



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2022 – 06:09 PM EDT

PDB ID : 7UCF
Title : Structure of the BG505 SOSIP.664 trimer in complex with neutralizing anti-body Fab fragments 10-1074 and BG24
Authors : Barnes, C.O.; Bjorkman, P.J.
Deposited on : 2022-03-16
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

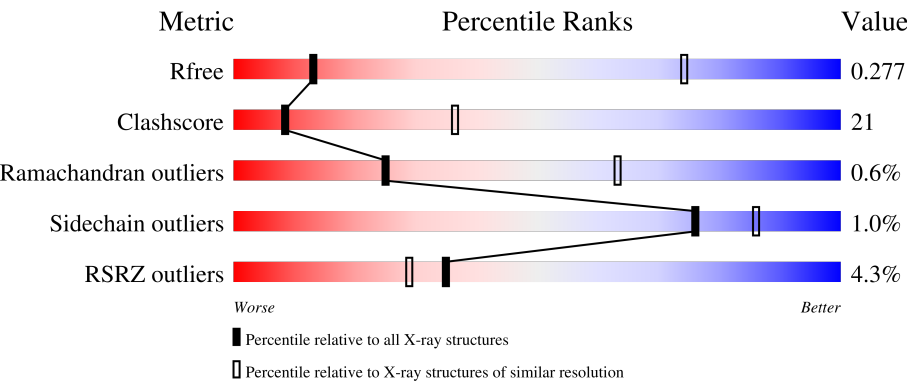
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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

Mol	Chain	Length	Quality of chain
1	B	153	<div><div>4%</div><div>55%</div><div>34%</div><div>10%</div></div>
2	D	234	<div><div>8%</div><div>49%</div><div>44%</div><div>6%</div></div>
3	E	205	<div><div>7%</div><div>61%</div><div>37%</div><div>2%</div></div>
4	G	501	<div><div>2%</div><div>52%</div><div>34%</div><div>10%</div></div>
5	H	243	<div><div>5%</div><div>63%</div><div>30%</div><div>6%</div></div>

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Mol	Chain	Length	Quality of chain
6	L	214	 67% 31%
7	A	2	 100%
8	F	2	 50% 50%
8	V	2	 50% 50%
8	W	2	 100%
9	I	5	 80% 20%
10	J	7	 71% 29%
11	K	4	 75% 25%
12	M	6	 17% 50% 33%
13	N	2	 100%
13	O	2	 100%
14	P	3	 67% 33%
14	U	3	 33% 67%
15	Q	4	 50% 50%
16	R	3	 100%
17	S	6	 83% 17%
18	T	7	 86% 14%
19	X	6	 83% 17%
20	Y	4	 50% 50%

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
11	MAN	K	4	-	-	-	X
14	NAG	P	2	-	-	-	X
22	FUC	G	602	-	-	X	X

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 12078 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	137	Total	C	N	O	S	0	0	0
			1089	687	190	206	6			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called BG24 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	220	Total	C	N	O	S	0	0	0
			1667	1050	289	319	9			

- Molecule 3 is a protein called BG24 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	202	Total	C	N	O	S	0	0	0
			1514	946	255	308	5			

- Molecule 4 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	451	Total	C	N	O	S	0	0	0
			3538	2222	625	664	27			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	6	MET	-	initiating methionine	UNP Q2N0S6
G	7	ASP	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	8	ALA	-	expression tag	UNP Q2N0S6
G	9	MET	-	expression tag	UNP Q2N0S6
G	10	LYS	-	expression tag	UNP Q2N0S6
G	11	ARG	-	expression tag	UNP Q2N0S6
G	12	GLY	-	expression tag	UNP Q2N0S6
G	13	LEU	-	expression tag	UNP Q2N0S6
G	14	CYS	-	expression tag	UNP Q2N0S6
G	15	CYS	-	expression tag	UNP Q2N0S6
G	16	VAL	-	expression tag	UNP Q2N0S6
G	17	LEU	-	expression tag	UNP Q2N0S6
G	18	LEU	-	expression tag	UNP Q2N0S6
G	19	LEU	-	expression tag	UNP Q2N0S6
G	20	CYS	-	expression tag	UNP Q2N0S6
G	21	GLY	-	expression tag	UNP Q2N0S6
G	22	ALA	-	expression tag	UNP Q2N0S6
G	23	VAL	-	expression tag	UNP Q2N0S6
G	24	PHE	-	expression tag	UNP Q2N0S6
G	25	VAL	-	expression tag	UNP Q2N0S6
G	26	SER	-	expression tag	UNP Q2N0S6
G	27	PRO	-	expression tag	UNP Q2N0S6
G	28	ALA	-	expression tag	UNP Q2N0S6
G	29	GLY	-	expression tag	UNP Q2N0S6
G	31	GLY	ALA	conflict	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 5 is a protein called 10-1074 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	229	Total	C	N	O	S	0	0	0
			1744	1103	291	343	7			

- Molecule 6 is a protein called 10-1074 Fab light chain.

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

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



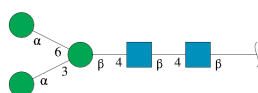
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	A	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



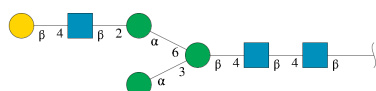
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	W	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 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
9	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 10 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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.



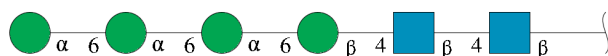
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	7	Total	C	N	O	0	0	0
			86	48	3	35			

- Molecule 11 is an oligosaccharide called 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	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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.



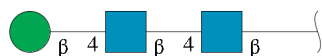
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	M	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
13	N	2	Total	C	O	0	0	0
			22	12	10			
13	O	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 14 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.



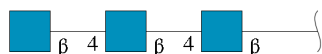
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	P	3	Total	C	N	O	0	0	0
			39	22	2	15			
14	U	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 15 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.



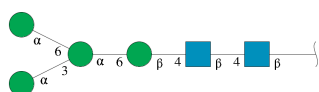
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 16 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



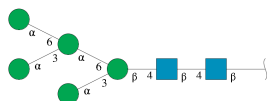
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	R	3	Total	C	N	O	0	0	0
			42	24	3	15			

- Molecule 17 is an oligosaccharide called 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.



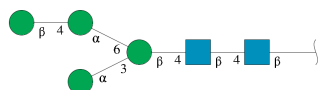
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	S	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 18 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.



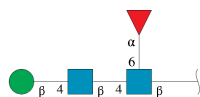
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	T	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 19 is an oligosaccharide called beta-D-mannopyranose-(1-4)-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	X	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



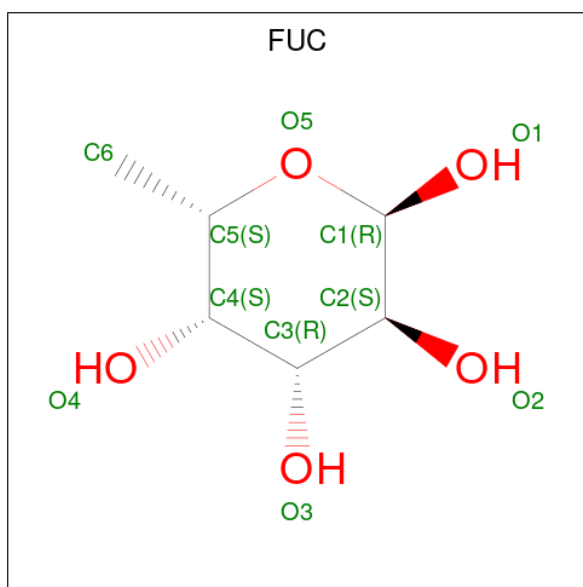
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	Y	4	Total	C	N	O	0	0	0
			49	28	2	19			

- 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	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		

- Molecule 22 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$).

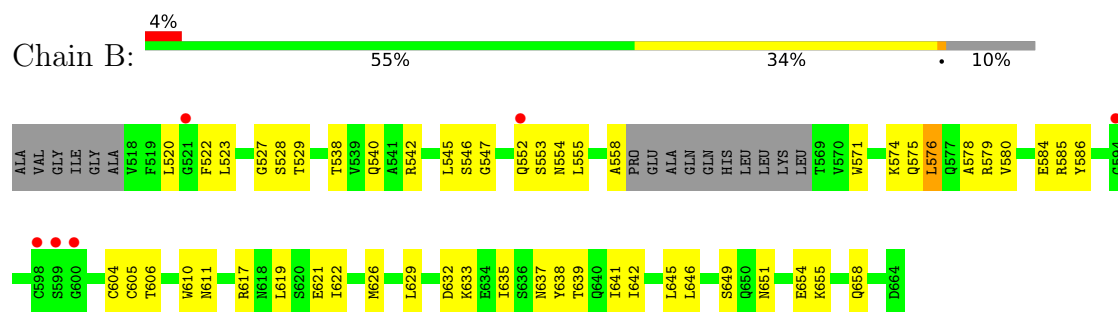


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	G	1	Total	C	O	0	0
			10	6	4		

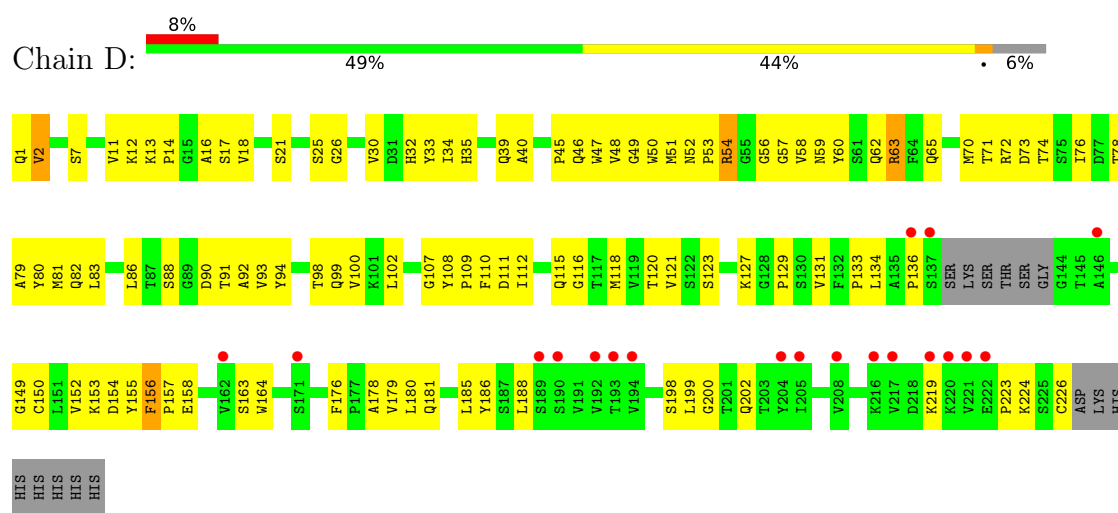
3 Residue-property plots

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

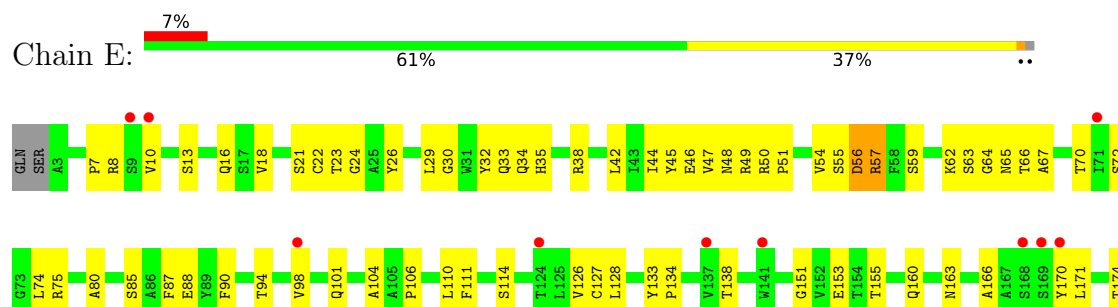
• Molecule 1: Envelope glycoprotein gp41



• Molecule 2: BG24 Fab heavy chain

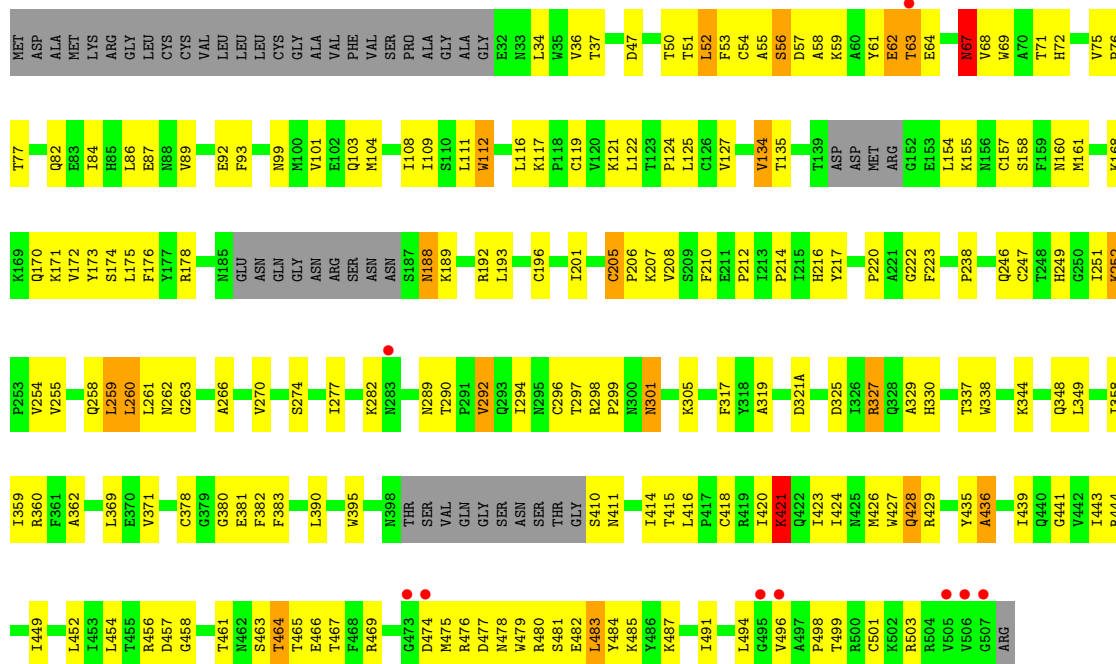


• Molecule 3: BG24 light chain

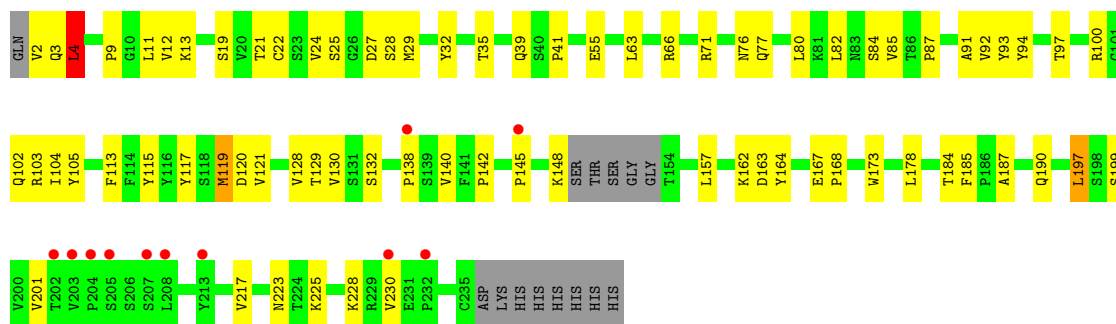




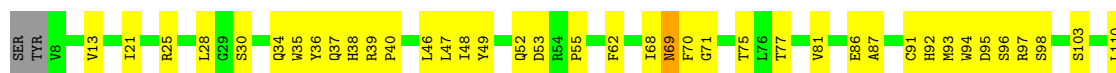
• Molecule 4: Envelope glycoprotein gp120



• Molecule 5: 10-1074 Fab heavy chain



• Molecule 6: 10-1074 Fab light chain





- Molecule 7: alpha-L-fucopyranose-(1-6)-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 F:  50%



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

Chain V:  50%




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

Chain W:  100%



- Molecule 9: 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 I:  80%




- Molecule 10: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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 J:  71%




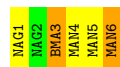
- Molecule 11: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  75% 25%



- Molecule 12: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  17% 50% 33%



- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain N:  100%



- Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose

Chain O:  100%



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

Chain P:  67% 33%



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

Chain U:  33% 67%



- Molecule 15: 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 Q:  50% 50%



- Molecule 16: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 100%



- Molecule 17: 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: 83% 17%



- Molecule 18: 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 T: 86% 14%



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

Chain X: 83% 17%



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

Chain Y: 50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	208.96Å 208.96Å 155.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.49 – 4.00 39.49 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.49-4.00) 99.7 (39.49-3.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.76Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.245 , 0.277 0.247 , 0.277	Depositor DCC
R_{free} test set	1250 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	191.6	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 197.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.059 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12078	wwPDB-VP
Average B, all atoms (Å ²)	264.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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: GAL, NAG, FUC, BMA, 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	0.61	0/1107	1.02	4/1501 (0.3%)
2	D	0.60	0/1709	0.79	0/2330
3	E	0.52	0/1551	0.68	0/2114
4	G	0.95	6/3611 (0.2%)	1.27	27/4903 (0.6%)
5	H	0.77	2/1787 (0.1%)	1.03	4/2438 (0.2%)
6	L	0.64	0/1649	0.96	1/2250 (0.0%)
All	All	0.75	8/11414 (0.1%)	1.03	36/15536 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
4	G	0	3
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	168	PRO	N-CD	-8.34	1.36	1.47
4	G	62	GLU	CG-CD	8.19	1.64	1.51
4	G	62	GLU	CA-CB	-7.53	1.37	1.53
4	G	205	CYS	CB-SG	-6.71	1.70	1.82
4	G	418	CYS	CB-SG	-6.31	1.71	1.82
4	G	67	ASN	CB-CG	6.06	1.65	1.51
4	G	112	TRP	CB-CG	-5.15	1.41	1.50
5	H	128	VAL	CB-CG2	5.02	1.63	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	62	GLU	OE1-CD-OE2	19.34	146.51	123.30
4	G	62	GLU	CG-CD-OE2	-15.47	87.36	118.30
6	L	38	HIS	C-N-CA	-8.45	100.57	121.70
1	B	576	LEU	CA-CB-CG	-8.14	96.58	115.30
4	G	255	VAL	CG1-CB-CG2	7.51	122.91	110.90
4	G	252	LYS	CD-CE-NZ	7.35	128.61	111.70
5	H	197	LEU	CA-CB-CG	7.30	132.09	115.30
4	G	154	LEU	CB-CG-CD2	-7.01	99.09	111.00
4	G	154	LEU	CB-CG-CD1	6.99	122.89	111.00
1	B	520	LEU	CA-CB-CG	6.90	131.17	115.30
4	G	62	GLU	CA-CB-CG	-6.89	98.24	113.40
4	G	371	VAL	CG1-CB-CG2	-6.83	99.96	110.90
1	B	555	LEU	CA-CB-CG	6.83	131.01	115.30
4	G	116	LEU	CA-CB-CG	-6.67	99.97	115.30
4	G	259	LEU	CA-CB-CG	6.62	130.52	115.30
1	B	574	LYS	CD-CE-NZ	6.54	126.74	111.70
5	H	80	LEU	CB-CG-CD2	-6.32	100.26	111.00
5	H	39	GLN	C-N-CA	-6.26	106.06	121.70
4	G	205	CYS	CA-CB-SG	-6.24	102.76	114.00
4	G	421	LYS	CD-CE-NZ	6.15	125.85	111.70
4	G	255	VAL	CA-CB-CG1	-5.98	101.92	110.90
4	G	428	GLN	CA-CB-CG	-5.87	100.48	113.40
4	G	483	LEU	CA-CB-CG	-5.83	101.90	115.30
4	G	321(A)	ASP	CB-CG-OD1	5.71	123.44	118.30
4	G	369	LEU	CB-CG-CD2	5.71	120.70	111.00
5	H	4	LEU	CA-CB-CG	5.64	128.26	115.30
4	G	452	LEU	CB-CG-CD2	-5.52	101.62	111.00
4	G	369	LEU	CB-CA-C	5.46	120.58	110.20
4	G	327	ARG	CG-CD-NE	-5.38	100.50	111.80
4	G	52	LEU	CB-CG-CD1	5.36	120.10	111.00
4	G	193	LEU	CB-CG-CD1	-5.29	102.00	111.00
4	G	260	LEU	CB-CG-CD2	5.25	119.92	111.00
4	G	435	TYR	CB-CG-CD2	-5.22	117.87	121.00
4	G	34	LEU	CA-CB-CG	5.20	127.25	115.30
4	G	292	VAL	CG1-CB-CG2	5.11	119.08	110.90
4	G	193	LEU	CA-CB-CG	-5.07	103.63	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	156	PHE	Peptide
4	G	301	ASN	Mainchain

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Mol	Chain	Res	Type	Group
4	G	421	LYS	Mainchain
4	G	436	ALA	Mainchain

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	1089	0	1071	49	0
2	D	1667	0	1628	106	0
3	E	1514	0	1458	76	0
4	G	3538	0	3474	182	0
5	H	1744	0	1710	52	1
6	L	1607	0	1550	49	0
7	A	24	0	22	0	0
8	F	28	0	25	0	0
8	V	28	0	25	0	0
8	W	28	0	25	0	0
9	I	61	0	52	1	0
10	J	86	0	73	3	0
11	K	50	0	43	4	0
12	M	72	0	61	2	0
13	N	22	0	19	1	1
13	O	22	0	19	3	0
14	P	39	0	34	1	0
14	U	39	0	33	1	0
15	Q	50	0	43	1	0
16	R	42	0	37	0	0
17	S	72	0	61	1	0
18	T	83	0	70	3	0
19	X	72	0	61	2	0
20	Y	49	0	43	4	0
21	B	14	0	13	1	0
21	G	28	0	26	0	0
22	G	10	0	10	6	0
All	All	12078	0	11686	493	1

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 21.

All (493) 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)
4:G:62:GLU:CG	4:G:63:THR:H	1.32	1.37
4:G:52:LEU:HD23	4:G:53:PHE:N	1.55	1.20
4:G:62:GLU:HG2	4:G:63:THR:N	1.10	1.10
4:G:298:ARG:NH2	4:G:441:GLY:O	1.92	1.03
2:D:2:VAL:H	2:D:26:GLY:HA3	1.27	1.00
4:G:52:LEU:HD23	4:G:53:PHE:H	0.85	0.98
4:G:55:ALA:HB3	4:G:216:HIS:HB2	1.51	0.93
4:G:474:ASP:OD1	4:G:476:ARG:HG3	1.72	0.90
1:B:529:THR:HG23	20:Y:1:NAG:H81	1.53	0.88
3:E:50:ARG:HD2	3:E:56:ASP:HA	1.56	0.87
6:L:37:GLN:HB2	6:L:47:LEU:HD11	1.56	0.86
2:D:179:VAL:HB	3:E:155:THR:HG22	1.58	0.85
4:G:52:LEU:CD2	4:G:53:PHE:H	1.80	0.85
4:G:52:LEU:CD2	4:G:53:PHE:N	2.40	0.84
2:D:178:ALA:HB2	2:D:188:LEU:HD23	1.61	0.83
4:G:62:GLU:CG	4:G:63:THR:N	2.03	0.83
1:B:585:ARG:NH2	4:G:491:ILE:O	2.12	0.82
1:B:553:SER:H	1:B:554:ASN:HA	1.45	0.81
4:G:117:LYS:O	4:G:121:LYS:NZ	2.11	0.81
3:E:10:VAL:HG11	3:E:18:VAL:HG13	1.61	0.81
3:E:26:TYR:HA	10:J:2:NAG:H83	1.61	0.81
2:D:81:MET:HG2	2:D:82:GLN:N	1.96	0.81
18:T:2:NAG:H81	18:T:5:MAN:H2	1.64	0.80
3:E:44:ILE:HG13	3:E:49:ARG:O	1.82	0.79
2:D:153:LYS:NZ	2:D:181:GLN:OE1	2.15	0.79
5:H:3:GLN:N	5:H:25:SER:O	2.14	0.78
1:B:610:TRP:HE3	4:G:36:VAL:HG22	1.50	0.76
6:L:166:VAL:HG22	6:L:185:LEU:HD13	1.68	0.75
3:E:46:GLU:HG2	3:E:47:VAL:H	1.50	0.75
2:D:33:TYR:CE1	2:D:52:ASN:HB3	2.21	0.74
5:H:163:ASP:OD1	5:H:190:GLN:NE2	2.18	0.73
6:L:152:THR:HB	6:L:203:THR:HB	1.69	0.73
4:G:59:LYS:HE3	4:G:59:LYS:HA	1.69	0.73
5:H:162:LYS:NZ	5:H:163:ASP:OD2	2.21	0.73
2:D:156:PHE:CD1	2:D:157:PRO:HD3	2.23	0.73
6:L:214:ALA:HB3	6:L:217:GLU:HG3	1.71	0.72
6:L:68:ILE:O	6:L:69:ASN:ND2	2.23	0.72
3:E:29:LEU:HD22	3:E:87:PHE:HD2	1.55	0.71
5:H:145:PRO:HD3	5:H:157:LEU:HB3	1.72	0.71
1:B:578:ALA:HB1	4:G:220:PRO:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:476:ARG:HA	4:G:479:TRP:CD1	2.26	0.71
1:B:538:THR:O	1:B:542:ARG:HG3	1.91	0.71
3:E:45:TYR:O	3:E:49:ARG:HB2	1.92	0.70
4:G:101:VAL:HG12	4:G:476:ARG:HB3	1.72	0.70
2:D:99:GLN:HB2	2:D:102:LEU:HD12	1.74	0.70
1:B:632:ASP:HA	1:B:635:ILE:HG12	1.72	0.70
2:D:86:LEU:HD22	2:D:121:VAL:HG21	1.74	0.70
5:H:97:THR:HG22	5:H:121:VAL:HG22	1.73	0.70
1:B:571:TRP:O	4:G:53:PHE:HE1	1.75	0.70
5:H:138:PRO:HB3	5:H:164:TYR:HB3	1.73	0.70
4:G:381:GLU:HG2	4:G:439:ILE:HG12	1.74	0.69
4:G:456:ARG:HD3	4:G:466:GLU:OE2	1.92	0.69
6:L:129:SER:O	6:L:133:GLN:HG3	1.94	0.68
5:H:164:TYR:OH	5:H:167:GLU:OE2	2.11	0.67
4:G:456:ARG:NE	4:G:457:ASP:O	2.28	0.67
2:D:60:TYR:HB2	2:D:65:GLN:HG3	1.77	0.67
2:D:91:THR:HB	2:D:121:VAL:H	1.60	0.67
5:H:2:VAL:HG22	5:H:27:ASP:HB2	1.76	0.67
4:G:158:SER:HB3	22:G:602:FUC:H62	1.77	0.67
3:E:44:ILE:HA	3:E:51:PRO:HD3	1.76	0.67
5:H:4:LEU:HB2	5:H:22:CYS:SG	2.34	0.66
2:D:11:VAL:HG22	2:D:120:THR:HB	1.78	0.66
2:D:33:TYR:CD1	2:D:52:ASN:HB3	2.30	0.66
3:E:50:ARG:NH1	3:E:54:VAL:O	2.29	0.66
3:E:111:PHE:HB2	3:E:126:VAL:HB	1.78	0.66
2:D:71:THR:O	2:D:80:TYR:N	2.28	0.66
4:G:119:CYS:SG	4:G:205:CYS:N	2.69	0.65
2:D:90:ASP:O	2:D:94:TYR:OH	2.13	0.65
3:E:87:PHE:HB3	3:E:88:GLU:HG3	1.77	0.65
3:E:64:GLY:HA3	10:J:5:NAG:H4	1.79	0.65
4:G:92:GLU:HA	4:G:238:PRO:HA	1.78	0.65
2:D:111:ASP:OD1	2:D:111:ASP:N	2.30	0.65
4:G:58:ALA:HB2	4:G:76:PRO:HB3	1.79	0.65
2:D:129:PRO:HB3	2:D:155:TYR:HB3	1.79	0.64
1:B:528:SER:HB3	20:Y:4:FUC:H4	1.77	0.64
6:L:49:TYR:O	6:L:53:ASP:HB2	1.96	0.64
2:D:109:PRO:HG3	3:E:29:LEU:HG	1.79	0.64
1:B:522:PHE:H	4:G:84:ILE:HD13	1.63	0.63
20:Y:1:NAG:H83	20:Y:1:NAG:H3	1.80	0.63
4:G:55:ALA:CB	4:G:216:HIS:HB2	2.25	0.63
2:D:7:SER:HB3	2:D:21:SER:OG	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:61:TYR:CG	4:G:61:TYR:O	2.51	0.63
4:G:68:VAL:HG13	4:G:111:LEU:HD22	1.81	0.63
4:G:292:VAL:HG12	4:G:337:THR:CG2	2.27	0.63
3:E:13:SER:O	3:E:16:GLN:HB2	1.98	0.62
2:D:51:MET:HE3	2:D:72:ARG:HB3	1.81	0.62
4:G:217:TYR:O	4:G:247:CYS:HA	2.00	0.62
4:G:301:ASN:HD22	18:T:1:NAG:H83	1.63	0.62
4:G:358:ILE:HB	4:G:465:THR:HB	1.82	0.62
3:E:62:LYS:HA	3:E:67:ALA:HA	1.82	0.62
2:D:54:ARG:HG3	4:G:428:GLN:HE21	1.64	0.62
4:G:62:GLU:HG2	4:G:63:THR:CA	2.23	0.61
6:L:25:ARG:NE	6:L:93:MET:HB3	2.16	0.61
2:D:13:LYS:HG2	2:D:123:SER:HA	1.82	0.61
2:D:108:TYR:HB3	3:E:29:LEU:HD21	1.83	0.61
4:G:104:MET:O	4:G:108:ILE:HG13	2.00	0.61
5:H:97:THR:CG2	5:H:121:VAL:HG22	2.29	0.61
1:B:638:TYR:HD2	1:B:641:ILE:HD12	1.66	0.61
2:D:47:TRP:CZ3	4:G:458:GLY:HA3	2.36	0.61
5:H:28:SER:OG	5:H:29:MET:N	2.34	0.60
6:L:35:TRP:CZ3	6:L:91:CYS:HB2	2.37	0.60
2:D:39:GLN:OE1	3:E:34:GLN:NE2	2.24	0.60
5:H:105:TYR:CE1	6:L:96:SER:HB2	2.36	0.60
4:G:210:PHE:HD1	4:G:380:GLY:HA2	1.66	0.60
6:L:92:HIS:CE1	6:L:94:TRP:HE1	2.19	0.60
5:H:102:GLN:HB3	12:M:6:MAN:H5	1.84	0.60
3:E:22:CYS:O	3:E:67:ALA:N	2.34	0.59
4:G:266:ALA:O	4:G:289:ASN:HA	2.02	0.59
6:L:86:GLU:HG3	6:L:110:LEU:O	2.01	0.59
2:D:88:SER:O	2:D:91:THR:HG22	2.02	0.59
15:Q:3:BMA:H2	15:Q:4:MAN:H3	1.83	0.59
2:D:51:MET:HA	2:D:57:GLY:O	2.02	0.59
4:G:252:LYS:HD2	4:G:262:ASN:O	2.02	0.59
4:G:205:CYS:O	4:G:208:VAL:HG22	2.03	0.59
4:G:212:PRO:HG3	4:G:254:VAL:HG22	1.84	0.59
2:D:133:PRO:HD3	2:D:219:LYS:HG2	1.84	0.58
3:E:44:ILE:HD11	3:E:48:ASN:HA	1.85	0.58
4:G:421:LYS:HE2	4:G:423:ILE:O	2.03	0.58
2:D:12:LYS:O	2:D:121:VAL:HA	2.04	0.58
5:H:217:VAL:O	5:H:225:LYS:HA	2.04	0.58
4:G:410:SER:OG	4:G:411:ASN:N	2.37	0.58
5:H:223:ASN:OD1	5:H:225:LYS:HE3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:GLY:HA3	2:D:72:ARG:NH1	2.18	0.58
4:G:122:LEU:HD22	4:G:125:LEU:HD23	1.86	0.57
4:G:82:GLN:O	4:G:84:ILE:HG13	2.04	0.57
1:B:642:ILE:O	1:B:646:LEU:HG	2.04	0.57
1:B:529:THR:HA	1:B:626:MET:O	2.03	0.57
4:G:296:CYS:O	4:G:444:ARG:HA	2.03	0.57
2:D:99:GLN:HA	2:D:111:ASP:OD1	2.05	0.57
1:B:610:TRP:CD2	4:G:498:PRO:HB3	2.40	0.57
4:G:390:LEU:HD23	4:G:414:ILE:HD12	1.87	0.57
4:G:101:VAL:HG11	4:G:480:ARG:HG3	1.87	0.56
2:D:134:LEU:N	2:D:149:GLY:O	2.38	0.56
3:E:32:TYR:HD1	3:E:42:LEU:HA	1.69	0.56
1:B:522:PHE:CE1	1:B:540:GLN:HA	2.41	0.56
4:G:112:TRP:CH2	4:G:426:MET:SD	2.98	0.56
2:D:181:GLN:HB2	2:D:185:LEU:O	2.06	0.56
4:G:69:TRP:HA	4:G:111:LEU:HD11	1.88	0.56
4:G:160:ASN:HA	4:G:170:GLN:O	2.06	0.56
3:E:57:ARG:HH22	3:E:75:ARG:CZ	2.19	0.56
3:E:32:TYR:HE1	3:E:42:LEU:HD13	1.70	0.55
3:E:32:TYR:CD1	3:E:42:LEU:HA	2.41	0.55
4:G:53:PHE:HE2	4:G:75:VAL:HG22	1.71	0.55
4:G:69:TRP:HE3	4:G:111:LEU:HD13	1.71	0.55
2:D:71:THR:OG1	2:D:80:TYR:HB2	2.05	0.55
2:D:93:VAL:HG22	2:D:118:MET:SD	2.47	0.55
4:G:499:THR:HG23	4:G:501:CYS:H	1.69	0.55
4:G:174:SER:HB3	4:G:176:PHE:CZ	2.41	0.55
5:H:100:ARG:HG3	5:H:117:TYR:CZ	2.41	0.55
6:L:174:GLN:HB2	6:L:176:ASN:OD1	2.06	0.55
4:G:338:TRP:CZ2	4:G:390:LEU:HB3	2.41	0.55
1:B:635:ILE:O	1:B:639:THR:HG23	2.07	0.55
2:D:32:HIS:ND1	2:D:100:VAL:HG22	2.21	0.55
2:D:33:TYR:CE2	2:D:50:TRP:CZ3	2.94	0.55
4:G:122:LEU:HB2	4:G:201:ILE:HG23	1.88	0.55
4:G:297:THR:HA	4:G:443:ILE:O	2.07	0.55
4:G:381:GLU:HG2	4:G:439:ILE:CG1	2.36	0.55
1:B:629:LEU:O	1:B:633:LYS:HG3	2.07	0.55
2:D:49:GLY:HA3	2:D:70:MET:CE	2.38	0.54
4:G:99:ASN:OD1	4:G:103:GLN:NE2	2.35	0.54
5:H:97:THR:HG23	5:H:120:ASP:OD1	2.07	0.54
1:B:617:ARG:HB3	1:B:621:GLU:HB2	1.89	0.54
3:E:32:TYR:CE1	3:E:42:LEU:HD13	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:53:PHE:CD2	4:G:54:CYS:N	2.76	0.54
4:G:55:ALA:HB3	4:G:216:HIS:CB	2.32	0.54
2:D:30:VAL:HA	2:D:53:PRO:HB2	1.89	0.54
3:E:23:THR:HG22	3:E:66:THR:HG23	1.89	0.54
4:G:57:ASP:OD2	4:G:59:LYS:HG2	2.07	0.54
5:H:105:TYR:CZ	6:L:96:SER:HB2	2.43	0.54
4:G:358:ILE:HB	4:G:465:THR:CB	2.36	0.54
2:D:34:ILE:O	2:D:50:TRP:HA	2.08	0.54
2:D:48:VAL:O	2:D:60:TYR:HA	2.07	0.54
2:D:72:ARG:HA	2:D:79:ALA:HA	1.89	0.54
2:D:134:LEU:HD22	3:E:111:PHE:HB3	1.90	0.54
3:E:185:SER:HB3	3:E:198:THR:HG22	1.88	0.54
22:G:602:FUC:O5	19:X:1:NAG:H61	2.08	0.54
1:B:522:PHE:HE1	1:B:540:GLN:HA	1.73	0.53
2:D:158:GLU:OE2	2:D:178:ALA:HB3	2.09	0.53
4:G:289:ASN:OD1	4:G:344:LYS:NZ	2.39	0.53
2:D:2:VAL:N	2:D:26:GLY:HA3	2.10	0.53
4:G:69:TRP:NE1	4:G:212:PRO:HA	2.22	0.53
3:E:45:TYR:HE2	3:E:51:PRO:HA	1.73	0.53
2:D:34:ILE:HD13	2:D:98:THR:HB	1.91	0.53
5:H:178:LEU:HD21	5:H:201:VAL:HG21	1.89	0.53
1:B:604:CYS:O	4:G:37:THR:HG23	2.09	0.53
3:E:46:GLU:HG2	3:E:47:VAL:N	2.21	0.53
4:G:58:ALA:HB2	4:G:76:PRO:CB	2.38	0.53
4:G:101:VAL:HG13	4:G:479:TRP:HB2	1.91	0.53
1:B:576:LEU:HD12	1:B:579:ARG:HD3	1.90	0.53
2:D:199:LEU:HD13	2:D:226:CYS:SG	2.48	0.53
3:E:23:THR:HA	3:E:66:THR:HA	1.91	0.53
4:G:362:ALA:HB3	4:G:469:ARG:HH11	1.73	0.53
1:B:638:TYR:CD2	1:B:641:ILE:HD12	2.42	0.52
6:L:62:PHE:HA	6:L:77:THR:O	2.08	0.52
4:G:298:ARG:HG3	4:G:420:ILE:HD12	1.91	0.52
2:D:14:PRO:HA	2:D:86:LEU:O	2.09	0.52
4:G:68:VAL:O	4:G:111:LEU:HD21	2.08	0.52
6:L:153:VAL:HG11	6:L:183:SER:HB2	1.90	0.52
1:B:553:SER:N	1:B:554:ASN:HA	2.13	0.52
5:H:24:VAL:HB	5:H:76:ASN:HB3	1.91	0.52
5:H:100:ARG:HG3	5:H:117:TYR:CE2	2.44	0.52
21:B:701:NAG:O7	21:B:701:NAG:O3	2.23	0.52
2:D:99:GLN:HB3	2:D:109:PRO:O	2.09	0.52
3:E:138:THR:HB	3:E:189:THR:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:53:PHE:CE2	4:G:75:VAL:HG22	2.45	0.52
5:H:173:TRP:HB3	5:H:178:LEU:HD23	1.92	0.52
2:D:133:PRO:HA	2:D:150:CYS:HA	1.92	0.52
4:G:254:VAL:HG11	4:G:261:LEU:HB2	1.91	0.52
5:H:21:THR:HG21	5:H:77:GLN:OE1	2.10	0.52
4:G:292:VAL:CG2	4:G:449:ILE:HD12	2.40	0.51
6:L:192:TRP:CZ2	6:L:215:PRO:HA	2.45	0.51
2:D:62:GLN:HA	2:D:65:GLN:OE1	2.09	0.51
1:B:658:GLN:OE1	1:B:658:GLN:HA	2.10	0.51
5:H:9:PRO:HD3	5:H:19:SER:O	2.10	0.51
2:D:48:VAL:HG12	2:D:70:MET:HE1	1.93	0.51
3:E:45:TYR:CZ	3:E:49:ARG:HB3	2.46	0.51
3:E:101:GLN:NE2	3:E:163:ASN:HB3	2.26	0.51
4:G:82:GLN:HB2	4:G:246:GLN:NE2	2.25	0.51
1:B:575:GLN:HB2	4:G:53:PHE:CE1	2.45	0.51
2:D:59:ASN:OD1	4:G:469:ARG:HD2	2.09	0.51
2:D:18:VAL:O	2:D:82:GLN:HA	2.10	0.51
18:T:2:NAG:H81	18:T:5:MAN:C2	2.38	0.51
2:D:156:PHE:HD1	2:D:157:PRO:HD3	1.73	0.51
5:H:142:PRO:HB2	5:H:230:VAL:HG13	1.93	0.51
2:D:176:PHE:CE1	3:E:128:LEU:HB3	2.47	0.51
6:L:68:ILE:O	6:L:68:ILE:HG13	2.10	0.51
6:L:13:VAL:HG13	6:L:81:VAL:HG11	1.93	0.50
6:L:214:ALA:HB3	6:L:217:GLU:CG	2.40	0.50
2:D:33:TYR:CD2	2:D:50:TRP:CE3	2.99	0.50
4:G:59:LYS:HA	4:G:59:LYS:CE	2.36	0.50
4:G:299:PRO:HD2	4:G:329:ALA:HA	1.93	0.50
6:L:25:ARG:NH1	6:L:103:SER:O	2.42	0.50
4:G:158:SER:HA	4:G:172:VAL:O	2.11	0.50
2:D:73:ASP:N	2:D:78:THR:O	2.39	0.50
4:G:270:VAL:HG22	4:G:348:GLN:HG3	1.93	0.50
4:G:484:TYR:CZ	4:G:485:LYS:HG3	2.47	0.50
6:L:86:GLU:HB3	6:L:173:LYS:HZ3	1.75	0.50
2:D:127:LYS:HD2	2:D:185:LEU:HD21	1.92	0.50
1:B:610:TRP:CE3	4:G:36:VAL:HG22	2.38	0.50
4:G:212:PRO:CG	4:G:254:VAL:HG22	2.40	0.50
4:G:317:PHE:CE2	4:G:319:ALA:HB2	2.47	0.50
5:H:41:PRO:HD3	5:H:91:ALA:HA	1.94	0.50
6:L:117:LYS:HA	6:L:147:TYR:O	2.12	0.49
1:B:571:TRP:CZ3	4:G:54:CYS:HB2	2.47	0.49
4:G:260:LEU:O	4:G:261:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:32:TYR:HB3	5:H:97:THR:OG1	2.13	0.49
5:H:187:ALA:HB2	5:H:197:LEU:HB3	1.94	0.49
14:U:1:NAG:O6	14:U:2:NAG:N2	2.42	0.49
2:D:127:LYS:HB2	2:D:185:LEU:HD21	1.94	0.49
4:G:263:GLY:HA2	4:G:482:GLU:OE2	2.12	0.49
5:H:104:ILE:HD13	5:H:113:PHE:HB3	1.93	0.49
1:B:651:ASN:OD1	1:B:655:LYS:NZ	2.45	0.49
3:E:7:PRO:HD3	3:E:21:SER:OG	2.11	0.49
3:E:63:SER:OG	3:E:66:THR:N	2.42	0.49
4:G:382:PHE:CD2	4:G:424:ILE:HD13	2.48	0.49
2:D:46:GLN:OE1	2:D:63:ARG:NH2	2.46	0.49
13:O:1:MAN:C2	13:O:2:MAN:H3	2.43	0.49
1:B:558:ALA:O	4:G:72:HIS:NE2	2.46	0.49
2:D:39:GLN:HG3	2:D:40:ALA:O	2.13	0.49
3:E:106:PRO:HD3	3:E:190:HIS:CG	2.48	0.49
5:H:2:VAL:HG13	5:H:27:ASP:HB3	1.95	0.49
3:E:160:GLN:OE1	3:E:166:ALA:HB2	2.12	0.48
4:G:68:VAL:O	4:G:111:LEU:HD11	2.13	0.48
6:L:173:LYS:HD3	6:L:177:ASN:HA	1.95	0.48
6:L:92:HIS:CE1	6:L:94:TRP:NE1	2.81	0.48
1:B:654:GLU:O	1:B:658:GLN:HG2	2.14	0.48
3:E:110:LEU:HD13	3:E:127:CYS:HB2	1.95	0.48
1:B:523:LEU:O	4:G:86:LEU:HD22	2.14	0.48
4:G:330:HIS:HA	4:G:416:LEU:O	2.13	0.48
4:G:362:ALA:CB	4:G:469:ARG:HH11	2.26	0.48
1:B:637:ASN:O	1:B:638:TYR:HB2	2.12	0.48
2:D:91:THR:OG1	2:D:120:THR:HA	2.13	0.48
1:B:645:LEU:O	1:B:649:SER:HB3	2.14	0.48
4:G:260:LEU:HD13	4:G:481:SER:CB	2.44	0.48
2:D:115:GLN:HG2	2:D:116:GLY:N	2.29	0.48
2:D:134:LEU:HB3	3:E:111:PHE:CD2	2.49	0.48
6:L:35:TRP:N	6:L:48:ILE:O	2.43	0.48
4:G:56:SER:C	4:G:77:THR:HG23	2.34	0.47
5:H:87:PRO:HA	5:H:130:VAL:HB	1.96	0.47
2:D:163:SER:OG	2:D:164:TRP:N	2.46	0.47
4:G:52:LEU:HD21	4:G:217:TYR:HB3	1.96	0.47
6:L:21:ILE:O	6:L:75:THR:HA	2.14	0.47
4:G:282:LYS:HA	4:G:282:LYS:HD3	1.36	0.47
1:B:576:LEU:HD12	1:B:576:LEU:HA	1.52	0.47
4:G:68:VAL:CG1	4:G:111:LEU:HD22	2.45	0.47
4:G:86:LEU:HB3	4:G:89:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:69:TRP:CE3	4:G:111:LEU:HD13	2.48	0.47
4:G:378:CYS:HB3	4:G:383:PHE:CE1	2.49	0.47
4:G:483:LEU:HA	4:G:483:LEU:HD23	1.62	0.47
9:I:1:NAG:H83	9:I:1:NAG:H3	1.97	0.47
1:B:575:GLN:O	1:B:579:ARG:HG3	2.15	0.47
2:D:12:LYS:HD2	2:D:17:SER:O	2.15	0.47
3:E:75:ARG:O	3:E:98:VAL:HG11	2.15	0.47
6:L:153:VAL:HG11	6:L:183:SER:CB	2.45	0.47
2:D:154:ASP:HA	2:D:185:LEU:HB3	1.97	0.47
4:G:477:ASP:OD1	4:G:480:ARG:NH1	2.47	0.47
6:L:36:TYR:CE2	6:L:46:LEU:HD13	2.50	0.47
6:L:151:VAL:HA	6:L:203:THR:O	2.15	0.47
6:L:155:TRP:CD1	6:L:166:VAL:HG13	2.50	0.47
2:D:115:GLN:O	3:E:38:ARG:HB3	2.14	0.46
3:E:13:SER:OG	3:E:16:GLN:HG3	2.15	0.46
1:B:610:TRP:CG	4:G:498:PRO:HB3	2.50	0.46
1:B:617:ARG:HB2	1:B:622:ILE:HG13	1.96	0.46
5:H:27:ASP:OD1	5:H:28:SER:N	2.49	0.46
5:H:148:LYS:HE3	6:L:218:CYS:SG	2.56	0.46
6:L:39:ARG:HG2	6:L:87:ALA:HB2	1.97	0.46
3:E:30:GLY:N	3:E:85:SER:OG	2.49	0.46
3:E:174:THR:H	3:E:177:GLN:HB2	1.81	0.46
4:G:109:ILE:HA	4:G:427:TRP:CH2	2.51	0.46
4:G:158:SER:HB3	22:G:602:FUC:C6	2.44	0.46
4:G:463:SER:O	4:G:464:THR:C	2.54	0.46
11:K:2:NAG:O7	11:K:2:NAG:O3	2.29	0.46
6:L:47:LEU:O	6:L:55:PRO:HD2	2.16	0.46
1:B:605:CYS:O	4:G:503:ARG:NE	2.47	0.46
4:G:220:PRO:HG2	4:G:223:PHE:CD1	2.51	0.46
4:G:290:THR:OG1	4:G:344:LYS:NZ	2.49	0.46
4:G:382:PHE:CE1	4:G:436:ALA:HB2	2.50	0.46
6:L:139:LEU:HD12	6:L:185:LEU:HD23	1.98	0.46
12:M:3:BMA:C3	13:O:1:MAN:H5	2.45	0.46
4:G:124:PRO:HG2	4:G:161:MET:HE1	1.98	0.46
4:G:206:PRO:HG2	4:G:207:LYS:HD3	1.97	0.46
4:G:157:CYS:O	4:G:173:TYR:HA	2.16	0.46
3:E:134:PRO:HD2	3:E:191:GLU:OE2	2.16	0.46
4:G:61:TYR:O	4:G:61:TYR:CD1	2.69	0.46
5:H:3:GLN:O	5:H:25:SER:N	2.33	0.46
1:B:580:VAL:O	1:B:584:GLU:HB2	2.16	0.46
2:D:219:LYS:HA	2:D:219:LYS:HD2	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:142:PRO:HB3	5:H:230:VAL:HA	1.98	0.46
2:D:49:GLY:HA3	2:D:70:MET:HE1	1.95	0.45
4:G:325:ASP:CG	6:L:30:SER:HG	2.20	0.45
4:G:54:CYS:SG	4:G:55:ALA:N	2.90	0.45
4:G:92:GLU:HG2	4:G:93:PHE:N	2.30	0.45
2:D:198:SER:HB2	2:D:202:GLN:HB2	1.98	0.45
4:G:62:GLU:H	4:G:62:GLU:CD	2.20	0.45
5:H:93:TYR:CD1	5:H:93:TYR:N	2.85	0.45
2:D:99:GLN:HG2	2:D:107:GLY:C	2.37	0.45
4:G:305:LYS:HB3	4:G:319:ALA:HB3	1.98	0.45
1:B:552:GLN:HG3	1:B:553:SER:H	1.82	0.45
4:G:292:VAL:HG21	4:G:449:ILE:HD12	1.99	0.45
14:P:1:NAG:H83	14:P:1:NAG:H3	1.98	0.45
1:B:606:THR:OG1	4:G:36:VAL:O	2.28	0.45
2:D:54:ARG:C	4:G:428:GLN:HE21	2.19	0.45
3:E:35:HIS:CD2	3:E:80:ALA:HB2	2.52	0.45
1:B:545:LEU:HD11	1:B:586:TYR:CE2	2.51	0.45
2:D:136:PRO:HD2	2:D:224:LYS:HE2	1.98	0.45
4:G:188:ASN:N	4:G:189:LYS:HA	2.32	0.45
4:G:294:ILE:HD13	4:G:294:ILE:HG21	1.68	0.45
6:L:34:GLN:HA	6:L:48:ILE:O	2.17	0.45
2:D:198:SER:HB2	2:D:202:GLN:CG	2.46	0.45
3:E:46:GLU:HB3	3:E:49:ARG:HG2	1.98	0.45
3:E:153:GLU:HB2	3:E:170:TYR:HB2	1.99	0.45
3:E:189:THR:HA	3:E:193:SER:O	2.17	0.45
4:G:52:LEU:CD2	4:G:53:PHE:O	2.65	0.45
4:G:134:VAL:HG23	4:G:135:THR:H	1.82	0.45
11:K:1:NAG:H83	11:K:1:NAG:H3	1.99	0.45
3:E:54:VAL:HG13	3:E:55:SER:O	2.17	0.45
2:D:102:LEU:HG	2:D:111:ASP:OD2	2.18	0.44
5:H:104:ILE:HD13	5:H:113:PHE:CB	2.47	0.44
3:E:111:PHE:N	3:E:126:VAL:O	2.46	0.44
4:G:50:THR:OG1	4:G:51:THR:N	2.50	0.44
4:G:158:SER:HB2	4:G:171:LYS:HE3	1.99	0.44
4:G:214:PRO:HG3	4:G:252:LYS:HG3	1.98	0.44
5:H:142:PRO:CB	5:H:230:VAL:HA	2.48	0.44
4:G:62:GLU:CD	4:G:62:GLU:N	2.70	0.44
4:G:108:ILE:HD12	4:G:479:TRP:CZ2	2.52	0.44
4:G:292:VAL:HG12	4:G:337:THR:HG22	1.97	0.44
3:E:74:LEU:HD23	3:E:74:LEU:HA	1.82	0.44
4:G:52:LEU:HD22	4:G:217:TYR:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:LEU:HD13	2:D:186:TYR:CZ	2.52	0.44
3:E:57:ARG:HD3	3:E:72:SER:O	2.17	0.44
4:G:359:ILE:O	4:G:395:TRP:HB2	2.18	0.44
2:D:180:LEU:HD13	2:D:186:TYR:CE1	2.52	0.44
3:E:44:ILE:HD11	3:E:48:ASN:CA	2.47	0.44
3:E:59:SER:O	3:E:70:THR:HG22	2.18	0.44
5:H:63:LEU:HD23	5:H:63:LEU:HA	1.83	0.44
3:E:101:GLN:HB2	3:E:133:TYR:CZ	2.52	0.44
4:G:475:MET:SD	4:G:478:ASN:ND2	2.91	0.44
6:L:70:PHE:CD1	6:L:71:GLY:N	2.82	0.44
3:E:33:GLN:NE2	3:E:35:HIS:CE1	2.86	0.43
4:G:175:LEU:O	4:G:176:PHE:CD2	2.71	0.43
4:G:249:HIS:O	4:G:251:ILE:HG13	2.18	0.43
4:G:69:TRP:O	4:G:71:THR:HG23	2.18	0.43
1:B:571:TRP:CE3	4:G:54:CYS:HB2	2.53	0.43
2:D:45:PRO:HG2	3:E:90:PHE:CB	2.48	0.43
5:H:92:VAL:HG12	5:H:94:TYR:CE1	2.52	0.43
11:K:2:NAG:H81	17:S:6:MAN:O4	2.18	0.43
2:D:156:PHE:H	2:D:156:PHE:HD2	1.65	0.43
3:E:44:ILE:CG1	3:E:49:ARG:H	2.31	0.43
4:G:214:PRO:HG3	4:G:252:LYS:CG	2.47	0.43
5:H:55:GLU:OE2	5:H:71:ARG:NH2	2.52	0.43
2:D:18:VAL:HG12	2:D:83:LEU:O	2.18	0.43
4:G:426:MET:O	4:G:429:ARG:HB3	2.19	0.43
5:H:184:THR:HA	5:H:199:SER:HA	1.99	0.43
1:B:527:GLY:N	4:G:89:VAL:HG22	2.34	0.43
1:B:528:SER:CB	20:Y:4:FUC:H4	2.47	0.43
3:E:26:TYR:CA	10:J:2:NAG:H83	2.42	0.43
3:E:44:ILE:HG13	3:E:49:ARG:C	2.38	0.43
4:G:36:VAL:HG13	4:G:496:VAL:HG13	2.01	0.43
2:D:54:ARG:O	4:G:428:GLN:NE2	2.52	0.43
4:G:222:GLY:O	4:G:491:ILE:HB	2.18	0.43
5:H:140:VAL:O	5:H:228:LYS:HE3	2.19	0.43
4:G:47:ASP:OD2	4:G:487:LYS:NZ	2.52	0.43
4:G:258:GLN:O	4:G:259:LEU:HD12	2.18	0.43
4:G:327:ARG:HE	4:G:327:ARG:HB3	1.53	0.43
1:B:619:LEU:HD23	1:B:619:LEU:HA	1.83	0.43
2:D:155:TYR:CZ	2:D:186:TYR:HB3	2.54	0.43
3:E:24:GLY:N	3:E:65:ASN:O	2.35	0.43
4:G:178:ARG:O	4:G:178:ARG:HG2	2.19	0.43
4:G:444:ARG:O	4:G:444:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:34:GLN:HG3	6:L:49:TYR:CB	2.49	0.43
6:L:35:TRP:CH2	6:L:91:CYS:HB2	2.54	0.43
2:D:127:LYS:CB	2:D:185:LEU:HD21	2.48	0.43
3:E:29:LEU:HD22	3:E:87:PHE:CD2	2.43	0.43
6:L:52:GLN:HG3	6:L:53:ASP:OD1	2.18	0.43
2:D:50:TRP:O	2:D:58:VAL:HG12	2.18	0.42
2:D:131:VAL:HG22	2:D:152:VAL:HG13	2.00	0.42
5:H:102:GLN:HB2	5:H:115:TYR:CE2	2.54	0.42
6:L:115:GLN:HB2	6:L:147:TYR:CD2	2.53	0.42
2:D:1:GLN:HG3	2:D:2:VAL:HG23	2.00	0.42
2:D:76:ILE:HG13	2:D:78:THR:HB	2.02	0.42
4:G:349:LEU:HD23	4:G:349:LEU:HA	1.76	0.42
4:G:382:PHE:CD2	4:G:424:ILE:CD1	3.02	0.42
1:B:546:SER:HA	1:B:547:GLY:HA3	1.59	0.42
4:G:168:LYS:HA	4:G:168:LYS:HD2	1.59	0.42
5:H:12:VAL:HG23	5:H:85:VAL:HG21	2.01	0.42
6:L:95:ASP:OD1	6:L:98:SER:HB2	2.20	0.42
2:D:200:GLY:CA	2:D:223:PRO:HB2	2.50	0.42
6:L:39:ARG:O	6:L:40:PRO:C	2.57	0.42
6:L:39:ARG:HG2	6:L:87:ALA:CB	2.49	0.42
6:L:124:LEU:HD12	6:L:140:VAL:O	2.19	0.42
11:K:1:NAG:C1	11:K:1:NAG:H82	2.50	0.42
2:D:154:ASP:CB	2:D:185:LEU:HD13	2.50	0.42
4:G:415:THR:O	4:G:416:LEU:HD23	2.20	0.42
5:H:35:THR:HG21	5:H:119:MET:HE2	2.00	0.42
5:H:185:PHE:CZ	6:L:142:LEU:HB3	2.55	0.42
3:E:45:TYR:CE2	3:E:51:PRO:HA	2.54	0.42
3:E:104:ALA:O	3:E:190:HIS:NE2	2.53	0.42
4:G:52:LEU:CD2	4:G:217:TYR:HB3	2.50	0.42
4:G:454:LEU:HD23	4:G:454:LEU:HA	1.77	0.42
2:D:86:LEU:HD23	2:D:86:LEU:HA	1.74	0.42
3:E:101:GLN:HE22	3:E:163:ASN:HB3	1.84	0.42
4:G:58:ALA:CB	4:G:76:PRO:HB3	2.49	0.42
5:H:66:ARG:HB3	5:H:82:LEU:HD12	2.02	0.42
3:E:32:TYR:CE1	3:E:42:LEU:HB2	2.55	0.41
3:E:44:ILE:HD11	3:E:49:ARG:N	2.35	0.41
2:D:35:HIS:ND1	2:D:50:TRP:HB3	2.35	0.41
1:B:629:LEU:H	1:B:629:LEU:HG	1.58	0.41
2:D:54:ARG:HG3	4:G:428:GLN:NE2	2.32	0.41
2:D:176:PHE:CZ	3:E:128:LEU:HB3	2.55	0.41
4:G:494:LEU:HD23	4:G:494:LEU:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:1:MAN:H2	13:N:2:MAN:H2	1.87	0.41
2:D:39:GLN:O	2:D:92:ALA:HB1	2.21	0.41
4:G:67:ASN:ND2	4:G:71:THR:O	2.53	0.41
4:G:68:VAL:HG13	4:G:111:LEU:CD2	2.49	0.41
4:G:449:ILE:HD13	4:G:449:ILE:HG21	1.91	0.41
1:B:632:ASP:HA	1:B:635:ILE:CG1	2.46	0.41
2:D:48:VAL:HG12	2:D:70:MET:CE	2.50	0.41
2:D:51:MET:O	2:D:51:MET:HG2	2.21	0.41
4:G:155:LYS:O	4:G:175:LEU:HA	2.20	0.41
4:G:158:SER:HB3	22:G:602:FUC:C5	2.51	0.41
4:G:173:TYR:HB3	22:G:602:FUC:H63	2.02	0.41
4:G:491:ILE:HD13	4:G:491:ILE:HA	1.91	0.41
2:D:129:PRO:CB	2:D:155:TYR:HB3	2.50	0.41
4:G:192:ARG:HD2	4:G:196:CYS:HB2	2.01	0.41
4:G:274:SER:OG	4:G:277:ILE:HG13	2.20	0.41
4:G:274:SER:OG	4:G:277:ILE:N	2.54	0.41
2:D:35:HIS:CD2	2:D:35:HIS:N	2.89	0.41
4:G:47:ASP:OD2	4:G:487:LYS:CE	2.69	0.41
4:G:124:PRO:O	4:G:127:VAL:HG13	2.21	0.41
6:L:117:LYS:HE2	6:L:205:GLU:OE1	2.21	0.41
2:D:99:GLN:HE21	2:D:107:GLY:HA2	1.85	0.41
2:D:156:PHE:CD1	2:D:157:PRO:CD	3.01	0.41
6:L:28:LEU:HD11	6:L:97:ARG:NH1	2.35	0.41
3:E:151:GLY:O	3:E:171:LEU:HA	2.20	0.40
4:G:205:CYS:HB3	4:G:207:LYS:HG2	2.03	0.40
4:G:416:LEU:HD23	4:G:416:LEU:HA	1.76	0.40
2:D:2:VAL:CG1	2:D:112:ILE:HD13	2.51	0.40
3:E:8:ARG:O	3:E:94:THR:HA	2.21	0.40
3:E:54:VAL:HG22	3:E:55:SER:H	1.86	0.40
5:H:11:LEU:HA	5:H:129:THR:O	2.21	0.40
13:O:1:MAN:H2	13:O:2:MAN:H3	2.04	0.40
2:D:99:GLN:HG2	2:D:107:GLY:O	2.21	0.40
4:G:87:GLU:O	4:G:89:VAL:HG23	2.22	0.40
5:H:13:LYS:HG2	5:H:132:SER:HA	2.03	0.40
19:X:1:NAG:O6	19:X:2:NAG:N2	2.55	0.40
2:D:16:ALA:O	2:D:86:LEU:HB2	2.22	0.40
2:D:133:PRO:O	3:E:114:SER:HB3	2.22	0.40
3:E:46:GLU:HB3	3:E:49:ARG:CG	2.51	0.40
4:G:62:GLU:C	4:G:64:GLU:N	2.74	0.40
4:G:173:TYR:HB3	22:G:602:FUC:C6	2.52	0.40
4:G:360:ARG:CG	4:G:467:THR:HG22	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:66:ARG:NH1	5:H:84:SER:O	2.54	0.40
5:H:145:PRO:HD3	5:H:157:LEU:CB	2.45	0.40

All (1) 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)
5:H:225:LYS:NZ	13:N:2:MAN:O6[8_544]	2.16	0.04

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	133/153 (87%)	125 (94%)	8 (6%)	0	100	100
2	D	216/234 (92%)	188 (87%)	26 (12%)	2 (1%)	17	55
3	E	200/205 (98%)	168 (84%)	32 (16%)	0	100	100
4	G	443/501 (88%)	411 (93%)	27 (6%)	5 (1%)	14	51
5	H	225/243 (93%)	220 (98%)	5 (2%)	0	100	100
6	L	209/214 (98%)	203 (97%)	5 (2%)	1 (0%)	29	67
All	All	1426/1550 (92%)	1315 (92%)	103 (7%)	8 (1%)	25	63

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	63	THR
4	G	464	THR
6	L	158	ASP
2	D	74	THR
4	G	461	THR
4	G	67	ASN

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Mol	Chain	Res	Type
2	D	2	VAL
4	G	134	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	118/129 (92%)	117 (99%)	1 (1%)	81	89
2	D	186/200 (93%)	182 (98%)	4 (2%)	52	71
3	E	169/173 (98%)	167 (99%)	2 (1%)	71	84
4	G	401/441 (91%)	399 (100%)	2 (0%)	88	93
5	H	201/213 (94%)	198 (98%)	3 (2%)	65	80
6	L	175/178 (98%)	174 (99%)	1 (1%)	86	92
All	All	1250/1334 (94%)	1237 (99%)	13 (1%)	76	86

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	611	ASN
2	D	25	SER
2	D	54	ARG
2	D	63	ARG
2	D	110	PHE
3	E	56	ASP
3	E	57	ARG
4	G	56	SER
4	G	188	ASN
5	H	4	LEU
5	H	103	ARG
5	H	119	MET
6	L	69	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	210	HIS
3	E	33	GLN
6	L	52	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 ⓘ

70 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	1	7,1	14,14,15	2.01	2 (14%)	17,19,21	1.52	3 (17%)
7	FUC	A	2	7	10,10,11	1.35	2 (20%)	14,14,16	0.89	2 (14%)
8	NAG	F	1	8,3	14,14,15	0.32	0	17,19,21	0.35	0
8	NAG	F	2	8	14,14,15	0.92	1 (7%)	17,19,21	0.51	0
9	NAG	I	1	9,4	14,14,15	1.57	2 (14%)	17,19,21	1.89	5 (29%)
9	NAG	I	2	9	14,14,15	0.59	0	17,19,21	1.50	3 (17%)
9	BMA	I	3	9	11,11,12	1.65	2 (18%)	15,15,17	3.22	4 (26%)
9	MAN	I	4	9	11,11,12	1.11	1 (9%)	15,15,17	1.24	3 (20%)
9	MAN	I	5	9	11,11,12	0.94	0	15,15,17	1.01	2 (13%)
10	NAG	J	1	10,4	14,14,15	0.90	1 (7%)	17,19,21	0.75	1 (5%)
10	NAG	J	2	10	14,14,15	0.73	1 (7%)	17,19,21	0.70	0
10	BMA	J	3	10	11,11,12	1.48	1 (9%)	15,15,17	0.97	0
10	MAN	J	4	10	11,11,12	1.67	3 (27%)	15,15,17	1.76	3 (20%)
10	NAG	J	5	10	14,14,15	0.77	1 (7%)	17,19,21	0.77	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GAL	J	6	10	11,11,12	0.93	1 (9%)	15,15,17	1.08	2 (13%)
10	MAN	J	7	10	11,11,12	0.72	0	15,15,17	0.99	1 (6%)
11	NAG	K	1	11,4	14,14,15	0.74	1 (7%)	17,19,21	1.30	2 (11%)
11	NAG	K	2	11	14,14,15	0.47	0	17,19,21	0.59	0
11	BMA	K	3	11	11,11,12	1.22	1 (9%)	15,15,17	0.99	0
11	MAN	K	4	11	11,11,12	1.06	0	15,15,17	0.97	1 (6%)
12	NAG	M	1	4,12	14,14,15	0.74	1 (7%)	17,19,21	0.57	0
12	NAG	M	2	12	14,14,15	0.44	0	17,19,21	0.66	0
12	BMA	M	3	12	11,11,12	1.60	2 (18%)	15,15,17	1.72	4 (26%)
12	MAN	M	4	12	11,11,12	0.49	0	15,15,17	1.81	3 (20%)
12	MAN	M	5	12	11,11,12	1.21	1 (9%)	15,15,17	1.49	3 (20%)
12	MAN	M	6	12	11,11,12	1.90	2 (18%)	15,15,17	1.48	2 (13%)
13	MAN	N	1	13	11,11,12	1.70	3 (27%)	15,15,17	1.74	3 (20%)
13	MAN	N	2	13	11,11,12	1.84	3 (27%)	15,15,17	1.11	2 (13%)
13	MAN	O	1	13	11,11,12	2.25	5 (45%)	15,15,17	2.34	4 (26%)
13	MAN	O	2	13	11,11,12	3.75	7 (63%)	15,15,17	2.61	8 (53%)
14	NAG	P	1	14,4	14,14,15	0.44	0	17,19,21	1.39	1 (5%)
14	NAG	P	2	14	14,14,15	0.87	1 (7%)	17,19,21	0.58	0
14	BMA	P	3	14	11,11,12	1.63	4 (36%)	15,15,17	1.15	1 (6%)
15	NAG	Q	1	15,4	14,14,15	0.61	0	17,19,21	1.36	2 (11%)
15	NAG	Q	2	15	14,14,15	0.42	0	17,19,21	1.71	3 (17%)
15	BMA	Q	3	15	11,11,12	2.33	4 (36%)	15,15,17	2.14	2 (13%)
15	MAN	Q	4	15	11,11,12	2.98	5 (45%)	15,15,17	2.91	4 (26%)
16	NAG	R	1	16,4	14,14,15	0.85	1 (7%)	17,19,21	0.88	0
16	NAG	R	2	16	14,14,15	0.68	1 (7%)	17,19,21	0.71	0
16	NAG	R	3	16	14,14,15	0.95	1 (7%)	17,19,21	0.64	0
17	NAG	S	1	17,4	14,14,15	0.60	0	17,19,21	1.09	1 (5%)
17	NAG	S	2	17	14,14,15	0.86	1 (7%)	17,19,21	0.59	0
17	BMA	S	3	17	11,11,12	1.23	1 (9%)	15,15,17	0.88	0
17	MAN	S	4	17	11,11,12	1.24	2 (18%)	15,15,17	1.74	3 (20%)
17	MAN	S	5	17	11,11,12	2.35	2 (18%)	15,15,17	2.22	4 (26%)
17	MAN	S	6	17	11,11,12	1.96	5 (45%)	15,15,17	1.54	2 (13%)
18	NAG	T	1	18,4	14,14,15	0.33	0	17,19,21	0.58	0
18	NAG	T	2	18	14,14,15	0.43	0	17,19,21	0.75	0
18	BMA	T	3	18	11,11,12	1.72	2 (18%)	15,15,17	1.33	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	MAN	T	4	18	11,11,12	1.08	1 (9%)	15,15,17	1.60	3 (20%)
18	MAN	T	5	18	11,11,12	2.11	4 (36%)	15,15,17	1.75	3 (20%)
18	MAN	T	6	18	11,11,12	1.49	4 (36%)	15,15,17	1.36	1 (6%)
18	MAN	T	7	18	11,11,12	1.41	2 (18%)	15,15,17	2.17	3 (20%)
14	NAG	U	1	14,4	14,14,15	0.65	1 (7%)	17,19,21	1.43	3 (17%)
14	NAG	U	2	14	14,14,15	0.84	1 (7%)	17,19,21	0.86	1 (5%)
14	BMA	U	3	14	11,11,12	1.37	1 (9%)	15,15,17	1.08	2 (13%)
8	NAG	V	1	8,4	14,14,15	0.63	0	17,19,21	0.77	1 (5%)
8	NAG	V	2	8	14,14,15	0.69	0	17,19,21	0.66	0
8	NAG	W	1	8,4	14,14,15	0.59	0	17,19,21	0.63	0
8	NAG	W	2	8	14,14,15	0.57	0	17,19,21	0.57	0
19	NAG	X	1	4,19	14,14,15	0.60	0	17,19,21	0.92	1 (5%)
19	NAG	X	2	19	14,14,15	0.37	0	17,19,21	0.40	0
19	BMA	X	3	19	11,11,12	1.46	2 (18%)	15,15,17	1.68	2 (13%)
19	MAN	X	4	19	11,11,12	1.94	3 (27%)	15,15,17	1.76	4 (26%)
19	BMA	X	5	19	11,11,12	1.72	3 (27%)	15,15,17	1.33	2 (13%)
19	MAN	X	6	19	11,11,12	2.01	4 (36%)	15,15,17	1.97	1 (6%)
20	NAG	Y	1	20,4	14,14,15	1.24	1 (7%)	17,19,21	1.31	1 (5%)
20	NAG	Y	2	20	14,14,15	1.03	2 (14%)	17,19,21	1.10	2 (11%)
20	BMA	Y	3	20	11,11,12	2.13	4 (36%)	15,15,17	1.39	1 (6%)
20	FUC	Y	4	20	10,10,11	1.01	0	14,14,16	1.35	1 (7%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	J	1	10,4	-	2/6/23/26	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	-	2/2/19/22	1/1/1/1
10	NAG	J	5	10	-	2/6/23/26	0/1/1/1
10	GAL	J	6	10	-	0/2/19/22	0/1/1/1
10	MAN	J	7	10	-	0/2/19/22	0/1/1/1
11	NAG	K	1	11,4	-	4/6/23/26	0/1/1/1
11	NAG	K	2	11	-	4/6/23/26	0/1/1/1
11	BMA	K	3	11	-	1/2/19/22	0/1/1/1
11	MAN	K	4	11	-	0/2/19/22	0/1/1/1
12	NAG	M	1	4,12	-	0/6/23/26	0/1/1/1
12	NAG	M	2	12	-	0/6/23/26	0/1/1/1
12	BMA	M	3	12	-	0/2/19/22	0/1/1/1
12	MAN	M	4	12	-	2/2/19/22	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	1/1/1/1
13	MAN	N	1	13	-	1/2/19/22	0/1/1/1
13	MAN	N	2	13	-	2/2/19/22	0/1/1/1
13	MAN	O	1	13	-	0/2/19/22	0/1/1/1
13	MAN	O	2	13	-	2/2/19/22	0/1/1/1
14	NAG	P	1	14,4	-	3/6/23/26	0/1/1/1
14	NAG	P	2	14	-	2/6/23/26	0/1/1/1
14	BMA	P	3	14	-	0/2/19/22	0/1/1/1
15	NAG	Q	1	15,4	-	3/6/23/26	0/1/1/1
15	NAG	Q	2	15	-	3/6/23/26	0/1/1/1
15	BMA	Q	3	15	-	0/2/19/22	0/1/1/1
15	MAN	Q	4	15	-	2/2/19/22	0/1/1/1
16	NAG	R	1	16,4	-	0/6/23/26	0/1/1/1
16	NAG	R	2	16	-	4/6/23/26	0/1/1/1
16	NAG	R	3	16	-	4/6/23/26	0/1/1/1
17	NAG	S	1	17,4	-	2/6/23/26	0/1/1/1
17	NAG	S	2	17	-	0/6/23/26	0/1/1/1
17	BMA	S	3	17	-	2/2/19/22	0/1/1/1
17	MAN	S	4	17	-	0/2/19/22	0/1/1/1
17	MAN	S	5	17	-	2/2/19/22	0/1/1/1
17	MAN	S	6	17	-	1/2/19/22	0/1/1/1
18	NAG	T	1	18,4	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	NAG	T	2	18	-	3/6/23/26	0/1/1/1
18	BMA	T	3	18	-	0/2/19/22	0/1/1/1
18	MAN	T	4	18	-	2/2/19/22	0/1/1/1
18	MAN	T	5	18	-	1/2/19/22	0/1/1/1
18	MAN	T	6	18	-	2/2/19/22	0/1/1/1
18	MAN	T	7	18	-	2/2/19/22	0/1/1/1
14	NAG	U	1	14,4	-	3/6/23/26	0/1/1/1
14	NAG	U	2	14	-	0/6/23/26	0/1/1/1
14	BMA	U	3	14	-	0/2/19/22	0/1/1/1
8	NAG	V	1	8,4	-	4/6/23/26	0/1/1/1
8	NAG	V	2	8	-	4/6/23/26	0/1/1/1
8	NAG	W	1	8,4	-	2/6/23/26	0/1/1/1
8	NAG	W	2	8	-	2/6/23/26	0/1/1/1
19	NAG	X	1	4,19	-	3/6/23/26	0/1/1/1
19	NAG	X	2	19	-	0/6/23/26	0/1/1/1
19	BMA	X	3	19	-	0/2/19/22	0/1/1/1
19	MAN	X	4	19	-	0/2/19/22	0/1/1/1
19	BMA	X	5	19	-	0/2/19/22	0/1/1/1
19	MAN	X	6	19	-	2/2/19/22	0/1/1/1
20	NAG	Y	1	20,4	-	3/6/23/26	0/1/1/1
20	NAG	Y	2	20	-	1/6/23/26	0/1/1/1
20	BMA	Y	3	20	-	2/2/19/22	0/1/1/1
20	FUC	Y	4	20	-	-	0/1/1/1

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1	NAG	O5-C1	6.82	1.54	1.43
13	O	2	MAN	O5-C1	6.07	1.53	1.43
13	O	2	MAN	C4-C3	5.93	1.67	1.52
15	Q	4	MAN	O5-C1	5.87	1.53	1.43
17	S	5	MAN	C1-C2	5.75	1.65	1.52
9	I	1	NAG	O5-C1	-5.35	1.35	1.43
19	X	4	MAN	C1-C2	5.12	1.63	1.52
15	Q	3	BMA	O5-C5	4.98	1.53	1.43
18	T	5	MAN	O5-C5	4.73	1.53	1.43
13	O	2	MAN	C2-C3	4.62	1.59	1.52
13	O	2	MAN	C6-C5	4.61	1.67	1.51
15	Q	4	MAN	C1-C2	4.52	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	S	5	MAN	O5-C1	4.51	1.50	1.43
13	O	2	MAN	O5-C5	4.50	1.52	1.43
19	X	6	MAN	O5-C5	4.48	1.52	1.43
10	J	3	BMA	C1-C2	4.21	1.61	1.52
13	N	1	MAN	C2-C3	4.17	1.58	1.52
20	Y	1	NAG	O5-C1	-4.16	1.37	1.43
20	Y	3	BMA	O5-C5	4.08	1.51	1.43
15	Q	4	MAN	C2-C3	4.07	1.58	1.52
9	I	3	BMA	C4-C5	3.99	1.61	1.53
18	T	3	BMA	C2-C3	3.86	1.58	1.52
13	N	2	MAN	C2-C3	3.80	1.58	1.52
20	Y	3	BMA	C1-C2	3.77	1.60	1.52
13	O	1	MAN	C2-C3	3.72	1.58	1.52
13	O	1	MAN	C4-C3	3.68	1.61	1.52
12	M	6	MAN	C2-C3	3.68	1.57	1.52
13	O	1	MAN	O5-C5	3.58	1.50	1.43
14	U	3	BMA	C1-C2	3.58	1.60	1.52
15	Q	3	BMA	O5-C1	3.57	1.49	1.43
15	Q	4	MAN	C4-C5	3.56	1.60	1.53
17	S	6	MAN	C2-C3	3.55	1.57	1.52
12	M	6	MAN	O5-C5	3.55	1.50	1.43
12	M	3	BMA	C2-C3	-3.55	1.47	1.52
16	R	3	NAG	O5-C1	3.33	1.49	1.43
13	O	2	MAN	C4-C5	3.32	1.60	1.53
11	K	3	BMA	C4-C5	3.24	1.59	1.53
17	S	6	MAN	C1-C2	3.22	1.59	1.52
18	T	3	BMA	O3-C3	3.21	1.50	1.43
17	S	4	MAN	C1-C2	3.19	1.59	1.52
14	P	3	BMA	C1-C2	3.09	1.59	1.52
18	T	7	MAN	C1-C2	3.02	1.59	1.52
9	I	3	BMA	C1-C2	2.99	1.59	1.52
18	T	5	MAN	O5-C1	2.97	1.48	1.43
10	J	4	MAN	O2-C2	2.94	1.49	1.43
10	J	1	NAG	O5-C1	2.88	1.48	1.43
13	O	1	MAN	O5-C1	2.88	1.48	1.43
8	F	2	NAG	C1-C2	2.85	1.56	1.52
18	T	5	MAN	C4-C3	2.85	1.59	1.52
17	S	2	NAG	C1-C2	2.85	1.56	1.52
10	J	4	MAN	C4-C3	2.84	1.59	1.52
20	Y	3	BMA	C2-C3	2.82	1.56	1.52
20	Y	2	NAG	O5-C1	2.79	1.48	1.43
13	N	2	MAN	C1-C2	2.74	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	X	5	BMA	C1-C2	2.74	1.58	1.52
20	Y	3	BMA	O5-C1	2.72	1.48	1.43
16	R	1	NAG	O5-C1	-2.71	1.39	1.43
19	X	5	BMA	C4-C3	2.68	1.59	1.52
17	S	3	BMA	C1-C2	2.68	1.58	1.52
19	X	3	BMA	O3-C3	2.67	1.49	1.43
18	T	7	MAN	O5-C5	2.65	1.48	1.43
14	U	2	NAG	O5-C1	-2.62	1.39	1.43
15	Q	4	MAN	O5-C5	2.57	1.48	1.43
14	P	2	NAG	C1-C2	2.54	1.56	1.52
12	M	1	NAG	C1-C2	2.52	1.56	1.52
10	J	2	NAG	C1-C2	2.49	1.56	1.52
14	P	3	BMA	O5-C1	2.49	1.47	1.43
17	S	6	MAN	O5-C1	2.49	1.47	1.43
7	A	2	FUC	C1-C2	2.48	1.57	1.52
14	P	3	BMA	O5-C5	2.47	1.48	1.43
19	X	4	MAN	O5-C1	-2.44	1.39	1.43
19	X	5	BMA	C4-C5	2.44	1.58	1.53
18	T	4	MAN	C2-C3	2.42	1.56	1.52
18	T	6	MAN	C4-C5	2.41	1.58	1.53
18	T	6	MAN	C1-C2	2.39	1.57	1.52
13	O	2	MAN	O4-C4	2.37	1.48	1.43
19	X	3	BMA	O5-C1	-2.36	1.39	1.43
11	K	1	NAG	O5-C1	-2.34	1.40	1.43
19	X	6	MAN	O5-C1	2.34	1.47	1.43
17	S	6	MAN	O5-C5	2.32	1.48	1.43
12	M	3	BMA	O5-C1	-2.32	1.40	1.43
14	U	1	NAG	C1-C2	2.32	1.55	1.52
13	O	1	MAN	O3-C3	2.30	1.48	1.43
19	X	6	MAN	C1-C2	2.29	1.57	1.52
12	M	5	MAN	O5-C5	2.27	1.48	1.43
10	J	4	MAN	C1-C2	2.27	1.57	1.52
19	X	4	MAN	C4-C5	2.27	1.57	1.53
18	T	6	MAN	C2-C3	2.27	1.55	1.52
15	Q	3	BMA	C1-C2	2.26	1.57	1.52
15	Q	3	BMA	C2-C3	2.25	1.55	1.52
18	T	6	MAN	O5-C5	2.24	1.48	1.43
7	A	2	FUC	O5-C1	2.24	1.47	1.43
20	Y	2	NAG	C1-C2	2.22	1.55	1.52
13	N	2	MAN	C4-C3	2.19	1.57	1.52
13	N	1	MAN	C1-C2	2.19	1.57	1.52
10	J	5	NAG	O5-C1	2.18	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	5	MAN	C6-C5	2.16	1.59	1.51
17	S	4	MAN	C4-C3	2.16	1.57	1.52
17	S	6	MAN	C4-C3	2.14	1.57	1.52
10	J	6	GAL	C1-C2	2.13	1.57	1.52
13	N	1	MAN	O5-C5	2.12	1.47	1.43
14	P	3	BMA	C2-C3	2.10	1.55	1.52
7	A	1	NAG	O7-C7	2.09	1.28	1.23
16	R	2	NAG	C1-C2	2.09	1.55	1.52
19	X	6	MAN	C4-C3	2.04	1.57	1.52
9	I	4	MAN	C4-C5	2.03	1.57	1.53
9	I	1	NAG	C1-C2	-2.02	1.49	1.52

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Q	4	MAN	C1-O5-C5	8.89	124.24	112.19
9	I	3	BMA	C1-C2-C3	-8.33	99.43	109.67
13	O	1	MAN	C1-O5-C5	7.22	121.98	112.19
18	T	7	MAN	C1-O5-C5	7.07	121.77	112.19
13	O	2	MAN	C1-O5-C5	6.69	121.25	112.19
19	X	6	MAN	C1-O5-C5	6.66	121.21	112.19
9	I	3	BMA	C1-O5-C5	-6.65	103.19	112.19
15	Q	3	BMA	C1-O5-C5	6.59	121.13	112.19
17	S	5	MAN	C1-O5-C5	6.55	121.06	112.19
9	I	1	NAG	C2-N2-C7	5.19	130.29	122.90
18	T	5	MAN	C1-O5-C5	5.02	118.99	112.19
10	J	4	MAN	C1-O5-C5	4.89	118.81	112.19
19	X	3	BMA	O3-C3-C2	4.86	119.30	109.99
15	Q	1	NAG	C1-O5-C5	4.61	118.44	112.19
14	P	1	NAG	C2-N2-C7	4.59	129.44	122.90
15	Q	2	NAG	C2-N2-C7	4.45	129.24	122.90
15	Q	4	MAN	C1-C2-C3	4.28	114.93	109.67
12	M	6	MAN	C1-O5-C5	4.23	117.92	112.19
9	I	3	BMA	O5-C1-C2	-4.21	104.27	110.77
20	Y	1	NAG	C2-N2-C7	4.13	128.78	122.90
12	M	4	MAN	C1-O5-C5	4.07	117.70	112.19
11	K	1	NAG	C2-N2-C7	4.02	128.63	122.90
9	I	2	NAG	O4-C4-C5	-4.00	99.36	109.30
18	T	6	MAN	C1-O5-C5	3.98	117.59	112.19
17	S	6	MAN	C1-O5-C5	3.96	117.56	112.19
17	S	4	MAN	O2-C2-C3	-3.91	102.31	110.14
17	S	4	MAN	C1-O5-C5	3.88	117.45	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	1	MAN	C1-O5-C5	3.84	117.40	112.19
17	S	5	MAN	C1-C2-C3	3.79	114.33	109.67
18	T	3	BMA	O3-C3-C2	3.67	117.02	109.99
7	A	1	NAG	C1-O5-C5	-3.64	107.26	112.19
12	M	3	BMA	C1-O5-C5	3.58	117.04	112.19
19	X	4	MAN	C1-C2-C3	3.49	113.96	109.67
15	Q	2	NAG	C1-O5-C5	3.43	116.84	112.19
15	Q	4	MAN	O5-C1-C2	3.37	115.97	110.77
18	T	4	MAN	C1-O5-C5	3.36	116.74	112.19
17	S	1	NAG	C1-O5-C5	3.29	116.64	112.19
15	Q	2	NAG	C1-C2-N2	3.26	116.06	110.49
19	X	4	MAN	O2-C2-C3	-3.23	103.68	110.14
13	O	2	MAN	C6-C5-C4	3.20	120.50	113.00
12	M	4	MAN	O2-C2-C3	-3.20	103.74	110.14
9	I	3	BMA	O3-C3-C2	3.15	116.03	109.99
12	M	4	MAN	O5-C1-C2	-3.14	105.93	110.77
13	O	1	MAN	O5-C1-C2	3.04	115.46	110.77
20	Y	4	FUC	C1-C2-C3	-3.03	105.94	109.67
9	I	1	NAG	C1-C2-N2	3.00	115.61	110.49
20	Y	3	BMA	C1-O5-C5	2.99	116.24	112.19
12	M	5	MAN	C1-O5-C5	2.98	116.23	112.19
19	X	3	BMA	C1-O5-C5	2.97	116.22	112.19
12	M	3	BMA	C2-C3-C4	2.97	116.03	110.89
13	N	1	MAN	O3-C3-C2	2.96	115.66	109.99
13	O	2	MAN	O5-C5-C6	2.84	111.65	107.20
7	A	1	NAG	O3-C3-C2	2.82	115.31	109.47
10	J	4	MAN	O5-C1-C2	2.79	115.07	110.77
18	T	4	MAN	C1-C2-C3	2.78	113.08	109.67
9	I	4	MAN	C1-O5-C5	2.76	115.94	112.19
18	T	5	MAN	O2-C2-C3	-2.70	104.73	110.14
20	Y	2	NAG	C1-O5-C5	2.69	115.84	112.19
14	U	1	NAG	C4-C3-C2	-2.66	107.12	111.02
14	P	3	BMA	C1-O5-C5	2.62	115.74	112.19
13	O	2	MAN	O3-C3-C4	2.60	116.35	110.35
14	U	1	NAG	C1-O5-C5	2.59	115.70	112.19
9	I	1	NAG	C1-O5-C5	-2.58	108.70	112.19
11	K	1	NAG	C1-O5-C5	-2.57	108.71	112.19
14	U	1	NAG	C1-C2-N2	2.55	114.84	110.49
9	I	2	NAG	C4-C3-C2	2.54	114.74	111.02
9	I	1	NAG	C3-C4-C5	2.53	114.75	110.24
19	X	5	BMA	C1-O5-C5	2.52	115.60	112.19
13	N	2	MAN	O3-C3-C2	2.50	114.79	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	U	3	BMA	C1-C2-C3	2.49	112.73	109.67
10	J	4	MAN	O2-C2-C1	2.47	114.21	109.15
18	T	7	MAN	O5-C1-C2	2.47	114.58	110.77
13	O	1	MAN	C2-C3-C4	2.46	115.15	110.89
12	M	3	BMA	O2-C2-C3	-2.45	105.23	110.14
18	T	5	MAN	O5-C5-C6	2.43	111.01	107.20
19	X	1	NAG	C2-N2-C7	2.43	126.36	122.90
18	T	7	MAN	O2-C2-C3	-2.43	105.27	110.14
9	I	1	NAG	O4-C4-C5	-2.42	103.28	109.30
9	I	5	MAN	O2-C2-C3	-2.42	105.29	110.14
13	O	2	MAN	O3-C3-C2	2.41	114.60	109.99
15	Q	3	BMA	O2-C2-C1	2.41	114.07	109.15
9	I	5	MAN	C1-O5-C5	2.40	115.45	112.19
10	J	6	GAL	O2-C2-C1	2.40	114.05	109.15
12	M	5	MAN	O2-C2-C1	2.39	114.05	109.15
12	M	3	BMA	O3-C3-C2	-2.39	105.42	109.99
15	Q	4	MAN	O3-C3-C2	2.38	114.56	109.99
10	J	5	NAG	C1-O5-C5	2.37	115.40	112.19
13	N	1	MAN	O5-C1-C2	2.36	114.42	110.77
20	Y	2	NAG	C2-N2-C7	2.36	126.26	122.90
9	I	2	NAG	C3-C4-C5	2.31	114.36	110.24
14	U	2	NAG	C3-C4-C5	2.30	114.34	110.24
17	S	6	MAN	C1-C2-C3	2.30	112.49	109.67
9	I	4	MAN	O2-C2-C3	-2.27	105.59	110.14
11	K	4	MAN	C1-O5-C5	2.26	115.25	112.19
13	O	1	MAN	O2-C2-C3	-2.25	105.64	110.14
13	O	2	MAN	O2-C2-C3	2.24	114.62	110.14
17	S	4	MAN	C1-C2-C3	2.23	112.41	109.67
19	X	4	MAN	C1-O5-C5	2.23	115.21	112.19
13	O	2	MAN	C2-C3-C4	2.20	114.70	110.89
7	A	1	NAG	O5-C5-C6	2.19	110.63	107.20
10	J	7	MAN	C1-O5-C5	2.17	115.14	112.19
19	X	5	BMA	O5-C1-C2	2.14	114.08	110.77
10	J	6	GAL	C1-O5-C5	2.14	115.08	112.19
10	J	1	NAG	C1-O5-C5	2.13	115.07	112.19
8	V	1	NAG	C2-N2-C7	2.11	125.91	122.90
7	A	2	FUC	O2-C2-C1	2.11	113.48	109.15
13	N	2	MAN	C1-O5-C5	2.11	115.06	112.19
12	M	6	MAN	O3-C3-C2	2.11	114.03	109.99
19	X	4	MAN	C6-C5-C4	2.10	117.93	113.00
14	U	3	BMA	O2-C2-C3	-2.10	105.93	110.14
13	O	2	MAN	O5-C1-C2	2.08	113.98	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Q	1	NAG	O5-C5-C6	-2.06	103.97	107.20
18	T	4	MAN	O2-C2-C3	-2.05	106.03	110.14
12	M	5	MAN	C1-C2-C3	-2.03	107.17	109.67
17	S	5	MAN	O5-C1-C2	2.01	113.88	110.77
17	S	5	MAN	O2-C2-C3	-2.01	106.11	110.14
9	I	4	MAN	O2-C2-C1	2.00	113.25	109.15
7	A	2	FUC	C1-O5-C5	2.00	117.31	112.78

There are no chirality outliers.

All (110) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
18	T	4	MAN	C4-C5-C6-O6
8	F	1	NAG	C8-C7-N2-C2
8	F	1	NAG	O7-C7-N2-C2
8	V	2	NAG	C8-C7-N2-C2
8	V	2	NAG	O7-C7-N2-C2
9	I	1	NAG	C8-C7-N2-C2
9	I	1	NAG	O7-C7-N2-C2
11	K	1	NAG	C8-C7-N2-C2
11	K	1	NAG	O7-C7-N2-C2
14	P	1	NAG	C8-C7-N2-C2
14	P	1	NAG	O7-C7-N2-C2
16	R	3	NAG	C8-C7-N2-C2
16	R	3	NAG	O7-C7-N2-C2
18	T	1	NAG	C8-C7-N2-C2
18	T	1	NAG	O7-C7-N2-C2
20	Y	1	NAG	C8-C7-N2-C2
20	Y	1	NAG	O7-C7-N2-C2
9	I	2	NAG	O5-C5-C6-O6
8	V	1	NAG	C4-C5-C6-O6
8	W	1	NAG	O5-C5-C6-O6
11	K	2	NAG	O5-C5-C6-O6
19	X	1	NAG	C1-C2-N2-C7
20	Y	2	NAG	C1-C2-N2-C7
17	S	3	BMA	O5-C5-C6-O6
9	I	3	BMA	C4-C5-C6-O6
18	T	7	MAN	C4-C5-C6-O6
12	M	5	MAN	O5-C5-C6-O6
8	W	1	NAG	C4-C5-C6-O6
15	Q	1	NAG	C1-C2-N2-C7
17	S	3	BMA	C4-C5-C6-O6
19	X	1	NAG	C4-C5-C6-O6
18	T	6	MAN	O5-C5-C6-O6
10	J	4	MAN	C4-C5-C6-O6
16	R	2	NAG	C4-C5-C6-O6
18	T	1	NAG	C4-C5-C6-O6
14	U	1	NAG	O5-C5-C6-O6
17	S	5	MAN	C4-C5-C6-O6
18	T	2	NAG	O5-C5-C6-O6
8	F	2	NAG	C1-C2-N2-C7
11	K	1	NAG	O5-C5-C6-O6
17	S	5	MAN	O5-C5-C6-O6
8	W	2	NAG	O5-C5-C6-O6

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

All (2) ring outliers are listed below:

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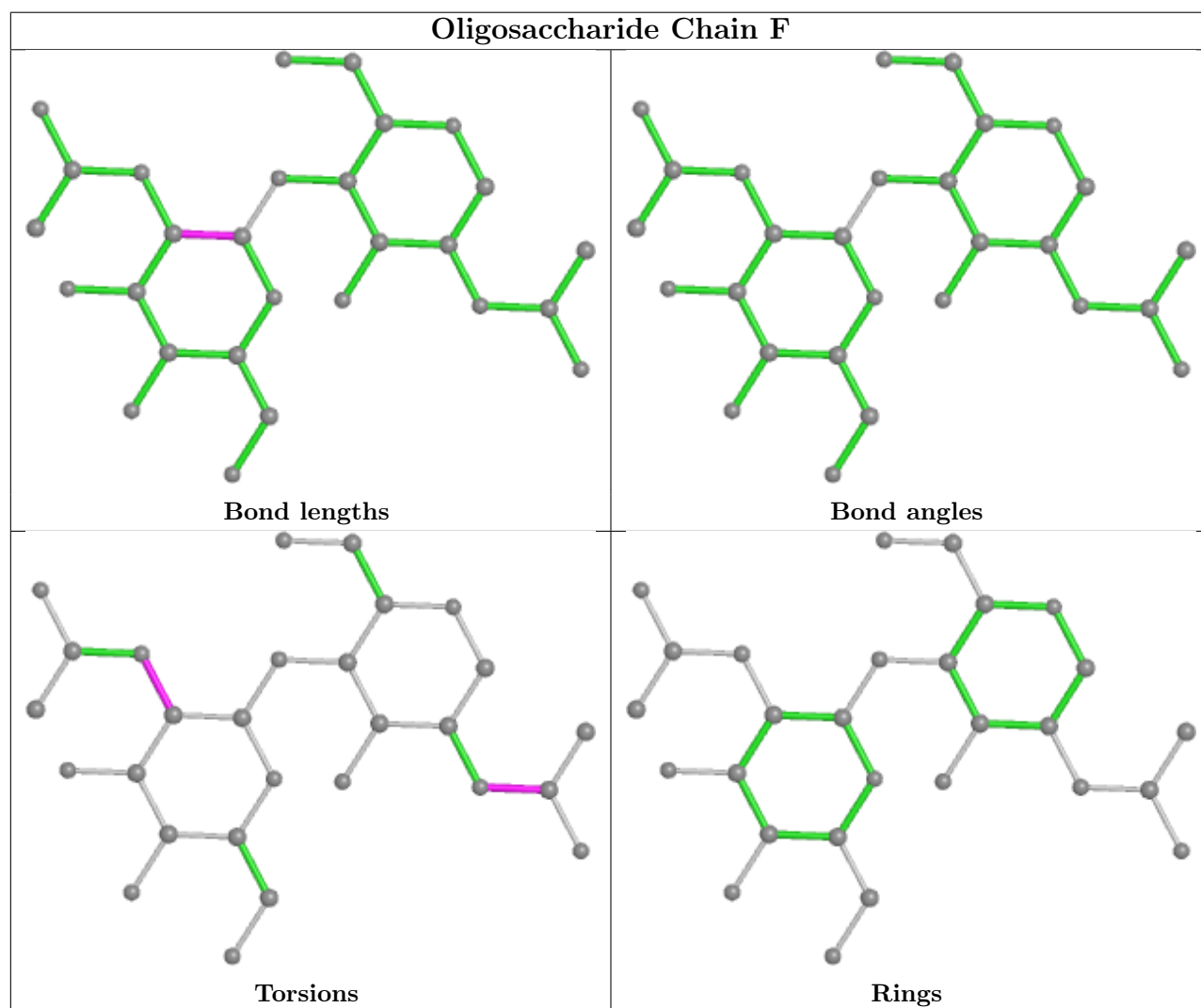
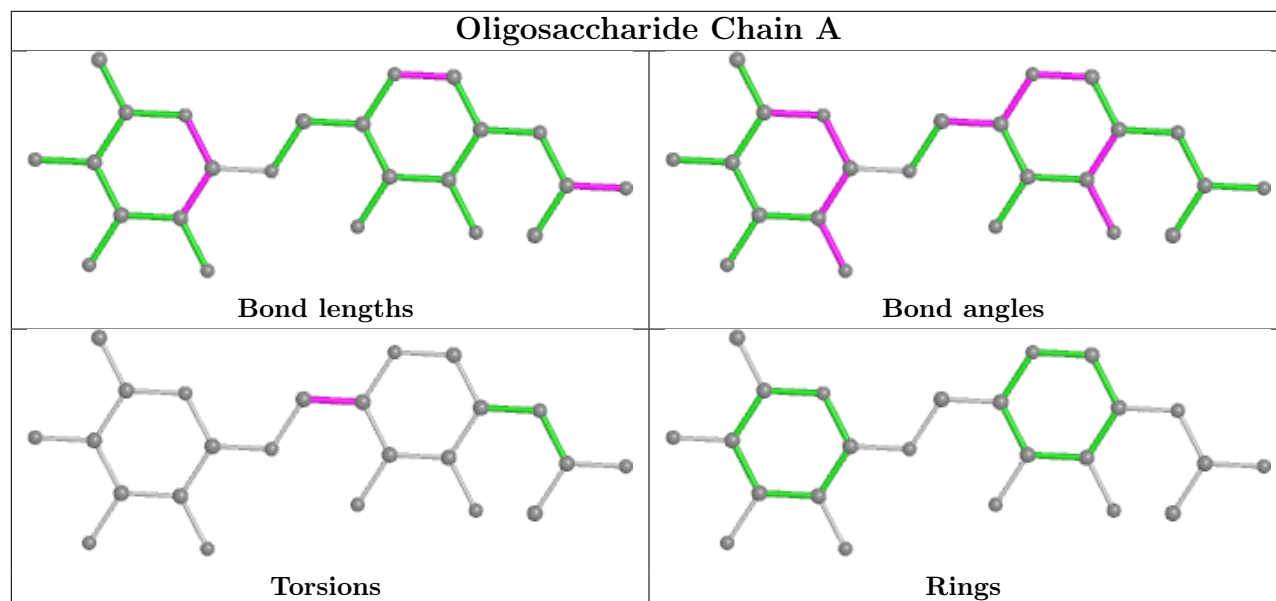
Mol	Chain	Res	Type	Atoms
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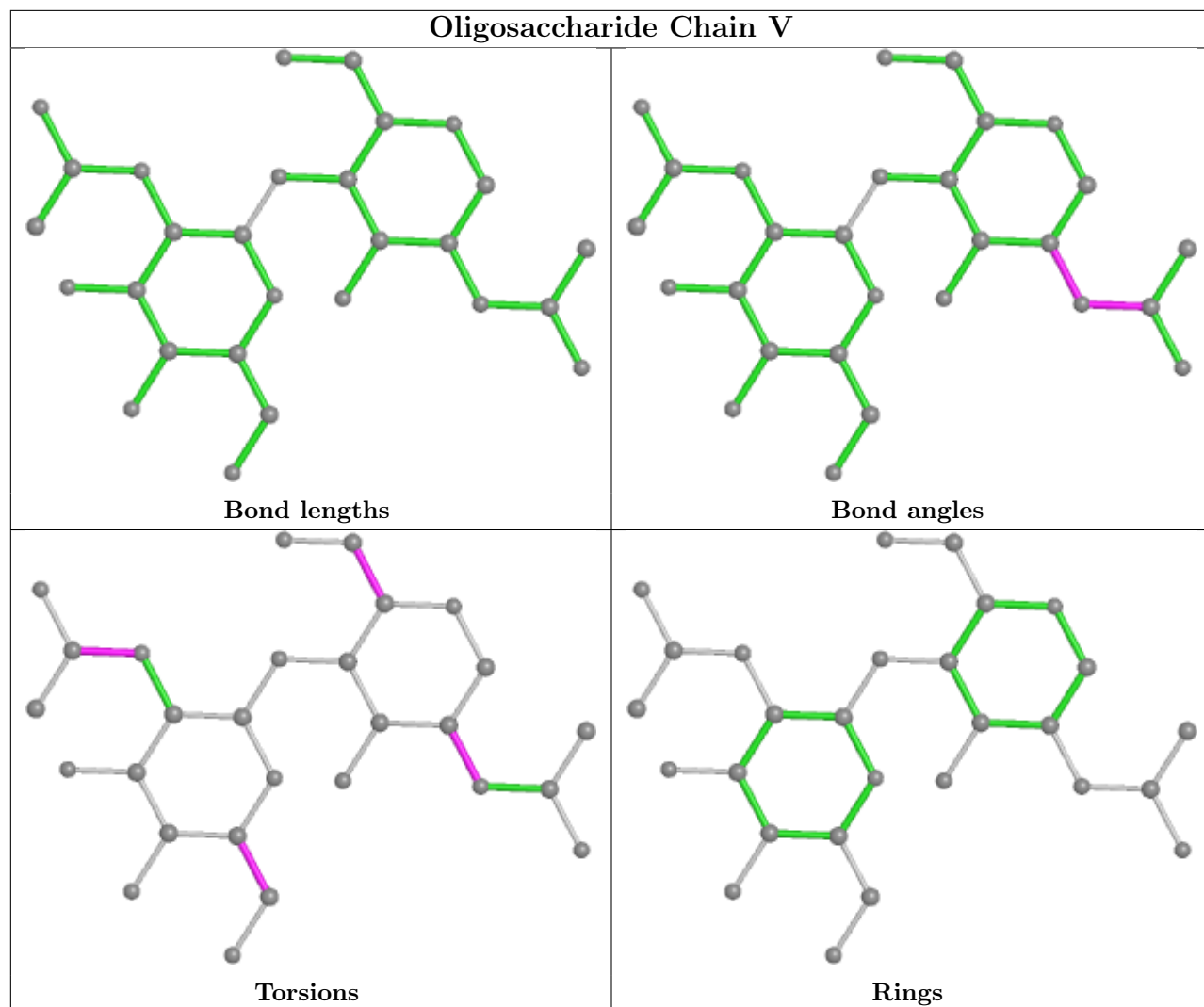
Mol	Chain	Res	Type	Atoms
10	J	4	MAN	C1-C2-C3-C4-C5-O5
12	M	6	MAN	C1-C2-C3-C4-C5-O5

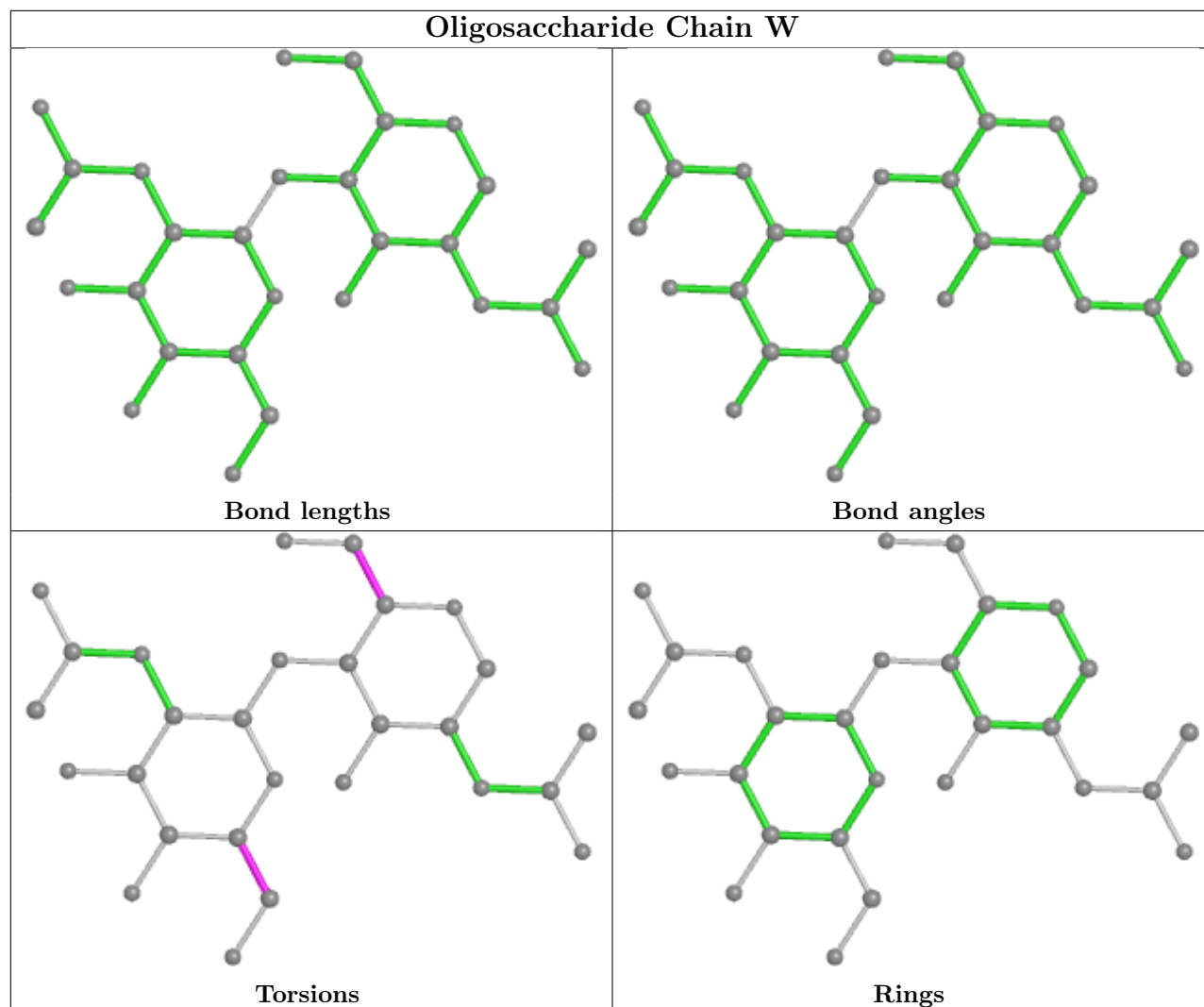
24 monomers are involved in 26 short contacts:

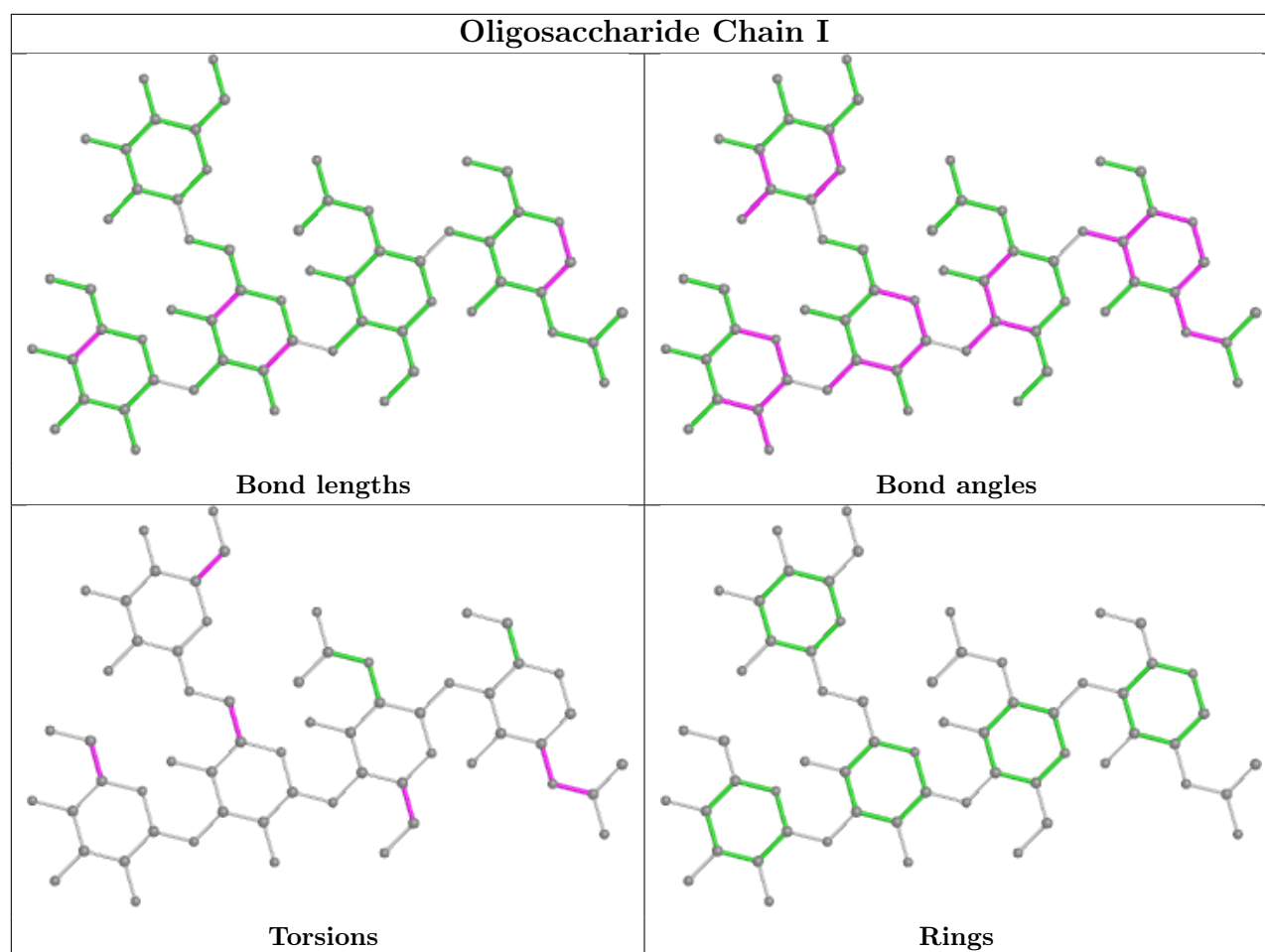
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	T	1	NAG	1	0
13	N	1	MAN	1	0
20	Y	4	FUC	2	0
14	U	1	NAG	1	0
15	Q	3	BMA	1	0
18	T	5	MAN	2	0
14	U	2	NAG	1	0
10	J	2	NAG	2	0
12	M	3	BMA	1	0
18	T	2	NAG	2	0
11	K	2	NAG	2	0
11	K	1	NAG	2	0
14	P	1	NAG	1	0
20	Y	1	NAG	2	0
15	Q	4	MAN	1	0
19	X	2	NAG	1	0
9	I	1	NAG	1	0
10	J	5	NAG	1	0
13	O	1	MAN	3	0
13	O	2	MAN	2	0
19	X	1	NAG	2	0
17	S	6	MAN	1	0
12	M	6	MAN	1	0
13	N	2	MAN	1	1

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

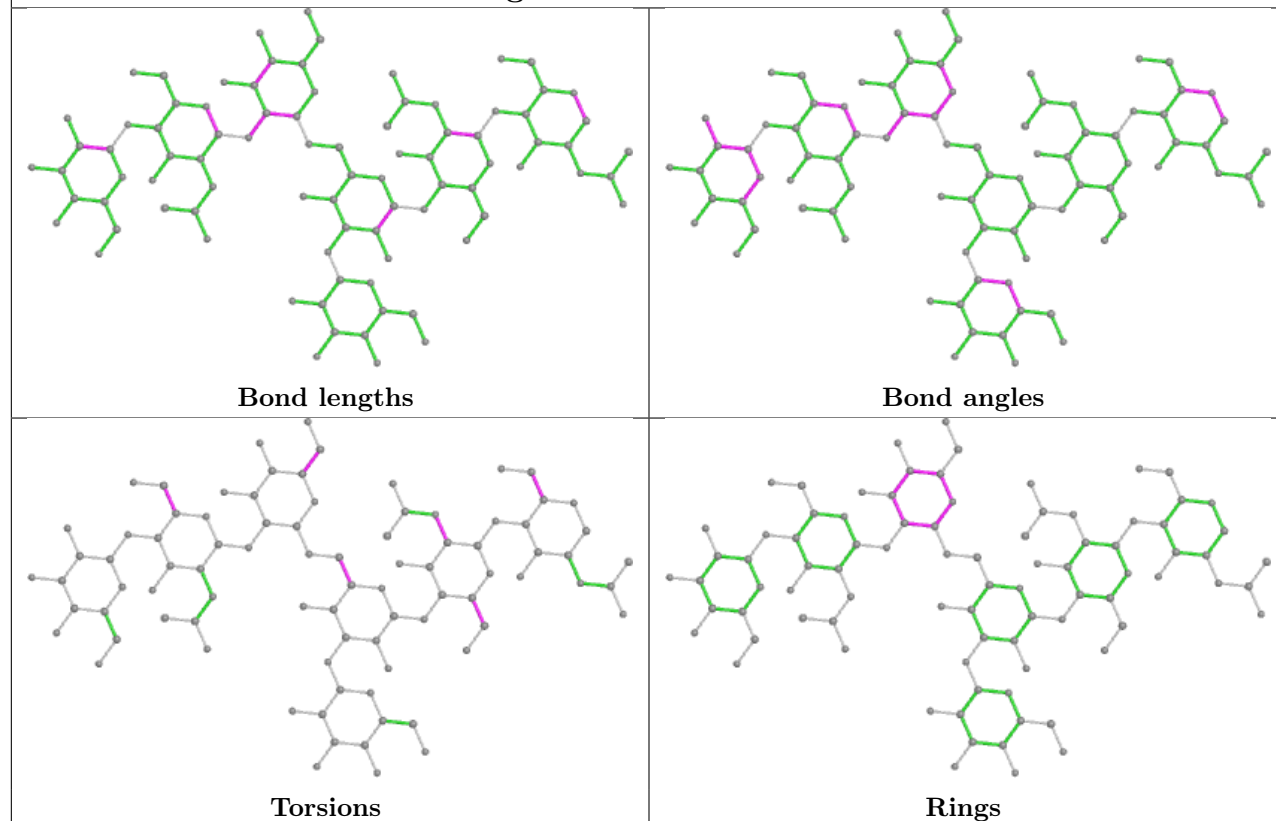




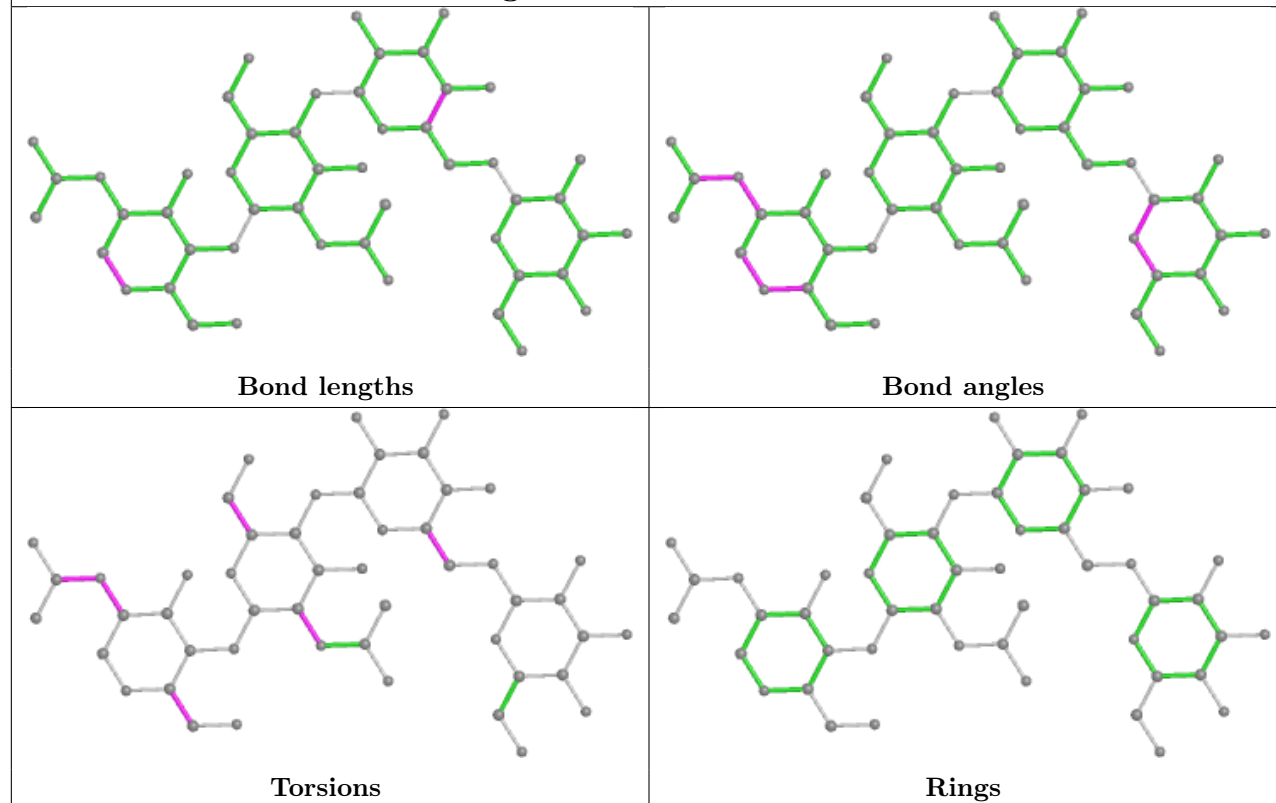


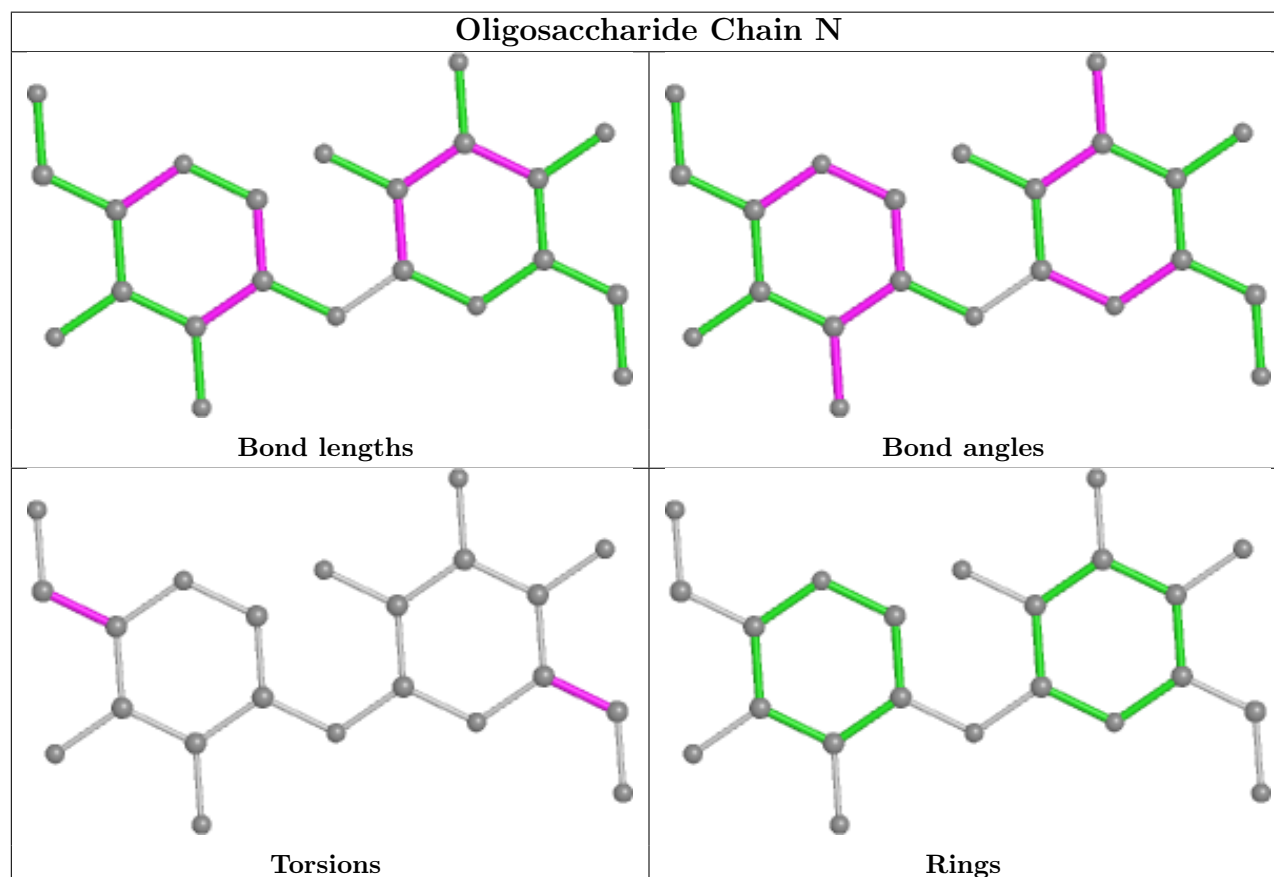
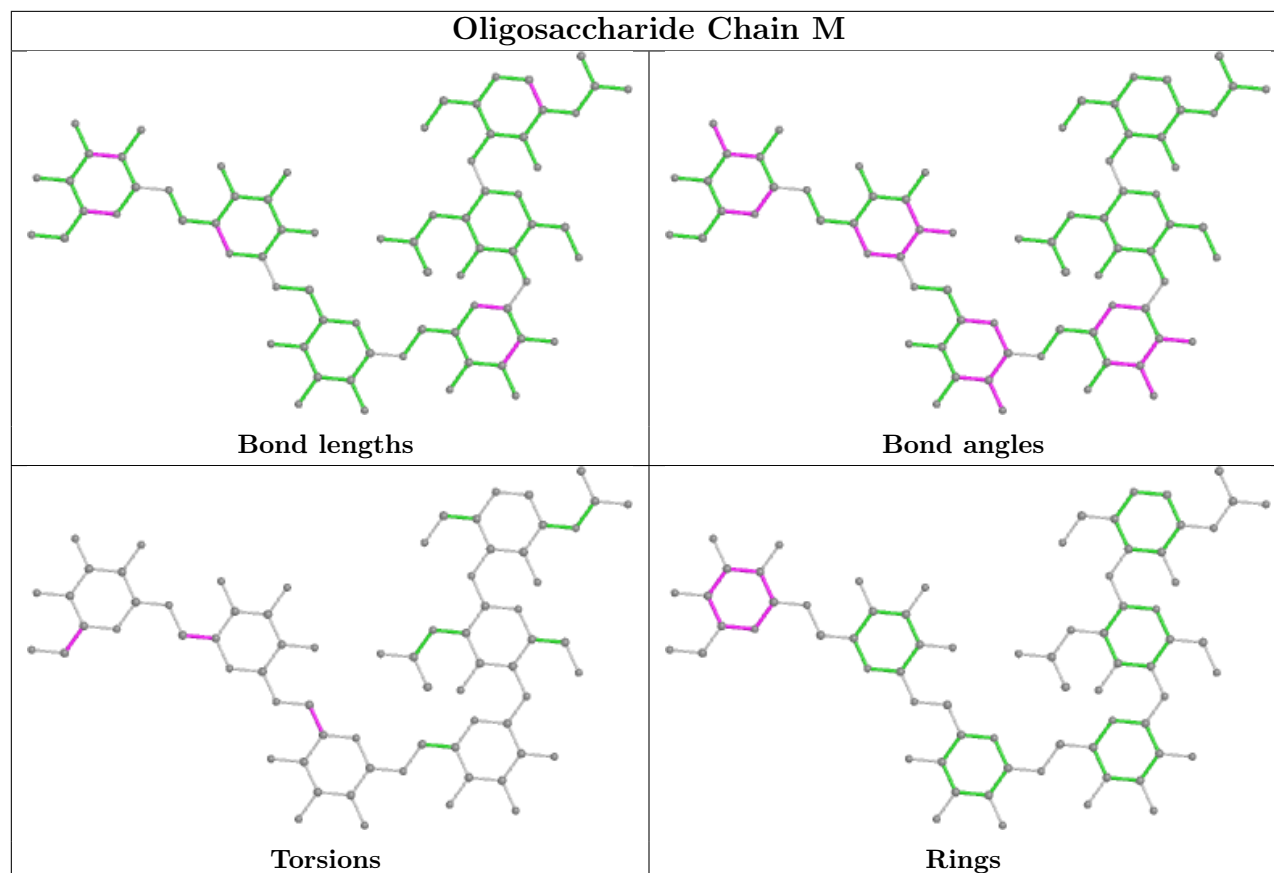


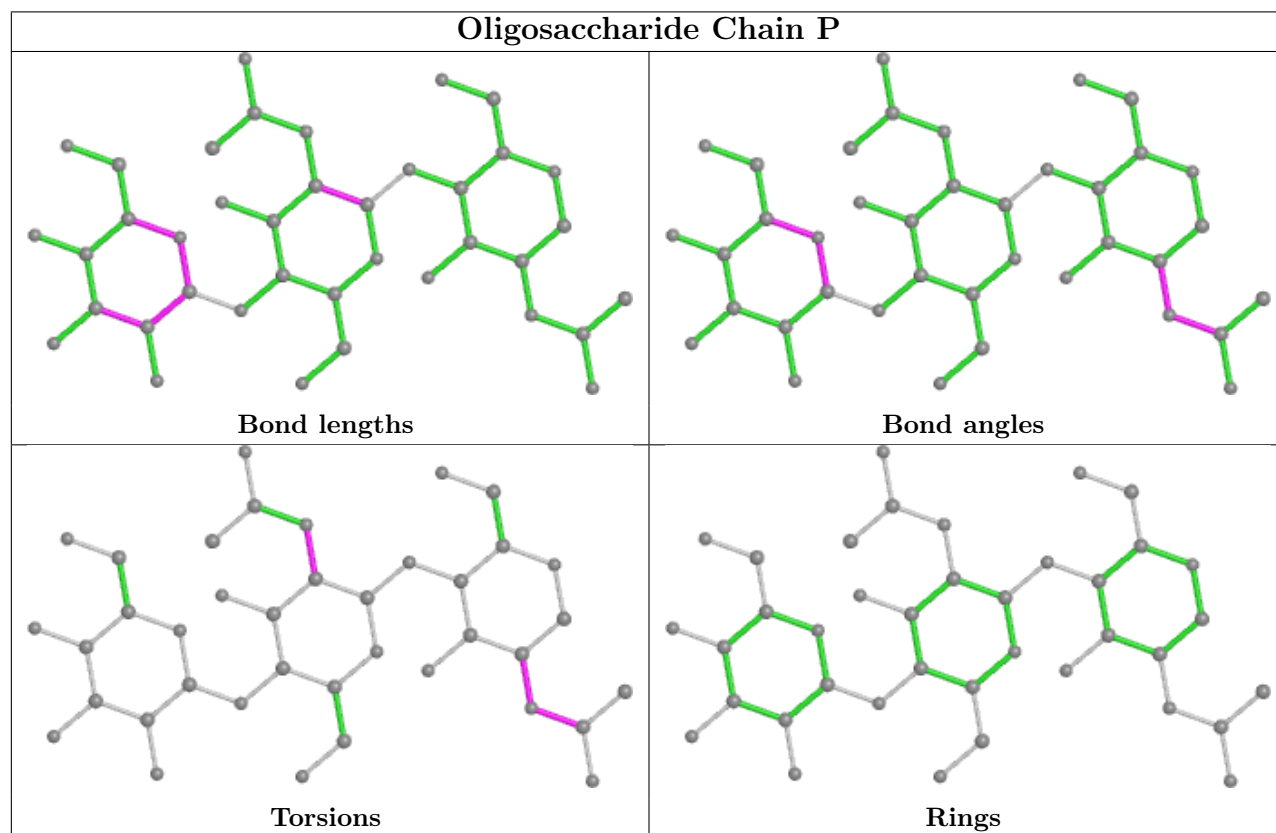
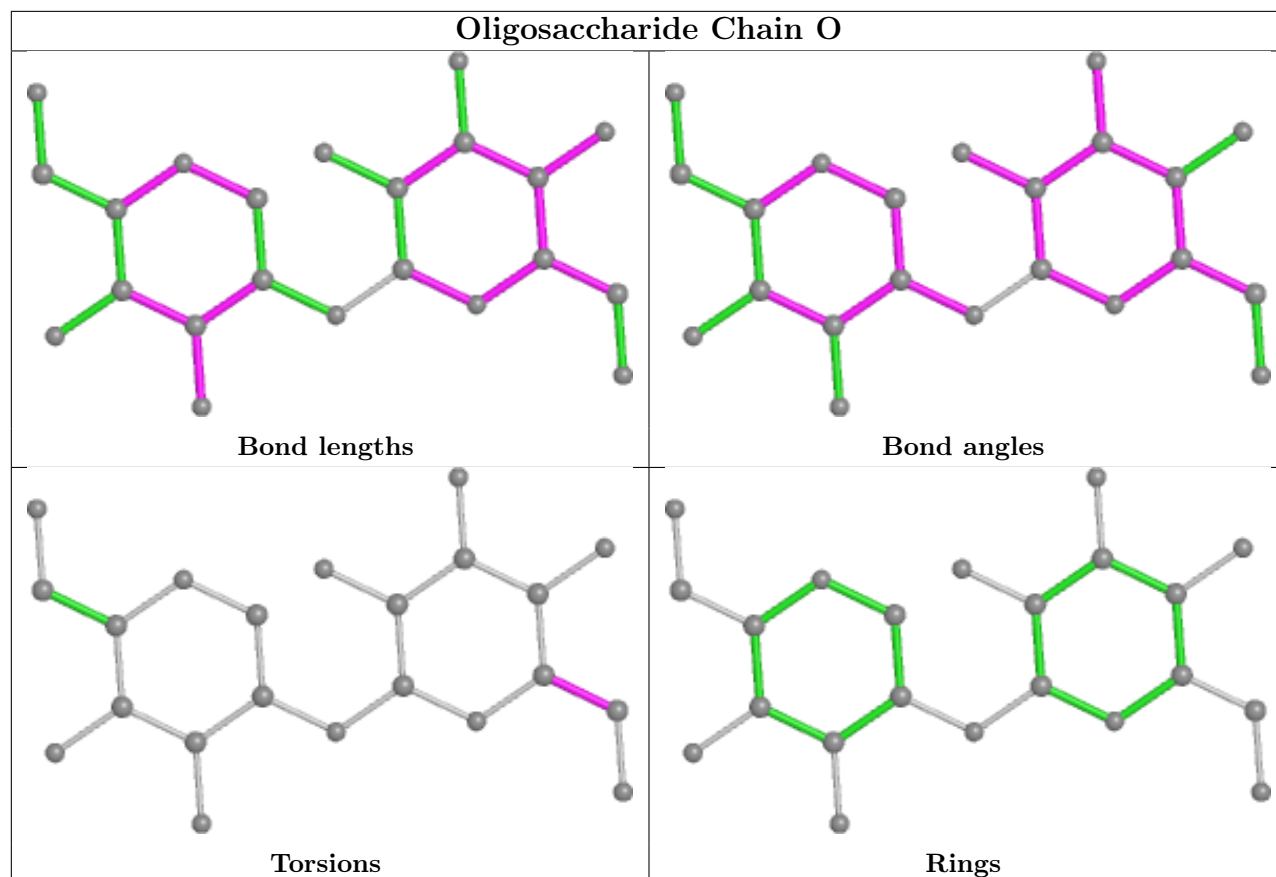
Oligosaccharide Chain J

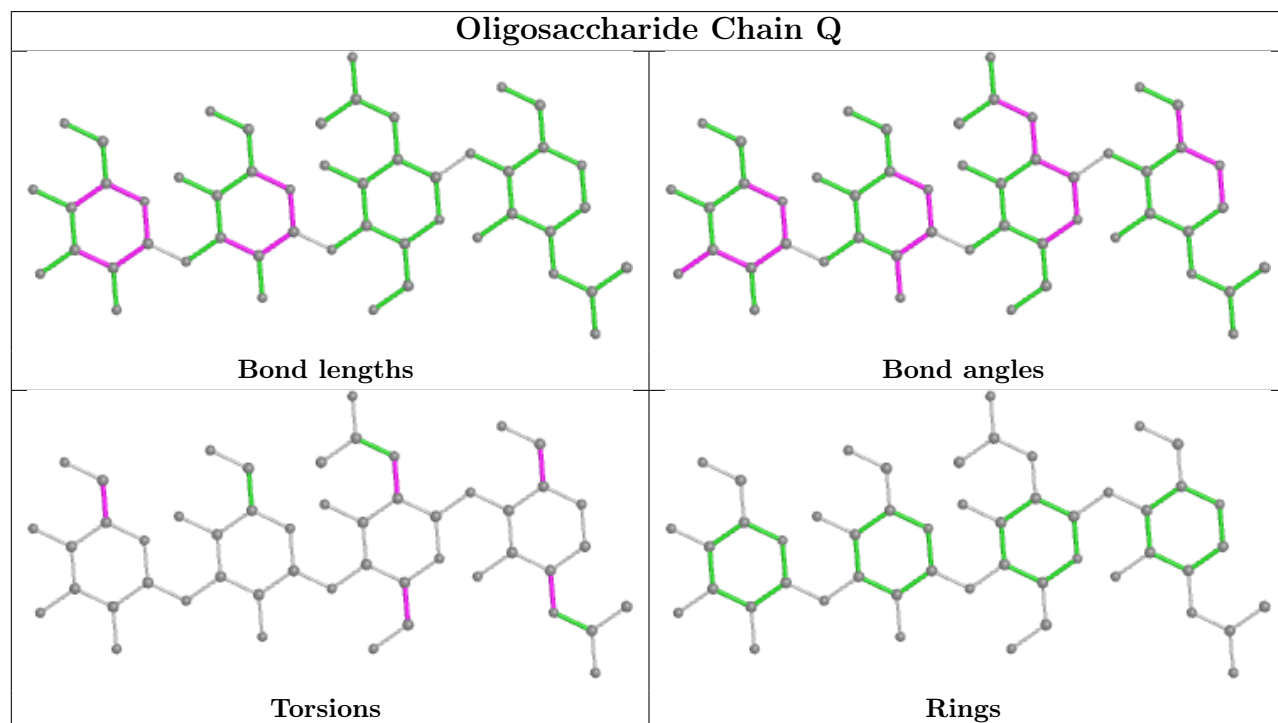
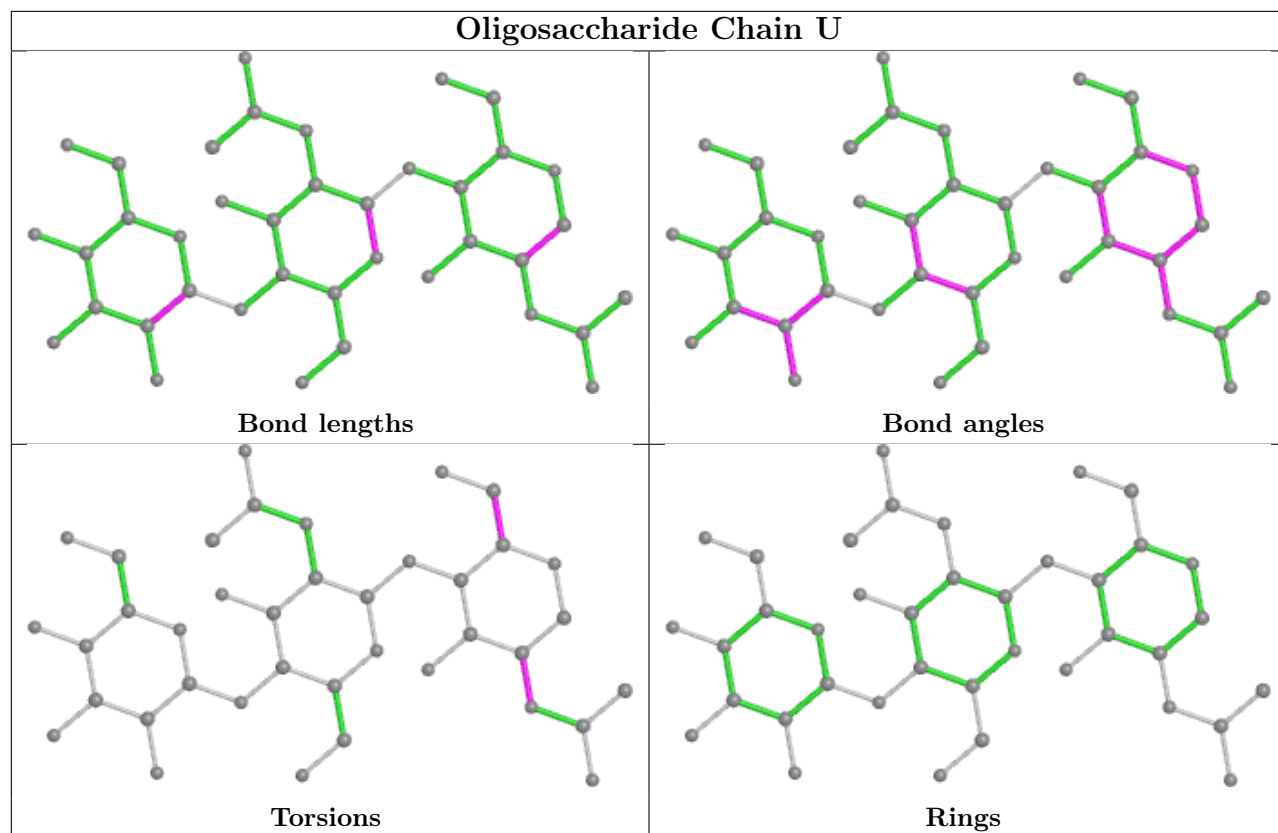


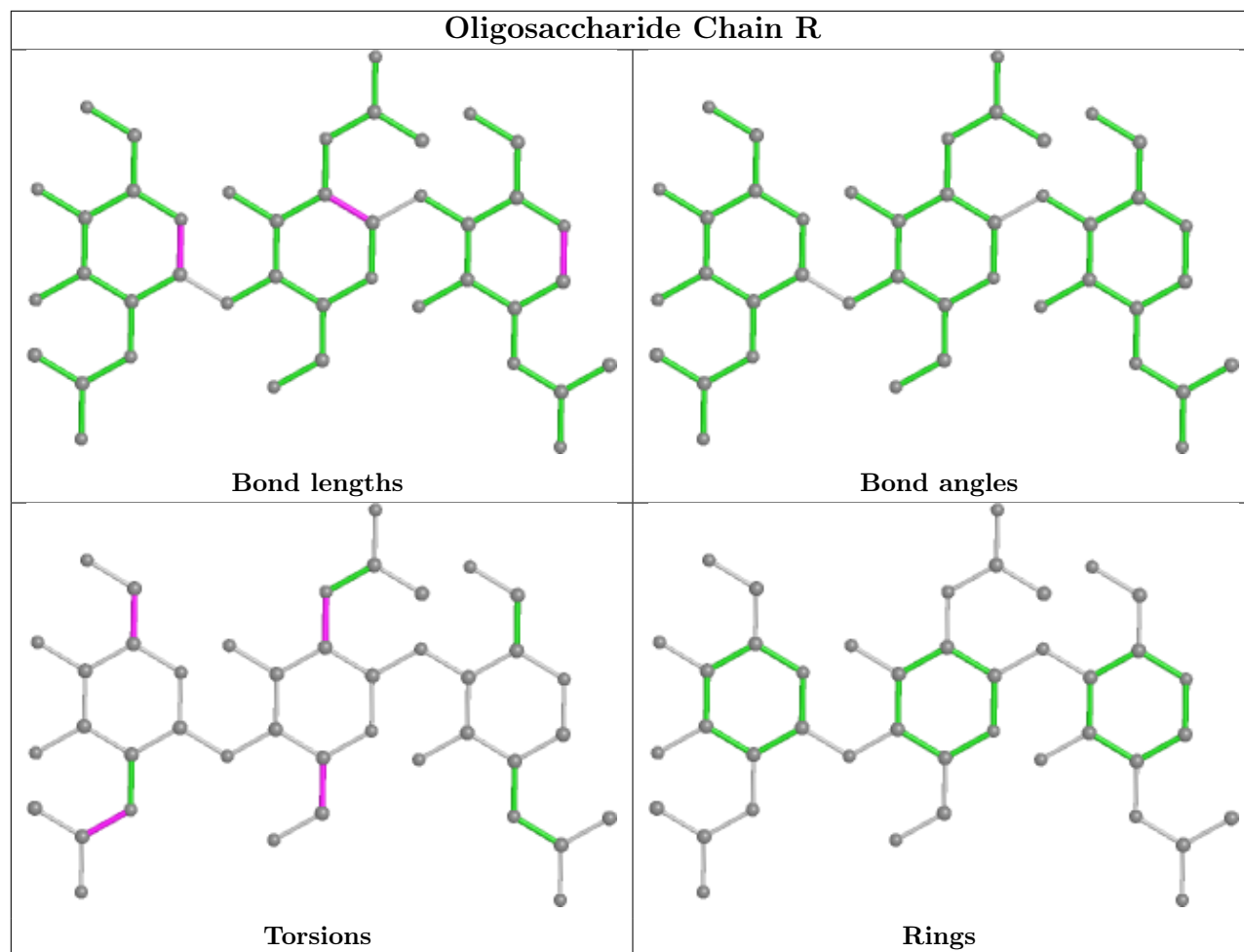
Oligosaccharide Chain K



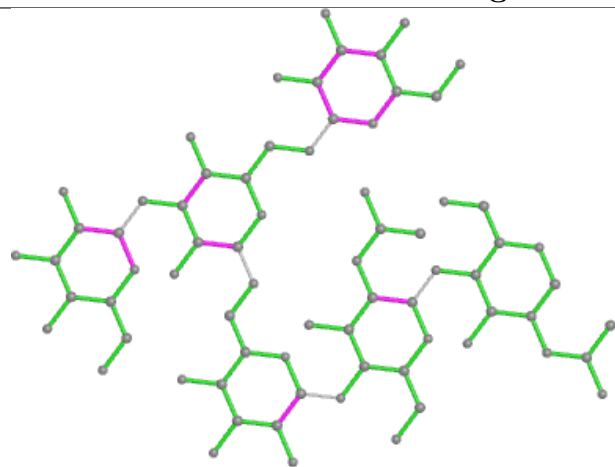




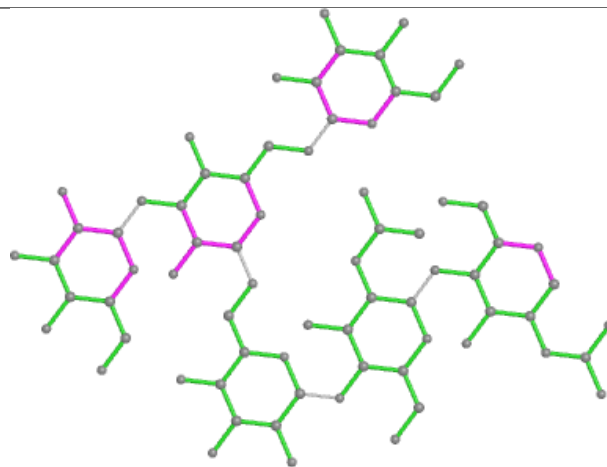




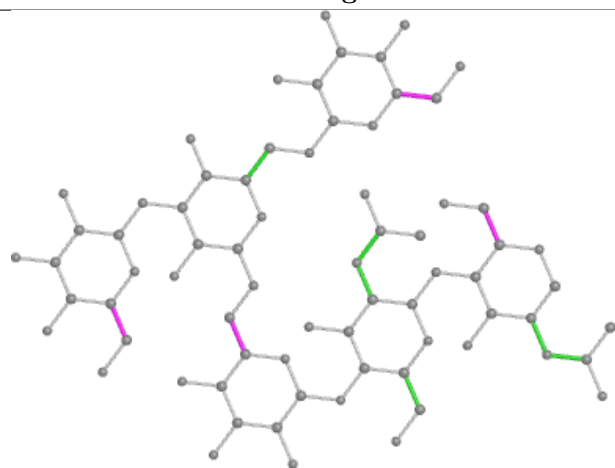
Oligosaccharide Chain S



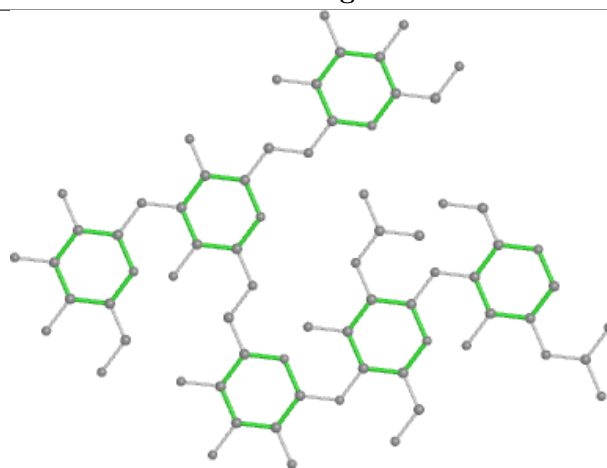
Bond lengths



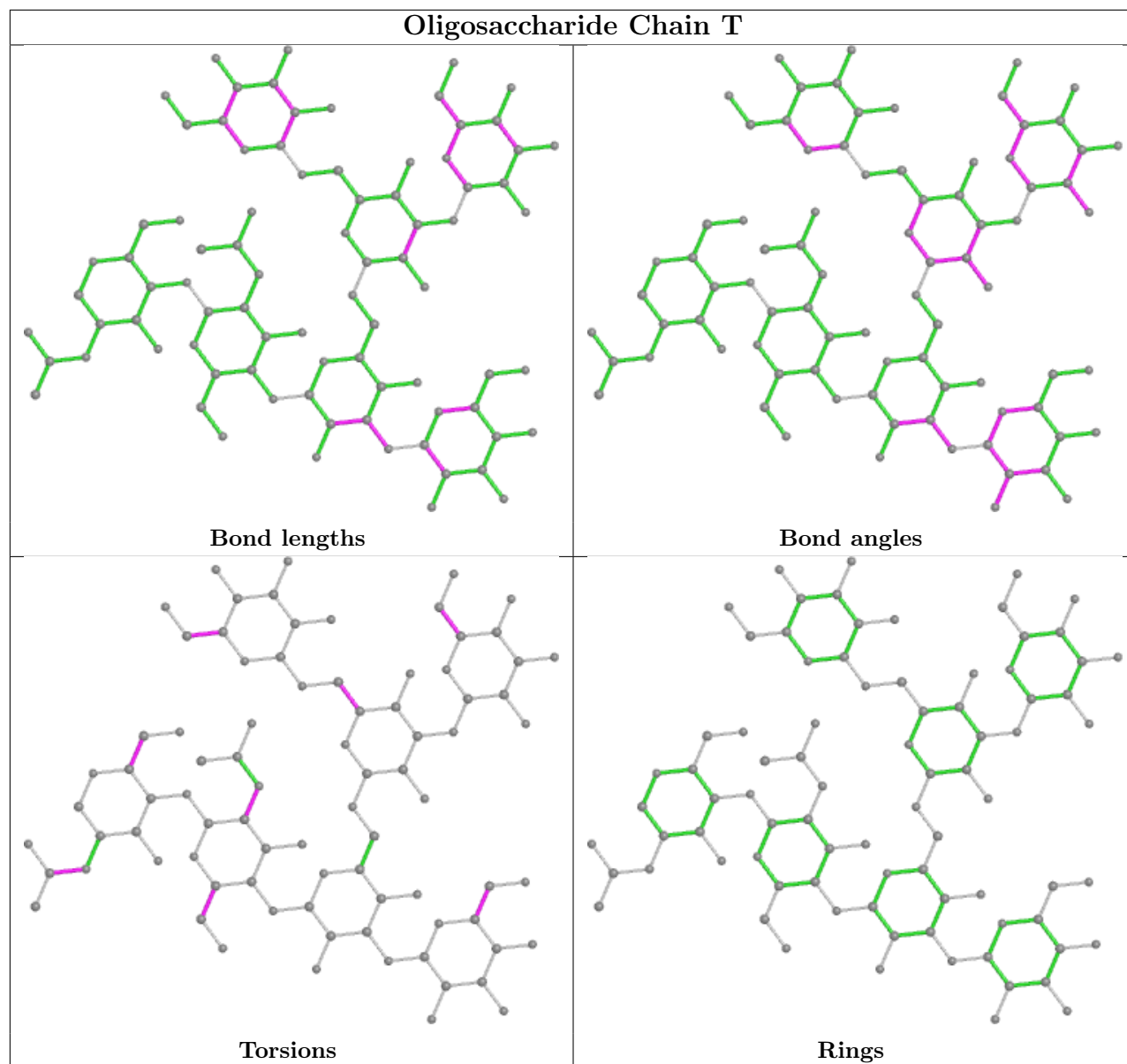
Bond angles

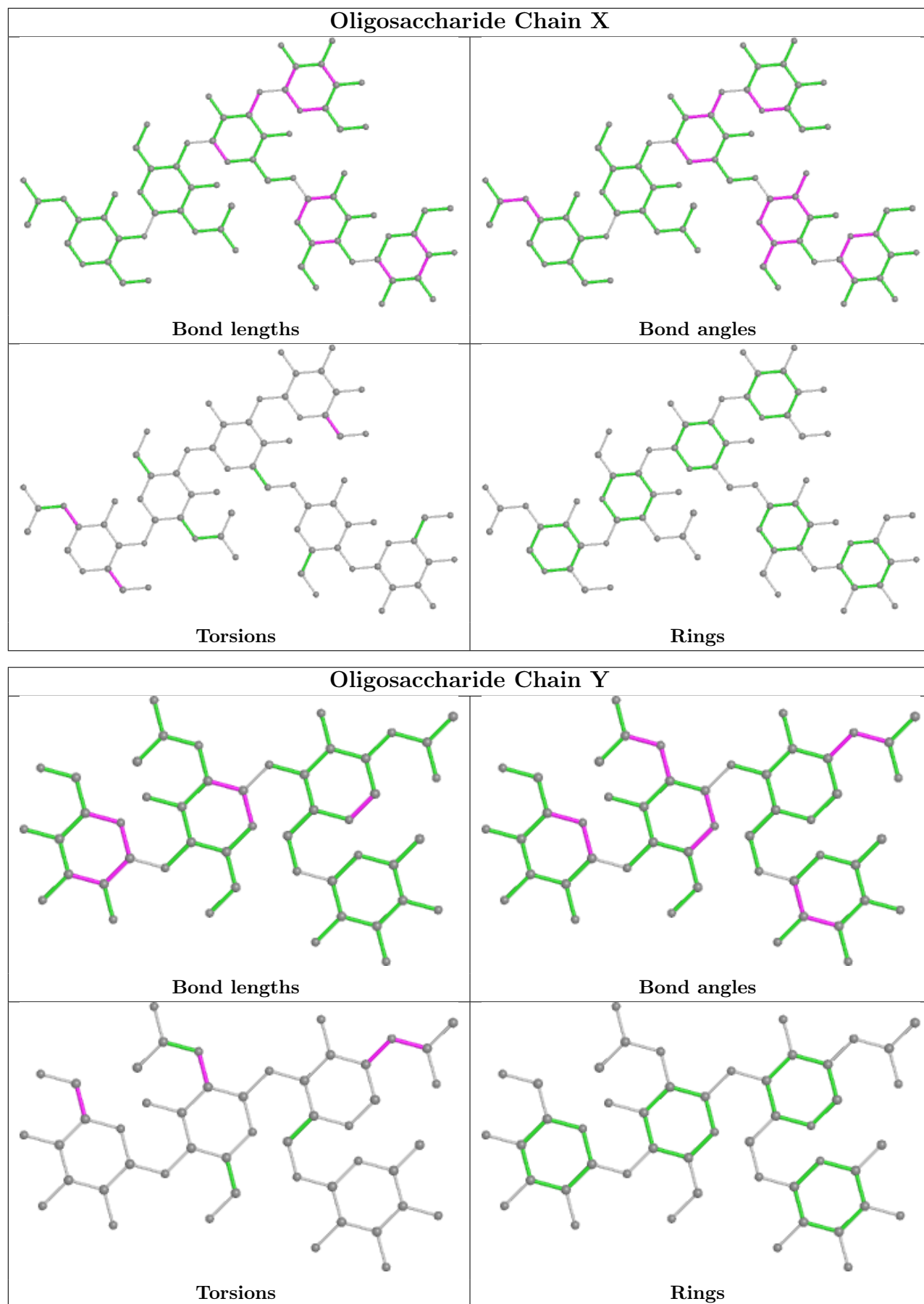


Torsions



Rings





5.6 Ligand geometry

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	G	601	4	14,14,15	0.85	1 (7%)	17,19,21	1.15	1 (5%)
21	NAG	B	701	1	14,14,15	0.49	0	17,19,21	1.34	1 (5%)
22	FUC	G	602	-	10,10,11	2.76	4 (40%)	14,14,16	1.71	5 (35%)
21	NAG	G	603	4	14,14,15	1.06	2 (14%)	17,19,21	1.18	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	G	601	4	-	2/6/23/26	0/1/1/1
21	NAG	B	701	1	-	3/6/23/26	0/1/1/1
22	FUC	G	602	-	-	-	0/1/1/1
21	NAG	G	603	4	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	602	FUC	C4-C3	5.69	1.66	1.52
22	G	602	FUC	C2-C3	4.00	1.58	1.52
22	G	602	FUC	C4-C5	3.66	1.61	1.52
21	G	601	NAG	O5-C1	2.80	1.48	1.43
22	G	602	FUC	O2-C2	2.67	1.49	1.43
21	G	603	NAG	C3-C2	2.30	1.57	1.52
21	G	603	NAG	C1-C2	2.18	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
21	B	701	NAG	C2-N2-C7	4.63	129.50	122.90
21	G	601	NAG	C1-O5-C5	3.58	117.05	112.19
21	G	603	NAG	C2-N2-C7	2.76	126.83	122.90
22	G	602	FUC	C6-C5-C4	2.74	118.13	113.07
22	G	602	FUC	O2-C2-C1	2.62	114.50	109.15
22	G	602	FUC	C1-O5-C5	2.46	118.36	112.78
22	G	602	FUC	O2-C2-C3	2.18	114.50	110.14
22	G	602	FUC	O5-C5-C4	2.09	113.28	109.52

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	B	701	NAG	C3-C2-N2-C7
21	G	601	NAG	C4-C5-C6-O6
21	G	601	NAG	O5-C5-C6-O6
21	B	701	NAG	O5-C5-C6-O6
21	G	603	NAG	C4-C5-C6-O6
21	G	603	NAG	O5-C5-C6-O6
21	B	701	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	701	NAG	1	0
22	G	602	FUC	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	B	137/153 (89%)	0.02	6 (4%)	34 28	218, 288, 324, 337	0
2	D	220/234 (94%)	0.23	19 (8%)	10 9	177, 255, 403, 439	0
3	E	202/205 (98%)	0.13	14 (6%)	16 13	207, 302, 381, 398	0
4	G	451/501 (90%)	-0.09	9 (1%)	65 56	136, 227, 315, 534	0
5	H	229/243 (94%)	0.02	11 (4%)	30 25	172, 254, 348, 408	0
6	L	211/214 (98%)	-0.22	3 (1%)	75 65	173, 251, 336, 360	0
All	All	1450/1550 (93%)	-0.00	62 (4%)	35 29	136, 259, 377, 534	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	507	GLY	9.4
2	D	136	PRO	7.3
2	D	146	ALA	7.2
3	E	169	SER	6.6
4	G	506	VAL	6.1
5	H	203	VAL	6.0
2	D	193	THR	6.0
5	H	204	PRO	5.9
3	E	168	SER	5.9
2	D	190	SER	5.5
1	B	600	GLY	5.4
2	D	220	LYS	4.8
1	B	521	GLY	4.5
2	D	192	VAL	4.5
5	H	208	LEU	4.4
2	D	137	SER	4.4
2	D	194	VAL	4.2
2	D	216	LYS	4.2
5	H	213	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
5	H	145	PRO	3.8
2	D	217	VAL	3.7
4	G	505	VAL	3.7
1	B	599	SER	3.5
2	D	222	GLU	3.5
5	H	230	VAL	3.4
1	B	594	GLY	3.3
3	E	184	TYR	3.3
2	D	205	ILE	3.2
4	G	473	GLY	3.2
2	D	189	SER	3.2
3	E	204	CYS	3.1
3	E	141	TRP	3.1
3	E	186	CYS	3.1
4	G	495	GLY	3.1
3	E	137	VAL	3.0
2	D	208	VAL	2.9
2	D	221	VAL	2.9
2	D	162	VAL	2.8
6	L	124	LEU	2.8
5	H	205	SER	2.8
4	G	63	THR	2.8
5	H	202	THR	2.7
4	G	496	VAL	2.7
5	H	207	SER	2.7
4	G	283	ASN	2.6
2	D	171	SER	2.6
6	L	125	PHE	2.5
2	D	204	TYR	2.5
3	E	170	TYR	2.5
3	E	203	GLU	2.4
1	B	598	CYS	2.4
3	E	98	VAL	2.3
2	D	219	LYS	2.3
5	H	138	PRO	2.2
3	E	124	THR	2.2
5	H	232	PRO	2.2
4	G	474	ASP	2.1
1	B	552	GLN	2.1
6	L	127	PRO	2.1
3	E	9	SER	2.0
3	E	71	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
3	E	10	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	GAL	J	6	11/12	0.39	0.33	340,340,340,340	0
19	MAN	X	6	11/12	0.58	0.30	351,351,351,351	0
9	MAN	I	4	11/12	0.60	0.35	356,356,356,356	0
9	BMA	I	3	11/12	0.65	0.23	358,358,358,358	0
10	BMA	J	3	11/12	0.67	0.12	287,287,287,287	0
17	BMA	S	3	11/12	0.68	0.19	299,299,299,299	0
11	BMA	K	3	11/12	0.68	0.16	308,308,308,308	0
8	NAG	V	2	14/15	0.70	0.25	286,286,286,286	0
19	BMA	X	3	11/12	0.73	0.16	336,336,336,336	0
13	MAN	N	2	11/12	0.74	0.22	280,280,280,280	0
9	MAN	I	5	11/12	0.74	0.33	377,377,377,377	0
14	NAG	P	2	14/15	0.75	0.47	345,345,345,345	0
9	NAG	I	2	14/15	0.75	0.30	313,313,313,313	0
11	MAN	K	4	11/12	0.76	0.42	348,348,348,348	0
18	MAN	T	7	11/12	0.76	0.26	333,333,333,333	0
17	MAN	S	6	11/12	0.77	0.18	316,316,316,316	0
17	MAN	S	4	11/12	0.77	0.14	315,315,315,315	0
14	BMA	P	3	11/12	0.78	0.29	326,326,326,326	0
17	MAN	S	5	11/12	0.80	0.20	305,305,305,305	0
14	NAG	P	1	14/15	0.81	0.26	311,311,311,311	0
16	NAG	R	3	14/15	0.81	0.18	296,296,296,296	0
19	BMA	X	5	11/12	0.81	0.33	344,344,344,344	0
8	NAG	V	1	14/15	0.81	0.25	260,260,260,260	0
14	BMA	U	3	11/12	0.82	0.24	297,297,297,297	0
19	MAN	X	4	11/12	0.82	0.19	338,338,338,338	0
8	NAG	F	1	14/15	0.83	0.20	328,328,328,328	0
7	FUC	A	2	10/11	0.83	0.50	321,321,321,321	0

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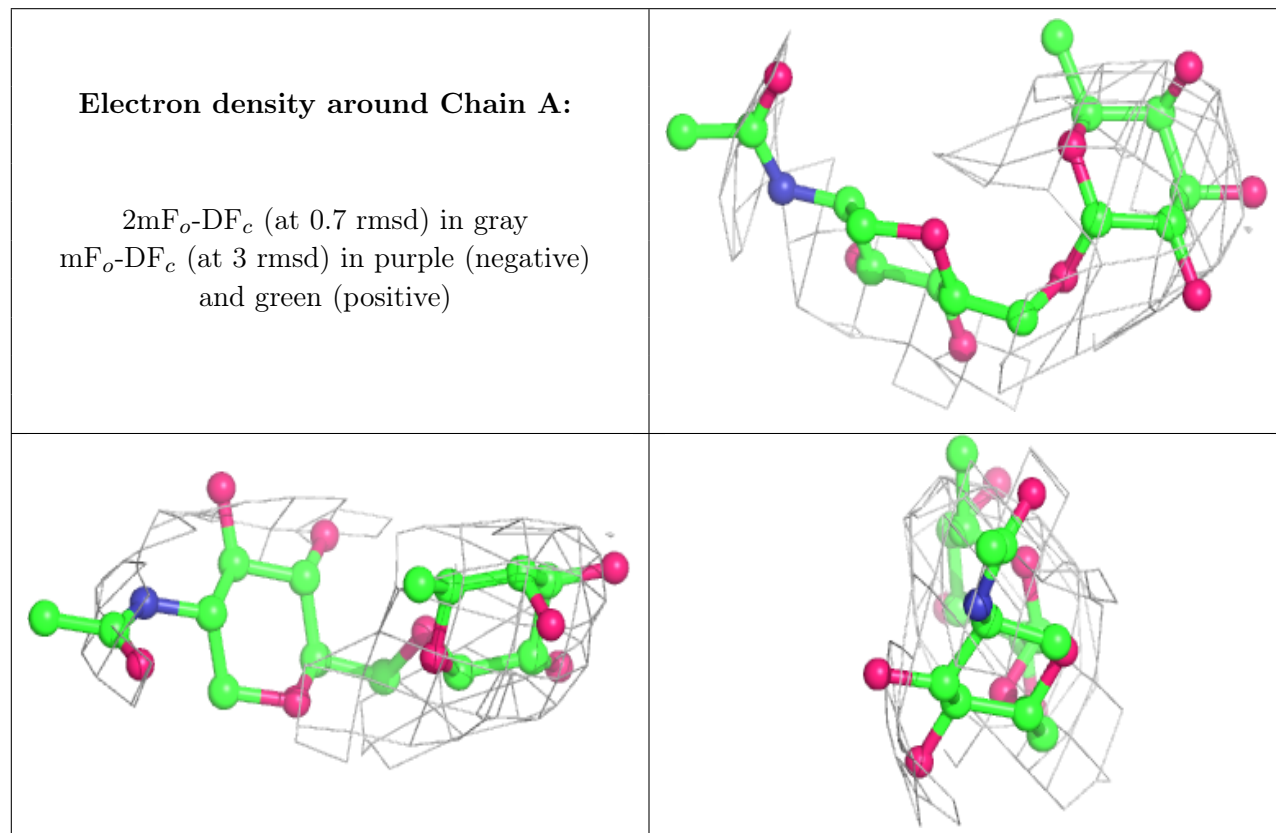
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	BMA	Y	3	11/12	0.83	0.12	305,305,305,305	0
18	BMA	T	3	11/12	0.84	0.23	318,318,318,318	0
10	NAG	J	5	14/15	0.84	0.41	332,332,332,332	0
19	NAG	X	1	14/15	0.84	0.19	232,232,232,232	0
7	NAG	A	1	14/15	0.84	0.38	322,322,322,322	0
18	MAN	T	5	11/12	0.85	0.28	291,291,291,291	0
18	MAN	T	6	11/12	0.85	0.17	272,272,272,272	0
20	NAG	Y	1	14/15	0.85	0.22	316,316,316,316	0
12	MAN	M	5	11/12	0.85	0.24	277,277,277,277	0
10	MAN	J	7	11/12	0.86	0.20	290,290,290,290	0
16	NAG	R	2	14/15	0.86	0.20	272,272,272,272	0
10	MAN	J	4	11/12	0.86	0.28	308,308,308,308	0
17	NAG	S	1	14/15	0.88	0.28	215,215,215,215	0
8	NAG	W	2	14/15	0.88	0.29	288,288,288,288	0
9	NAG	I	1	14/15	0.89	0.29	266,266,266,266	0
18	MAN	T	4	11/12	0.89	0.10	290,290,290,290	0
12	MAN	M	6	11/12	0.89	0.27	273,273,273,273	0
20	FUC	Y	4	10/11	0.89	0.62	313,313,313,313	0
8	NAG	W	1	14/15	0.90	0.13	246,246,246,246	0
13	MAN	N	1	11/12	0.90	0.11	258,258,258,258	0
20	NAG	Y	2	14/15	0.90	0.20	336,336,336,336	0
18	NAG	T	2	14/15	0.90	0.23	303,303,303,303	0
10	NAG	J	1	14/15	0.90	0.20	273,273,273,273	0
15	NAG	Q	2	14/15	0.91	0.18	239,239,239,239	0
15	BMA	Q	3	11/12	0.91	0.14	267,267,267,267	0
8	NAG	F	2	14/15	0.91	0.50	347,347,347,347	0
12	MAN	M	4	11/12	0.91	0.16	248,248,248,248	0
13	MAN	O	1	11/12	0.92	0.15	204,204,204,204	0
16	NAG	R	1	14/15	0.92	0.27	213,213,213,213	0
12	NAG	M	1	14/15	0.93	0.24	200,200,200,200	0
12	NAG	M	2	14/15	0.93	0.18	203,203,203,203	0
11	NAG	K	1	14/15	0.93	0.13	238,238,238,238	0
14	NAG	U	1	14/15	0.93	0.21	234,234,234,234	0
14	NAG	U	2	14/15	0.93	0.15	264,264,264,264	0
11	NAG	K	2	14/15	0.93	0.08	282,282,282,282	0
15	NAG	Q	1	14/15	0.93	0.24	230,230,230,230	0
13	MAN	O	2	11/12	0.93	0.13	202,202,202,202	0
19	NAG	X	2	14/15	0.94	0.11	280,280,280,280	0
17	NAG	S	2	14/15	0.94	0.32	282,282,282,282	0
10	NAG	J	2	14/15	0.94	0.11	281,281,281,281	0
15	MAN	Q	4	11/12	0.95	0.12	245,245,245,245	0
12	BMA	M	3	11/12	0.96	0.12	213,213,213,213	0

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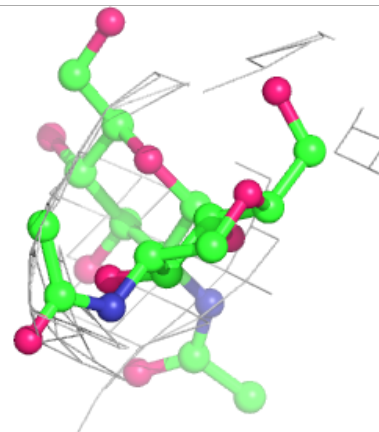
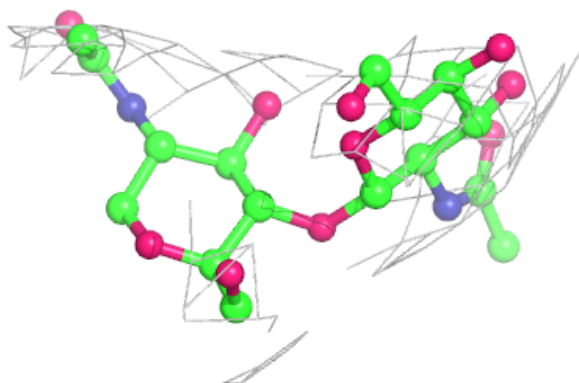
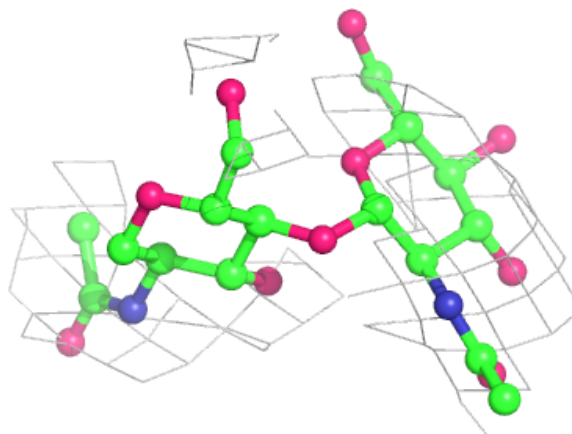
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	NAG	T	1	14/15	0.97	0.14	250,250,250,250	0

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



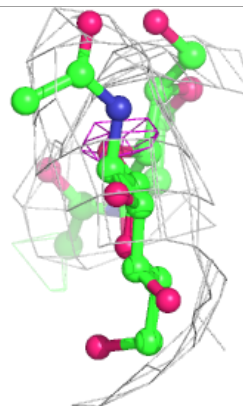
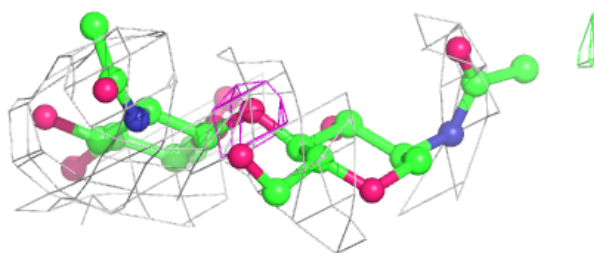
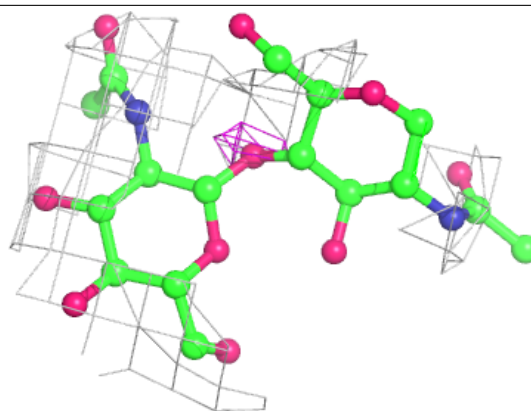
Electron density around Chain F:

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

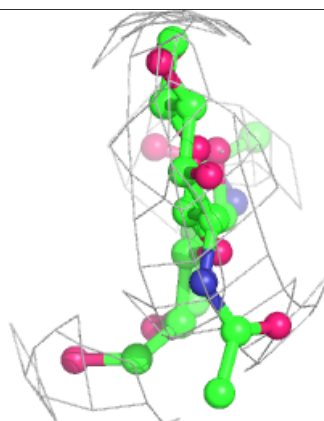
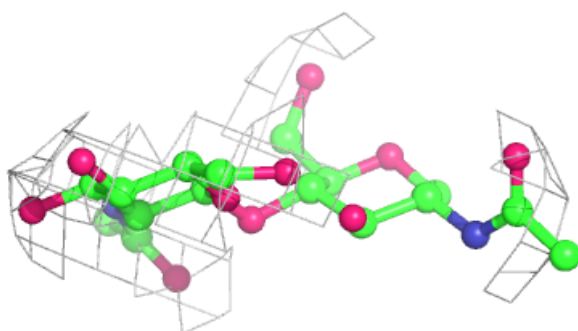
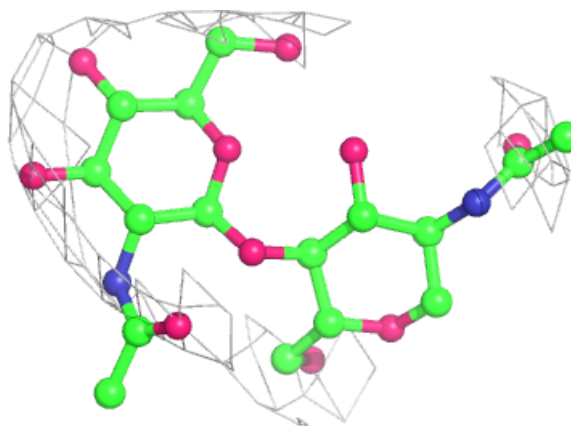


Electron density around Chain V:

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

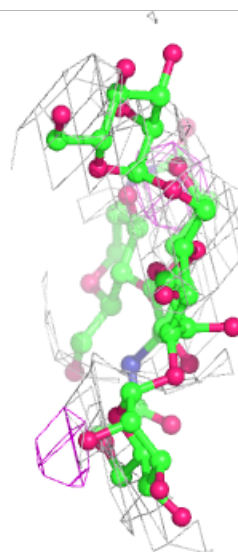
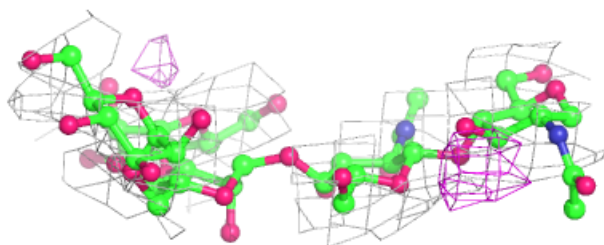
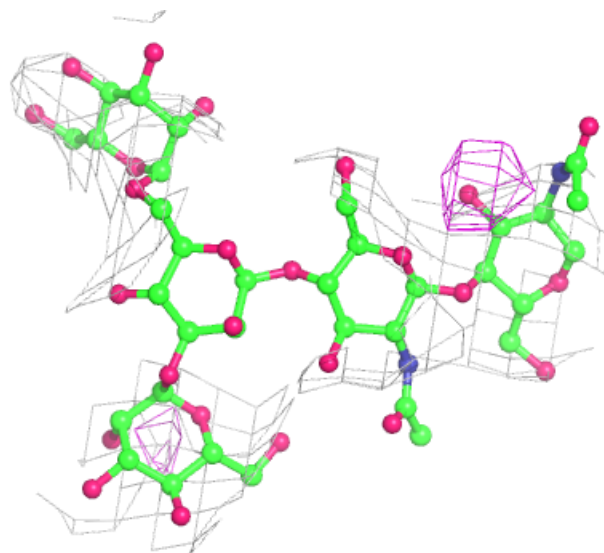
**Electron density around Chain W:**

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



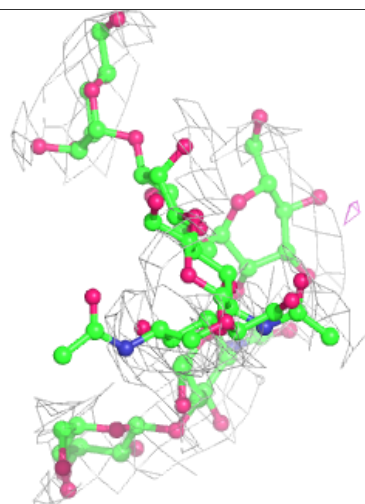
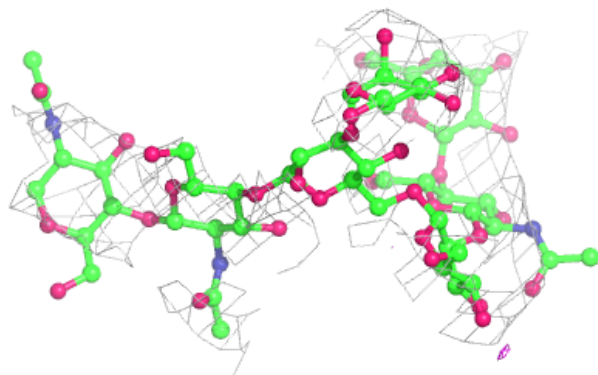
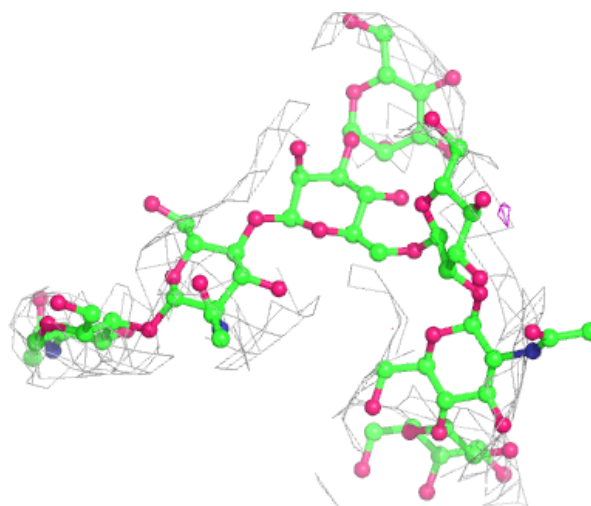
Electron density around Chain I:

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



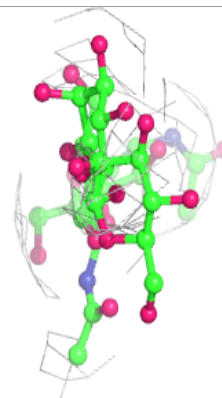
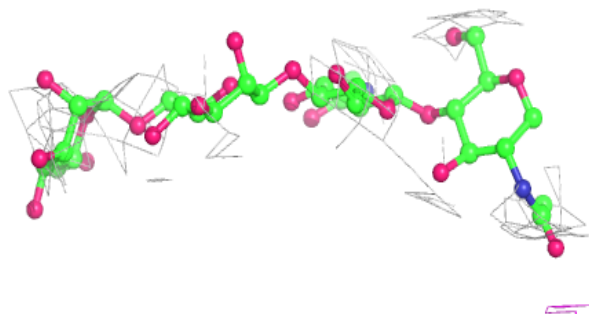
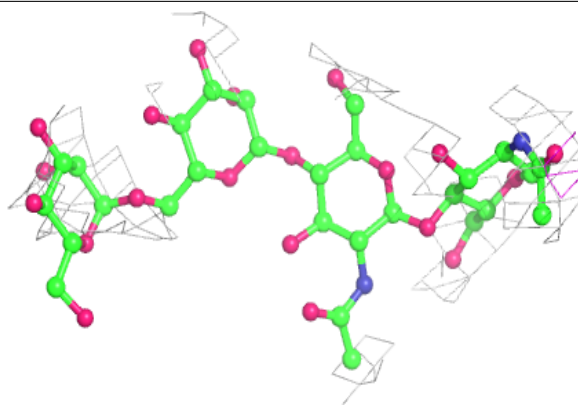
Electron density around Chain J:

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

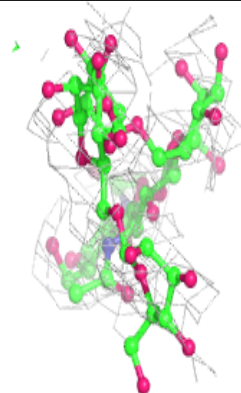
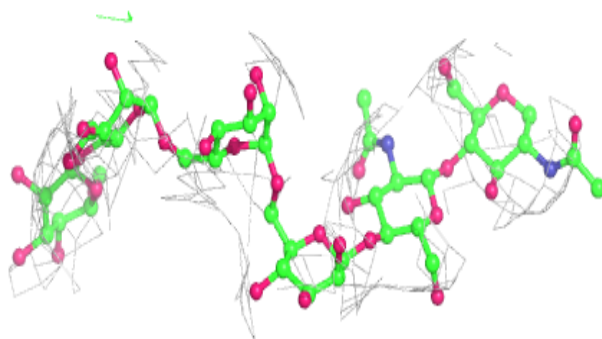
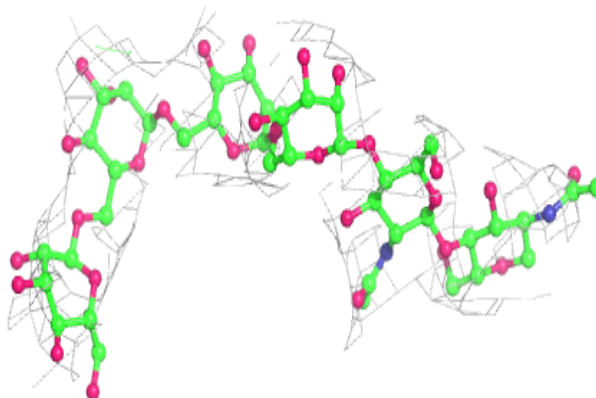


Electron density around Chain K:

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

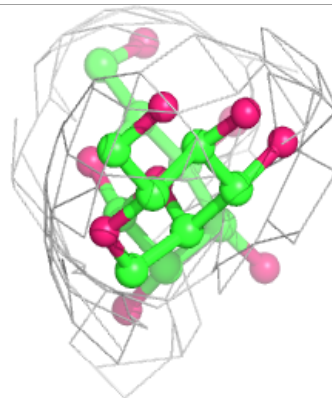
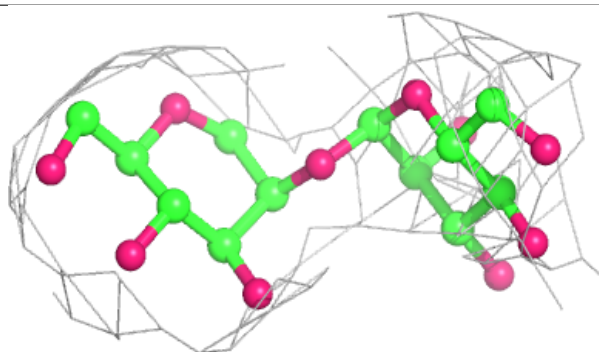
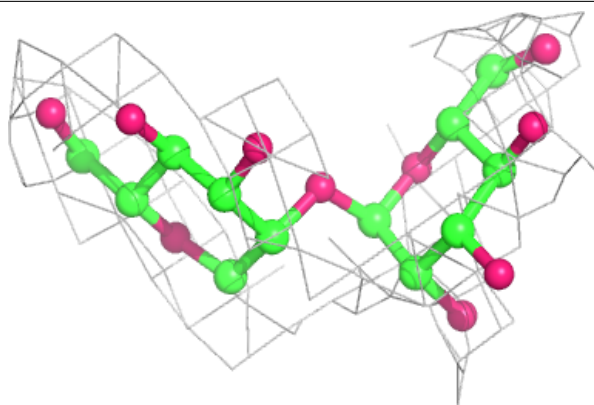
**Electron density around Chain M:**

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

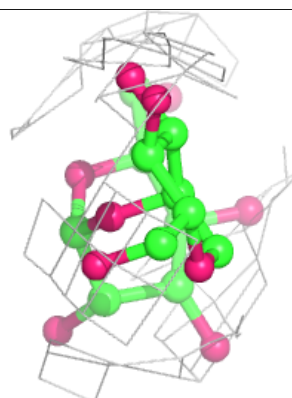
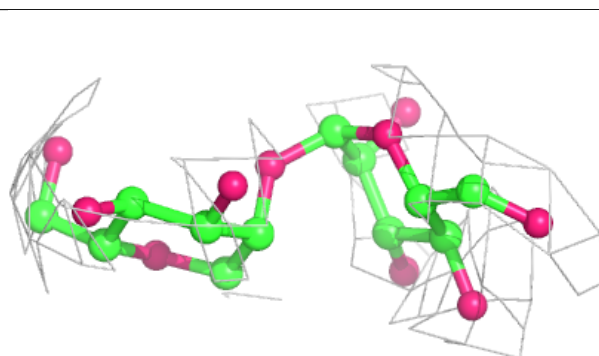
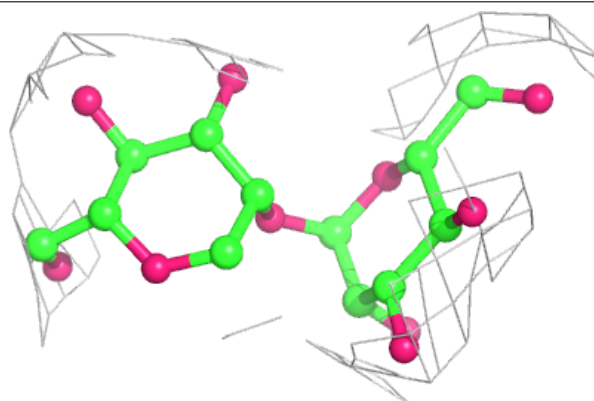


Electron density around Chain N:

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

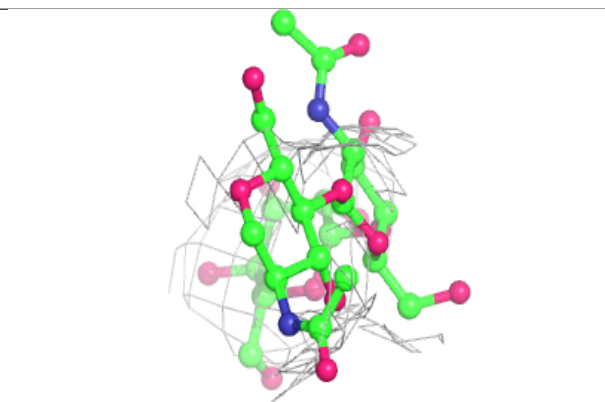
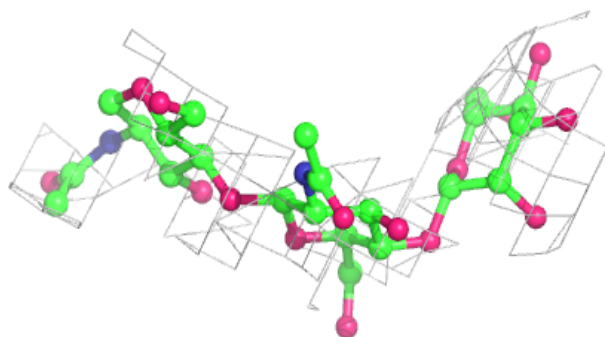
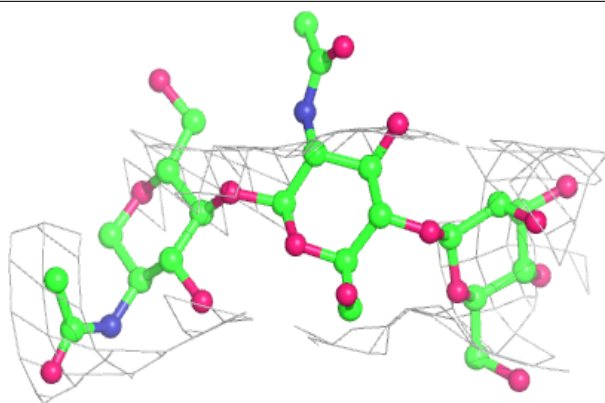
**Electron density around Chain O:**

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

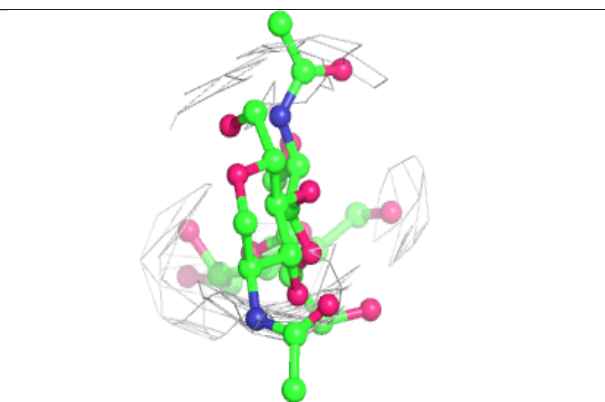
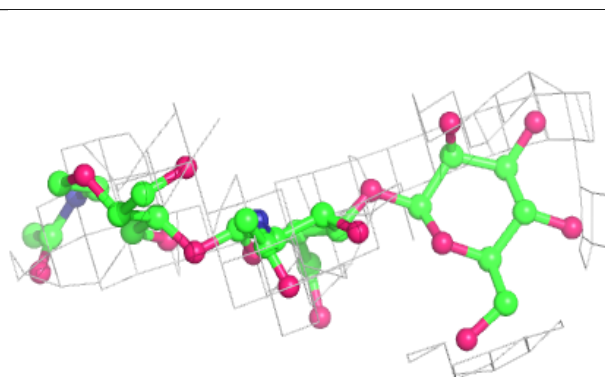
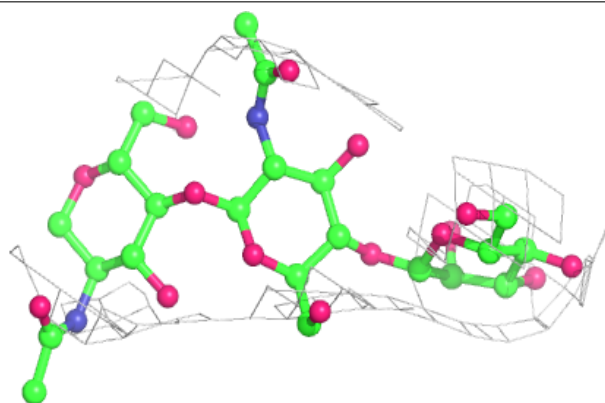


Electron density around Chain P:

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

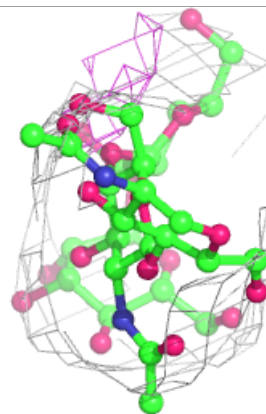
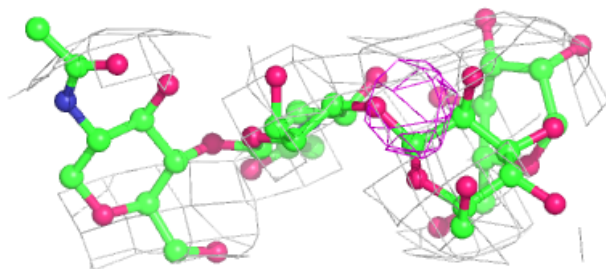
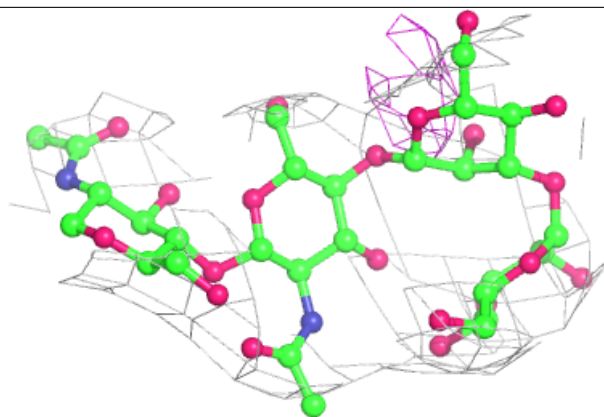
**Electron density around Chain U:**

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

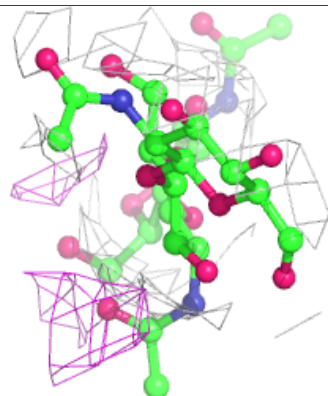
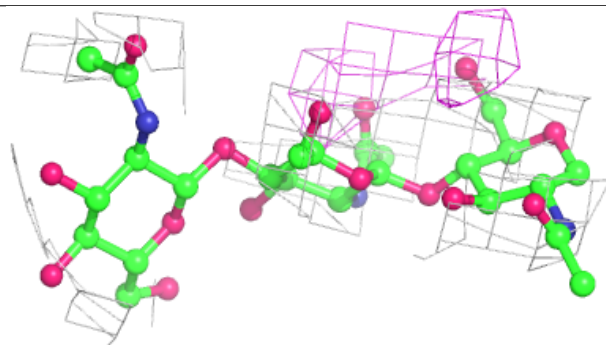
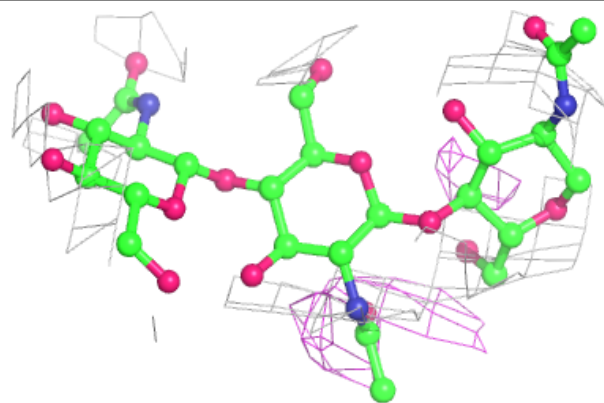


Electron density around Chain Q:

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

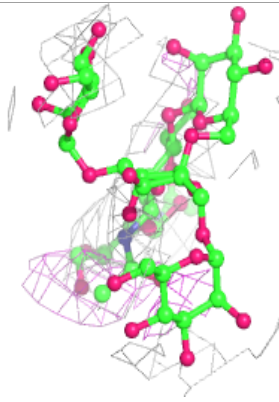
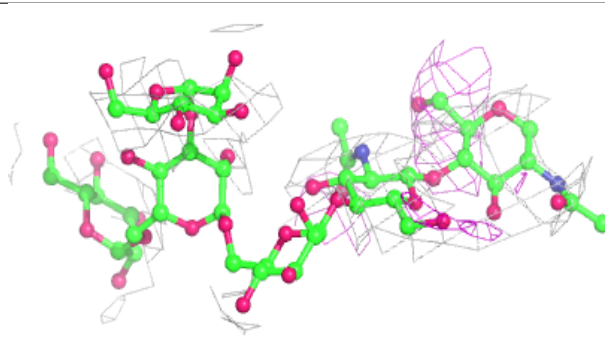
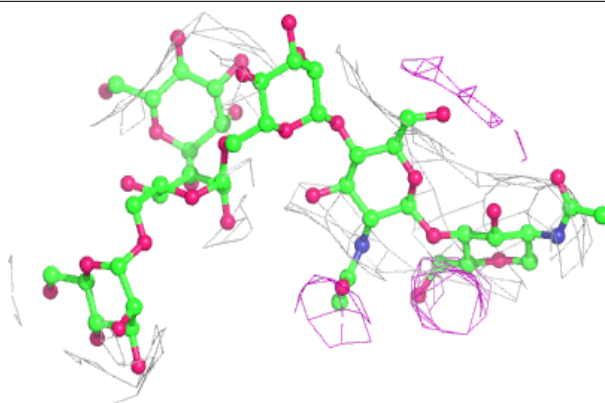
**Electron density around Chain R:**

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



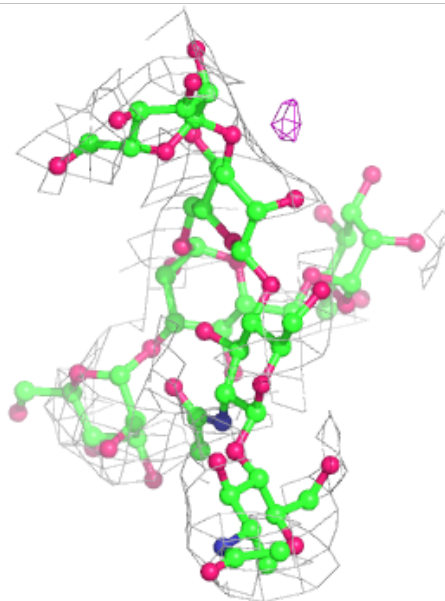
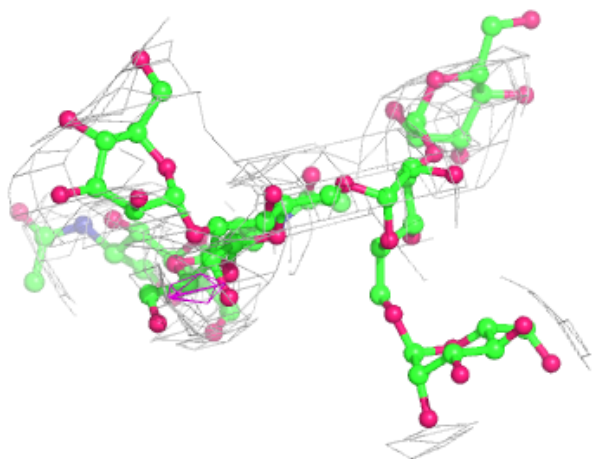
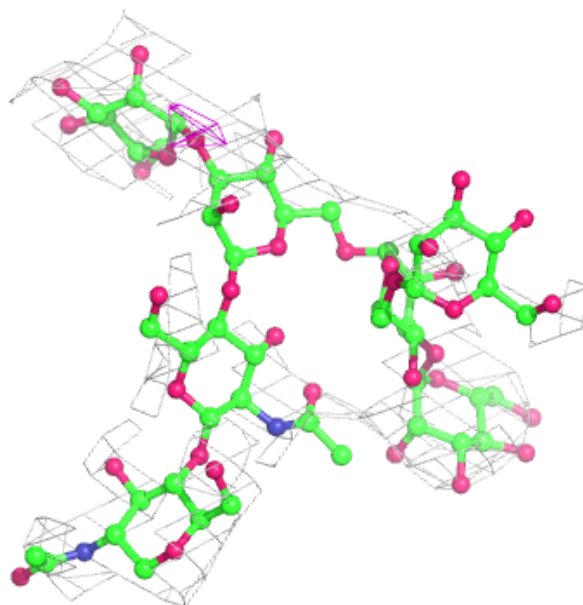
Electron density around Chain S:

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



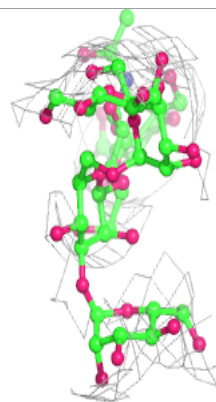
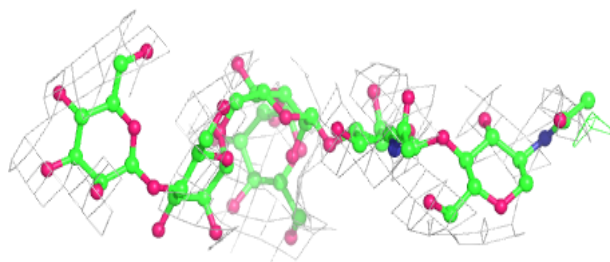
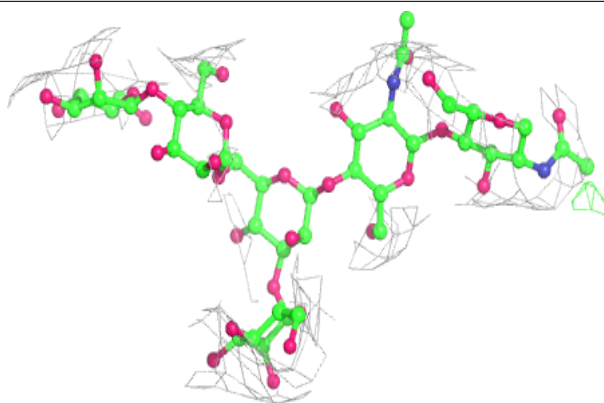
Electron density around Chain T:

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

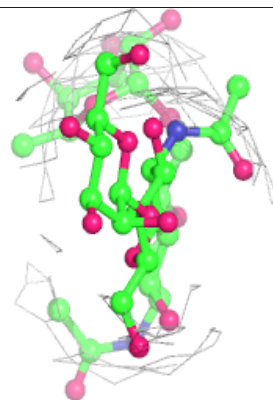
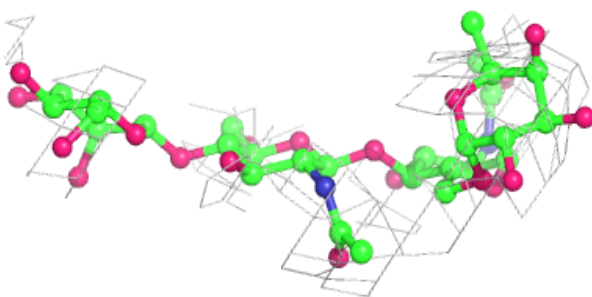
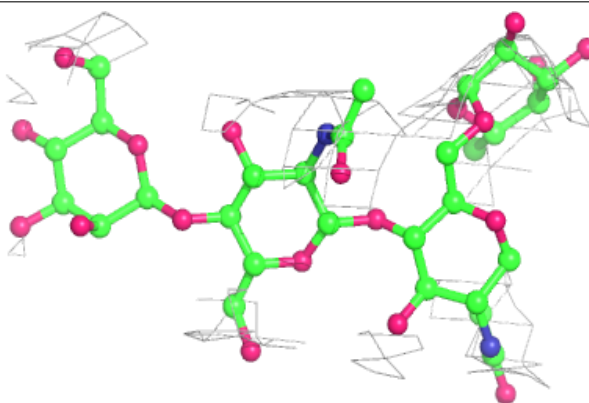


Electron density around Chain X:

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

**Electron density around Chain Y:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	FUC	G	602	10/11	0.40	1.02	262,262,262,262	0
21	NAG	G	601	14/15	0.75	0.36	268,268,268,268	0
21	NAG	B	701	14/15	0.76	0.34	309,309,309,309	0
21	NAG	G	603	14/15	0.88	0.15	262,262,262,262	0

6.5 Other polymers [i](#)

There are no such residues in this entry.