



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:03 PM BST

PDB ID : 5FYL
Title : Crystal Structure at 3.7 Å Resolution of Fully Glycosylated HIV-1 Clade A BG505 SOSIP.664 Prefusion Env Trimer in Complex with Broadly Neutralizing Antibodies PGT122 and 35O22
Authors : Stewart-Jones, G.B.E.; Zhou, T.; Thomas, P.V.; Kwong, P.D.
Deposited on : 2016-03-08
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

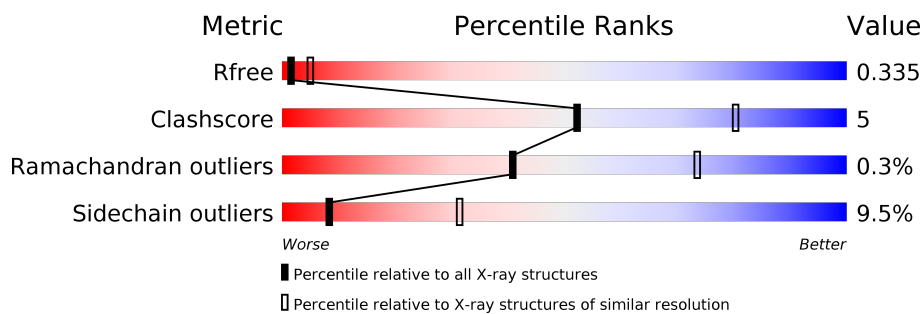
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.




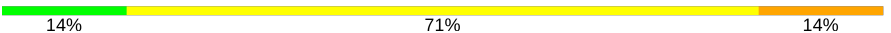
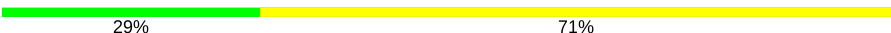
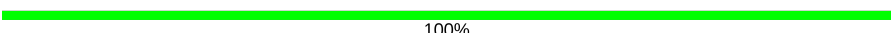

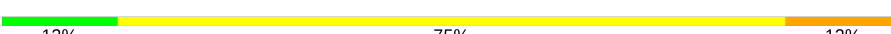
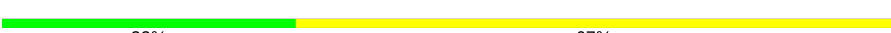




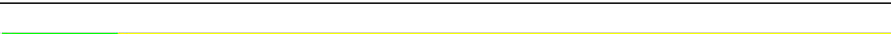



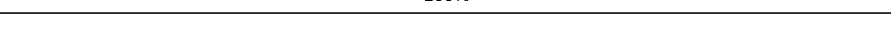

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	B	153	
2	D	243	
3	E	216	
4	G	481	
5	H	244	
6	L	213	
7	A	3	

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Mol	Chain	Length	Quality of chain
7	T	3	 33%67%
8	C	7	 14%71%14%
8	I	7	 29%71%
9	F	2	 100%
10	J	9	 33%67%
11	K	8	 13%75%13%
12	M	6	 33%67%
13	N	5	 40%60%
13	P	5	 40%60%
14	O	8	 25%75%
15	Q	7	 43%57%
16	R	8	 13%88%
17	S	10	 30%70%
18	U	6	 17%83%
18	V	6	 100%
19	W	6	 33%67%
20	X	4	 50%50%

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 12718 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 BG505 GP120 ENV ECTODOMAIN.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called 35O22 ANTIBODY FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	242	Total	C	N	O	S	0	0	0
			1832	1165	306	353	8			

- Molecule 3 is a protein called 35O22 ANTIBODY FAB LIGHT CHAIN.

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 BG505 GP120 ENV ECTODOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	453	Total	C	N	O	S	0	0	0
			3565	2236	630	671	28			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 5 is a protein called PGT122 ANTIBODY FAB HEAVY CHAIN.

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 ANTIBODY FAB LIGHT CHAIN.

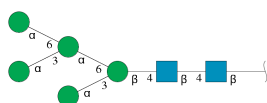
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	210	Total	C	N	O	S	0	0	0
			1589	998	267	320	4			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



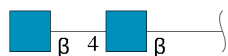
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	A	3	Total	C	N	O		0	0	0
			39	22	2	15				
7	T	3	Total	C	N	O		0	0	0
			39	22	2	15				

- Molecule 8 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.



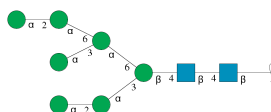
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	C	7	Total	C	N	O	0	0	0
			83	46	2	35			
8	I	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



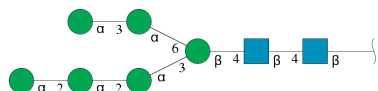
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 10 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.



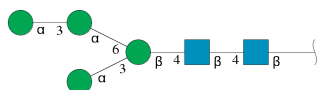
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	9	Total	C	N	O	0	0	0
			105	58	2	45			

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



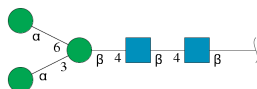
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	K	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 12 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.



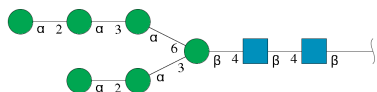
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	M	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 13 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.



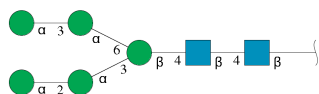
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	N	5	Total	C	N	O	0	0	0
			61	34	2	25			
13	P	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 14 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.



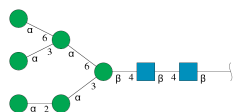
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	O	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 15 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.



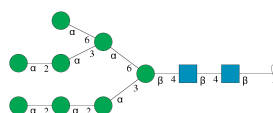
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	Q	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 16 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.



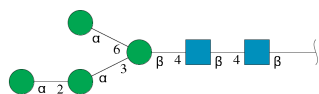
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	R	8	Total	C	N	O	0	0	0
			94	52	2	40			

- 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.



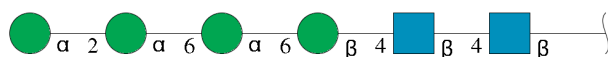
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	S	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 18 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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	U	6	Total	C	N	O	0	0	0
			72	40	2	30			
18	V	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 19 is an oligosaccharide called 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.



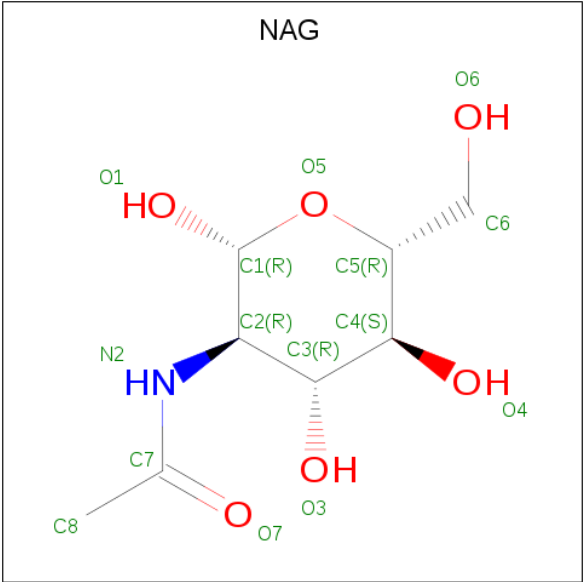
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	W	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 20 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
20	X	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 21 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

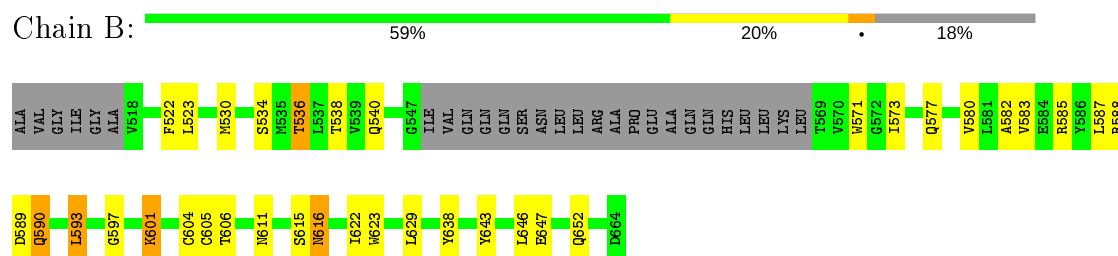


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	B	1	Total	C	N	O	0	0
			14	8	1	5		
21	B	1	Total	C	N	O	0	0
			14	8	1	5		
21	G	1	Total	C	N	O	0	0
			14	8	1	5		
21	G	1	Total	C	N	O	0	0
			14	8	1	5		

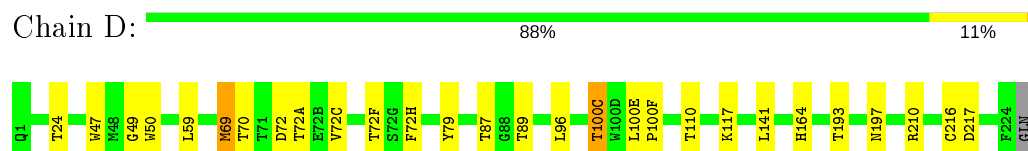
3 Residue-property plots [i](#)

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.

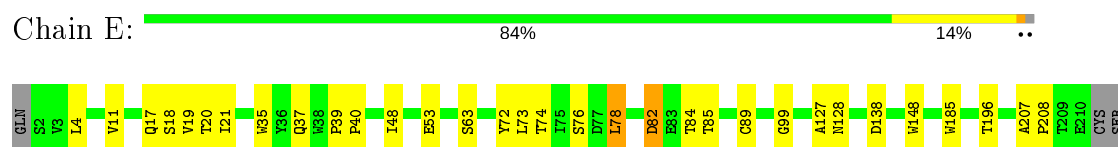
- Molecule 1: BG505 GP120 ENV ECTODOMAIN



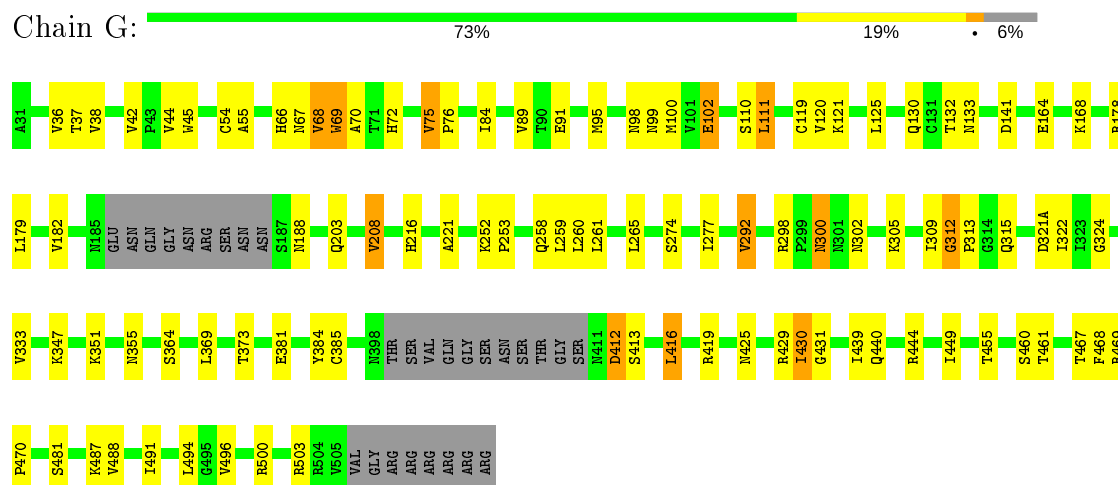
- Molecule 2: 35O22 ANTIBODY FAB HEAVY CHAIN



- Molecule 3: 35O22 ANTIBODY FAB LIGHT CHAIN

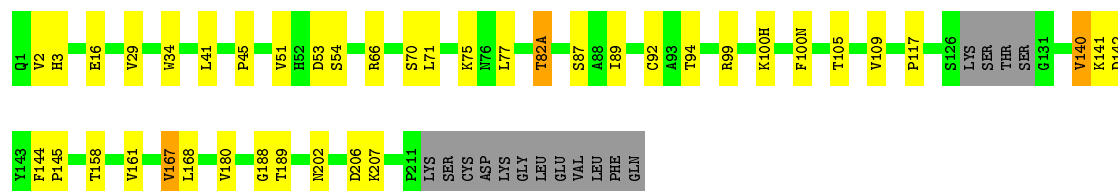


- Molecule 4: BG505 GP120 ENV ECTODOMAIN



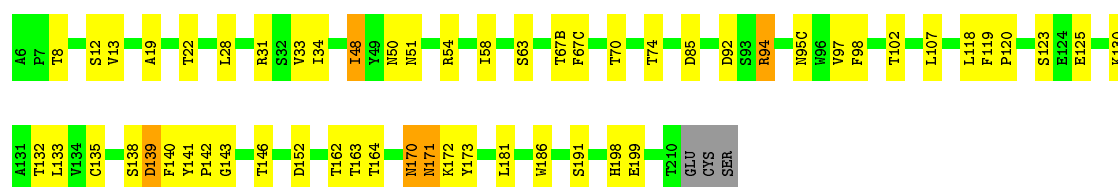
- Molecule 5: PGT122 ANTIBODY FAB HEAVY CHAIN

Chain H: 



- Molecule 6: PGT122 ANTIBODY FAB LIGHT CHAIN

Chain L: 



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 

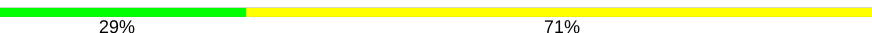


- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 



- Molecule 8: 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 I: 



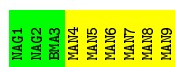
- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



- Molecule 10: 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 J:



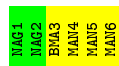
- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



- Molecule 12: 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 M:



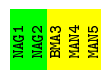
- Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



- Molecule 13: 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:  40% 60%



- Molecule 14: 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 O:  25% 75%



- Molecule 15: 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:  43% 57%



- Molecule 16: 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 R:  13% 88%



- 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 S:  30% 70%



- Molecule 18: 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 U:  17% 83%



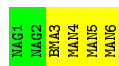
- Molecule 18: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%



- Molecule 19: 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

Chain W:  33% 67%



- Molecule 20: 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:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	129.78Å 129.78Å 313.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.00 – 3.10 41.00 – 2.91	Depositor EDS
% Data completeness (in resolution range)	58.5 (41.00-3.10) 49.3 (41.00-2.91)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.90Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.250 , 0.307 0.304 , 0.335	Depositor DCC
R_{free} test set	1619 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.085 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	12718	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.25	0/1019	0.46	0/1382
2	D	0.23	0/1880	0.43	0/2560
3	E	0.23	0/1659	0.42	0/2269
4	G	0.27	0/3639	0.48	1/4941 (0.0%)
5	H	0.23	0/1789	0.45	0/2443
6	L	0.24	0/1632	0.46	0/2236
All	All	0.25	0/11618	0.45	1/15831 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	111	LEU	CA-CB-CG	5.80	128.63	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1001	0	975	18	0
2	D	1832	0	1806	11	0
3	E	1615	0	1542	14	0
4	G	3565	0	3495	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	1742	0	1715	22	0
6	L	1589	0	1530	28	0
7	A	39	0	34	0	0
7	T	39	0	34	1	0
8	C	83	0	70	2	0
8	I	83	0	70	0	0
9	F	28	0	25	0	0
10	J	105	0	88	0	0
11	K	94	0	79	3	0
12	M	72	0	61	0	0
13	N	61	0	52	0	0
13	P	61	0	52	0	0
14	O	94	0	79	0	0
15	Q	83	0	70	0	0
16	R	94	0	79	0	0
17	S	116	0	97	0	0
18	U	72	0	61	2	0
18	V	72	0	61	1	0
19	W	72	0	61	0	0
20	X	50	0	43	3	0
21	B	28	0	26	1	0
21	G	28	0	26	1	0
All	All	12718	0	12231	137	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 (137) 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)
11:K:3:BMA:H3	11:K:4:MAN:H5	1.23	1.14
11:K:3:BMA:H3	11:K:4:MAN:C5	2.00	0.92
5:H:77:LEU:HD22	20:X:2:NAG:H83	1.62	0.82
1:B:615:SER:O	1:B:616:ASN:ND2	2.17	0.75
6:L:139:ASP:H	6:L:172:LYS:HE3	1.57	0.69
4:G:274:SER:HB3	4:G:277:ILE:HG13	1.75	0.68
3:E:127:ALA:H	3:E:128:ASN:HA	1.59	0.67
4:G:412:ASP:OD1	4:G:412:ASP:N	2.29	0.65
5:H:29:VAL:HA	5:H:34:TRP:CZ2	2.33	0.63
5:H:77:LEU:HD22	20:X:2:NAG:C8	2.29	0.62
4:G:132:THR:OG1	4:G:133:ASN:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:258:GLN:HG3	4:G:470:PRO:HB2	1.81	0.62
4:G:292:VAL:HG13	4:G:449:ILE:HB	1.81	0.61
4:G:75:VAL:HG22	4:G:76:PRO:HD2	1.83	0.59
4:G:67:ASN:HA	4:G:208:VAL:HA	1.85	0.59
4:G:322:ILE:O	6:L:94:ARG:NH2	2.35	0.59
4:G:309:ILE:HB	4:G:315:GLN:HB2	1.85	0.59
6:L:118:LEU:HD13	6:L:135:CYS:HB3	1.85	0.58
5:H:167:VAL:HB	6:L:163:THR:HG22	1.84	0.58
21:B:1666:NAG:H62	3:E:53:GLU:HA	1.83	0.58
5:H:141:LYS:HZ1	6:L:130:LYS:HD3	1.68	0.58
3:E:17:GLN:HG3	3:E:18:SER:H	1.69	0.57
4:G:55:ALA:HB3	4:G:216:HIS:HB2	1.84	0.57
6:L:170:ASN:O	6:L:172:LYS:N	2.38	0.57
4:G:351:LYS:HA	21:G:1583:NAG:H82	1.86	0.57
3:E:82:ASP:OD1	3:E:82:ASP:N	2.37	0.57
4:G:430:ILE:HD12	4:G:431:GLY:H	1.71	0.56
8:C:3:BMA:H61	8:C:4:MAN:H3	1.88	0.56
4:G:258:GLN:HE21	4:G:470:PRO:HB2	1.71	0.56
5:H:34:TRP:CZ3	5:H:94:THR:HG22	2.41	0.56
1:B:643:TYR:HA	1:B:646:LEU:HD12	1.88	0.55
5:H:45:PRO:HD2	6:L:98:PHE:HB2	1.88	0.55
6:L:171:ASN:N	6:L:171:ASN:OD1	2.38	0.55
2:D:87:THR:HG23	2:D:110:THR:HA	1.89	0.54
4:G:164:GLU:HA	4:G:312:GLY:HA3	1.88	0.54
6:L:198:HIS:CG	6:L:199:GLU:H	2.25	0.54
4:G:430:ILE:HD12	4:G:431:GLY:N	2.23	0.54
4:G:119:CYS:HB3	4:G:203:GLN:O	2.07	0.54
3:E:84:THR:OG1	3:E:85:THR:N	2.39	0.53
4:G:373:THR:HG21	4:G:384:TYR:HB3	1.91	0.53
4:G:369:LEU:O	4:G:373:THR:HG22	2.08	0.53
1:B:605:CYS:HA	4:G:37:THR:HG22	1.91	0.53
6:L:152:ASP:OD1	6:L:191:SER:N	2.39	0.52
20:X:2:NAG:O3	20:X:3:BMA:O5	2.23	0.52
4:G:460:SER:O	4:G:461:THR:OG1	2.28	0.51
2:D:100(C):THR:HG21	8:C:2:NAG:H3	1.91	0.51
5:H:29:VAL:HA	5:H:34:TRP:HZ2	1.75	0.51
6:L:33:VAL:HG12	6:L:51:ASN:ND2	2.26	0.51
1:B:590:GLN:OE1	1:B:601:LYS:NZ	2.44	0.50
2:D:96:LEU:HD22	2:D:100(E):LEU:HD23	1.93	0.50
5:H:34:TRP:HB2	5:H:51:VAL:HG13	1.95	0.48
4:G:460:SER:OG	4:G:461:THR:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:117:PRO:HA	5:H:142:ASP:O	2.12	0.48
1:B:582:ALA:HB1	4:G:221:ALA:HB3	1.95	0.48
4:G:385:CYS:HB3	4:G:416:LEU:HD12	1.95	0.48
4:G:69:TRP:CE3	4:G:111:LEU:HD21	2.48	0.48
4:G:98:ASN:OD1	4:G:100:MET:N	2.47	0.48
4:G:425:ASN:HA	4:G:429:ARG:HD2	1.94	0.48
1:B:604:CYS:SG	4:G:503:ARG:NH2	2.87	0.47
6:L:63:SER:HB2	6:L:74:THR:HB	1.96	0.47
4:G:455:THR:N	4:G:469:ARG:O	2.48	0.47
3:E:4:LEU:HB3	3:E:99:GLY:HA2	1.96	0.47
6:L:143:GLY:HA3	6:L:173:TYR:CD2	2.50	0.47
1:B:530:MET:O	1:B:534:SER:OG	2.21	0.47
4:G:120:VAL:HG23	4:G:315:GLN:NE2	2.30	0.46
4:G:381:GLU:HB2	4:G:439:ILE:HD11	1.97	0.46
4:G:300:ASN:OD1	4:G:300:ASN:N	2.49	0.46
1:B:536:THR:O	1:B:540:GLN:NE2	2.45	0.46
3:E:20:THR:HG22	3:E:74:THR:HG22	1.97	0.46
1:B:571:TRP:CD1	4:G:70:ALA:HB1	2.51	0.46
4:G:69:TRP:CD2	4:G:111:LEU:HD21	2.50	0.46
4:G:252:LYS:HA	4:G:253:PRO:HD3	1.69	0.46
4:G:321(A):ASP:OD1	4:G:322:ILE:N	2.49	0.46
5:H:141:LYS:NZ	6:L:130:LYS:HD3	2.31	0.45
1:B:589:ASP:O	1:B:593:LEU:HD22	2.17	0.45
5:H:53:ASP:O	5:H:54:SER:OG	2.25	0.45
4:G:324:GLY:HA2	6:L:67(C):PHE:CD1	2.52	0.45
4:G:298:ARG:NH2	4:G:439:ILE:O	2.48	0.45
6:L:140:PHE:CE2	6:L:143:GLY:HA2	2.51	0.45
6:L:139:ASP:N	6:L:172:LYS:HE3	2.27	0.45
1:B:629:LEU:HA	4:G:44:VAL:HG23	1.99	0.45
1:B:522:PHE:N	4:G:84:ILE:HD13	2.32	0.44
6:L:13:VAL:HG21	6:L:19:ALA:HB2	1.98	0.44
1:B:577:GLN:HA	1:B:580:VAL:HG22	1.99	0.44
2:D:47:TRP:CZ2	2:D:49:GLY:HA2	2.52	0.44
4:G:42:VAL:HG12	4:G:44:VAL:HG12	1.99	0.44
2:D:100(E):LEU:HD12	2:D:100(F):PRO:HD2	2.00	0.44
3:E:19:VAL:HG12	3:E:78:LEU:HD21	1.99	0.44
1:B:571:TRP:NE1	4:G:70:ALA:HB1	2.33	0.44
18:U:2:NAG:H82	18:V:1:NAG:H83	1.99	0.44
5:H:141:LYS:HZ1	6:L:130:LYS:CD	2.30	0.44
3:E:35:TRP:HB2	3:E:48:ILE:HG22	2.00	0.43
2:D:216:CYS:SG	2:D:217:ASP:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:78:LEU:HA	3:E:78:LEU:HD13	1.90	0.43
6:L:13:VAL:O	6:L:107:LEU:N	2.51	0.43
6:L:31:ARG:HG2	6:L:92:ASP:HA	2.00	0.43
3:E:35:TRP:CE2	3:E:73:LEU:HB2	2.54	0.43
5:H:117:PRO:HB3	5:H:140:VAL:HG23	2.00	0.43
2:D:193:THR:HG23	2:D:210:ARG:HH12	1.83	0.42
6:L:170:ASN:OD1	6:L:172:LYS:HB3	2.19	0.42
3:E:207:ALA:HA	3:E:208:PRO:HD3	1.92	0.42
1:B:522:PHE:O	1:B:523:LEU:HB2	2.18	0.42
2:D:59:LEU:HD11	2:D:69:MET:HG3	2.00	0.42
6:L:48:ILE:HG23	6:L:50:ASN:O	2.20	0.42
4:G:67:ASN:OD1	4:G:68:VAL:HG22	2.19	0.42
5:H:89:ILE:O	5:H:89:ILE:HG13	2.20	0.42
2:D:70:THR:HB	2:D:79:TYR:HB2	2.02	0.42
6:L:125:GLU:OE2	6:L:132:THR:N	2.53	0.42
6:L:141:TYR:HA	6:L:142:PRO:HA	1.85	0.42
6:L:199:GLU:HA	6:L:199:GLU:OE1	2.20	0.42
4:G:99:ASN:O	4:G:102:GLU:N	2.53	0.42
2:D:72(F):THR:HG23	2:D:72(H):PHE:H	1.85	0.42
4:G:130:GLN:HG3	11:K:1:NAG:H82	2.01	0.41
4:G:45:TRP:HB3	4:G:491:ILE:HD13	2.02	0.41
4:G:300:ASN:HB2	4:G:302:ASN:OD1	2.20	0.41
5:H:75:LYS:O	5:H:77:LEU:HD12	2.20	0.41
5:H:141:LYS:NZ	6:L:130:LYS:CD	2.83	0.41
4:G:91:GLU:HG3	4:G:487:LYS:HZ2	1.86	0.41
2:D:47:TRP:HZ2	2:D:50:TRP:CD1	2.38	0.41
5:H:144:PHE:HA	5:H:145:PRO:HA	1.83	0.41
5:H:70:SER:OG	5:H:71:LEU:N	2.53	0.41
3:E:127:ALA:N	3:E:128:ASN:HA	2.25	0.41
3:E:39:PRO:HA	3:E:40:PRO:HD3	1.94	0.41
4:G:261:LEU:HD23	4:G:449:ILE:HA	2.03	0.41
6:L:119:PHE:HA	6:L:120:PRO:HD3	1.88	0.41
5:H:161:VAL:HG12	5:H:180:VAL:HG12	2.03	0.41
4:G:179:LEU:HD21	4:G:419:ARG:HD3	2.01	0.41
4:G:385:CYS:HB3	4:G:416:LEU:CD1	2.51	0.41
4:G:98:ASN:OD1	4:G:99:ASN:N	2.54	0.41
7:T:2:NAG:O4	18:U:2:NAG:H61	2.21	0.41
1:B:622:ILE:HG13	1:B:623:TRP:N	2.36	0.40
5:H:188:GLY:HA3	5:H:189:THR:HA	1.88	0.40
4:G:54:CYS:SG	4:G:55:ALA:N	2.94	0.40
5:H:66:ARG:HB2	5:H:82(A):THR:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:467:THR:OG1	4:G:468:PHE:N	2.55	0.40
1:B:536:THR:OG1	1:B:536:THR:O	2.36	0.40
1:B:597:GLY:HA3	4:G:503:ARG:HH12	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	122/153 (80%)	109 (89%)	13 (11%)	0	100	100
2	D	240/243 (99%)	212 (88%)	27 (11%)	1 (0%)	34	69
3	E	211/216 (98%)	189 (90%)	22 (10%)	0	100	100
4	G	447/481 (93%)	406 (91%)	39 (9%)	2 (0%)	34	69
5	H	224/244 (92%)	203 (91%)	20 (9%)	1 (0%)	34	69
6	L	208/213 (98%)	183 (88%)	24 (12%)	1 (0%)	29	64
All	All	1452/1550 (94%)	1302 (90%)	145 (10%)	5 (0%)	41	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	H	202	ASN
6	L	171	ASN
4	G	500	ARG
2	D	197	ASN
4	G	312	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	108/129 (84%)	92 (85%)	16 (15%)	3	13
2	D	205/206 (100%)	195 (95%)	10 (5%)	25	57
3	E	186/189 (98%)	173 (93%)	13 (7%)	15	45
4	G	404/428 (94%)	364 (90%)	40 (10%)	8	29
5	H	198/213 (93%)	180 (91%)	18 (9%)	9	33
6	L	178/181 (98%)	153 (86%)	25 (14%)	3	15
All	All	1279/1346 (95%)	1157 (90%)	122 (10%)	8	31

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	536	THR
1	B	538	THR
1	B	573	ILE
1	B	583	VAL
1	B	585	ARG
1	B	587	LEU
1	B	588	ARG
1	B	590	GLN
1	B	593	LEU
1	B	601	LYS
1	B	606	THR
1	B	611	ASN
1	B	616	ASN
1	B	638	TYR
1	B	647	GLU
1	B	652	GLN
2	D	24	THR
2	D	69	MET
2	D	72	ASP
2	D	72(A)	THR
2	D	72(C)	VAL
2	D	89	THR

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Mol	Chain	Res	Type
2	D	100(C)	THR
2	D	117	LYS
2	D	141	LEU
2	D	164	HIS
3	E	11	VAL
3	E	21	ILE
3	E	37	GLN
3	E	63	SER
3	E	72	TYR
3	E	76	SER
3	E	78	LEU
3	E	82	ASP
3	E	89	CYS
3	E	138	ASP
3	E	148	TRP
3	E	185	TRP
3	E	196	THR
4	G	36	VAL
4	G	38	VAL
4	G	66	HIS
4	G	68	VAL
4	G	69	TRP
4	G	72	HIS
4	G	75	VAL
4	G	89	VAL
4	G	95	MET
4	G	102	GLU
4	G	110	SER
4	G	121	LYS
4	G	125	LEU
4	G	141	ASP
4	G	168	LYS
4	G	178	ARG
4	G	182	VAL
4	G	188	ASN
4	G	208	VAL
4	G	259	LEU
4	G	260	LEU
4	G	265	LEU
4	G	292	VAL
4	G	300	ASN
4	G	305	LYS

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Mol	Chain	Res	Type
4	G	313	PRO
4	G	333	VAL
4	G	347	LYS
4	G	355	ASN
4	G	364	SER
4	G	412	ASP
4	G	413	SER
4	G	416	LEU
4	G	430	ILE
4	G	440	GLN
4	G	444	ARG
4	G	481	SER
4	G	488	VAL
4	G	494	LEU
4	G	496	VAL
5	H	2	VAL
5	H	3	HIS
5	H	16	GLU
5	H	41	LEU
5	H	82(A)	THR
5	H	87	SER
5	H	92	CYS
5	H	99	ARG
5	H	100(H)	LYS
5	H	100(N)	PHE
5	H	105	THR
5	H	109	VAL
5	H	140	VAL
5	H	158	THR
5	H	167	VAL
5	H	168	LEU
5	H	206	ASP
5	H	207	LYS
6	L	8	THR
6	L	12	SER
6	L	22	THR
6	L	28	LEU
6	L	34	ILE
6	L	48	ILE
6	L	54	ARG
6	L	58	ILE
6	L	67(B)	THR

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Mol	Chain	Res	Type
6	L	70	THR
6	L	85	ASP
6	L	94	ARG
6	L	95(C)	ASN
6	L	97	VAL
6	L	102	THR
6	L	123	SER
6	L	133	LEU
6	L	138	SER
6	L	139	ASP
6	L	146	THR
6	L	162	THR
6	L	164	THR
6	L	170	ASN
6	L	181	LEU
6	L	186	TRP

Some 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
4	G	258	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 ⓘ

110 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	1	1,7	14,14,15	0.27	0	17,19,21	0.38	0
7	NAG	A	2	7	14,14,15	0.32	0	17,19,21	0.52	0
7	BMA	A	3	7	11,11,12	0.66	0	15,15,17	0.79	0
8	NAG	C	1	8,4	14,14,15	0.22	0	17,19,21	0.47	0
8	NAG	C	2	8	14,14,15	0.41	0	17,19,21	0.55	0
8	BMA	C	3	8	11,11,12	0.57	0	15,15,17	0.71	0
8	MAN	C	4	8	11,11,12	0.84	0	15,15,17	1.43	2 (13%)
8	MAN	C	5	8	11,11,12	0.64	0	15,15,17	0.92	1 (6%)
8	MAN	C	6	8	11,11,12	0.63	0	15,15,17	0.92	2 (13%)
8	MAN	C	7	8	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
9	NAG	F	1	9,4	14,14,15	0.34	0	17,19,21	0.61	0
9	NAG	F	2	9	14,14,15	0.37	0	17,19,21	0.39	0
8	NAG	I	1	8,4	14,14,15	0.40	0	17,19,21	0.49	0
8	NAG	I	2	8	14,14,15	0.33	0	17,19,21	0.65	0
8	BMA	I	3	8	11,11,12	1.16	1 (9%)	15,15,17	1.01	1 (6%)
8	MAN	I	4	8	11,11,12	1.16	1 (9%)	15,15,17	1.49	2 (13%)
8	MAN	I	5	8	11,11,12	0.59	0	15,15,17	1.14	2 (13%)
8	MAN	I	6	8	11,11,12	0.68	0	15,15,17	0.92	2 (13%)
8	MAN	I	7	8	11,11,12	0.68	0	15,15,17	1.18	2 (13%)
10	NAG	J	1	10,4	14,14,15	0.26	0	17,19,21	0.45	0
10	NAG	J	2	10	14,14,15	0.18	0	17,19,21	0.44	0
10	BMA	J	3	10	11,11,12	0.65	0	15,15,17	0.81	0
10	MAN	J	4	10	11,11,12	0.58	0	15,15,17	1.23	2 (13%)
10	MAN	J	5	10	11,11,12	0.55	0	15,15,17	1.11	1 (6%)
10	MAN	J	6	10	11,11,12	0.73	0	15,15,17	1.28	2 (13%)
10	MAN	J	7	10	11,11,12	0.68	0	15,15,17	1.00	2 (13%)
10	MAN	J	8	10	11,11,12	0.65	0	15,15,17	1.21	2 (13%)
10	MAN	J	9	10	11,11,12	0.65	0	15,15,17	0.96	2 (13%)
11	NAG	K	1	11,4	14,14,15	0.31	0	17,19,21	0.54	0
11	NAG	K	2	11	14,14,15	0.25	0	17,19,21	0.39	0
11	BMA	K	3	11	11,11,12	0.57	0	15,15,17	0.90	0
11	MAN	K	4	11	11,11,12	0.44	0	15,15,17	1.18	2 (13%)
11	MAN	K	5	11	11,11,12	0.76	1 (9%)	15,15,17	1.11	1 (6%)
11	MAN	K	6	11	11,11,12	0.71	1 (9%)	15,15,17	1.14	2 (13%)
11	MAN	K	7	11	11,11,12	1.07	1 (9%)	15,15,17	0.93	1 (6%)
11	MAN	K	8	11	11,11,12	0.96	1 (9%)	15,15,17	1.55	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	M	1	12,4	14,14,15	0.24	0	17,19,21	0.48	0
12	NAG	M	2	12	14,14,15	0.33	0	17,19,21	0.67	0
12	BMA	M	3	12	11,11,12	1.08	1 (9%)	15,15,17	1.23	2 (13%)
12	MAN	M	4	12	11,11,12	0.93	1 (9%)	15,15,17	1.16	2 (13%)
12	MAN	M	5	12	11,11,12	0.80	0	15,15,17	0.84	1 (6%)
12	MAN	M	6	12	11,11,12	0.83	1 (9%)	15,15,17	1.27	1 (6%)
13	NAG	N	1	13,4	14,14,15	0.33	0	17,19,21	0.57	0
13	NAG	N	2	13	14,14,15	0.21	0	17,19,21	0.46	0
13	BMA	N	3	13	11,11,12	0.72	0	15,15,17	1.01	1 (6%)
13	MAN	N	4	13	11,11,12	0.67	0	15,15,17	1.00	2 (13%)
13	MAN	N	5	13	11,11,12	0.65	0	15,15,17	1.13	2 (13%)
14	NAG	O	1	4,14	14,14,15	0.33	0	17,19,21	0.39	0
14	NAG	O	2	14	14,14,15	0.30	0	17,19,21	0.39	0
14	BMA	O	3	14	11,11,12	1.07	1 (9%)	15,15,17	0.87	0
14	MAN	O	4	14	11,11,12	1.26	2 (18%)	15,15,17	1.40	3 (20%)
14	MAN	O	5	14	11,11,12	0.82	0	15,15,17	0.91	1 (6%)
14	MAN	O	6	14	11,11,12	0.77	1 (9%)	15,15,17	1.23	2 (13%)
14	MAN	O	7	14	11,11,12	0.82	0	15,15,17	1.16	3 (20%)
14	MAN	O	8	14	11,11,12	0.87	1 (9%)	15,15,17	1.44	2 (13%)
13	NAG	P	1	13,4	14,14,15	0.33	0	17,19,21	0.50	0
13	NAG	P	2	13	14,14,15	0.24	0	17,19,21	0.53	0
13	BMA	P	3	13	11,11,12	1.05	0	15,15,17	1.21	2 (13%)
13	MAN	P	4	13	11,11,12	0.71	0	15,15,17	1.20	2 (13%)
13	MAN	P	5	13	11,11,12	0.71	1 (9%)	15,15,17	1.14	2 (13%)
15	NAG	Q	1	15,4	14,14,15	0.41	0	17,19,21	0.50	0
15	NAG	Q	2	15	14,14,15	0.23	0	17,19,21	0.40	0
15	BMA	Q	3	15	11,11,12	1.05	0	15,15,17	0.88	0
15	MAN	Q	4	15	11,11,12	0.75	0	15,15,17	1.06	2 (13%)
15	MAN	Q	5	15	11,11,12	0.85	1 (9%)	15,15,17	1.12	2 (13%)
15	MAN	Q	6	15	11,11,12	0.90	1 (9%)	15,15,17	1.15	2 (13%)
15	MAN	Q	7	15	11,11,12	0.72	1 (9%)	15,15,17	1.18	2 (13%)
16	NAG	R	1	4,16	14,14,15	0.34	0	17,19,21	0.54	0
16	NAG	R	2	16	14,14,15	0.40	0	17,19,21	1.32	2 (11%)
16	BMA	R	3	16	11,11,12	1.02	0	15,15,17	1.74	2 (13%)
16	MAN	R	4	16	11,11,12	0.66	0	15,15,17	1.07	2 (13%)
16	MAN	R	5	16	11,11,12	0.62	0	15,15,17	1.02	2 (13%)
16	MAN	R	6	16	11,11,12	1.03	0	15,15,17	1.35	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	MAN	R	7	16	11,11,12	0.63	0	15,15,17	0.99	2 (13%)
16	MAN	R	8	16	11,11,12	0.90	1 (9%)	15,15,17	1.36	2 (13%)
17	NAG	S	1	4,17	14,14,15	0.32	0	17,19,21	0.45	0
17	MAN	S	10	17	11,11,12	0.68	0	15,15,17	1.04	2 (13%)
17	NAG	S	2	17	14,14,15	0.38	0	17,19,21	0.64	0
17	BMA	S	3	17	11,11,12	0.64	0	15,15,17	0.87	0
17	MAN	S	4	17	11,11,12	0.64	0	15,15,17	1.40	2 (13%)
17	MAN	S	5	17	11,11,12	0.66	0	15,15,17	1.13	2 (13%)
17	MAN	S	6	17	11,11,12	0.74	0	15,15,17	1.14	2 (13%)
17	MAN	S	7	17	11,11,12	0.73	0	15,15,17	1.00	2 (13%)
17	MAN	S	8	17	11,11,12	0.79	1 (9%)	15,15,17	1.13	1 (6%)
17	MAN	S	9	17	11,11,12	0.68	0	15,15,17	0.87	1 (6%)
7	NAG	T	1	4,7	14,14,15	0.24	0	17,19,21	0.43	0
7	NAG	T	2	7	14,14,15	0.28	0	17,19,21	0.52	0
7	BMA	T	3	7	11,11,12	0.80	0	15,15,17	1.09	1 (6%)
18	NAG	U	1	18,4	14,14,15	0.52	0	17,19,21	0.67	1 (5%)
18	NAG	U	2	18	14,14,15	0.25	0	17,19,21	0.63	0
18	BMA	U	3	18	11,11,12	0.66	0	15,15,17	0.83	0
18	MAN	U	4	18	11,11,12	1.26	1 (9%)	15,15,17	1.36	2 (13%)
18	MAN	U	5	18	11,11,12	0.63	0	15,15,17	1.02	2 (13%)
18	MAN	U	6	18	11,11,12	0.64	0	15,15,17	0.97	2 (13%)
18	NAG	V	1	18,4	14,14,15	0.51	0	17,19,21	0.60	0
18	NAG	V	2	18	14,14,15	0.34	0	17,19,21	0.90	1 (5%)
18	BMA	V	3	18	11,11,12	1.03	1 (9%)	15,15,17	1.05	1 (6%)
18	MAN	V	4	18	11,11,12	0.89	1 (9%)	15,15,17	1.11	1 (6%)
18	MAN	V	5	18	11,11,12	0.68	0	15,15,17	1.16	2 (13%)
18	MAN	V	6	18	11,11,12	0.73	0	15,15,17	1.04	2 (13%)
19	NAG	W	1	19,4	14,14,15	0.27	0	17,19,21	0.52	0
19	NAG	W	2	19	14,14,15	0.32	0	17,19,21	0.48	0
19	BMA	W	3	19	11,11,12	0.64	0	15,15,17	1.18	1 (6%)
19	MAN	W	4	19	11,11,12	0.96	1 (9%)	15,15,17	1.58	2 (13%)
19	MAN	W	5	19	11,11,12	0.83	1 (9%)	15,15,17	1.11	1 (6%)
19	MAN	W	6	19	11,11,12	0.68	0	15,15,17	1.11	2 (13%)
20	NAG	X	1	20,5	14,14,15	0.64	1 (7%)	17,19,21	0.64	0
20	NAG	X	2	20	14,14,15	0.42	0	17,19,21	0.74	1 (5%)
20	BMA	X	3	20	11,11,12	0.89	1 (9%)	15,15,17	1.03	1 (6%)
20	MAN	X	4	20	11,11,12	0.69	0	15,15,17	0.86	1 (6%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	0/2/19/22	0/1/1/1
12	MAN	M	6	12	-	2/2/19/22	0/1/1/1
13	NAG	N	1	13,4	-	2/6/23/26	0/1/1/1
13	NAG	N	2	13	-	0/6/23/26	0/1/1/1
13	BMA	N	3	13	-	0/2/19/22	0/1/1/1
13	MAN	N	4	13	-	0/2/19/22	0/1/1/1
13	MAN	N	5	13	-	0/2/19/22	0/1/1/1
14	NAG	O	1	4,14	-	0/6/23/26	0/1/1/1
14	NAG	O	2	14	-	0/6/23/26	0/1/1/1
14	BMA	O	3	14	-	2/2/19/22	0/1/1/1
14	MAN	O	4	14	-	0/2/19/22	0/1/1/1
14	MAN	O	5	14	-	0/2/19/22	0/1/1/1
14	MAN	O	6	14	-	0/2/19/22	0/1/1/1
14	MAN	O	7	14	-	1/2/19/22	0/1/1/1
14	MAN	O	8	14	-	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	-	1/6/23/26	0/1/1/1
13	BMA	P	3	13	-	1/2/19/22	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
15	NAG	Q	1	15,4	-	2/6/23/26	0/1/1/1
15	NAG	Q	2	15	-	1/6/23/26	0/1/1/1
15	BMA	Q	3	15	-	0/2/19/22	0/1/1/1
15	MAN	Q	4	15	-	0/2/19/22	0/1/1/1
15	MAN	Q	5	15	-	0/2/19/22	0/1/1/1
15	MAN	Q	6	15	-	0/2/19/22	0/1/1/1
15	MAN	Q	7	15	-	0/2/19/22	0/1/1/1
16	NAG	R	1	4,16	-	2/6/23/26	0/1/1/1
16	NAG	R	2	16	-	0/6/23/26	0/1/1/1
16	BMA	R	3	16	-	1/2/19/22	0/1/1/1
16	MAN	R	4	16	-	0/2/19/22	0/1/1/1
16	MAN	R	5	16	-	0/2/19/22	0/1/1/1
16	MAN	R	6	16	-	1/2/19/22	0/1/1/1
16	MAN	R	7	16	-	1/2/19/22	0/1/1/1
16	MAN	R	8	16	-	0/2/19/22	0/1/1/1
17	NAG	S	1	4,17	-	2/6/23/26	0/1/1/1
17	MAN	S	10	17	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	NAG	S	2	17	-	3/6/23/26	0/1/1/1
17	BMA	S	3	17	-	0/2/19/22	0/1/1/1
17	MAN	S	4	17	-	1/2/19/22	0/1/1/1
17	MAN	S	5	17	-	0/2/19/22	0/1/1/1
17	MAN	S	6	17	-	0/2/19/22	0/1/1/1
17	MAN	S	7	17	-	2/2/19/22	0/1/1/1
17	MAN	S	8	17	-	1/2/19/22	0/1/1/1
17	MAN	S	9	17	-	1/2/19/22	0/1/1/1
7	NAG	T	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	T	2	7	-	0/6/23/26	0/1/1/1
7	BMA	T	3	7	-	1/2/19/22	0/1/1/1
18	NAG	U	1	18,4	-	2/6/23/26	0/1/1/1
18	NAG	U	2	18	-	0/6/23/26	0/1/1/1
18	BMA	U	3	18	-	2/2/19/22	0/1/1/1
18	MAN	U	4	18	-	0/2/19/22	0/1/1/1
18	MAN	U	5	18	-	0/2/19/22	0/1/1/1
18	MAN	U	6	18	-	0/2/19/22	0/1/1/1
18	NAG	V	1	18,4	-	0/6/23/26	0/1/1/1
18	NAG	V	2	18	-	0/6/23/26	0/1/1/1
18	BMA	V	3	18	-	1/2/19/22	0/1/1/1
18	MAN	V	4	18	-	0/2/19/22	0/1/1/1
18	MAN	V	5	18	-	0/2/19/22	0/1/1/1
18	MAN	V	6	18	-	0/2/19/22	0/1/1/1
19	NAG	W	1	19,4	-	2/6/23/26	0/1/1/1
19	NAG	W	2	19	-	0/6/23/26	0/1/1/1
19	BMA	W	3	19	-	1/2/19/22	0/1/1/1
19	MAN	W	4	19	-	0/2/19/22	0/1/1/1
19	MAN	W	5	19	-	2/2/19/22	0/1/1/1
19	MAN	W	6	19	-	0/2/19/22	0/1/1/1
20	NAG	X	1	20,5	-	3/6/23/26	0/1/1/1
20	NAG	X	2	20	-	2/6/23/26	0/1/1/1
20	BMA	X	3	20	-	0/2/19/22	0/1/1/1
20	MAN	X	4	20	-	1/2/19/22	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	V	3	BMA	C1-C2	2.81	1.58	1.52
19	W	4	MAN	C1-C2	2.77	1.58	1.52
8	I	3	BMA	C1-C2	2.77	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	R	8	MAN	C1-C2	2.76	1.58	1.52
11	K	8	MAN	C1-C2	2.74	1.58	1.52
18	U	4	MAN	O2-C2	2.46	1.48	1.43
15	Q	6	MAN	C1-C2	2.45	1.57	1.52
12	M	6	MAN	C1-C2	2.38	1.57	1.52
14	O	4	MAN	C2-C3	2.38	1.56	1.52
14	O	8	MAN	C1-C2	2.29	1.57	1.52
8	I	4	MAN	C2-C3	2.28	1.55	1.52
15	Q	5	MAN	C1-C2	2.23	1.57	1.52
14	O	6	MAN	C1-C2	2.20	1.57	1.52
12	M	4	MAN	C1-C2	2.20	1.57	1.52
11	K	7	MAN	C4-C3	2.19	1.57	1.52
20	X	3	BMA	C2-C3	2.19	1.55	1.52
12	M	3	BMA	C2-C3	2.18	1.55	1.52
14	O	4	MAN	C1-C2	2.15	1.57	1.52
14	O	3	BMA	C4-C5	2.15	1.57	1.53
19	W	5	MAN	C1-C2	2.14	1.57	1.52
20	X	1	NAG	C1-C2	2.13	1.55	1.52
11	K	5	MAN	C1-C2	2.08	1.56	1.52
18	V	4	MAN	C1-C2	2.06	1.56	1.52
17	S	8	MAN	C1-C2	2.05	1.56	1.52
13	P	5	MAN	C1-C2	2.04	1.56	1.52
11	K	6	MAN	C1-C2	2.04	1.56	1.52
15	Q	7	MAN	C1-C2	2.03	1.56	1.52

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	R	3	BMA	C1-O5-C5	5.34	119.42	112.19
19	W	4	MAN	C1-O5-C5	4.68	118.53	112.19
14	O	8	MAN	C1-O5-C5	4.57	118.38	112.19
17	S	4	MAN	C1-O5-C5	4.38	118.13	112.19
11	K	8	MAN	C1-O5-C5	4.34	118.08	112.19
16	R	6	MAN	C1-O5-C5	4.29	118.01	112.19
8	C	4	MAN	C1-C2-C3	3.98	114.55	109.67
16	R	2	NAG	C1-O5-C5	3.92	117.50	112.19
19	W	3	BMA	C1-O5-C5	3.86	117.42	112.19
18	U	4	MAN	O2-C2-C1	3.85	117.02	109.15
10	J	6	MAN	C1-O5-C5	3.81	117.35	112.19
12	M	3	BMA	C1-O5-C5	3.77	117.29	112.19
8	I	4	MAN	C1-O5-C5	3.62	117.10	112.19
16	R	8	MAN	C1-O5-C5	3.61	117.08	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	4	MAN	O3-C3-C2	3.53	116.76	109.99
13	P	4	MAN	C1-O5-C5	3.51	116.95	112.19
12	M	6	MAN	C1-O5-C5	3.51	116.95	112.19
8	I	7	MAN	C1-O5-C5	3.48	116.91	112.19
10	J	5	MAN	C1-O5-C5	3.36	116.75	112.19
10	J	4	MAN	C1-O5-C5	3.36	116.75	112.19
10	J	8	MAN	C1-O5-C5	3.31	116.68	112.19
15	Q	7	MAN	C1-O5-C5	3.28	116.64	112.19
8	I	5	MAN	C1-O5-C5	3.28	116.63	112.19
11	K	5	MAN	C1-O5-C5	3.24	116.58	112.19
14	O	6	MAN	C1-O5-C5	3.22	116.56	112.19
14	O	4	MAN	C1-O5-C5	3.22	116.55	112.19
13	N	5	MAN	C1-O5-C5	3.19	116.51	112.19
18	V	5	MAN	C1-O5-C5	3.18	116.50	112.19
13	P	3	BMA	O3-C3-C2	3.09	115.91	109.99
13	P	5	MAN	C1-O5-C5	3.07	116.36	112.19
16	R	3	BMA	O3-C3-C2	3.07	115.88	109.99
13	P	3	BMA	C1-O5-C5	3.06	116.33	112.19
16	R	2	NAG	O4-C4-C5	3.04	116.84	109.30
11	K	6	MAN	C1-O5-C5	2.95	116.19	112.19
8	C	4	MAN	O3-C3-C2	2.92	115.58	109.99
19	W	6	MAN	C1-O5-C5	2.90	116.12	112.19
17	S	5	MAN	C1-O5-C5	2.89	116.11	112.19
18	V	2	NAG	C1-O5-C5	2.84	116.04	112.19
17	S	6	MAN	C1-O5-C5	2.83	116.03	112.19
16	R	4	MAN	C1-O5-C5	2.82	116.01	112.19
17	S	5	MAN	O2-C2-C3	-2.80	104.53	110.14
11	K	4	MAN	C1-C2-C3	2.73	113.02	109.67
19	W	5	MAN	C1-O5-C5	2.71	115.86	112.19
18	V	3	BMA	O2-C2-C3	-2.64	104.86	110.14
14	O	4	MAN	C1-C2-C3	2.62	112.89	109.67
18	V	6	MAN	C1-O5-C5	2.60	115.72	112.19
8	C	7	MAN	C1-O5-C5	2.59	115.71	112.19
10	J	8	MAN	O2-C2-C3	-2.59	104.94	110.14
15	Q	4	MAN	O2-C2-C3	-2.58	104.98	110.14
10	J	7	MAN	C1-O5-C5	2.57	115.68	112.19
12	M	3	BMA	O3-C3-C2	2.54	114.86	109.99
18	U	5	MAN	C1-O5-C5	2.53	115.62	112.19
18	V	4	MAN	C1-O5-C5	2.52	115.61	112.19
15	Q	6	MAN	C1-O5-C5	2.52	115.61	112.19
16	R	5	MAN	C1-O5-C5	2.51	115.60	112.19
17	S	7	MAN	C1-O5-C5	2.51	115.59	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	7	MAN	C1-O5-C5	2.51	115.59	112.19
12	M	4	MAN	C1-C2-C3	2.50	112.73	109.67
16	R	7	MAN	C1-O5-C5	2.45	115.51	112.19
18	U	6	MAN	C1-O5-C5	2.42	115.47	112.19
17	S	10	MAN	C1-O5-C5	2.40	115.44	112.19
15	Q	4	MAN	C1-O5-C5	2.39	115.43	112.19
17	S	4	MAN	O2-C2-C3	-2.37	105.39	110.14
10	J	4	MAN	O2-C2-C3	-2.37	105.39	110.14
11	K	7	MAN	O2-C2-C3	-2.36	105.41	110.14
14	O	7	MAN	O3-C3-C2	2.32	114.44	109.99
11	K	4	MAN	O5-C1-C2	2.32	114.35	110.77
10	J	9	MAN	C1-O5-C5	2.31	115.32	112.19
14	O	5	MAN	O2-C2-C3	-2.29	105.55	110.14
13	P	4	MAN	O2-C2-C3	-2.28	105.56	110.14
17	S	6	MAN	O2-C2-C3	-2.28	105.57	110.14
20	X	3	BMA	C1-O5-C5	2.28	115.28	112.19
13	N	4	MAN	C1-O5-C5	2.27	115.27	112.19
18	U	5	MAN	O2-C2-C3	-2.27	105.59	110.14
13	N	4	MAN	O2-C2-C3	-2.27	105.59	110.14
8	C	7	MAN	O2-C2-C3	-2.27	105.59	110.14
18	V	5	MAN	O2-C2-C3	-2.26	105.61	110.14
17	S	10	MAN	O2-C2-C3	-2.25	105.62	110.14
18	V	6	MAN	O2-C2-C3	-2.25	105.63	110.14
16	R	5	MAN	O2-C2-C3	-2.25	105.63	110.14
18	U	4	MAN	C1-O5-C5	2.25	115.24	112.19
17	S	7	MAN	O2-C2-C3	-2.24	105.64	110.14
13	N	5	MAN	O2-C2-C3	-2.24	105.64	110.14
8	I	6	MAN	O2-C2-C3	-2.24	105.64	110.14
12	M	5	MAN	O2-C2-C3	-2.24	105.65	110.14
8	I	5	MAN	O2-C2-C3	-2.23	105.66	110.14
12	M	4	MAN	O2-C2-C3	-2.23	105.67	110.14
10	J	7	MAN	O2-C2-C3	-2.22	105.69	110.14
18	U	6	MAN	O2-C2-C3	-2.22	105.69	110.14
15	Q	7	MAN	O2-C2-C3	-2.21	105.70	110.14
16	R	7	MAN	O2-C2-C3	-2.21	105.71	110.14
7	T	3	BMA	O2-C2-C3	-2.20	105.72	110.14
8	C	6	MAN	O2-C2-C3	-2.20	105.72	110.14
8	C	5	MAN	O2-C2-C3	-2.20	105.72	110.14
17	S	9	MAN	O2-C2-C3	-2.20	105.73	110.14
16	R	8	MAN	O2-C2-C3	-2.20	105.74	110.14
10	J	6	MAN	O2-C2-C3	-2.19	105.76	110.14
11	K	6	MAN	O2-C2-C3	-2.18	105.77	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	3	BMA	C1-O5-C5	2.18	115.14	112.19
20	X	2	NAG	C1-O5-C5	2.17	115.13	112.19
15	Q	6	MAN	O2-C2-C3	-2.16	105.81	110.14
8	I	7	MAN	O2-C2-C3	-2.16	105.81	110.14
10	J	9	MAN	O2-C2-C3	-2.16	105.82	110.14
13	P	5	MAN	O2-C2-C3	-2.15	105.83	110.14
19	W	4	MAN	O2-C2-C3	-2.14	105.85	110.14
15	Q	5	MAN	O2-C2-C3	-2.14	105.86	110.14
20	X	4	MAN	O2-C2-C3	-2.13	105.86	110.14
8	C	6	MAN	C1-O5-C5	2.13	115.08	112.19
14	O	7	MAN	C1-C2-C3	-2.12	107.06	109.67
11	K	8	MAN	O2-C2-C3	-2.11	105.91	110.14
15	Q	5	MAN	C1-O5-C5	2.11	115.05	112.19
19	W	6	MAN	O2-C2-C3	-2.11	105.92	110.14
14	O	6	MAN	O2-C2-C3	-2.10	105.92	110.14
8	I	3	BMA	O2-C2-C3	-2.10	105.93	110.14
14	O	4	MAN	O3-C3-C4	2.10	115.19	110.35
14	O	8	MAN	O2-C2-C3	-2.08	105.96	110.14
17	S	8	MAN	O2-C2-C3	-2.08	105.97	110.14
18	U	1	NAG	C1-O5-C5	2.07	115.00	112.19
16	R	4	MAN	O2-C2-C3	-2.04	106.05	110.14
8	I	6	MAN	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	6	MAN	O5-C5-C6-O6
17	S	2	NAG	O5-C5-C6-O6
11	K	6	MAN	O5-C5-C6-O6
8	I	1	NAG	O5-C5-C6-O6
8	I	3	BMA	O5-C5-C6-O6
17	S	2	NAG	C4-C5-C6-O6
7	T	1	NAG	O5-C5-C6-O6
8	I	1	NAG	C4-C5-C6-O6
8	I	3	BMA	C4-C5-C6-O6
11	K	6	MAN	C4-C5-C6-O6
8	C	6	MAN	C4-C5-C6-O6
19	W	5	MAN	C4-C5-C6-O6
15	Q	1	NAG	O5-C5-C6-O6
10	J	4	MAN	O5-C5-C6-O6
14	O	8	MAN	O5-C5-C6-O6

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

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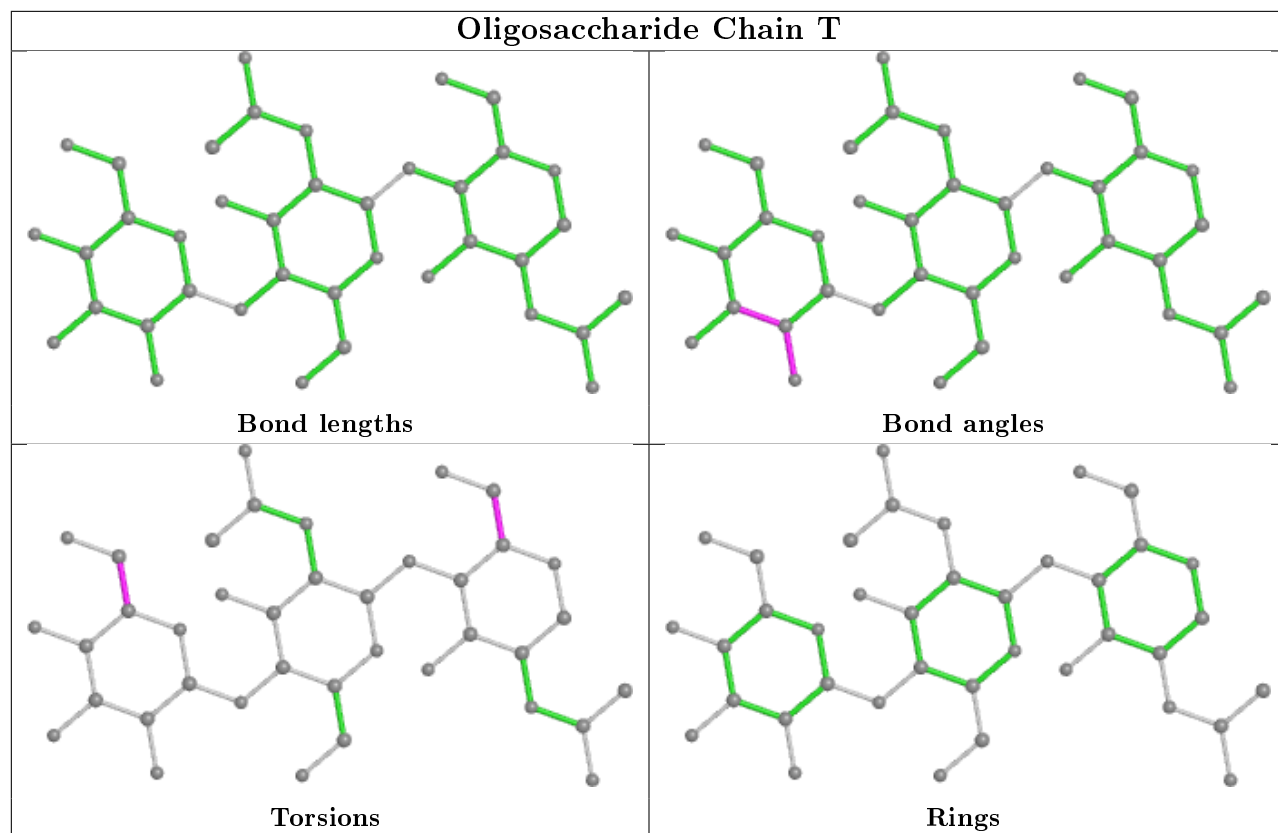
Mol	Chain	Res	Type	Atoms
8	C	1	NAG	O5-C5-C6-O6
17	S	7	MAN	C4-C5-C6-O6
20	X	2	NAG	C3-C2-N2-C7
9	F	1	NAG	C3-C2-N2-C7
20	X	1	NAG	C3-C2-N2-C7
17	S	2	NAG	C3-C2-N2-C7
16	R	1	NAG	O5-C5-C6-O6
13	N	1	NAG	C4-C5-C6-O6
20	X	2	NAG	C4-C5-C6-O6
17	S	1	NAG	C4-C5-C6-O6
9	F	1	NAG	C1-C2-N2-C7
13	P	2	NAG	O5-C5-C6-O6
17	S	1	NAG	O5-C5-C6-O6
17	S	7	MAN	O5-C5-C6-O6
11	K	1	NAG	C1-C2-N2-C7
18	U	1	NAG	C3-C2-N2-C7
19	W	1	NAG	C3-C2-N2-C7
11	K	1	NAG	C3-C2-N2-C7
10	J	3	BMA	C4-C5-C6-O6
19	W	1	NAG	C1-C2-N2-C7

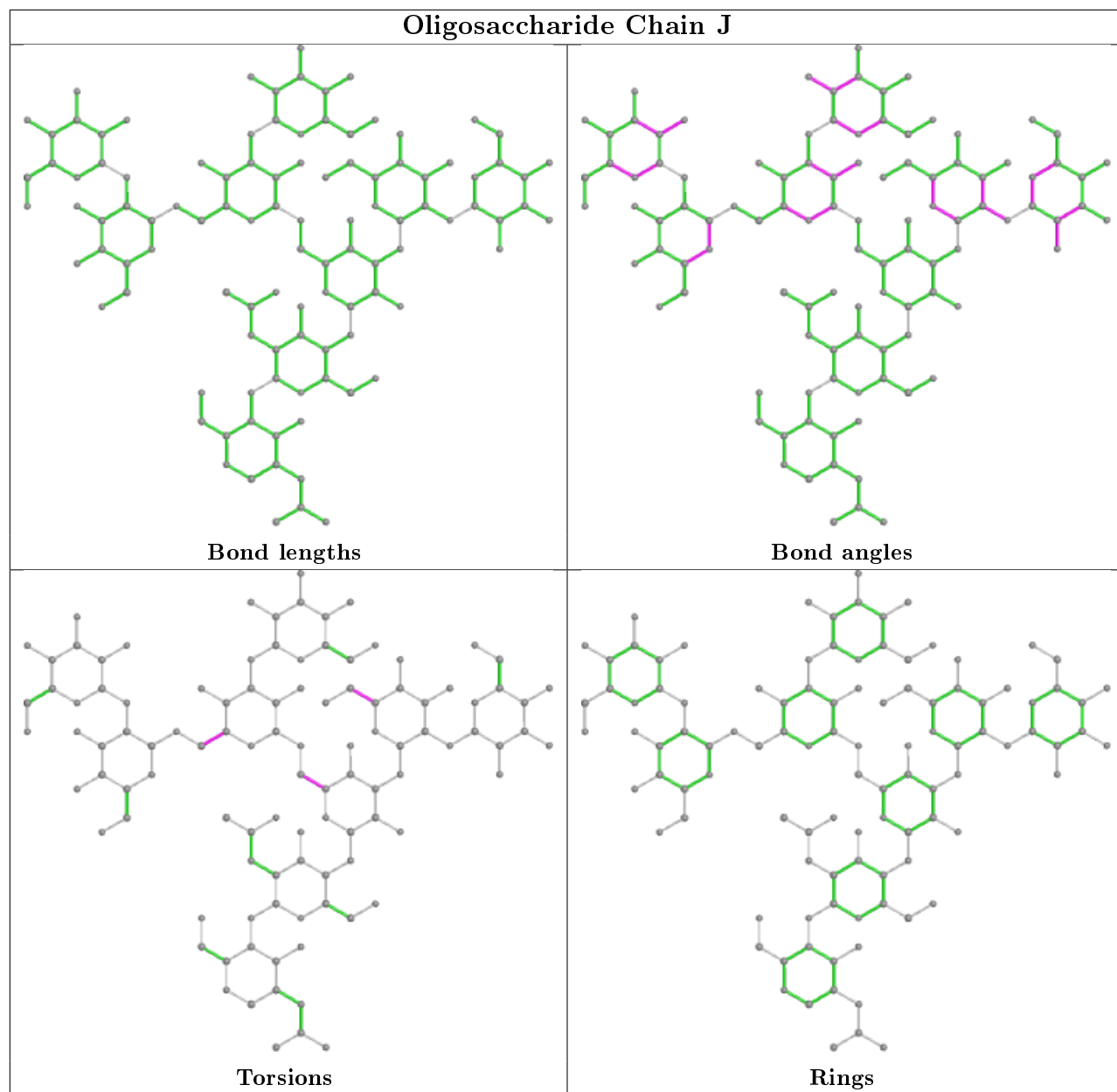
There are no ring outliers.

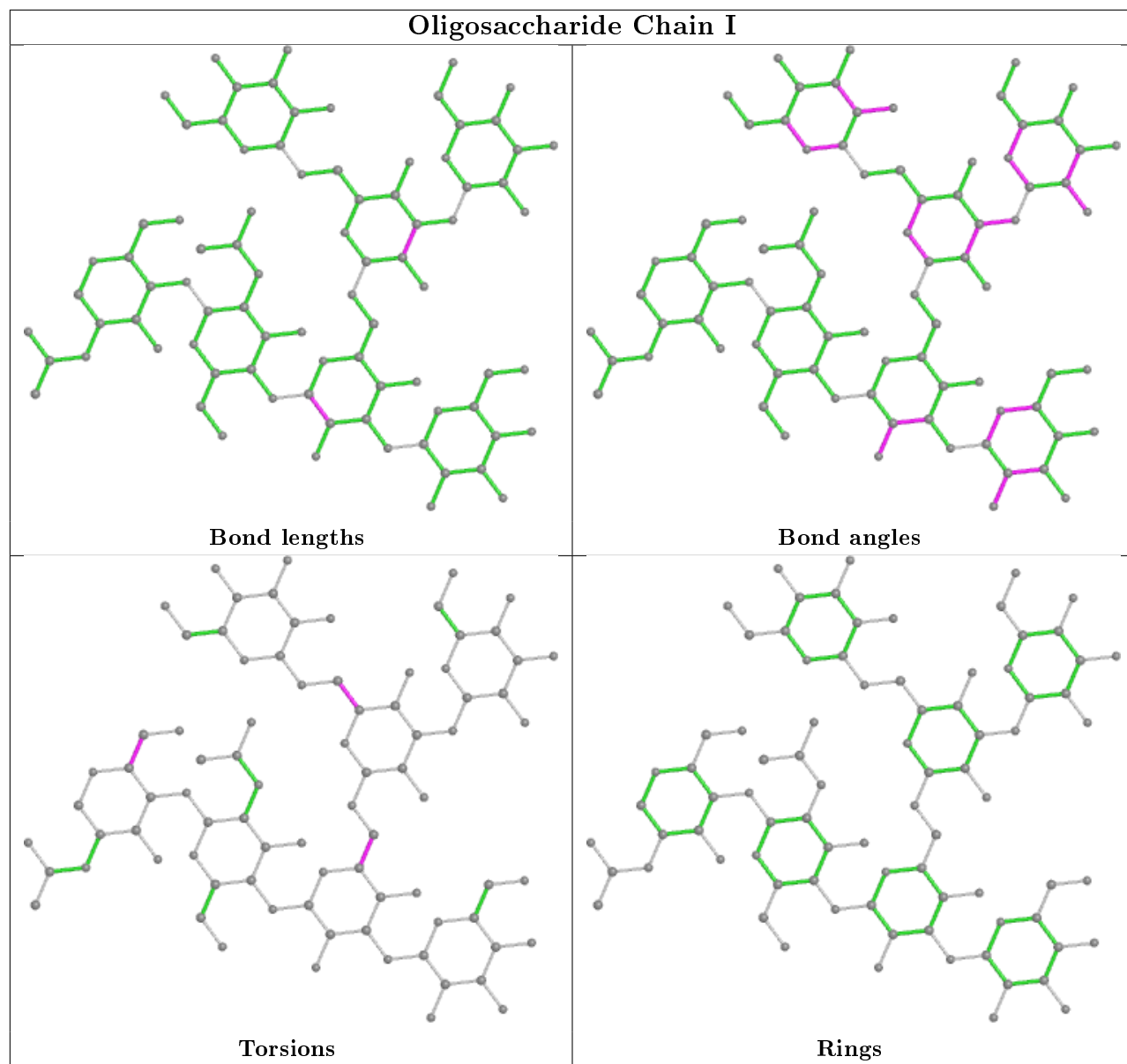
11 monomers are involved in 10 short contacts:

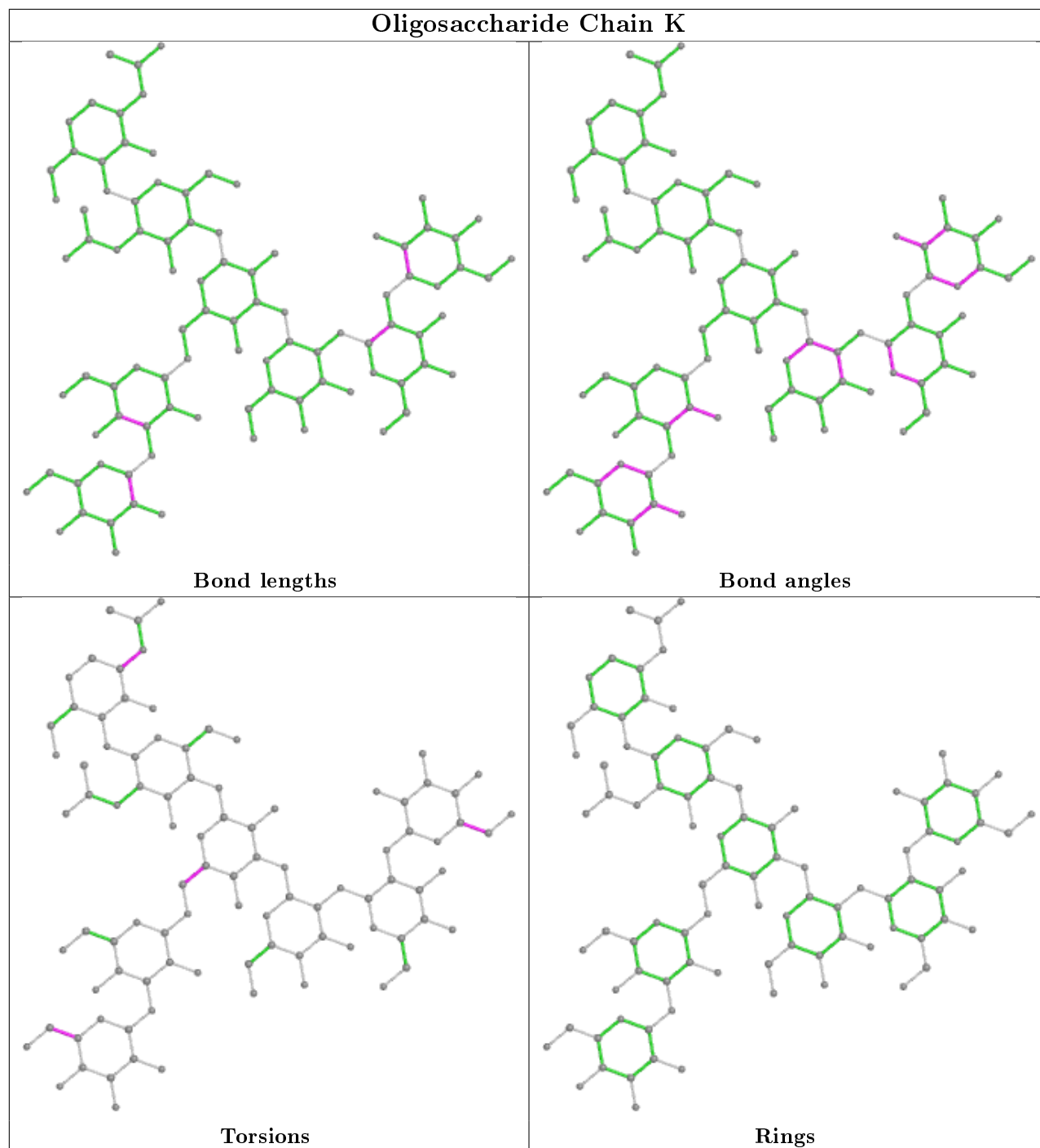
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	V	1	NAG	1	0
18	U	2	NAG	2	0
20	X	2	NAG	3	0
7	T	2	NAG	1	0
8	C	4	MAN	1	0
8	C	3	BMA	1	0
11	K	3	BMA	2	0
11	K	1	NAG	1	0
11	K	4	MAN	2	0
8	C	2	NAG	1	0
20	X	3	BMA	1	0

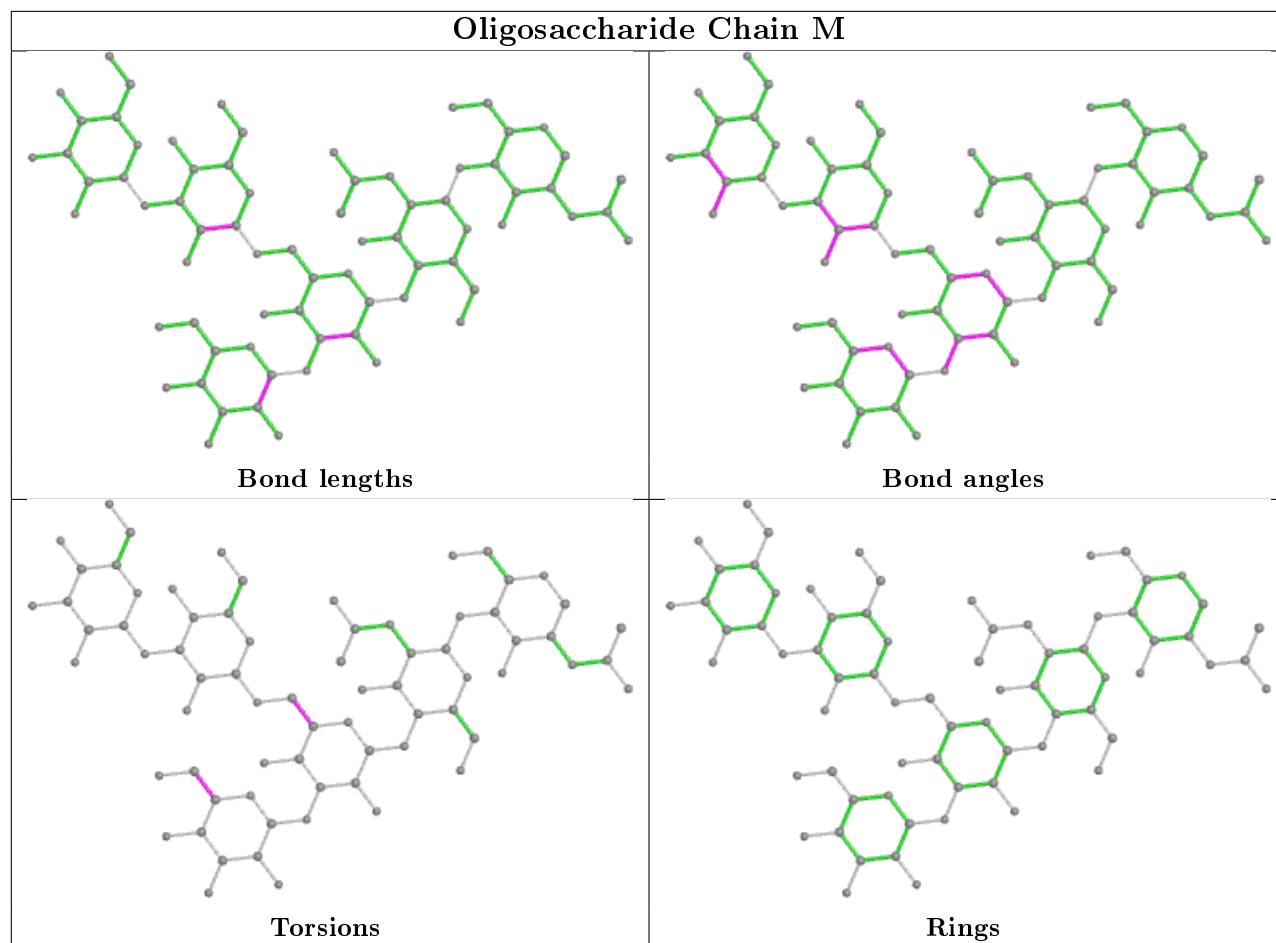
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

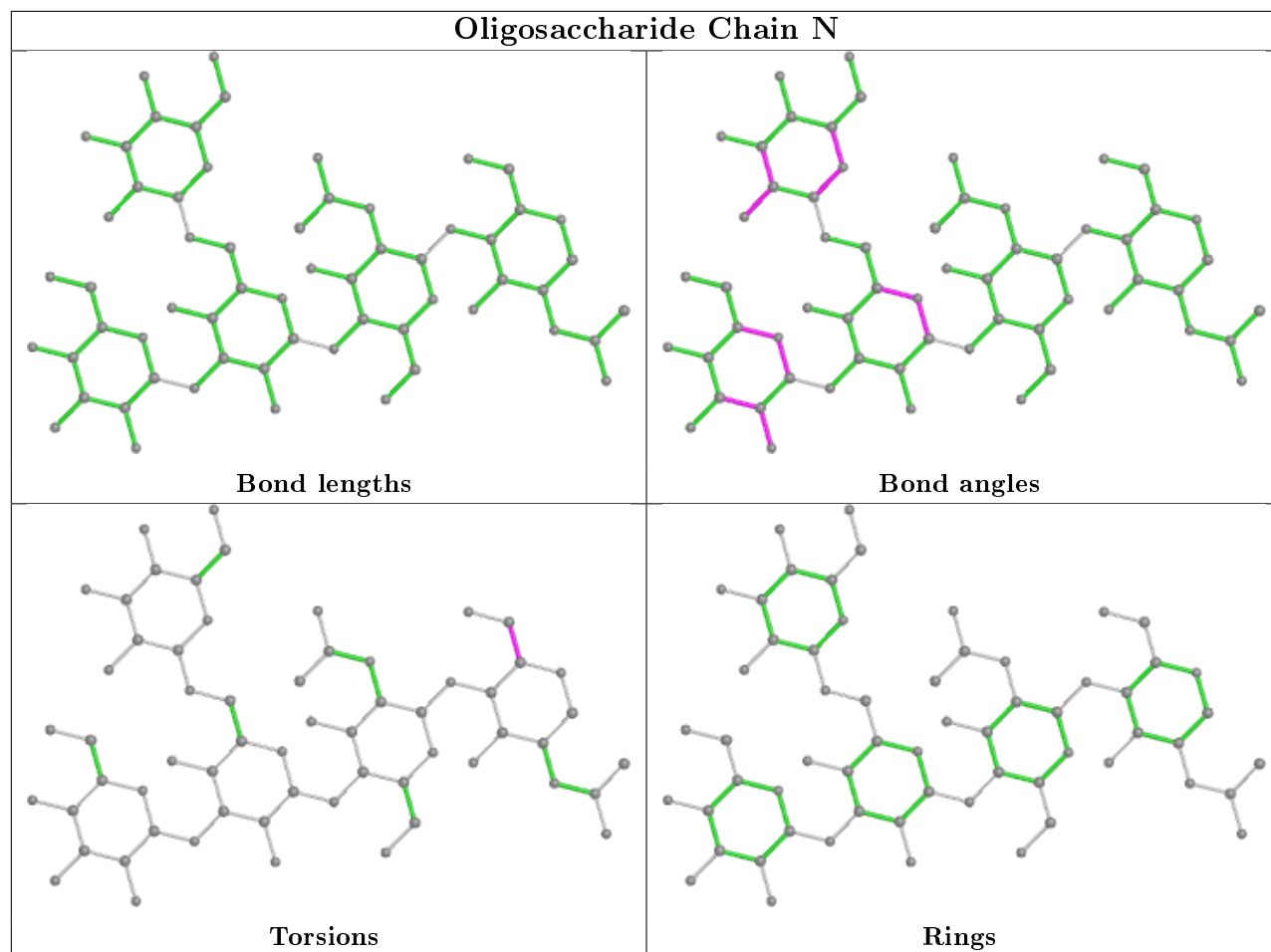


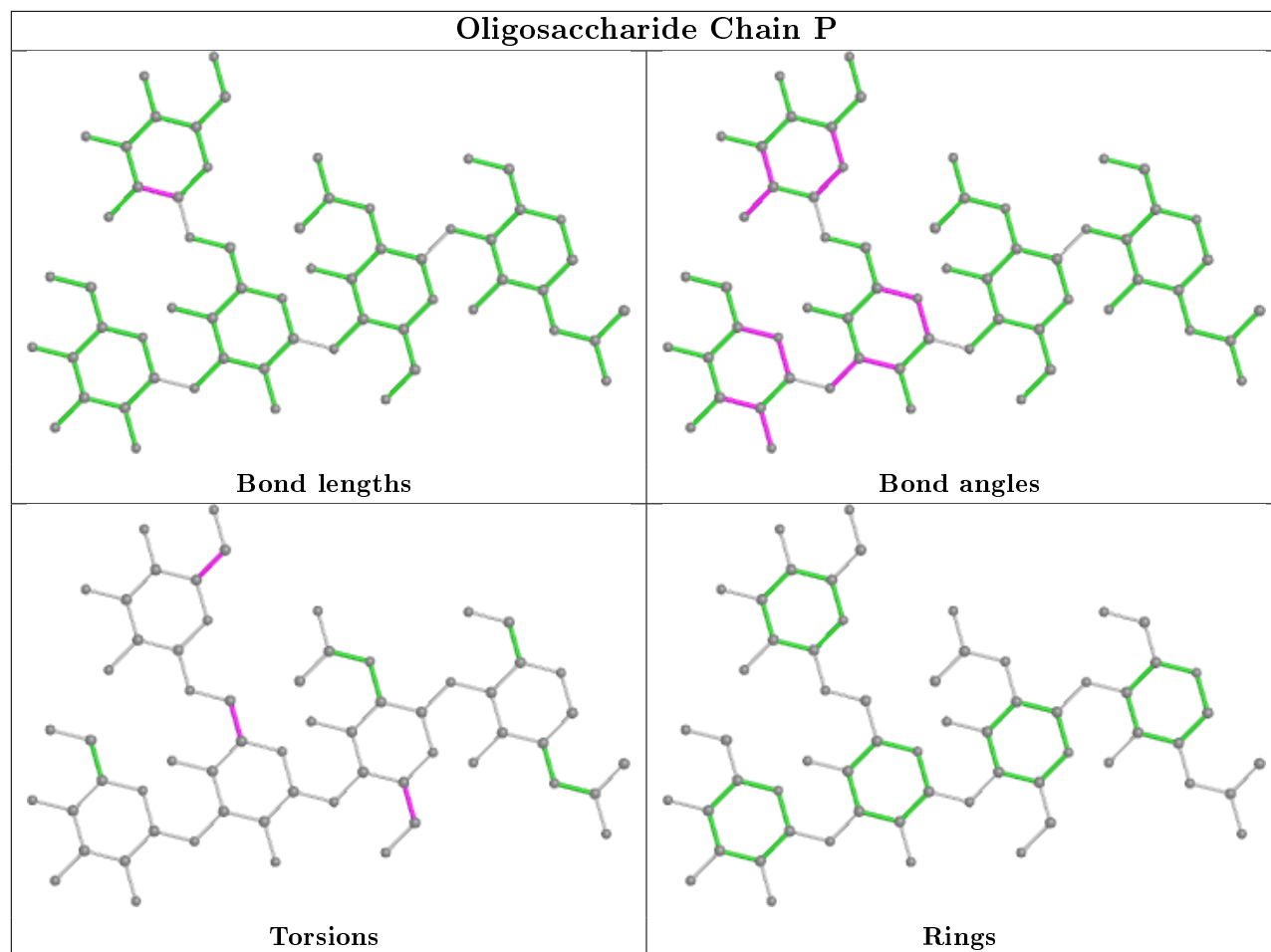


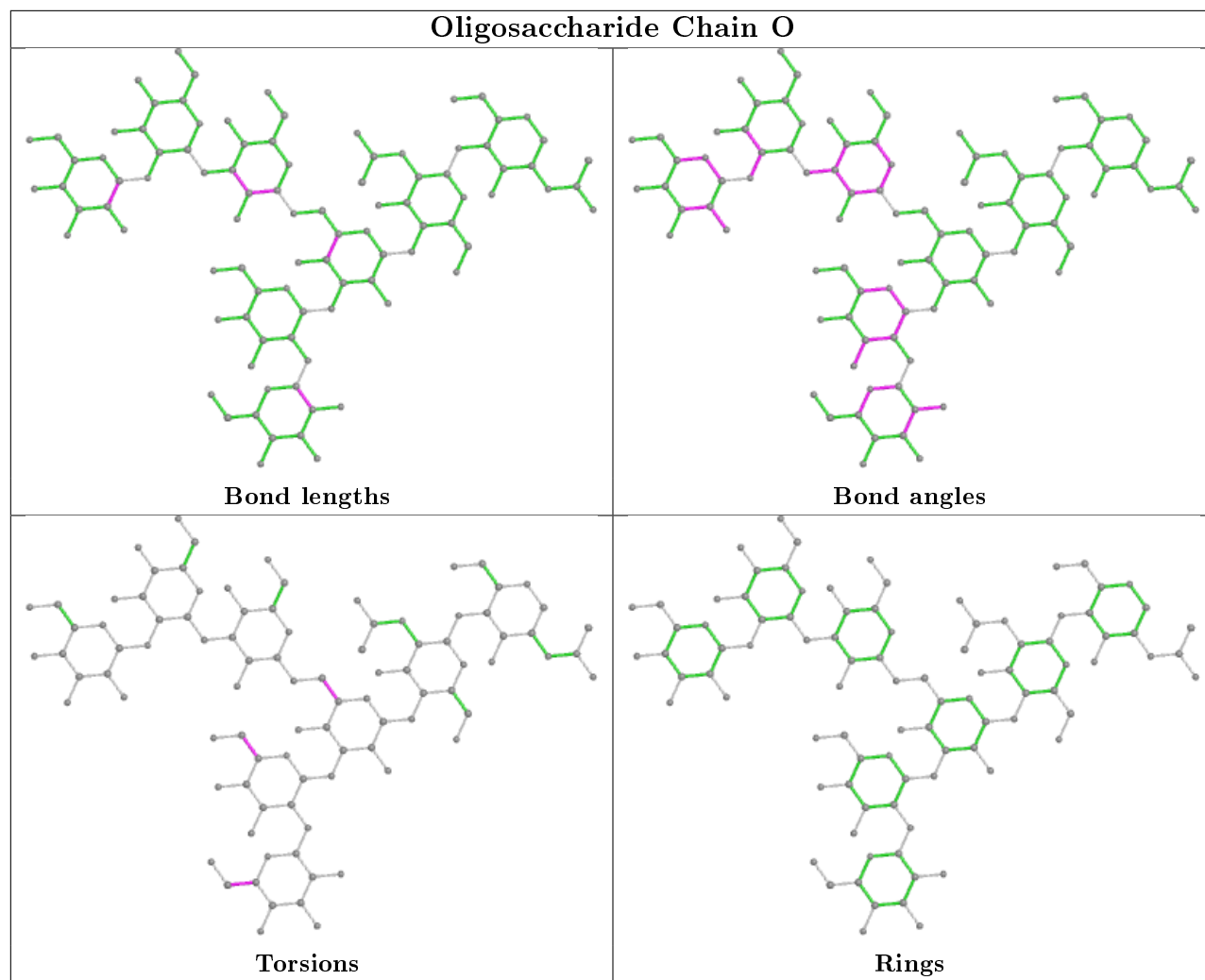


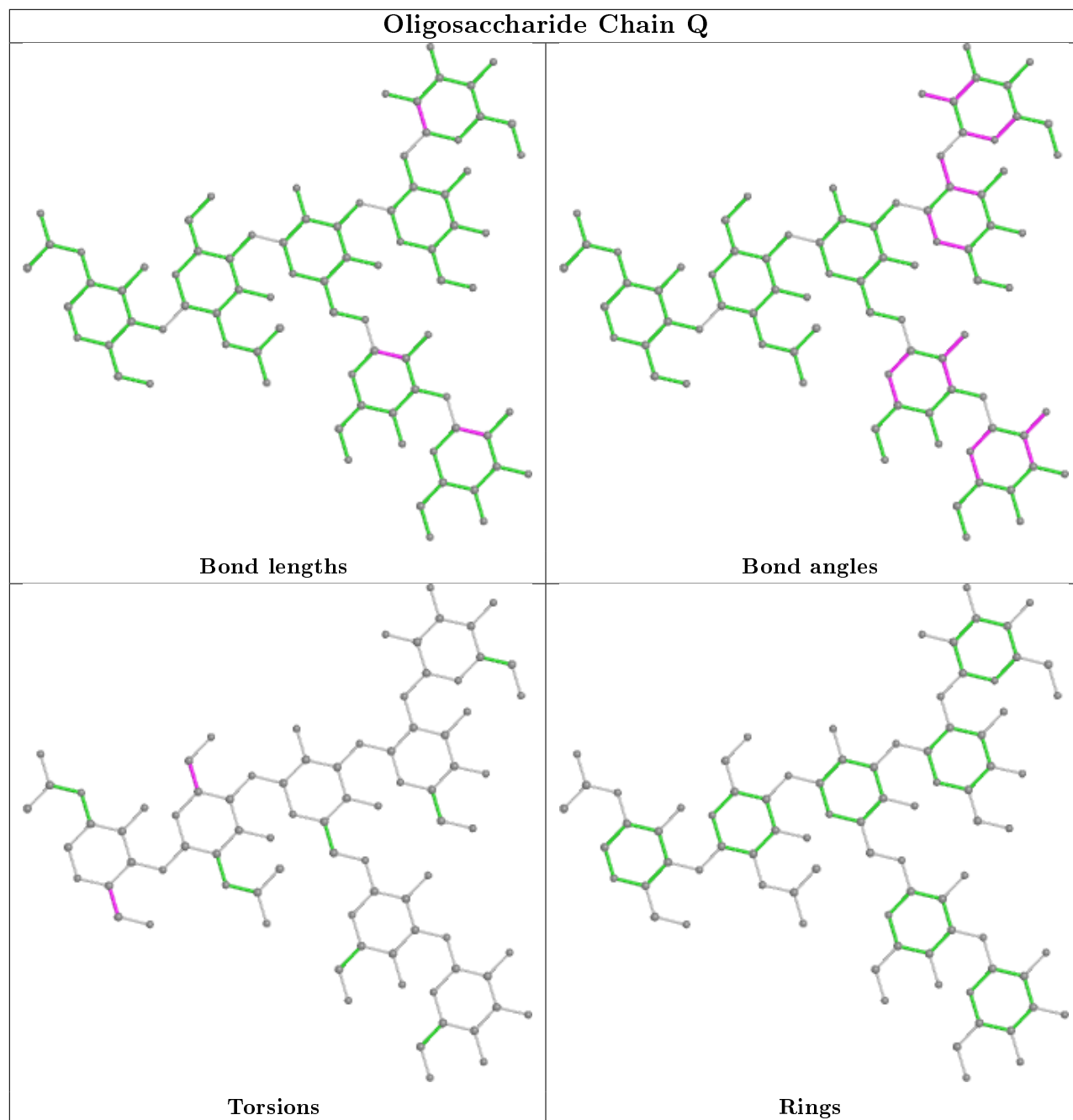


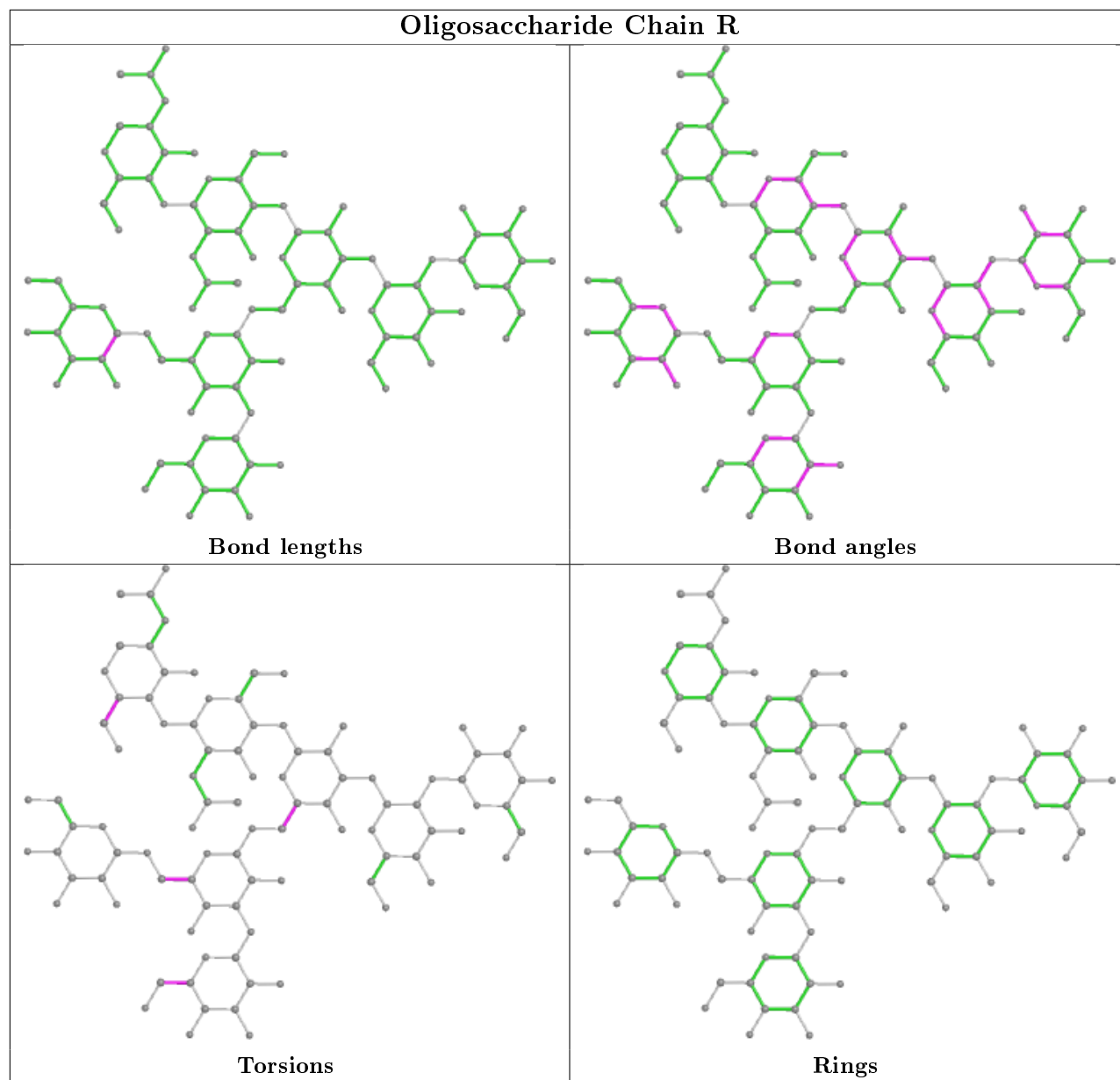


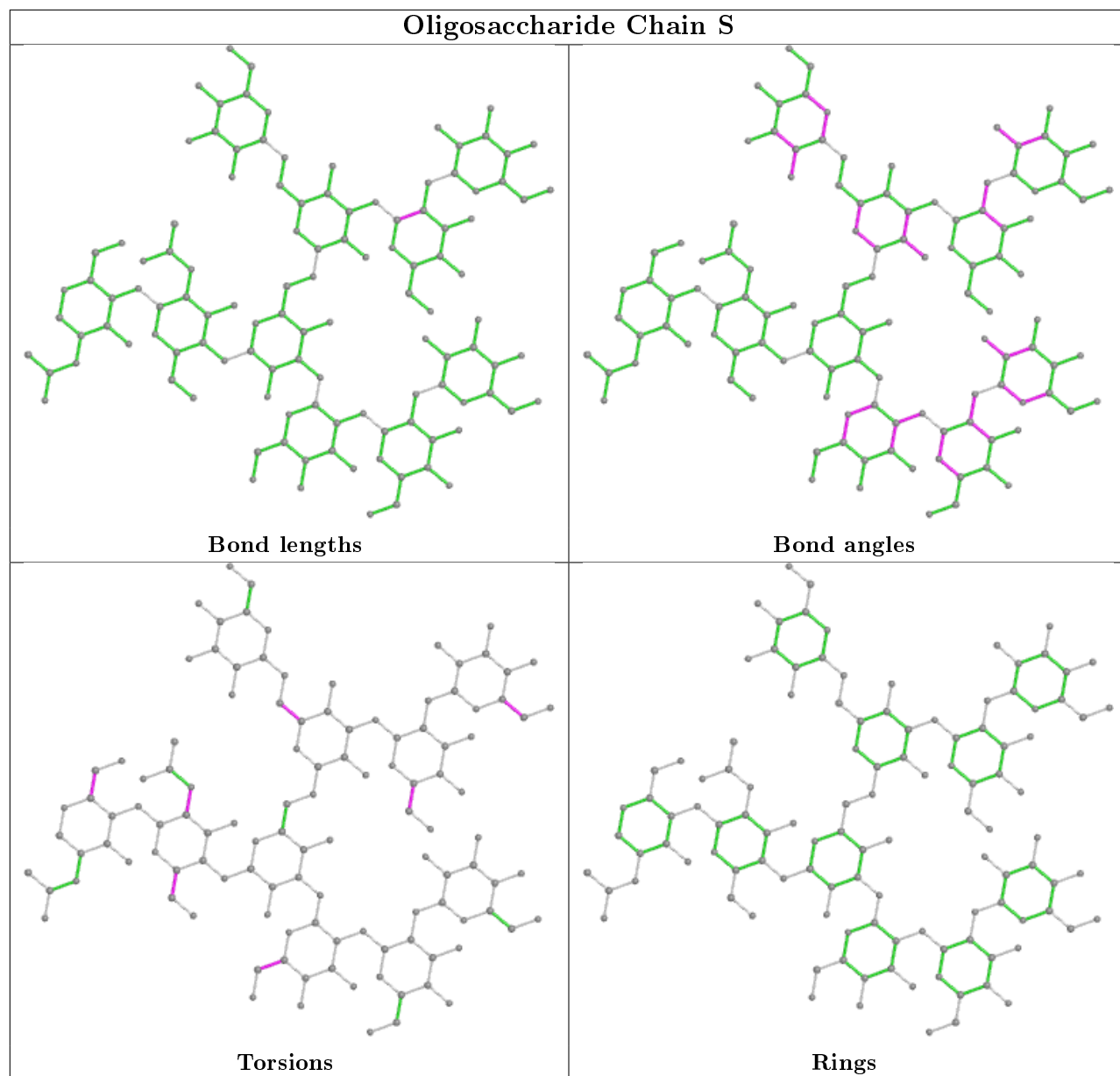


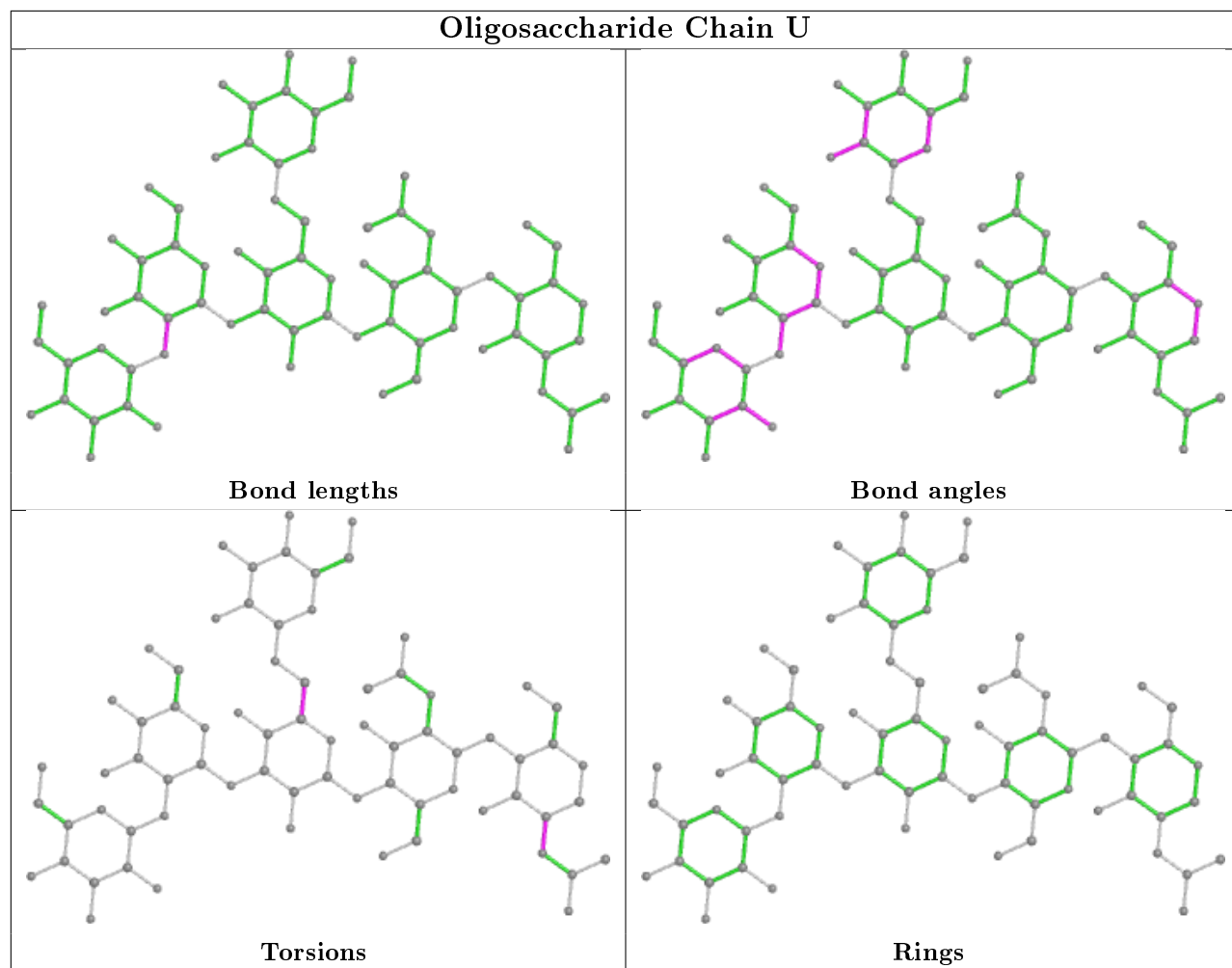


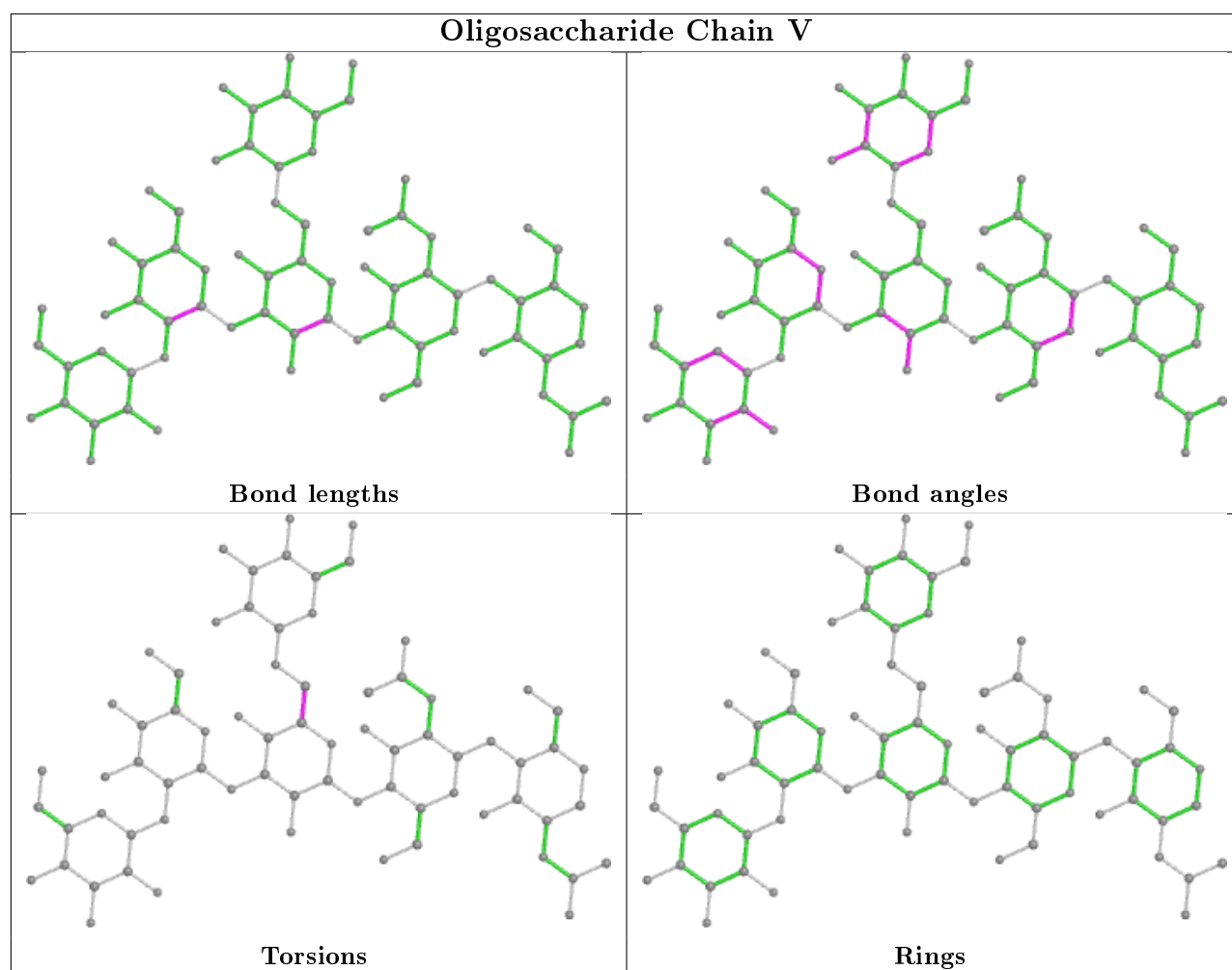


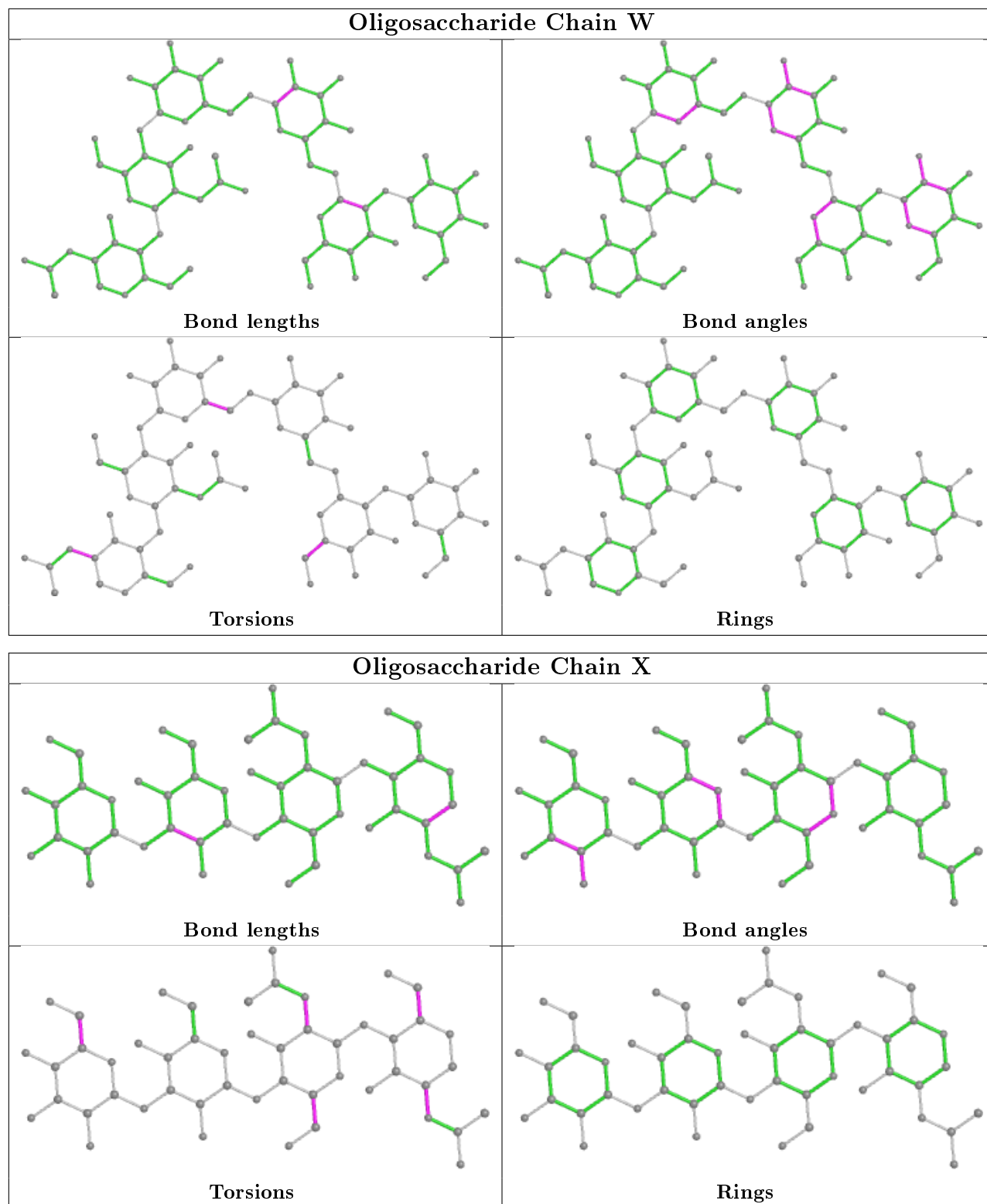












5.6 Ligand geometry [i](#)

4 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
21	NAG	B	1665	1	14,14,15	0.24	0	17,19,21	0.41	0
21	NAG	B	1666	1	14,14,15	0.23	0	17,19,21	0.36	0
21	NAG	G	1583	4	14,14,15	0.23	0	17,19,21	0.40	0
21	NAG	G	1582	4	14,14,15	0.73	1 (7%)	17,19,21	0.99	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
21	NAG	B	1665	1	-	2/6/23/26	0/1/1/1
21	NAG	B	1666	1	-	1/6/23/26	0/1/1/1
21	NAG	G	1583	4	-	1/6/23/26	0/1/1/1
21	NAG	G	1582	4	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	G	1582	NAG	C1-C2	2.29	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	G	1582	NAG	C1-O5-C5	3.40	116.80	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	G	1582	NAG	O5-C5-C6-O6
21	B	1665	NAG	O5-C5-C6-O6
21	G	1582	NAG	C1-C2-N2-C7
21	G	1583	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
21	B	1666	NAG	O5-C5-C6-O6
21	B	1665	NAG	C4-C5-C6-O6
21	G	1582	NAG	C4-C5-C6-O6
21	G	1582	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	1666	NAG	1	0
21	G	1583	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

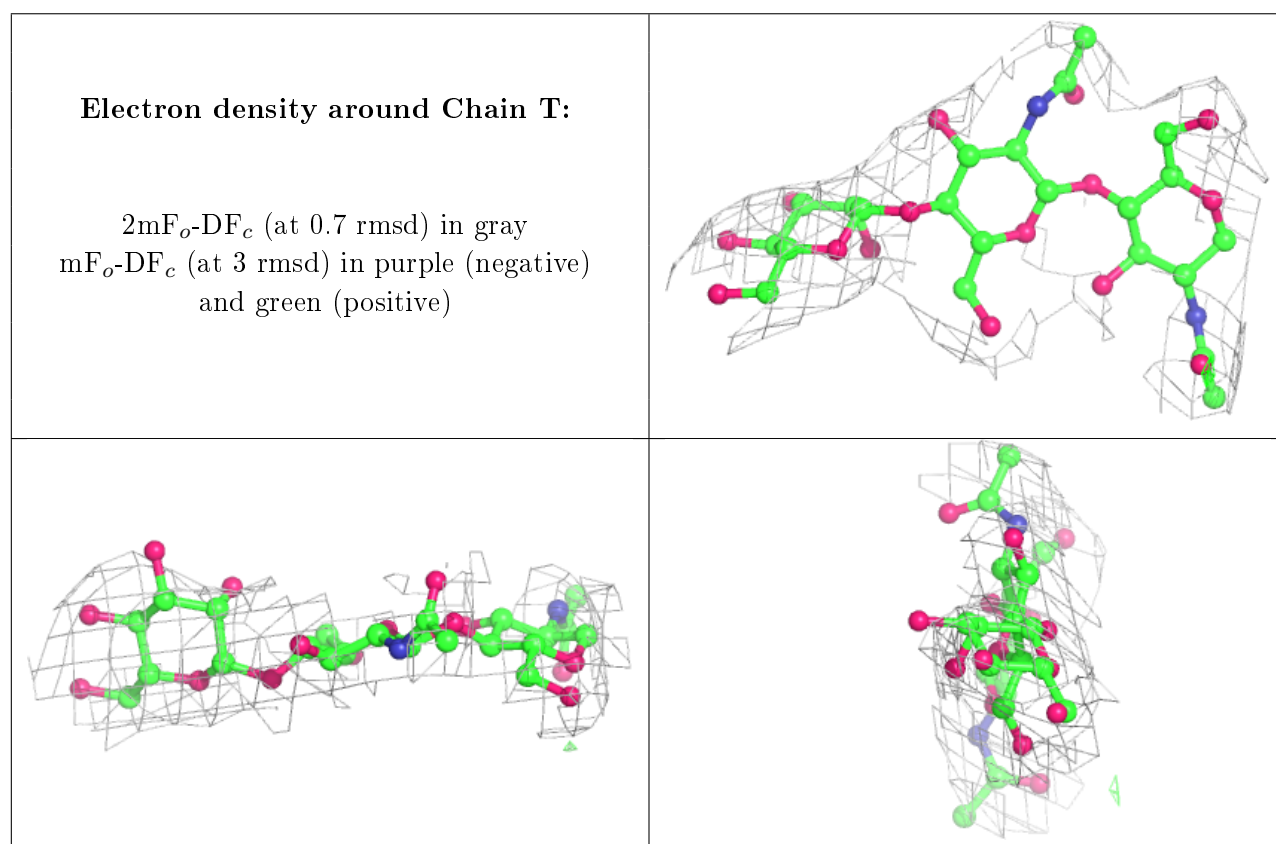
6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

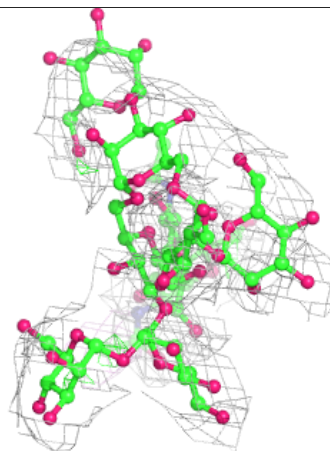
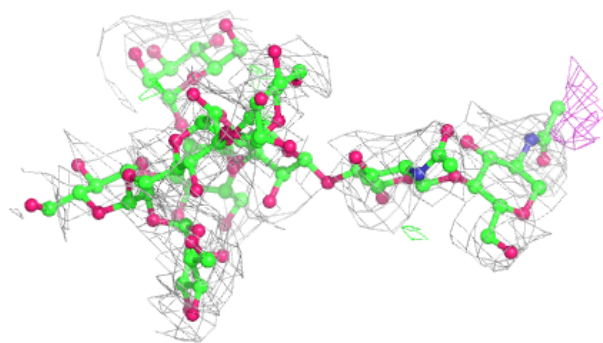
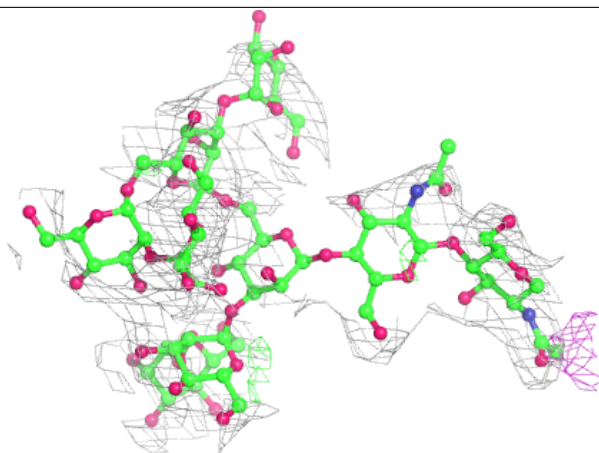
Unable to reproduce the depositors R factor - this section is therefore empty.

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.



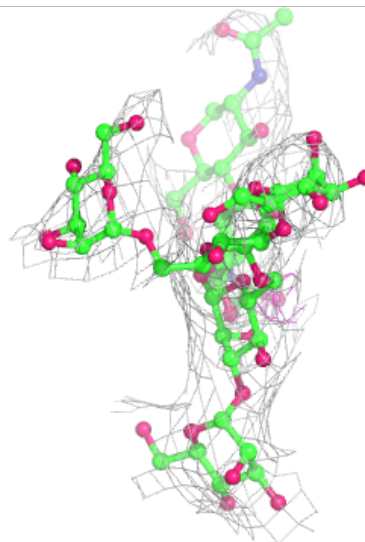
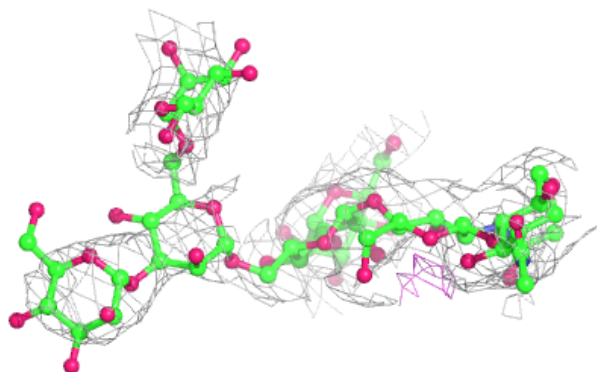
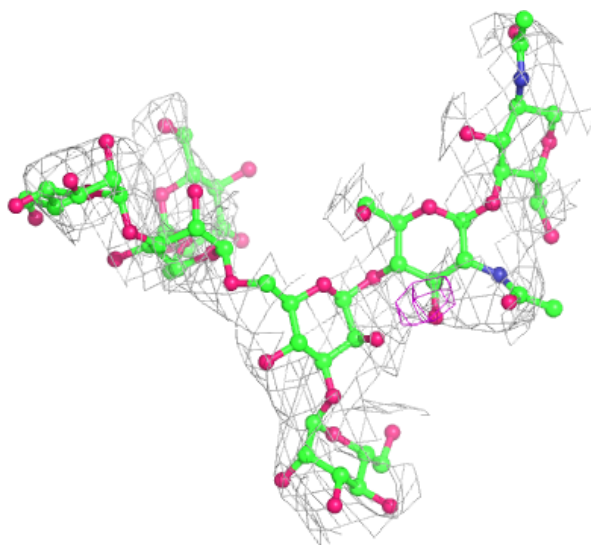
Electron density around Chain J:

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



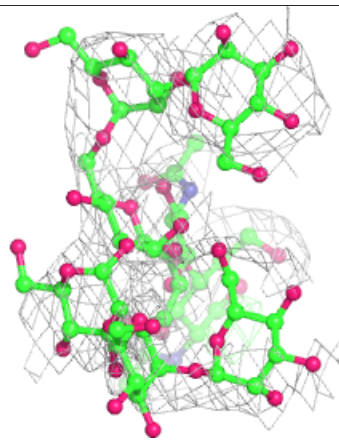
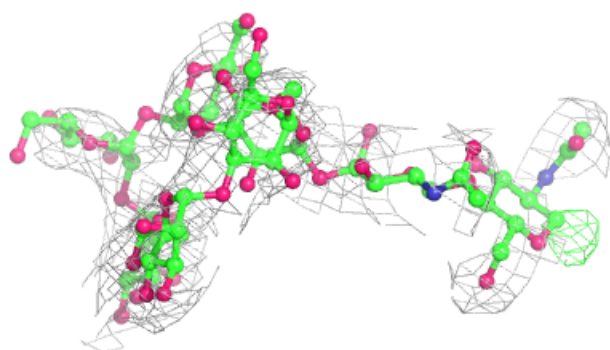
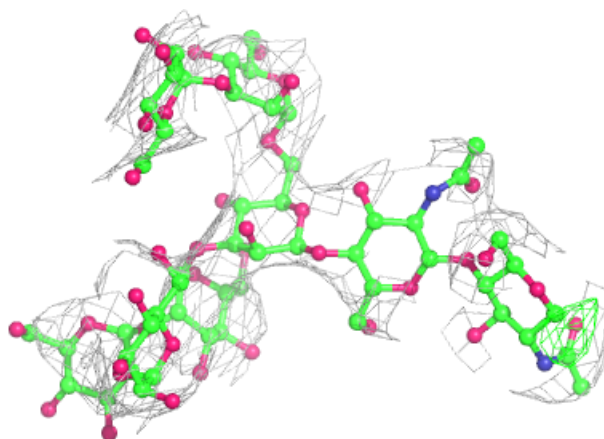
Electron density around Chain I:

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



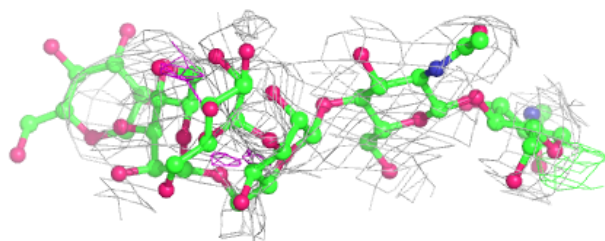
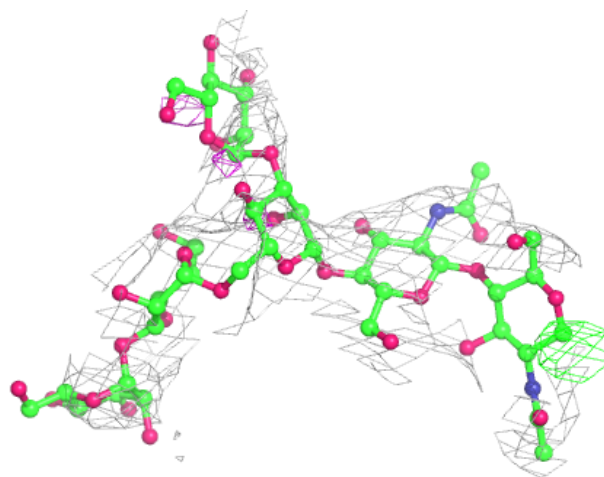
Electron density around Chain K:

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



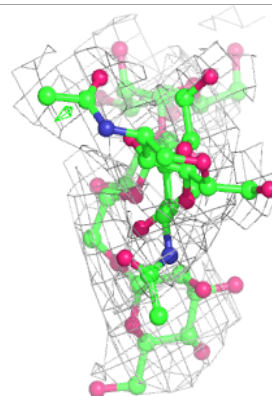
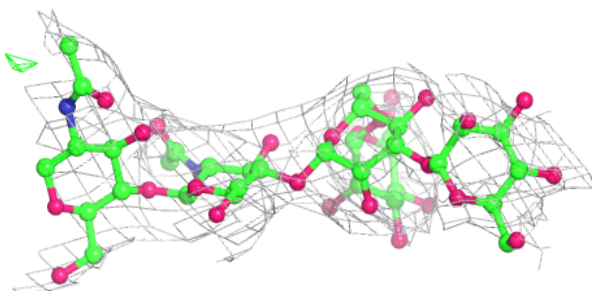
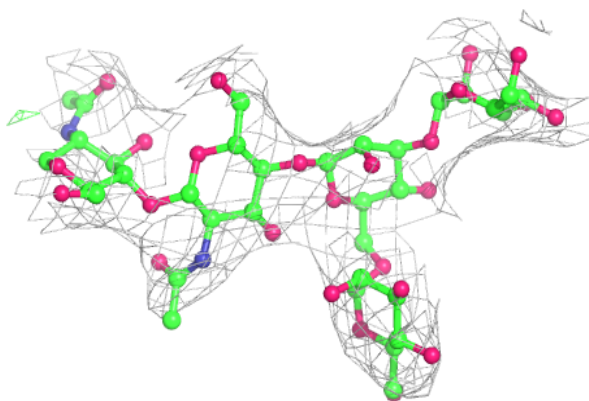
Electron density around Chain M:

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

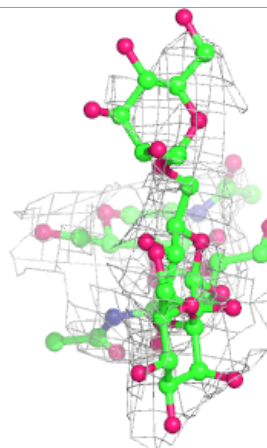
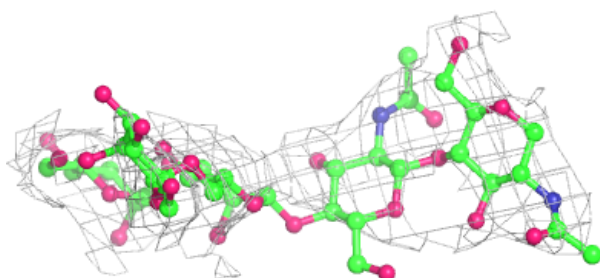
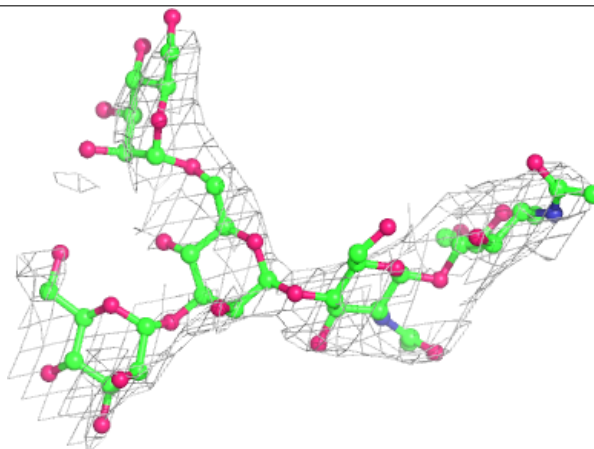


Electron density around Chain N:

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

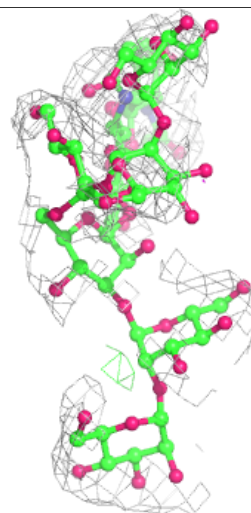
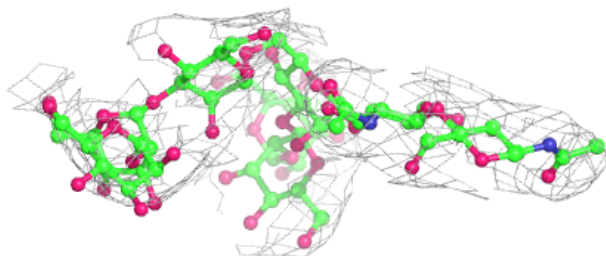
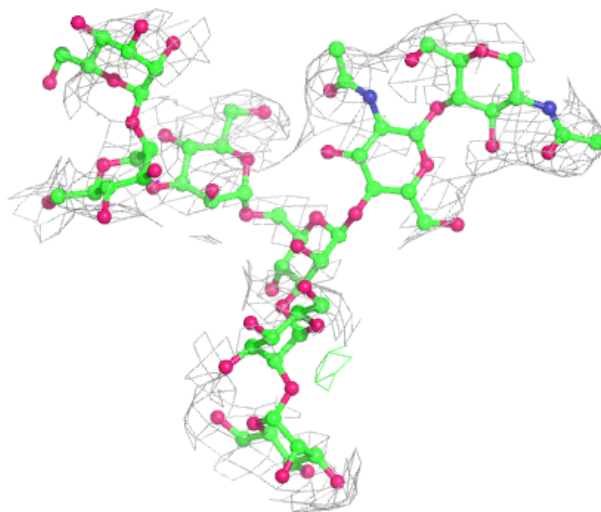
**Electron density around Chain P:**

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



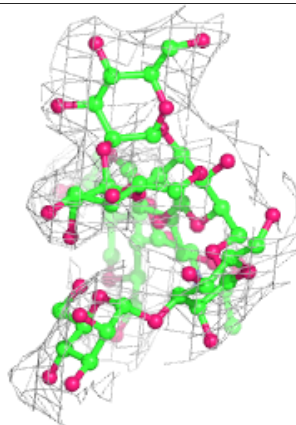
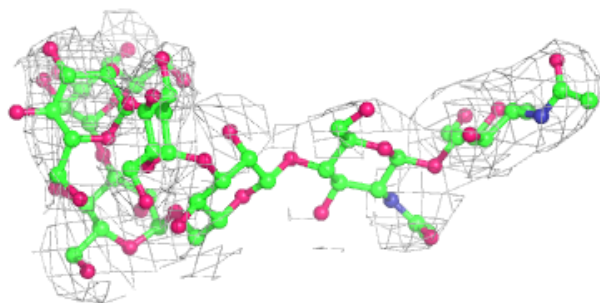
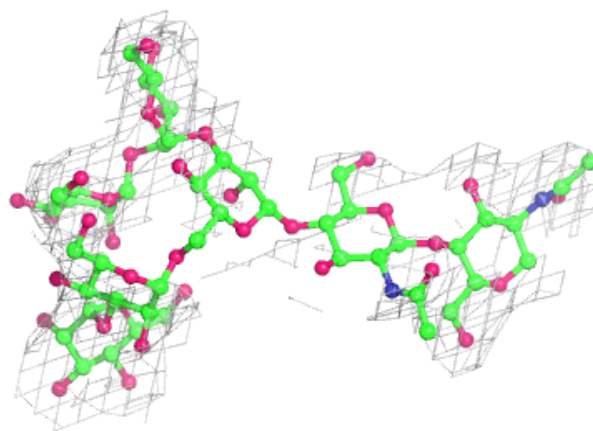
Electron density around Chain O:

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

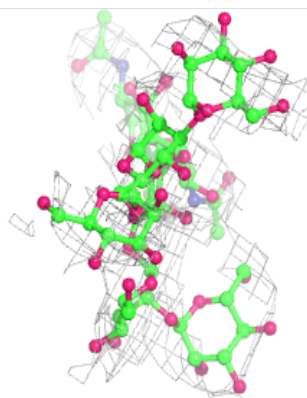
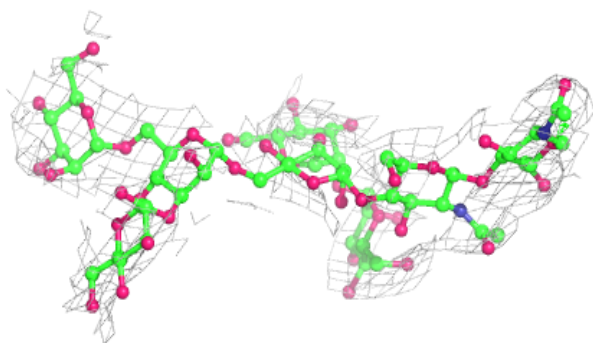
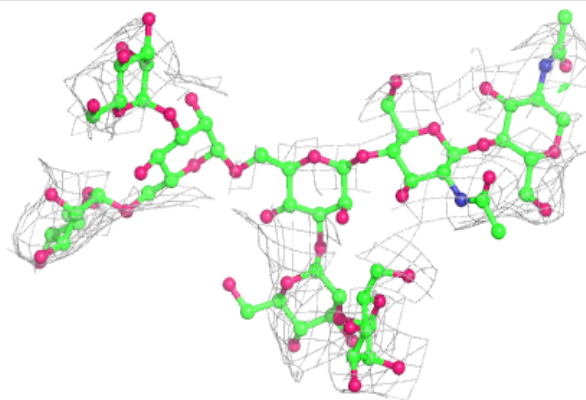


Electron density around Chain Q:

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

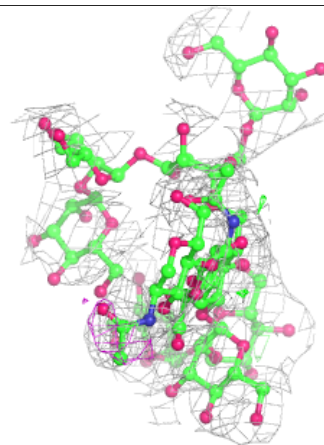
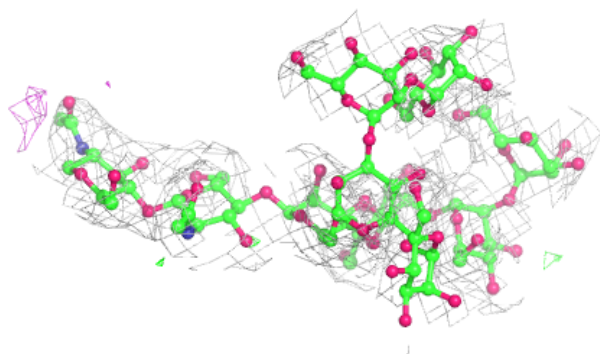
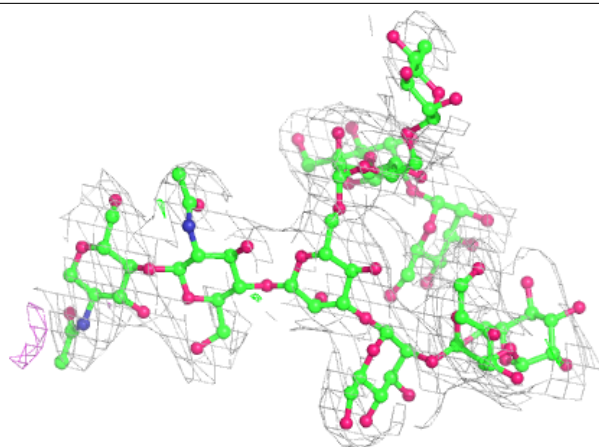
**Electron density around Chain R:**

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



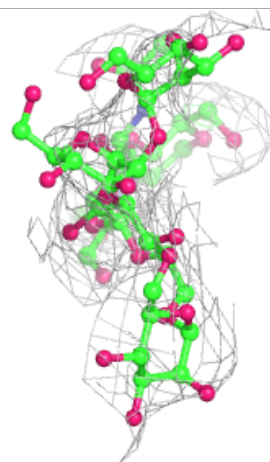
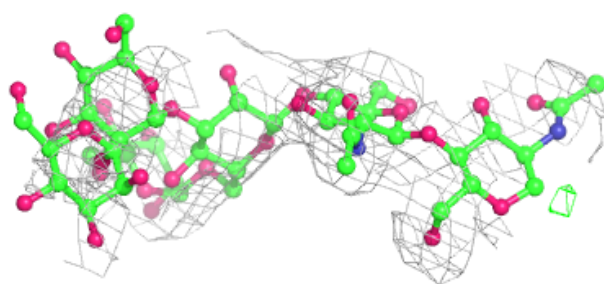
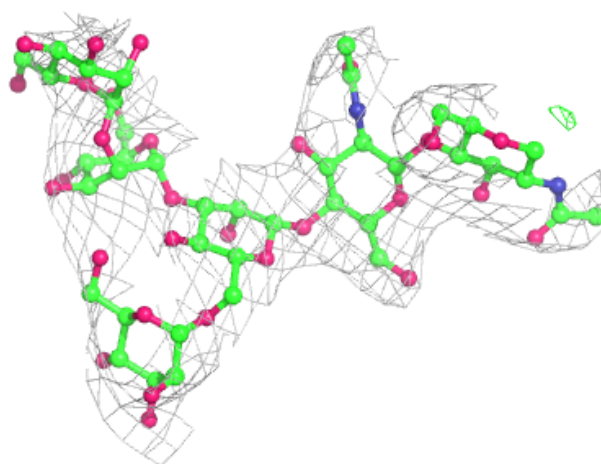
Electron density around Chain S:

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



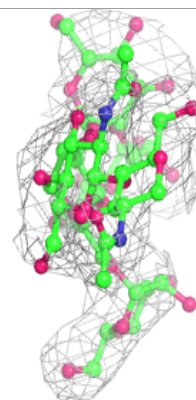
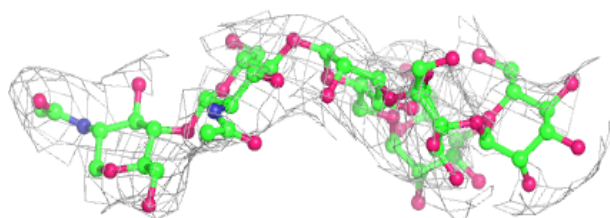
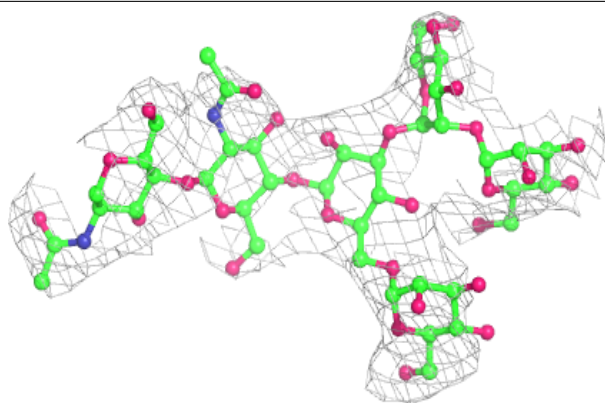
Electron density around Chain U:

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

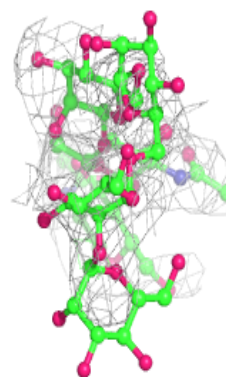
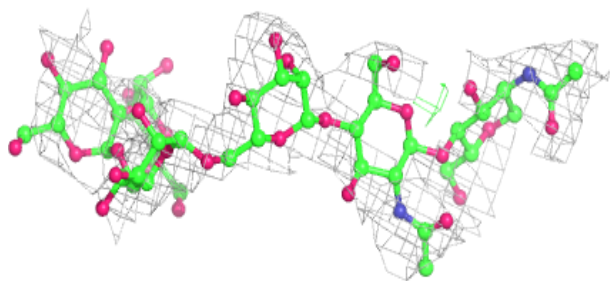
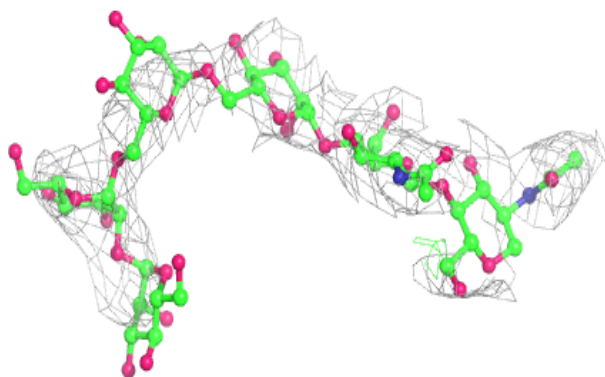


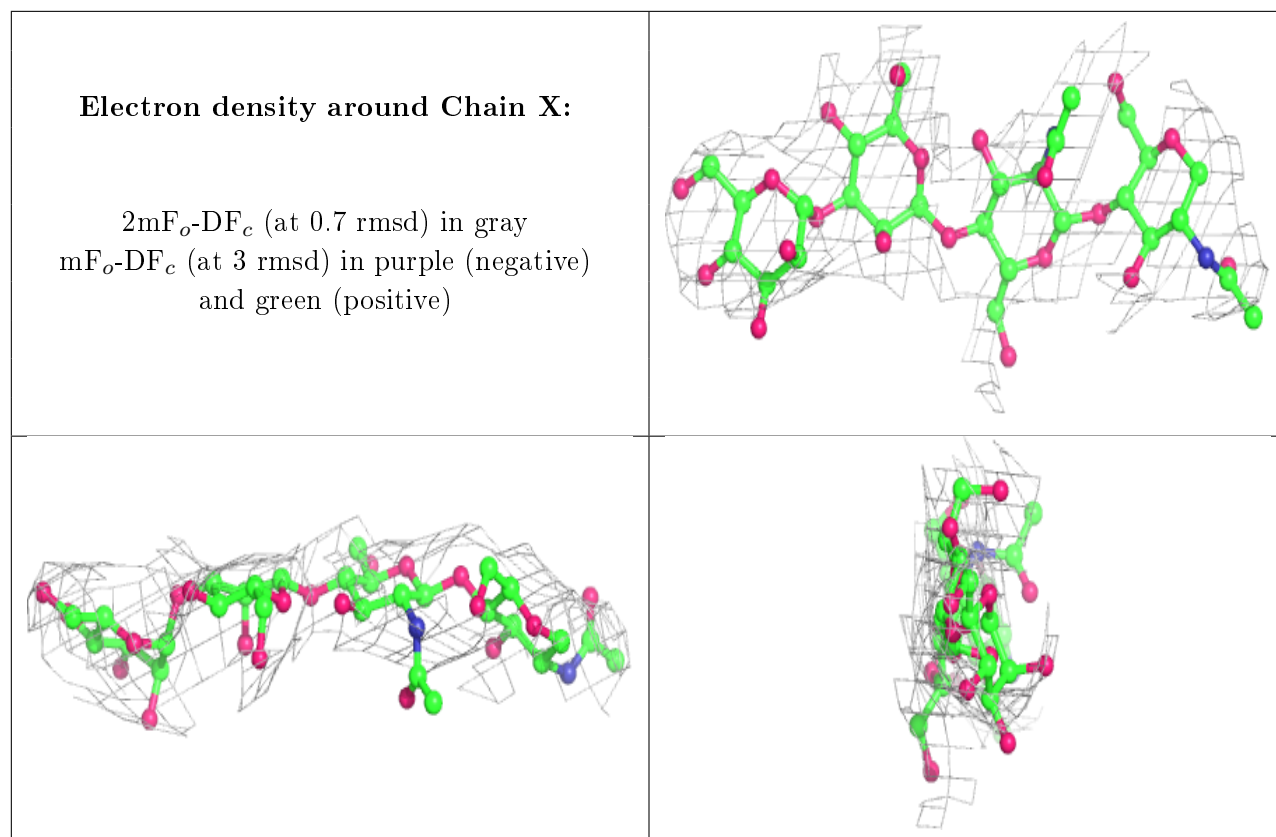
Electron density around Chain V:

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

**Electron density around Chain W:**

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





6.4 Ligands [i](#)

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.