14,14,15	0.38	0	17,19,21	0.40	0
23	EDO	D	1225	-	3,3,3	0.47	0	2,2,2	0.37	0
24	NAG	G	1421	4	14,14,15	0.26	0	17,19,21	0.43	0
22	CIT	G	1513	-	3,12,12	1.32	0	3,17,17	1.14	0
22	CIT	B	1666	-	3,12,12	1.18	0	3,17,17	1.71	1 (33%)

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
22	CIT	G	1511	-	-	1/6/16/16	-
23	EDO	G	1512	-	-	0/1/1/1	-
24	NAG	G	3921	4	-	2/6/23/26	0/1/1/1
24	NAG	G	1331	4	-	1/6/23/26	0/1/1/1
23	EDO	D	1225	-	-	0/1/1/1	-
24	NAG	G	1421	4	-	2/6/23/26	0/1/1/1
22	CIT	G	1513	-	-	0/6/16/16	-
22	CIT	B	1666	-	-	6/6/16/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1666	CIT	C3-C4-C5	-2.81	110.48	114.98

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	1666	CIT	C1-C2-C3-O7
22	B	1666	CIT	C1-C2-C3-C4
22	B	1666	CIT	C1-C2-C3-C6
22	B	1666	CIT	C2-C3-C4-C5
22	B	1666	CIT	C6-C3-C4-C5
24	G	3921	NAG	O5-C5-C6-O6
24	G	1331	NAG	O5-C5-C6-O6
22	B	1666	CIT	O7-C3-C4-C5
24	G	3921	NAG	C4-C5-C6-O6
22	G	1511	CIT	C1-C2-C3-C6
24	G	1421	NAG	C4-C5-C6-O6
24	G	1421	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	G	1331	NAG	1	0
22	G	1513	CIT	2	0
22	B	1666	CIT	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 [i](#)

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

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

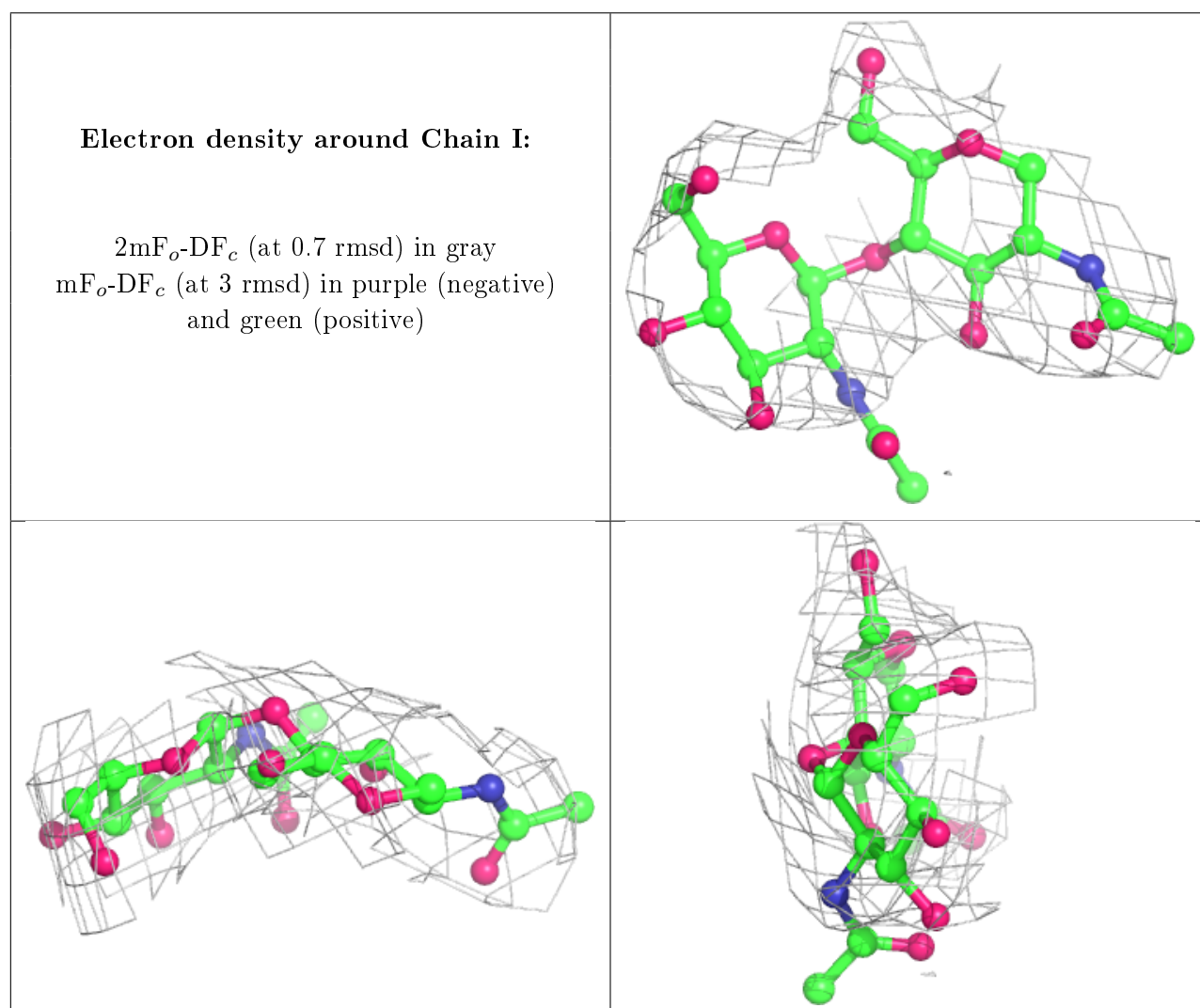
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

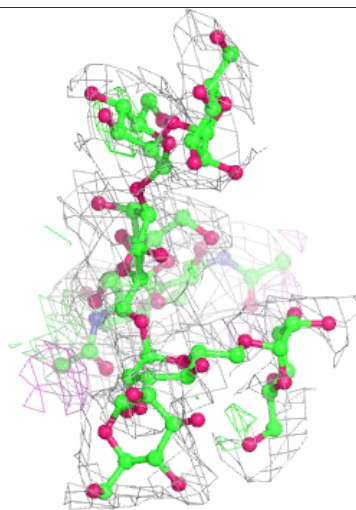
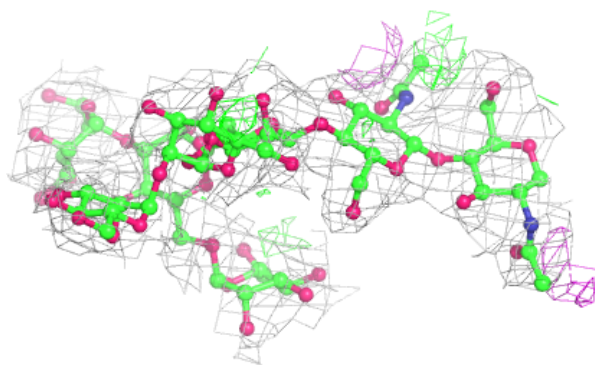
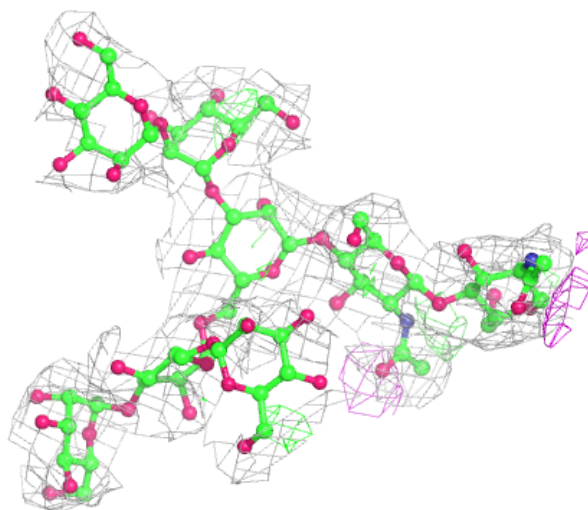
Unable to reproduce the depositors R factor - this section is therefore empty.

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



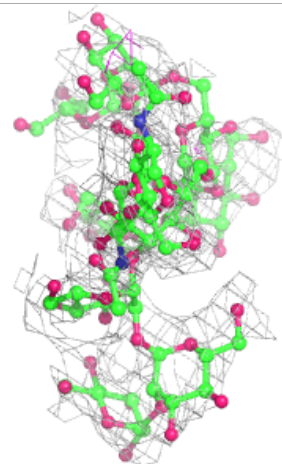
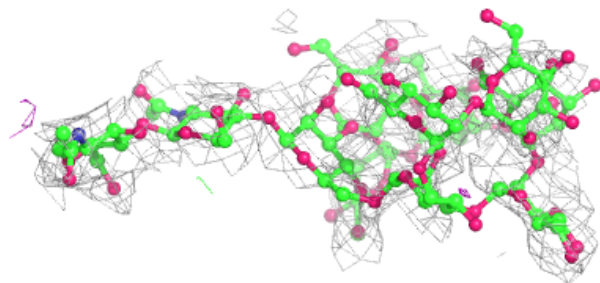
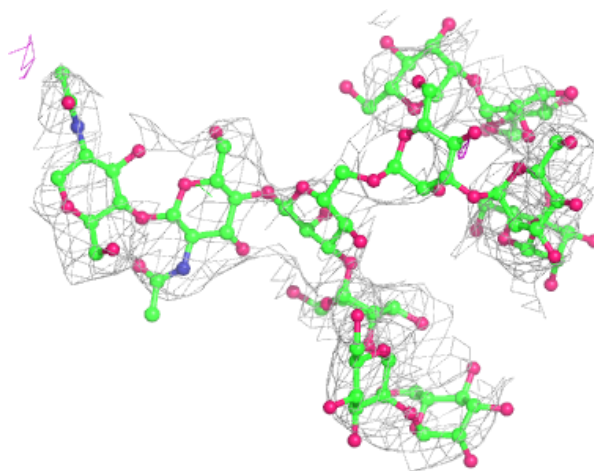
**Electron density around Chain J:**

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



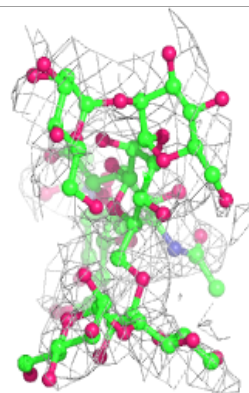
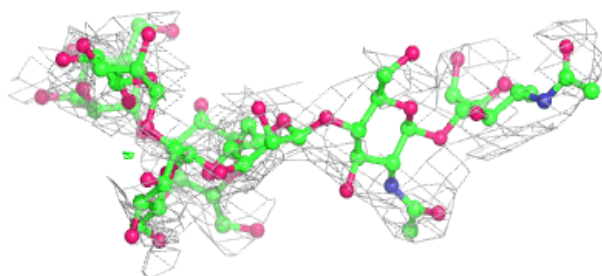
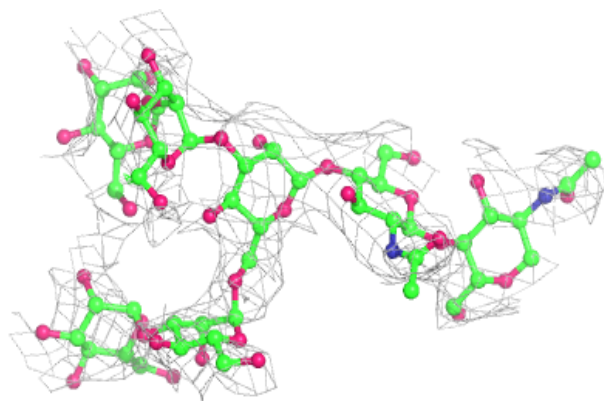
**Electron density around Chain K:**

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

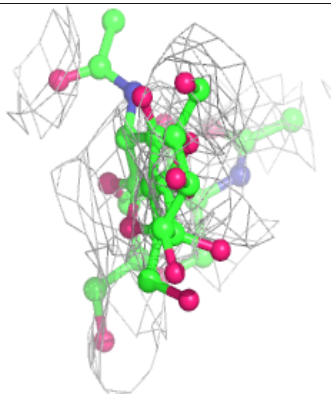
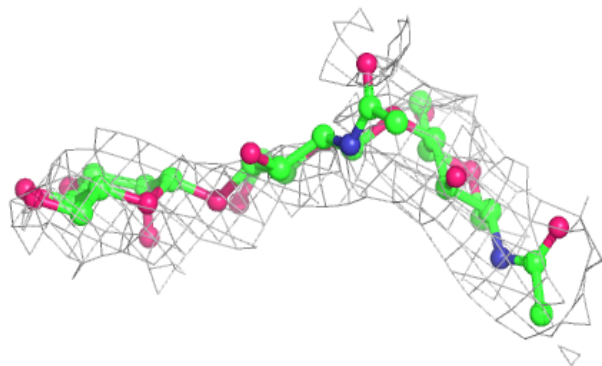
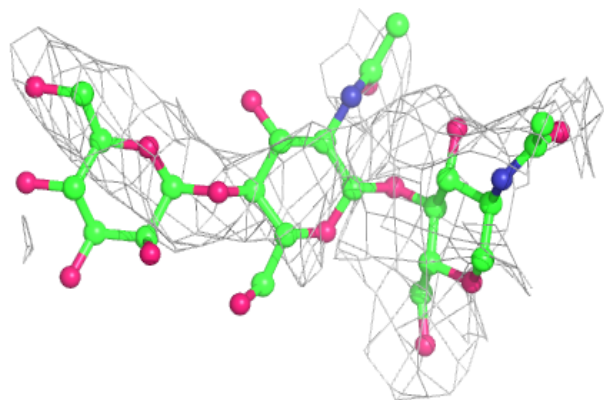


**Electron density around Chain Q:**

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

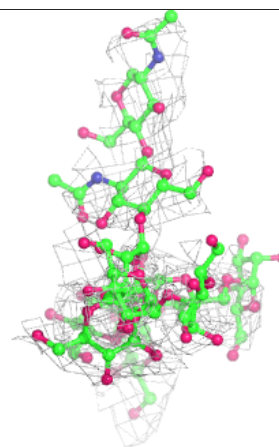
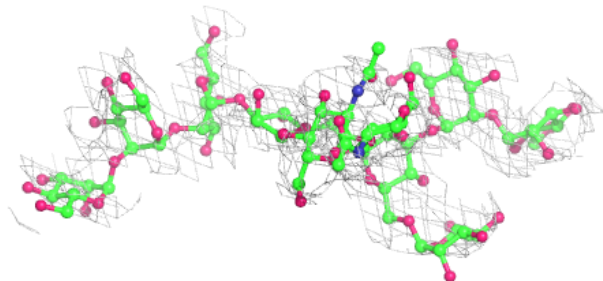
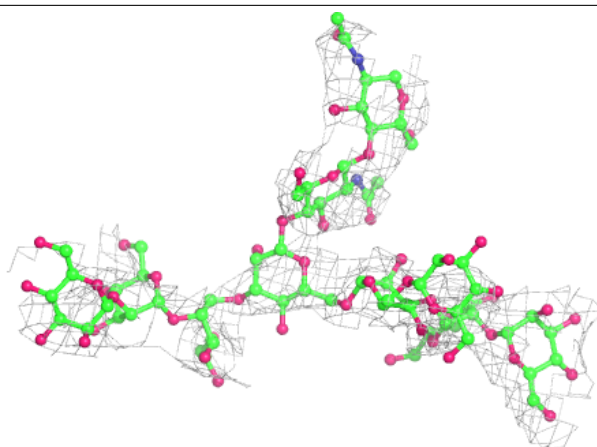
**Electron density around Chain Z:**

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



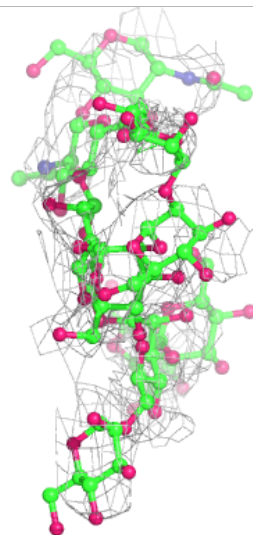
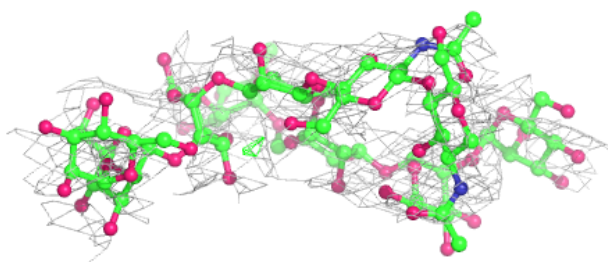
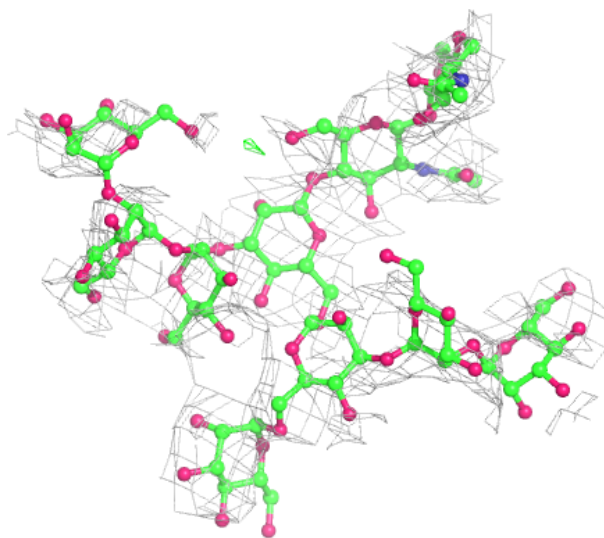
**Electron density around Chain M:**

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



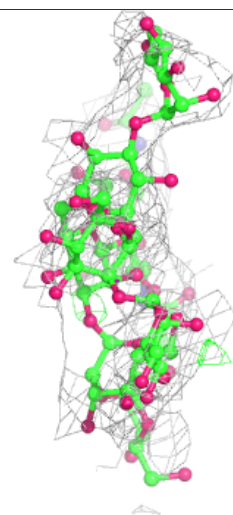
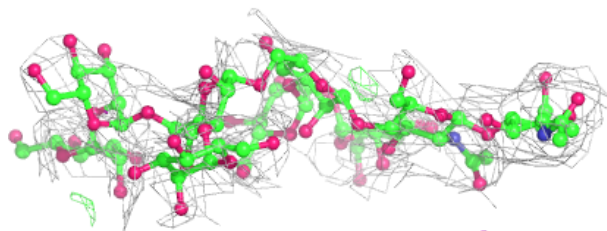
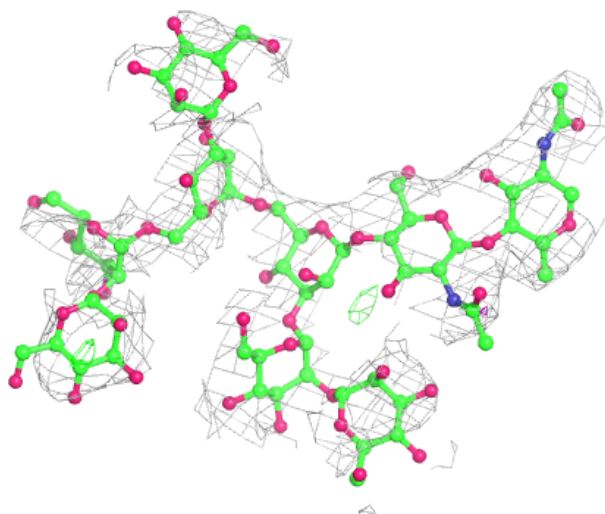
**Electron density around Chain N:**

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



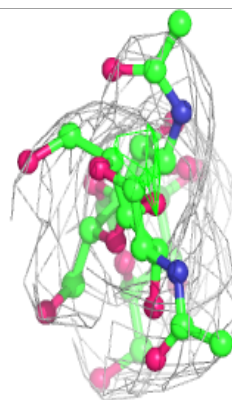
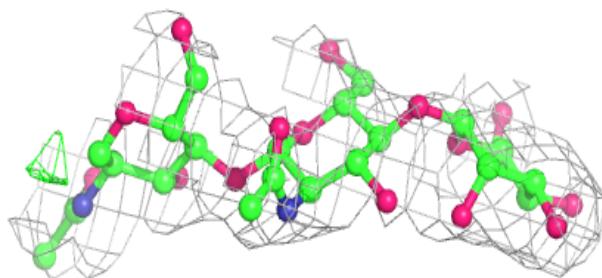
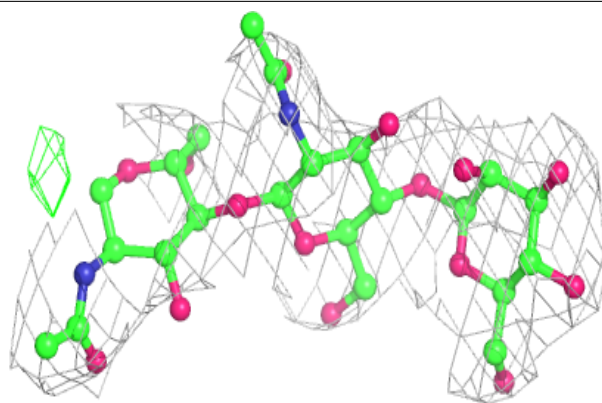
**Electron density around Chain T:**

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

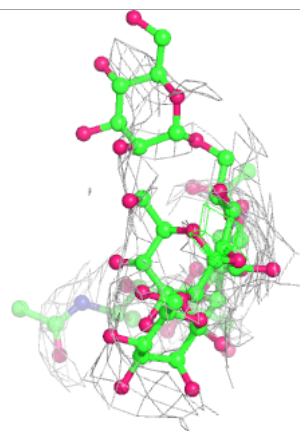
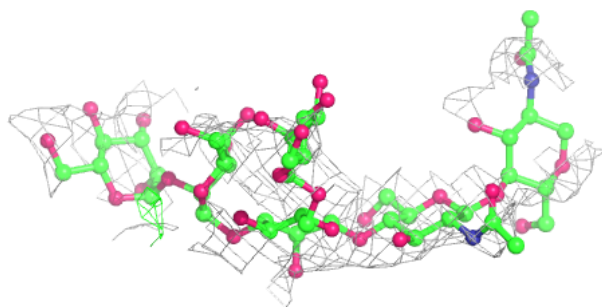
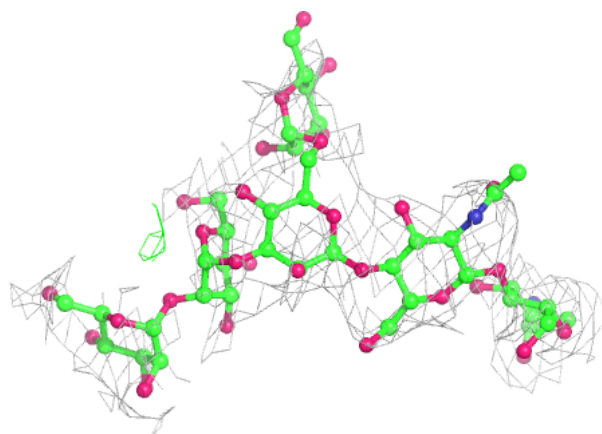


**Electron density around Chain O:**

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

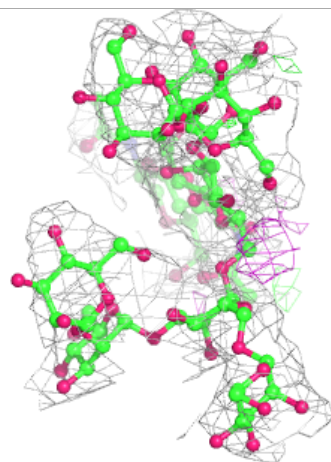
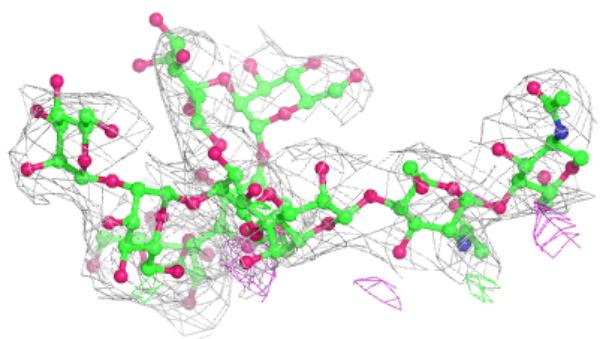
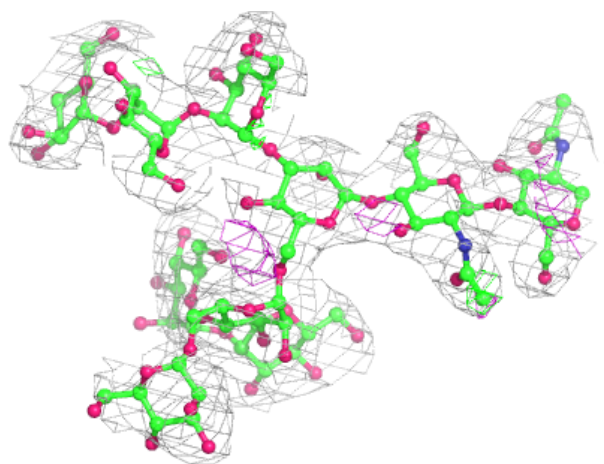
**Electron density around Chain P:**

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



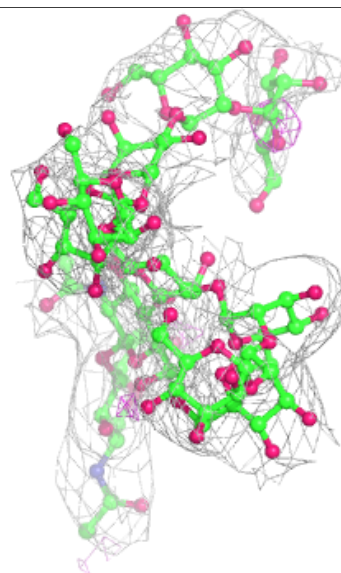
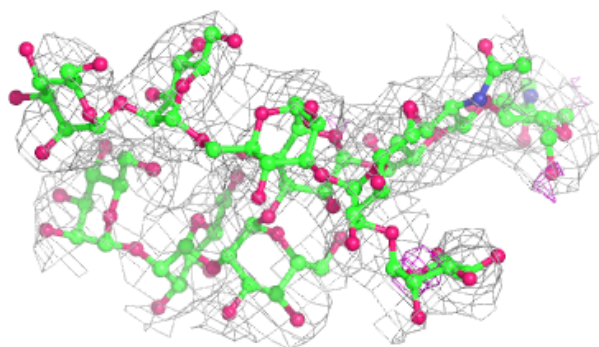
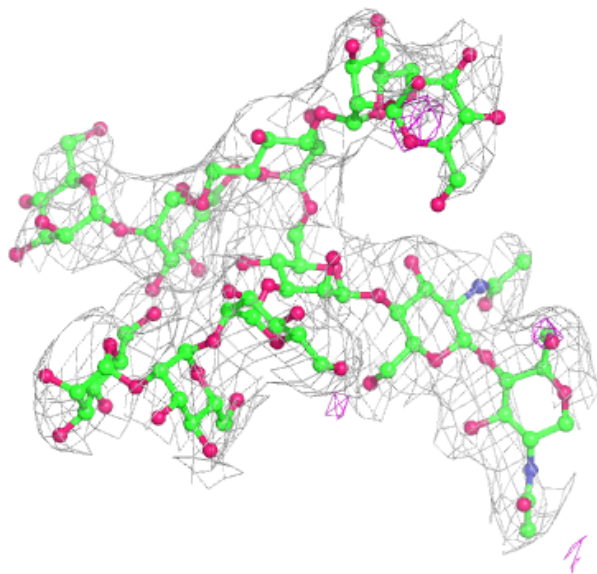
**Electron density around Chain X:**

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



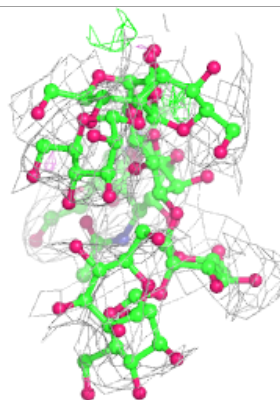
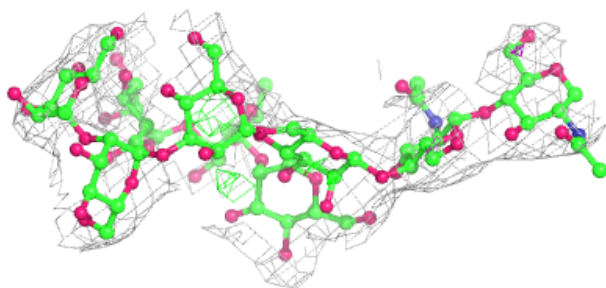
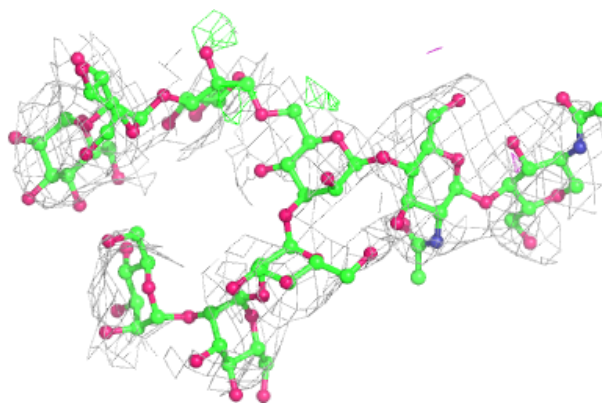
**Electron density around Chain R:**

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

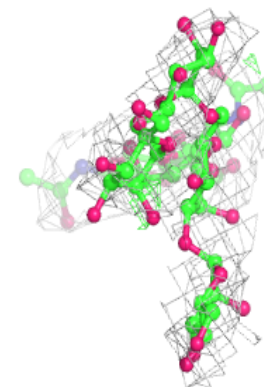
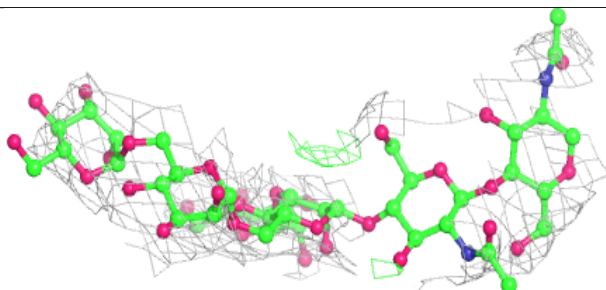
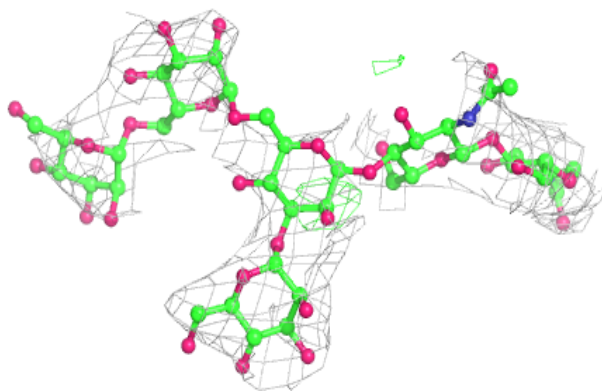


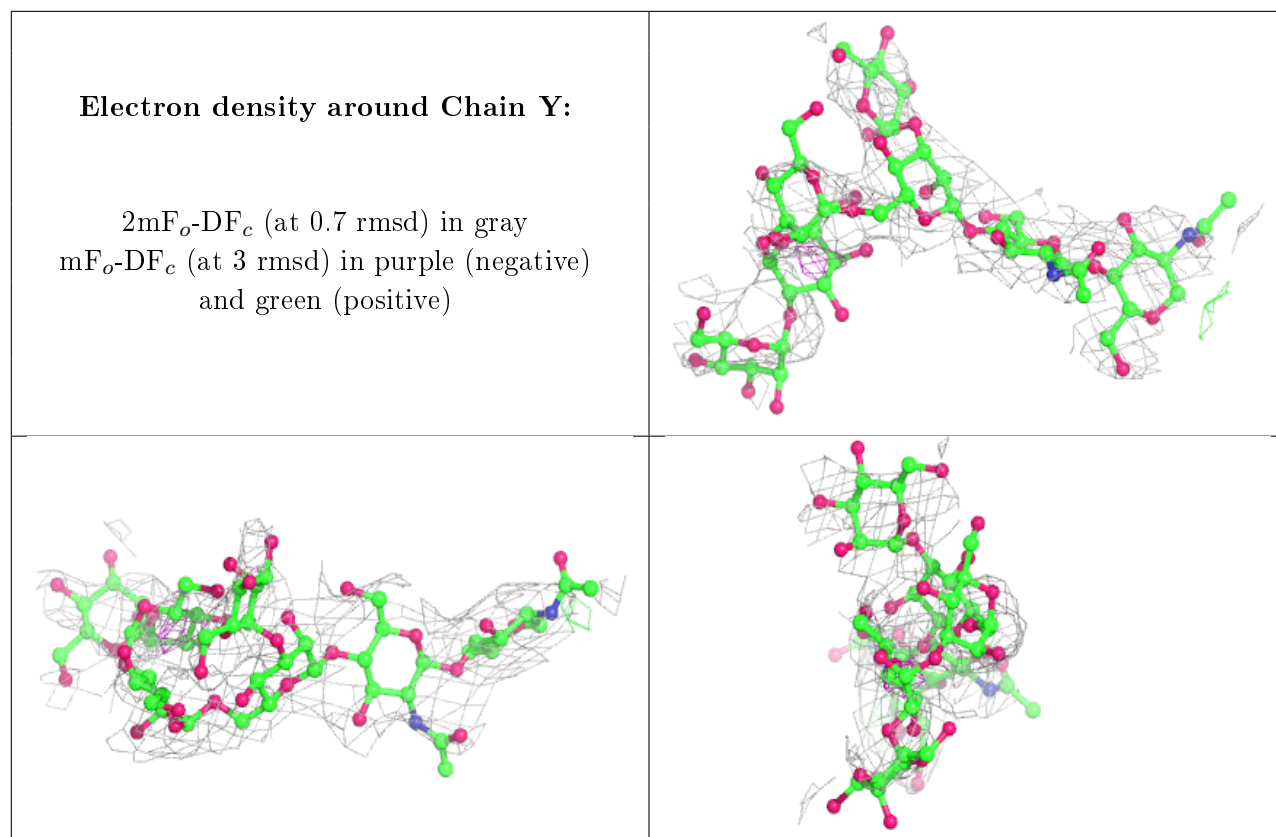
**Electron density around Chain S:**

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

**Electron density around Chain 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](#)

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

## 6.5 Other polymers [i](#)

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