



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:11 AM UTC

PDB ID : 6CH7 / pdb_00006ch7
Title : XFEL crystal structure of a natively-glycosylated BG505 SOSIP.664 HIV-1 Envelope Trimer in complex with the broadly-neutralizing antibodies BG18 and 35O22
Authors : Barnes, C.O.; Bjorkman, P.J.
Deposited on : 2018-02-22
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

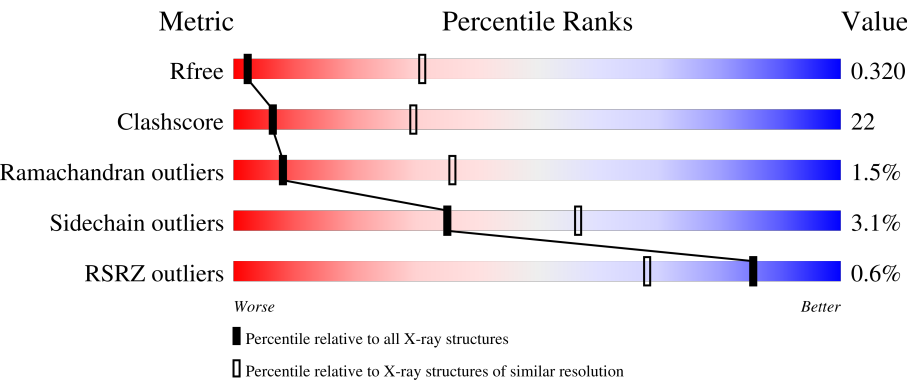
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	61%23%•12%
2	D	243	58%32%•7%
3	E	216	% 63%32%••
4	G	479	58%34%•6%
5	Q	241	64%29%••

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Mol	Chain	Length	Quality of chain
6	R	215	 2% 59% 34% 5%
7	A	5	 100%
8	C	8	 12% 62% 25%
9	F	8	 25% 75%
10	H	3	 33% 33% 33%
10	J	3	 67% 33%
10	M	3	 67% 33%
11	I	4	 50% 50%
12	K	7	 29% 57% 14%
13	L	6	 33% 17% 50%
14	N	2	 50% 50%
15	O	7	 29% 29% 43%
16	P	7	 57% 43%
17	S	6	 33% 50% 17%
18	T	9	 22% 67% 11%

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 12160 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	134	Total	C	N	O	S	0	0	0
			1068	675	186	201	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	engineered mutation	UNP Q2N0S7

- Molecule 2 is a protein called 35O22 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	226	Total	C	N	O	S	0	0	0
			1708	1086	287	328	7			

- Molecule 3 is a protein called 35O22 Light Chain.

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

- Molecule 4 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	452	Total	C	N	O	S	0	0	0
			3546	2224	628	667	27			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	152	THR	GLY	conflict	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6

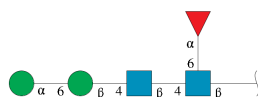
- Molecule 5 is a protein called BG18 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Q	231	Total	C	N	O	S	0	0	0
			1709	1077	291	333	8			

- Molecule 6 is a protein called BG18 Light Chain.

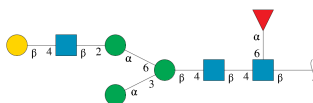
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	R	211	Total	C	N	O	S	0	0	0
			1527	958	255	308	6			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



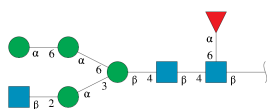
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	A	5	Total	C	N	O	0	0	0
			60	34	2	24			

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



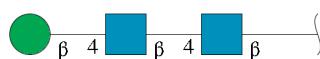
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	C	8	Total	C	N	O	0	0	0
			96	54	3	39			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	F	8	Total	C	N	O	0	0	0
			96	54	3	39			

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



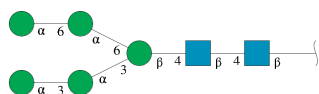
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
10	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
10	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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.



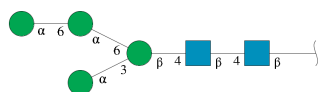
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



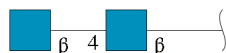
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	K	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



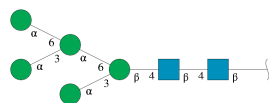
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



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

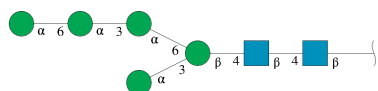
- Molecule 15 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

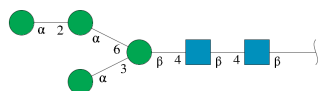
- Molecule 16 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

ucopyranose.



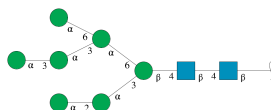
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	P	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 17 is an oligosaccharide called alpha-D-mannopyranose-(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.



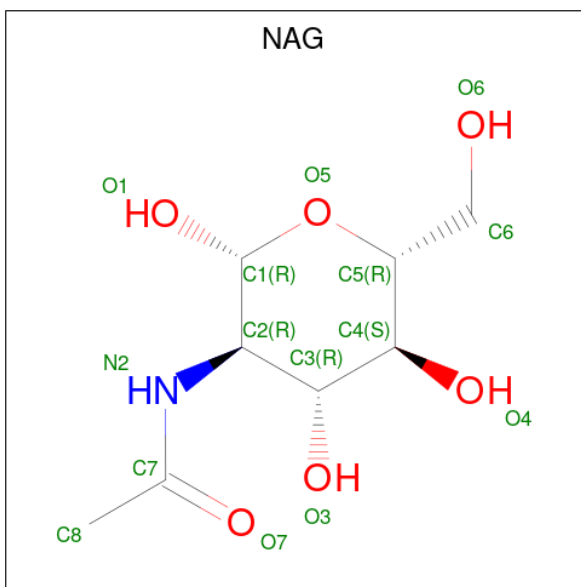
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	S	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



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

- Molecule 19 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



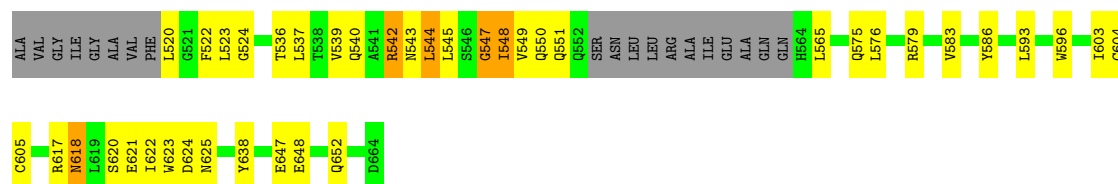
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	B	1	Total	C	N	O	0	0
			14	8	1	5		
19	G	1	Total	C	N	O	0	0
			14	8	1	5		
19	G	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

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

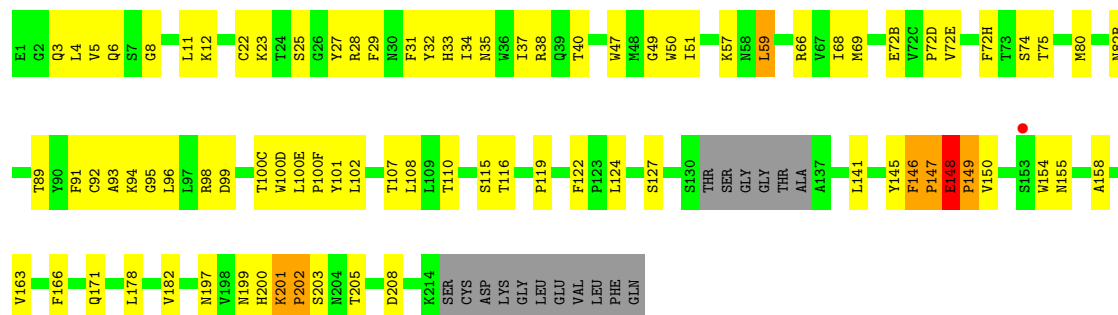
• Molecule 1: Envelope glycoprotein gp41

Chain B: 



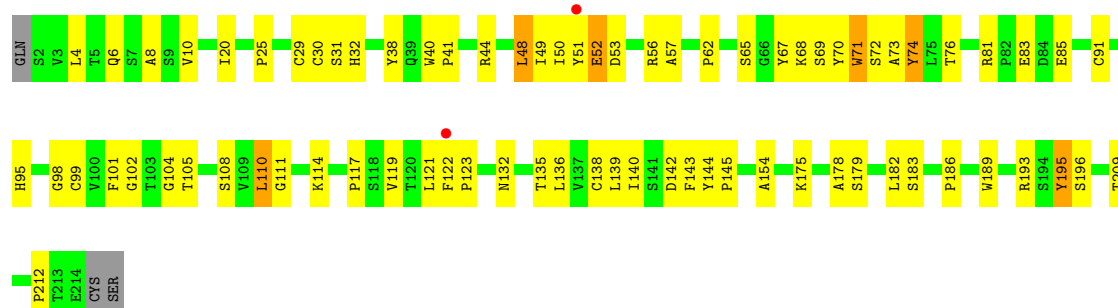
• Molecule 2: 35O22 Heavy Chain

Chain D: 

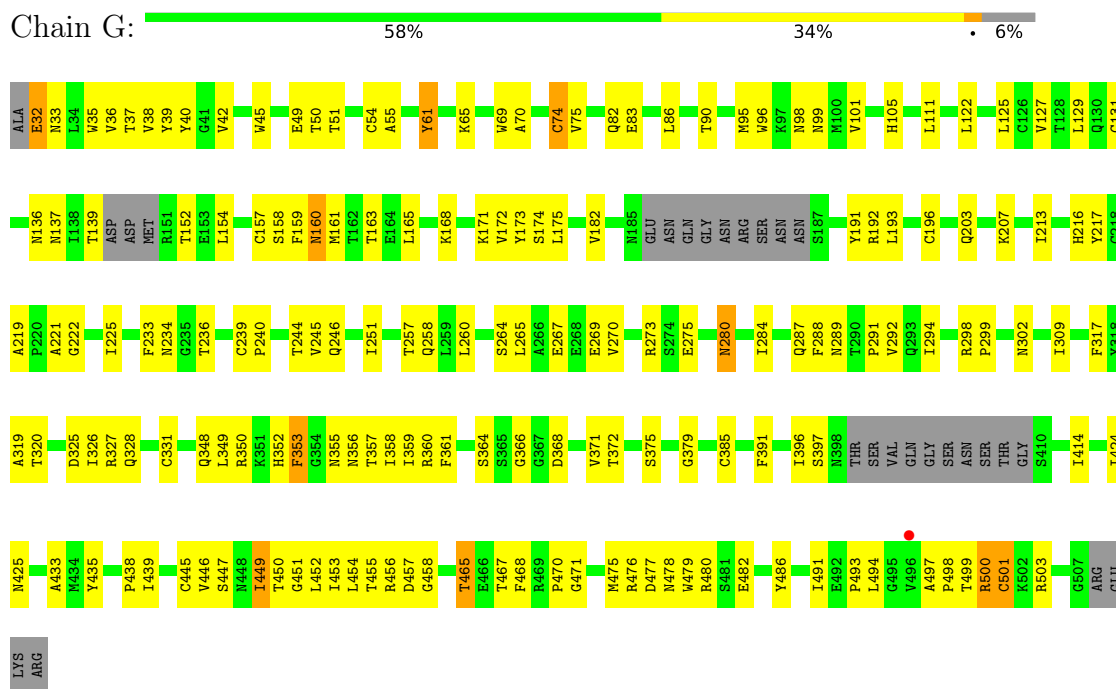


• Molecule 3: 35O22 Light Chain

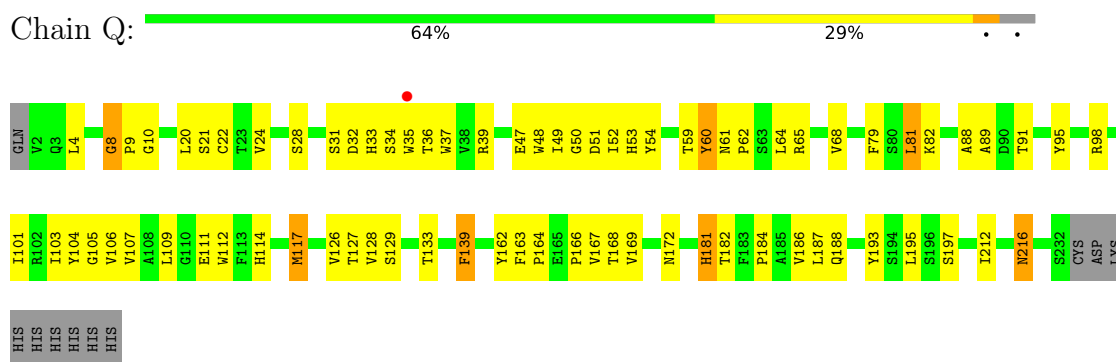
Chain E: 



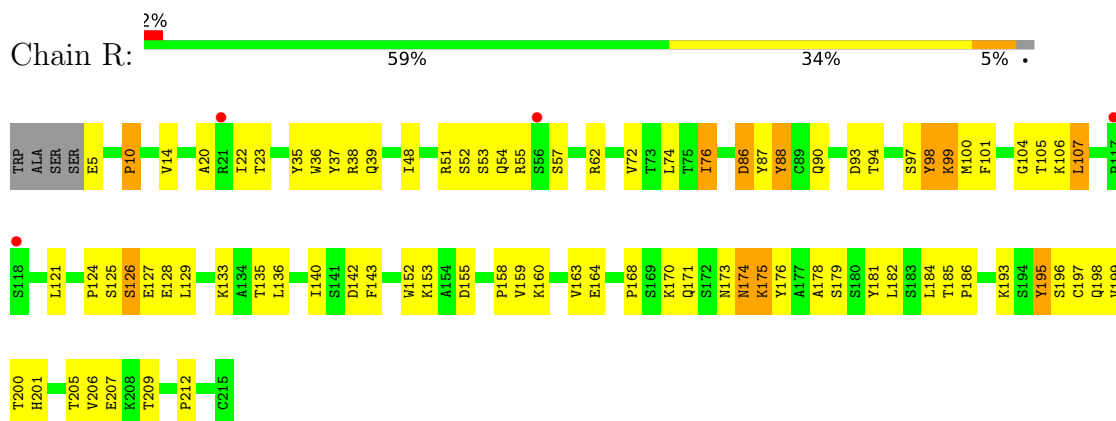
• Molecule 4: Envelope glycoprotein gp120



• Molecule 5: BG18 Heavy Chain



• Molecule 6: BG18 Light Chain

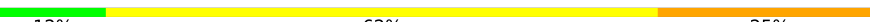


- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:  100%

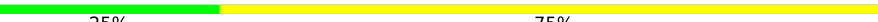


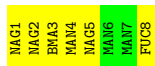
- Molecule 8: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  12% 62% 25%



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

Chain F:  25% 75%



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

Chain H:  33% 33% 33%



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

Chain J:  67% 33%



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

Chain M:  67% 33%



- 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 I: 



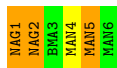
- Molecule 12: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 



- Molecule 13: 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 L: 



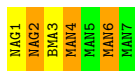
- Molecule 14: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 



- Molecule 15: 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 O: 

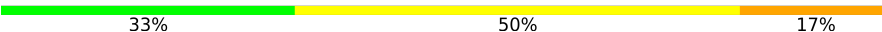


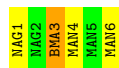
- Molecule 16: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 

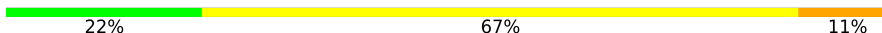


- Molecule 17: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain S:  33% 50% 17%



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

Chain T:  22% 67% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	238.94Å 238.94Å 354.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.03 – 3.80 24.03 – 3.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (24.03-3.80) 93.4 (24.03-3.80)	Depositor EDS
R_{merge}	0.54	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.84Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.232 , 0.262 0.301 , 0.320	Depositor DCC
R_{free} test set	1809 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	175.6	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 178.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12160	wwPDB-VP
Average B, all atoms (Å ²)	213.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: MAN, FUC, NAG, GAL, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	B	0.33	0/1086	0.68	5/1472 (0.3%)
2	D	0.17	0/1752	0.53	5/2385 (0.2%)
3	E	0.14	0/1659	0.34	0/2269
4	G	0.18	0/3619	0.46	1/4914 (0.0%)
5	Q	0.16	0/1753	0.46	2/2397 (0.1%)
6	R	0.22	0/1567	0.63	2/2149 (0.1%)
All	All	0.20	0/11436	0.51	15/15586 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	547	GLY	N-CA-C	10.64	123.81	111.36
4	G	500	ARG	N-CA-C	-8.17	97.93	110.10
6	R	126	SER	N-CA-C	7.47	126.70	110.80
2	D	146	PHE	N-CA-C	7.37	122.23	112.35
1	B	542	ARG	N-CA-C	6.89	118.44	111.07
1	B	544	LEU	N-CA-C	6.86	118.41	111.07
1	B	543	ASN	N-CA-C	6.63	118.51	111.28
2	D	148	GLU	CA-C-N	5.78	127.06	119.84
2	D	148	GLU	C-N-CA	5.78	127.06	119.84
2	D	202	PRO	N-CA-C	-5.78	105.21	113.47
2	D	100(C)	THR	N-CA-C	-5.73	108.09	114.62
5	Q	8	GLY	CA-C-N	5.69	126.95	119.84
5	Q	8	GLY	C-N-CA	5.69	126.95	119.84
1	B	539	VAL	CB-CA-C	-5.58	104.60	112.14
6	R	175	LYS	N-CA-C	-5.36	99.20	108.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1068	0	1055	73	0
2	D	1708	0	1682	82	0
3	E	1615	0	1548	56	0
4	G	3546	0	3468	149	0
5	Q	1709	0	1639	72	0
6	R	1527	0	1428	112	0
7	A	60	0	52	0	0
8	C	96	0	81	3	0
9	F	96	0	82	2	0
10	H	39	0	34	2	0
10	J	39	0	34	3	0
10	M	39	0	34	0	0
11	I	50	0	43	3	0
12	K	83	0	70	1	0
13	L	72	0	61	3	0
14	N	28	0	25	3	0
15	O	83	0	70	4	0
16	P	83	0	70	2	0
17	S	72	0	61	1	0
18	T	105	0	86	3	0
19	B	14	0	13	1	0
19	G	28	0	26	0	0
All	All	12160	0	11662	521	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (521) 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)
1:B:545:LEU:HD12	1:B:586:TYR:CE2	1.25	1.61
1:B:545:LEU:HD12	1:B:586:TYR:CD2	1.42	1.52
6:R:142:ASP:CG	6:R:175:LYS:HZ1	1.05	1.52
1:B:545:LEU:CD1	1:B:586:TYR:CE2	1.94	1.47
6:R:98:TYR:CE2	6:R:100:MET:HG2	1.54	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:LEU:CD1	1:B:586:TYR:CD2	2.05	1.38
5:Q:48:TRP:CE2	6:R:99:LYS:HG3	1.63	1.33
1:B:550:GLN:OE1	1:B:579:ARG:HD2	1.28	1.30
6:R:142:ASP:CG	6:R:175:LYS:NZ	1.89	1.27
1:B:547:GLY:O	1:B:548:ILE:CG2	1.87	1.22
6:R:98:TYR:HE2	6:R:100:MET:CG	1.57	1.18
2:D:148:GLU:HB3	2:D:149:PRO:CD	1.76	1.15
6:R:163:VAL:HG11	6:R:182:LEU:HD22	1.24	1.15
1:B:536:THR:O	1:B:540:GLN:NE2	1.81	1.14
1:B:547:GLY:O	1:B:548:ILE:HG23	0.98	1.13
1:B:550:GLN:OE1	1:B:579:ARG:CD	2.00	1.08
4:G:391:PHE:CE2	4:G:470:PRO:HG3	1.90	1.07
2:D:148:GLU:HB3	2:D:149:PRO:HD3	1.35	1.05
6:R:142:ASP:CB	6:R:175:LYS:NZ	2.20	1.04
1:B:547:GLY:C	1:B:548:ILE:HG23	1.83	0.99
6:R:142:ASP:HA	6:R:175:LYS:CE	1.92	0.97
6:R:163:VAL:HG11	6:R:182:LEU:CD2	1.93	0.97
5:Q:48:TRP:NE1	6:R:99:LYS:HG3	1.79	0.97
1:B:545:LEU:CD1	1:B:586:TYR:HE2	1.77	0.96
1:B:545:LEU:HD11	1:B:586:TYR:CD2	2.03	0.93
6:R:142:ASP:CB	6:R:175:LYS:HZ1	1.78	0.93
2:D:148:GLU:CB	2:D:149:PRO:CD	2.46	0.92
5:Q:168:THR:H	5:Q:216:ASN:HB2	1.35	0.91
3:E:6:GLN:HG3	3:E:104:GLY:H	1.36	0.91
1:B:537:LEU:HA	1:B:540:GLN:NE2	1.87	0.89
4:G:391:PHE:HE2	4:G:470:PRO:HG3	1.33	0.89
4:G:391:PHE:HE2	4:G:470:PRO:CG	1.87	0.88
2:D:146:PHE:HB3	2:D:147:PRO:HD3	1.58	0.84
6:R:142:ASP:OD1	6:R:175:LYS:NZ	1.98	0.84
4:G:236:THR:H	10:J:1:NAG:H81	1.42	0.83
5:Q:91:THR:HB	5:Q:127:THR:HA	1.61	0.83
1:B:545:LEU:HD11	1:B:586:TYR:CE2	2.09	0.83
5:Q:48:TRP:CE2	6:R:99:LYS:CG	2.55	0.83
1:B:537:LEU:HA	1:B:540:GLN:CD	2.04	0.82
1:B:536:THR:C	1:B:540:GLN:HE22	1.89	0.81
2:D:110:THR:OG1	2:D:148:GLU:OE2	1.97	0.81
6:R:173:ASN:C	6:R:174:ASN:ND2	2.40	0.80
1:B:548:ILE:O	1:B:549:VAL:HG12	1.81	0.80
6:R:36:TRP:HB2	6:R:48:ILE:HG21	1.63	0.80
4:G:298:ARG:NH2	4:G:439:ILE:O	2.14	0.79
6:R:142:ASP:CB	6:R:175:LYS:HZ3	1.91	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:50:GLY:HA3	5:Q:60:TYR:HA	1.63	0.79
4:G:391:PHE:CE2	4:G:470:PRO:CG	2.62	0.79
4:G:55:ALA:HB3	4:G:216:HIS:HB2	1.64	0.79
6:R:198:GLN:HA	6:R:207:GLU:HB3	1.65	0.79
2:D:116:THR:HA	2:D:146:PHE:HD2	1.48	0.78
2:D:148:GLU:HB3	2:D:149:PRO:HD2	1.61	0.78
1:B:537:LEU:C	1:B:540:GLN:OE1	2.26	0.78
5:Q:48:TRP:CZ2	6:R:99:LYS:HG3	2.19	0.78
6:R:142:ASP:HB2	6:R:175:LYS:HZ3	1.50	0.76
4:G:33:ASN:O	4:G:500:ARG:HG2	1.86	0.76
6:R:52:SER:O	18:T:9:MAN:O3	2.03	0.76
4:G:90:THR:HG22	4:G:240:PRO:HA	1.68	0.76
2:D:201:LYS:H	2:D:202:PRO:CD	1.99	0.75
2:D:124:LEU:HB2	2:D:141:LEU:HB2	1.67	0.75
4:G:270:VAL:HG12	4:G:289:ASN:H	1.49	0.74
1:B:540:GLN:OE1	1:B:540:GLN:N	2.19	0.74
4:G:35:TRP:HD1	4:G:501:CYS:H	1.33	0.73
6:R:98:TYR:HE2	6:R:100:MET:HG2	0.67	0.73
1:B:544:LEU:HG	4:G:222:GLY:HA2	1.68	0.73
4:G:129:LEU:HD23	4:G:159:PHE:HB3	1.71	0.73
1:B:540:GLN:CD	1:B:540:GLN:H	1.97	0.73
6:R:142:ASP:HA	6:R:175:LYS:HE3	1.71	0.73
4:G:258:GLN:NE2	4:G:371:VAL:O	2.21	0.72
6:R:155:ASP:HA	6:R:193:LYS:HG2	1.73	0.71
1:B:545:LEU:O	1:B:545:LEU:HD23	1.89	0.71
4:G:475:MET:SD	4:G:478:ASN:ND2	2.64	0.70
1:B:544:LEU:C	1:B:544:LEU:HD23	2.16	0.70
4:G:70:ALA:HB2	4:G:213:ILE:HD11	1.73	0.70
4:G:98:ASN:ND2	4:G:486:TYR:O	2.24	0.70
1:B:625:ASN:OD1	2:D:32:TYR:OH	2.09	0.69
2:D:37:ILE:HG22	2:D:47:TRP:HA	1.72	0.69
1:B:545:LEU:CD1	1:B:586:TYR:HD2	1.95	0.69
2:D:163:VAL:HG12	2:D:182:VAL:HG23	1.73	0.69
1:B:548:ILE:HD11	1:B:550:GLN:HB3	1.74	0.68
4:G:265:LEU:HD12	4:G:287:GLN:HB3	1.76	0.68
4:G:258:GLN:HG2	4:G:470:PRO:HB2	1.75	0.68
2:D:146:PHE:CB	2:D:147:PRO:HD3	2.21	0.68
5:Q:48:TRP:HB2	6:R:101:PHE:CE1	2.29	0.67
5:Q:112:TRP:HH2	16:P:6:MAN:H2	1.58	0.67
2:D:200:HIS:HD2	2:D:205:THR:HB	1.60	0.67
4:G:500:ARG:O	4:G:501:CYS:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:GLN:OE1	1:B:579:ARG:NH1	2.28	0.67
3:E:196:SER:HA	3:E:209:THR:HG23	1.77	0.67
6:R:152:TRP:CD1	6:R:163:VAL:HG21	2.30	0.66
4:G:264:SER:O	4:G:287:GLN:NE2	2.29	0.66
1:B:545:LEU:HD23	1:B:545:LEU:C	2.21	0.66
2:D:66:ARG:HD2	2:D:82(B):ASN:HB2	1.78	0.65
2:D:72(D):PRO:HG3	4:G:240:PRO:HG3	1.78	0.65
1:B:548:ILE:O	1:B:549:VAL:CG1	2.44	0.65
2:D:66:ARG:NH2	2:D:82(B):ASN:O	2.29	0.65
6:R:88:TYR:HA	6:R:104:GLY:HA3	1.78	0.65
4:G:269:GLU:HB2	4:G:348:GLN:HG3	1.78	0.65
6:R:142:ASP:OD1	6:R:175:LYS:CE	2.45	0.65
1:B:550:GLN:HB2	1:B:579:ARG:HD3	1.78	0.64
4:G:325:ASP:HA	6:R:54:GLN:HE22	1.62	0.64
4:G:360:ARG:O	4:G:467:THR:OG1	2.14	0.64
3:E:41:PRO:HB2	3:E:44:ARG:HB2	1.77	0.64
4:G:273:ARG:NH1	4:G:287:GLN:OE1	2.31	0.64
4:G:219:ALA:HB2	4:G:225:ILE:HG13	1.80	0.64
6:R:142:ASP:CA	6:R:175:LYS:NZ	2.60	0.63
6:R:142:ASP:HA	6:R:175:LYS:NZ	2.13	0.63
6:R:163:VAL:CG1	6:R:182:LEU:CD2	2.74	0.63
6:R:10:PRO:HA	6:R:105:THR:HA	1.80	0.63
4:G:455:THR:HG22	4:G:456:ARG:H	1.64	0.63
5:Q:166:PRO:O	5:Q:216:ASN:ND2	2.32	0.63
2:D:201:LYS:H	2:D:202:PRO:HD3	1.64	0.62
4:G:125:LEU:HG	4:G:193:LEU:HD11	1.82	0.62
4:G:391:PHE:CD2	4:G:470:PRO:HD3	2.34	0.62
4:G:454:LEU:HB3	4:G:468:PHE:HB3	1.80	0.62
6:R:22:ILE:HB	6:R:74:LEU:HB3	1.81	0.62
4:G:391:PHE:CD2	4:G:470:PRO:HG3	2.32	0.62
6:R:90:GLN:HG2	6:R:101:PHE:CE1	2.35	0.62
1:B:544:LEU:CG	4:G:222:GLY:HA2	2.30	0.61
2:D:6:GLN:HE21	2:D:92:CYS:H	1.47	0.61
6:R:160:LYS:O	6:R:163:VAL:HG22	1.99	0.61
3:E:4:LEU:HB3	3:E:102:GLY:HA2	1.82	0.61
4:G:49:GLU:HG2	4:G:99:ASN:HB3	1.82	0.61
1:B:550:GLN:CD	1:B:579:ARG:HD2	2.20	0.61
1:B:550:GLN:HB2	1:B:579:ARG:CD	2.29	0.61
6:R:196:SER:HB2	6:R:209:THR:HG23	1.80	0.61
1:B:547:GLY:C	1:B:548:ILE:CG2	2.57	0.61
4:G:236:THR:N	10:J:1:NAG:H81	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:93:ASP:OD1	6:R:94:THR:N	2.33	0.61
6:R:153:LYS:HA	6:R:158:PRO:HA	1.83	0.60
6:R:152:TRP:CD2	6:R:182:LEU:HD21	2.36	0.60
6:R:153:LYS:NZ	6:R:196:SER:O	2.35	0.60
5:Q:28:SER:HB2	18:T:7:MAN:H61	1.83	0.60
2:D:37:ILE:HD11	2:D:91:PHE:HB2	1.84	0.60
1:B:549:VAL:HG13	1:B:549:VAL:O	2.02	0.60
2:D:146:PHE:CD2	2:D:147:PRO:HG3	2.37	0.60
3:E:195:TYR:HB2	3:E:212:PRO:HD3	1.84	0.60
5:Q:33:HIS:HA	5:Q:101:ILE:HG22	1.83	0.60
3:E:31:SER:O	3:E:32:HIS:ND1	2.35	0.60
4:G:39:TYR:HE2	4:G:497:ALA:HB3	1.67	0.60
6:R:175:LYS:HG3	6:R:175:LYS:O	2.01	0.60
4:G:35:TRP:CD1	4:G:501:CYS:H	2.17	0.59
5:Q:133:THR:OG1	5:Q:163:PHE:HB3	2.02	0.59
5:Q:32:ASP:O	5:Q:53:HIS:NE2	2.34	0.59
2:D:201:LYS:N	2:D:202:PRO:CD	2.64	0.59
4:G:95:MET:H	4:G:236:THR:HG21	1.67	0.59
2:D:37:ILE:HD13	3:E:40:TRP:HH2	1.67	0.59
4:G:325:ASP:OD1	4:G:326:ILE:N	2.33	0.59
4:G:350:ARG:HH22	4:G:397:SER:H	1.49	0.59
5:Q:22:CYS:HB2	5:Q:37:TRP:HZ2	1.68	0.58
5:Q:88:ALA:HA	5:Q:128:VAL:HG11	1.85	0.58
1:B:547:GLY:O	1:B:548:ILE:CB	2.51	0.58
6:R:90:GLN:HG2	6:R:101:PHE:CZ	2.39	0.58
4:G:292:VAL:O	4:G:449:ILE:HG22	2.04	0.58
5:Q:187:LEU:HA	5:Q:193:TYR:HD1	1.69	0.58
2:D:171:GLN:OE1	3:E:183:SER:OG	2.20	0.58
3:E:122:PHE:HE2	3:E:139:LEU:HB2	1.68	0.58
4:G:358:ILE:HB	4:G:465:THR:HG22	1.86	0.58
6:R:206:VAL:HG12	6:R:207:GLU:H	1.68	0.58
2:D:5:VAL:HG13	2:D:23:LYS:HB2	1.85	0.57
4:G:171:LYS:HE2	10:H:1:NAG:H2	1.85	0.57
5:Q:61:ASN:ND2	6:R:98:TYR:HE1	2.01	0.57
1:B:648:GLU:HA	1:B:652:GLN:HB3	1.85	0.57
4:G:359:ILE:H	4:G:396:ILE:CG2	2.18	0.57
2:D:47:TRP:HB2	3:E:101:PHE:HE2	1.69	0.57
4:G:74:CYS:SG	4:G:75:VAL:N	2.78	0.57
5:Q:114:HIS:NE2	16:P:6:MAN:O3	2.33	0.57
4:G:291:PRO:HB3	4:G:450:THR:HG22	1.85	0.57
5:Q:48:TRP:CZ2	6:R:99:LYS:CG	2.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:CYS:O	4:G:503:ARG:HG3	2.05	0.57
4:G:328:GLN:HB3	5:Q:109:LEU:HD21	1.87	0.57
6:R:126:SER:O	6:R:126:SER:OG	2.22	0.57
3:E:6:GLN:HG3	3:E:104:GLY:N	2.15	0.57
3:E:6:GLN:HB3	3:E:105:THR:HG23	1.87	0.57
5:Q:39:ARG:HG2	5:Q:47:GLU:HB3	1.87	0.57
4:G:357:THR:OG1	4:G:465:THR:N	2.37	0.56
2:D:116:THR:HA	2:D:146:PHE:CD2	2.35	0.56
4:G:82:GLN:HG2	4:G:246:GLN:HB2	1.87	0.56
4:G:160:ASN:N	4:G:160:ASN:OD1	2.39	0.56
4:G:476:ARG:HA	4:G:479:TRP:CE3	2.40	0.56
2:D:47:TRP:HZ2	2:D:50:TRP:HD1	1.53	0.56
3:E:110:LEU:HD23	3:E:111:GLY:H	1.69	0.56
4:G:391:PHE:HE2	4:G:470:PRO:CB	2.18	0.56
5:Q:181:HIS:O	5:Q:197:SER:OG	2.20	0.56
6:R:142:ASP:HA	6:R:175:LYS:HE2	1.85	0.56
2:D:122:PHE:HB2	2:D:141:LEU:HD22	1.86	0.56
6:R:168:PRO:HA	6:R:178:ALA:HB2	1.87	0.56
2:D:89:THR:HA	2:D:108:LEU:HA	1.88	0.56
4:G:368:ASP:H	4:G:371:VAL:HG12	1.71	0.56
3:E:48:LEU:HD12	3:E:49:ILE:H	1.70	0.56
4:G:95:MET:N	4:G:236:THR:HG21	2.21	0.56
2:D:197:ASN:HB2	2:D:208:ASP:HB3	1.88	0.55
6:R:98:TYR:CE2	6:R:100:MET:CG	2.49	0.55
5:Q:104:TYR:CZ	5:Q:111:GLU:HA	2.41	0.55
6:R:5:GLU:N	6:R:100:MET:SD	2.80	0.55
2:D:96:LEU:HA	2:D:101:TYR:HB2	1.88	0.55
2:D:150:VAL:HG22	2:D:178:LEU:HD21	1.88	0.55
4:G:173:TYR:CG	9:F:1:NAG:H62	2.42	0.55
5:Q:167:VAL:HG21	5:Q:195:LEU:HD23	1.88	0.55
6:R:142:ASP:HB2	6:R:175:LYS:NZ	2.11	0.55
1:B:537:LEU:HA	1:B:540:GLN:OE1	2.06	0.55
1:B:548:ILE:C	1:B:549:VAL:HG12	2.31	0.55
1:B:545:LEU:CG	1:B:586:TYR:CD2	2.87	0.55
3:E:135:THR:HA	3:E:182:LEU:HB3	1.88	0.55
2:D:108:LEU:HD21	2:D:149:PRO:HG3	1.89	0.55
4:G:298:ARG:NH1	4:G:302:ASN:OD1	2.40	0.55
4:G:101:VAL:HG21	4:G:480:ARG:HG2	1.89	0.54
4:G:137:ASN:ND2	6:R:55:ARG:O	2.40	0.54
10:J:3:BMA:H5	13:L:1:NAG:H81	1.90	0.54
4:G:445:CYS:C	4:G:446:VAL:HG22	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:45:TRP:HB3	4:G:491:ILE:HD13	1.90	0.54
4:G:317:PHE:CE2	4:G:319:ALA:HB2	2.43	0.54
5:Q:62:PRO:HA	5:Q:65:ARG:HG3	1.89	0.54
6:R:51:ARG:HA	6:R:57:SER:OG	2.08	0.54
3:E:51:TYR:O	3:E:53:ASP:N	2.40	0.54
6:R:121:LEU:HD11	6:R:140:ILE:HG23	1.89	0.54
4:G:129:LEU:O	4:G:191:TYR:N	2.37	0.54
5:Q:36:THR:OG1	5:Q:49:ILE:O	2.26	0.54
6:R:98:TYR:CE2	6:R:100:MET:HA	2.42	0.54
5:Q:168:THR:N	5:Q:216:ASN:HB2	2.15	0.53
4:G:83:GLU:HA	4:G:245:VAL:HG12	1.90	0.53
4:G:165:LEU:HD22	4:G:168:LYS:HE3	1.91	0.53
4:G:55:ALA:HA	4:G:75:VAL:O	2.09	0.53
4:G:158:SER:HB2	4:G:173:TYR:CD2	2.43	0.53
4:G:359:ILE:HA	4:G:467:THR:HG23	1.90	0.53
2:D:115:SER:O	2:D:146:PHE:CD2	2.62	0.53
5:Q:81:LEU:HD23	5:Q:82:LYS:H	1.72	0.53
6:R:98:TYR:CE2	6:R:100:MET:CA	2.91	0.53
1:B:620:SER:OG	1:B:624:ASP:OD2	2.25	0.53
3:E:189:TRP:HE1	3:E:212:PRO:HB2	1.74	0.53
4:G:61:TYR:O	4:G:65:LYS:HB3	2.09	0.53
2:D:110:THR:HG23	2:D:148:GLU:OE2	2.09	0.53
3:E:69:SER:OG	3:E:72:SER:OG	2.27	0.53
5:Q:129:SER:HB3	5:Q:163:PHE:HZ	1.74	0.53
6:R:86:ASP:OD1	6:R:86:ASP:N	2.33	0.52
2:D:98:ARG:HB2	8:C:1:NAG:H83	1.91	0.52
5:Q:9:PRO:HD2	5:Q:20:LEU:CD1	2.40	0.52
6:R:152:TRP:CE2	6:R:182:LEU:HD21	2.43	0.52
4:G:101:VAL:HG11	4:G:480:ARG:HE	1.75	0.52
6:R:163:VAL:HB	6:R:182:LEU:HD23	1.92	0.52
1:B:550:GLN:O	1:B:551:GLN:C	2.52	0.52
2:D:119:PRO:HG3	2:D:145:TYR:HB2	1.92	0.52
4:G:453:ILE:HG22	4:G:471:GLY:O	2.09	0.52
1:B:545:LEU:HD11	1:B:586:TYR:HD2	1.61	0.52
6:R:97:SER:O	6:R:98:TYR:HB3	2.09	0.52
2:D:69:MET:HE2	2:D:80:MET:HB2	1.93	0.51
4:G:175:LEU:HB2	4:G:320:THR:OG1	2.10	0.51
6:R:86:ASP:HA	6:R:106:LYS:HA	1.91	0.51
13:L:4:MAN:H62	13:L:5:MAN:H3	1.92	0.51
2:D:200:HIS:HB3	2:D:202:PRO:HD2	1.93	0.51
5:Q:61:ASN:ND2	6:R:98:TYR:CE1	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:110:THR:CG2	2:D:148:GLU:OE2	2.58	0.51
1:B:603:ILE:HG12	4:G:39:TYR:HD1	1.76	0.51
4:G:193:LEU:HB2	4:G:196:CYS:SG	2.50	0.51
1:B:593:LEU:HD21	4:G:40:TYR:HB2	1.92	0.51
6:R:133:LYS:HA	6:R:186:PRO:HG3	1.92	0.51
4:G:96:TRP:CD1	4:G:275:GLU:HB2	2.46	0.50
4:G:391:PHE:CD2	4:G:470:PRO:CD	2.93	0.50
6:R:155:ASP:HB2	6:R:193:LYS:HE3	1.92	0.50
5:Q:50:GLY:CA	5:Q:60:TYR:HA	2.39	0.50
6:R:201:HIS:H	6:R:205:THR:HG21	1.76	0.50
1:B:537:LEU:CA	1:B:540:GLN:OE1	2.58	0.50
4:G:172:VAL:HG11	4:G:309:ILE:HG12	1.93	0.50
5:Q:188:GLN:HA	6:R:164:GLU:OE1	2.11	0.50
6:R:142:ASP:OD1	6:R:175:LYS:HE3	2.11	0.50
3:E:121:LEU:HD11	3:E:136:LEU:HD21	1.93	0.50
4:G:320:THR:HG23	4:G:438:PRO:HG3	1.94	0.50
2:D:119:PRO:HG2	2:D:200:HIS:ND1	2.27	0.50
4:G:129:LEU:HB3	4:G:157:CYS:SG	2.52	0.50
4:G:158:SER:HB2	4:G:173:TYR:CG	2.47	0.50
6:R:174:ASN:ND2	6:R:174:ASN:N	2.60	0.50
3:E:30:CYS:SG	3:E:73:ALA:HB2	2.51	0.50
5:Q:48:TRP:CH2	6:R:98:TYR:HA	2.47	0.50
5:Q:4:LEU:HD13	5:Q:24:VAL:HB	1.92	0.49
1:B:545:LEU:C	1:B:545:LEU:CD2	2.86	0.49
4:G:267:GLU:HA	4:G:267:GLU:OE1	2.11	0.49
5:Q:31:SER:HA	5:Q:54:TYR:CD1	2.47	0.49
1:B:544:LEU:C	1:B:544:LEU:CD2	2.86	0.49
2:D:38:ARG:NH1	2:D:40:THR:OG1	2.45	0.49
2:D:72(E):VAL:HG23	2:D:74:SER:HA	1.95	0.49
2:D:93:ALA:HB3	2:D:100(F):PRO:HB3	1.94	0.49
4:G:96:TRP:HZ2	4:G:273:ARG:HB3	1.77	0.49
5:Q:103:ILE:HD11	18:T:3:BMA:H5	1.94	0.49
6:R:152:TRP:O	6:R:159:VAL:N	2.30	0.49
4:G:96:TRP:CZ2	4:G:273:ARG:HB3	2.48	0.49
5:Q:172:ASN:HA	5:Q:212:ILE:HG13	1.95	0.49
11:I:1:NAG:H3	11:I:2:NAG:H2	1.94	0.49
6:R:163:VAL:CB	6:R:182:LEU:HD23	2.43	0.49
4:G:203:GLN:HG3	4:G:435:TYR:HD2	1.77	0.49
4:G:299:PRO:HB2	4:G:327:ARG:HB2	1.93	0.49
4:G:361:PHE:HB3	4:G:391:PHE:O	2.13	0.48
1:B:522:PHE:CD2	1:B:523:LEU:HG	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:67:TYR:HB3	3:E:74:TYR:HE1	1.78	0.48
3:E:70:TYR:HB3	3:E:71:TRP:CE3	2.48	0.48
6:R:170:LYS:HE3	6:R:176:TYR:CZ	2.48	0.48
2:D:100(E):LEU:HD23	2:D:100(E):LEU:H	1.79	0.48
6:R:129:LEU:H	6:R:129:LEU:HD12	1.79	0.48
1:B:545:LEU:HD13	1:B:586:TYR:CE2	2.30	0.48
3:E:25:PRO:C	3:E:29:CYS:HB3	2.39	0.48
6:R:133:LYS:HD3	6:R:186:PRO:HD3	1.96	0.48
2:D:108:LEU:HG	2:D:148:GLU:OE1	2.14	0.48
5:Q:51:ASP:OD2	5:Q:52:ILE:N	2.47	0.48
5:Q:48:TRP:CZ3	6:R:98:TYR:HA	2.48	0.48
4:G:159:PHE:CE1	4:G:161:MET:HE2	2.49	0.48
15:O:1:NAG:H62	15:O:2:NAG:H82	1.95	0.48
2:D:25:SER:HA	2:D:75:THR:HG22	1.95	0.48
4:G:182:VAL:HG23	4:G:192:ARG:NH1	2.29	0.48
2:D:93:ALA:CB	2:D:100(F):PRO:HB3	2.44	0.48
4:G:54:CYS:SG	4:G:55:ALA:N	2.87	0.48
6:R:136:LEU:HD11	6:R:184:LEU:HB2	1.96	0.48
1:B:622:ILE:HG13	1:B:623:TRP:CD1	2.49	0.47
2:D:127:SER:HB2	3:E:123:PRO:HD3	1.95	0.47
4:G:391:PHE:HE2	4:G:470:PRO:HB3	1.79	0.47
6:R:23:THR:HA	6:R:72:VAL:O	2.14	0.47
6:R:36:TRP:CD2	6:R:74:LEU:HD22	2.49	0.47
1:B:520:LEU:HA	1:B:524:GLY:HA3	1.95	0.47
1:B:617:ARG:NH1	1:B:621:GLU:OE1	2.48	0.47
3:E:65:SER:HB2	3:E:76:THR:HB	1.96	0.47
5:Q:162:TYR:CE2	5:Q:195:LEU:HD13	2.49	0.47
6:R:173:ASN:C	6:R:174:ASN:CG	2.81	0.47
4:G:152:THR:O	4:G:154:LEU:N	2.46	0.47
4:G:359:ILE:H	4:G:396:ILE:HG21	1.79	0.47
5:Q:162:TYR:CE2	5:Q:193:TYR:HB2	2.49	0.47
4:G:280:ASN:C	4:G:456:ARG:HG3	2.40	0.47
4:G:391:PHE:CE2	4:G:470:PRO:HD3	2.49	0.47
6:R:153:LYS:HD3	6:R:198:GLN:HE22	1.80	0.47
15:O:1:NAG:O6	15:O:2:NAG:N2	2.44	0.47
2:D:199:ASN:HA	2:D:205:THR:HG21	1.96	0.47
4:G:331:CYS:HB2	4:G:385:CYS:SG	2.55	0.47
3:E:85:GLU:HG3	3:E:108:SER:HA	1.97	0.47
6:R:128:GLU:HG3	6:R:135:THR:H	1.79	0.47
5:Q:21:SER:HA	5:Q:79:PHE:O	2.15	0.46
6:R:51:ARG:HH11	6:R:54:GLN:HA	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:10:VAL:HG21	3:E:20:ILE:HG13	1.96	0.46
4:G:265:LEU:HD13	4:G:288:PHE:O	2.15	0.46
1:B:544:LEU:CD1	4:G:222:GLY:HA2	2.45	0.46
2:D:31:PHE:HD2	8:C:1:NAG:HN2	1.62	0.46
2:D:34:ILE:HD11	2:D:92:CYS:HB2	1.97	0.46
6:R:38:ARG:HB3	6:R:87:TYR:CE1	2.49	0.46
14:N:1:NAG:H61	14:N:2:NAG:O5	2.15	0.46
2:D:102:LEU:HD23	2:D:102:LEU:HA	1.73	0.46
3:E:140:ILE:HD11	3:E:178:ALA:HB3	1.97	0.46
1:B:548:ILE:CD1	1:B:550:GLN:HB3	2.43	0.46
3:E:91:CYS:HB3	3:E:101:PHE:HA	1.98	0.46
4:G:42:VAL:HG12	4:G:493:PRO:C	2.41	0.46
1:B:522:PHE:CE2	1:B:523:LEU:HG	2.51	0.46
2:D:35:ASN:ND2	2:D:100(D):TRP:O	2.49	0.46
3:E:56:ARG:HD2	3:E:62:PRO:HA	1.98	0.46
4:G:163:THR:HG23	4:G:165:LEU:H	1.81	0.46
1:B:544:LEU:HD23	1:B:544:LEU:O	2.15	0.46
2:D:94:LYS:O	2:D:101:TYR:N	2.49	0.46
2:D:155:ASN:ND2	2:D:208:ASP:OD2	2.49	0.46
4:G:294:ILE:HG13	4:G:447:SER:O	2.15	0.46
4:G:391:PHE:CE2	4:G:470:PRO:CD	2.99	0.46
3:E:132:ASN:HB3	3:E:186:PRO:HG3	1.98	0.46
4:G:105:HIS:CD2	4:G:476:ARG:HB3	2.51	0.46
6:R:163:VAL:CG1	6:R:182:LEU:HD23	2.46	0.46
2:D:8:GLY:HA2	2:D:107:THR:HB	1.98	0.45
5:Q:49:ILE:HG22	5:Q:50:GLY:H	1.79	0.45
5:Q:98:ARG:O	5:Q:117:MET:HA	2.16	0.45
5:Q:169:VAL:HG11	5:Q:182:THR:OG1	2.16	0.45
14:N:1:NAG:H4	14:N:2:NAG:H2	1.65	0.45
1:B:544:LEU:HG	4:G:222:GLY:CA	2.41	0.45
2:D:57:LYS:NZ	2:D:68:ILE:HG13	2.31	0.45
4:G:379:GLY:O	4:G:439:ILE:HG13	2.16	0.45
5:Q:186:VAL:HG22	5:Q:187:LEU:H	1.81	0.45
6:R:152:TRP:CD1	6:R:163:VAL:CG2	2.98	0.45
4:G:499:THR:O	4:G:500:ARG:C	2.55	0.45
6:R:35:TYR:HB2	6:R:90:GLN:HB2	1.99	0.45
17:S:3:BMA:H3	17:S:6:MAN:H2	1.81	0.45
1:B:604:CYS:HB2	4:G:38:VAL:CG2	2.47	0.45
1:B:604:CYS:HB2	4:G:38:VAL:HG22	1.98	0.45
1:B:622:ILE:HG13	1:B:623:TRP:HD1	1.81	0.45
4:G:182:VAL:HG21	11:I:1:NAG:H82	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:62:ARG:H	6:R:62:ARG:HG2	1.48	0.45
6:R:98:TYR:CZ	6:R:100:MET:HA	2.52	0.45
2:D:146:PHE:O	2:D:146:PHE:CD1	2.70	0.45
5:Q:10:GLY:HA2	5:Q:126:VAL:HG22	1.99	0.45
5:Q:50:GLY:HA3	5:Q:59:THR:O	2.17	0.45
5:Q:101:ILE:HD11	5:Q:112:TRP:O	2.16	0.45
1:B:604:CYS:O	4:G:37:THR:HG23	2.16	0.45
2:D:47:TRP:CZ2	3:E:98:GLY:HA3	2.51	0.45
3:E:30:CYS:SG	3:E:68:LYS:HG3	2.57	0.45
4:G:127:VAL:HG23	4:G:159:PHE:HB2	1.99	0.45
5:Q:8:GLY:HA3	5:Q:20:LEU:HD12	1.99	0.45
6:R:153:LYS:HG2	6:R:158:PRO:HA	1.97	0.45
6:R:171:GLN:O	6:R:175:LYS:HG2	2.16	0.45
1:B:596:TRP:HE1	1:B:647:GLU:HG3	1.82	0.44
2:D:201:LYS:H	2:D:202:PRO:HD2	1.81	0.44
3:E:20:ILE:O	3:E:74:TYR:HA	2.17	0.44
5:Q:163:PHE:N	5:Q:164:PRO:CD	2.80	0.44
6:R:37:TYR:H	6:R:48:ILE:HB	1.82	0.44
5:Q:48:TRP:HB2	6:R:101:PHE:CD1	2.51	0.44
3:E:121:LEU:HD21	3:E:136:LEU:HD21	1.98	0.44
4:G:349:LEU:O	4:G:353:PHE:N	2.50	0.44
4:G:350:ARG:HG3	4:G:355:ASN:HA	1.99	0.44
6:R:173:ASN:OD1	6:R:173:ASN:N	2.51	0.44
1:B:537:LEU:HA	1:B:540:GLN:HE22	1.65	0.44
2:D:3:GLN:N	2:D:3:GLN:OE1	2.50	0.44
4:G:445:CYS:C	4:G:446:VAL:CG2	2.90	0.44
5:Q:64:LEU:O	5:Q:68:VAL:HG22	2.18	0.44
6:R:152:TRP:CE3	6:R:182:LEU:HD11	2.53	0.44
4:G:36:VAL:HA	4:G:498:PRO:HA	2.00	0.44
5:Q:139:PHE:CZ	6:R:128:GLU:HB3	2.53	0.44
3:E:8:ALA:N	3:E:105:THR:HG22	2.32	0.44
4:G:260:LEU:HD12	4:G:451:GLY:HA3	1.99	0.44
5:Q:101:ILE:HD12	5:Q:114:HIS:HA	1.98	0.44
6:R:128:GLU:HB2	6:R:133:LYS:O	2.17	0.44
9:F:4:MAN:H2	9:F:5:NAG:H2	1.58	0.44
3:E:114:LYS:HA	3:E:144:TYR:HD2	1.83	0.44
4:G:366:GLY:O	4:G:372:THR:HG21	2.18	0.44
4:G:494:LEU:HD23	4:G:494:LEU:HA	1.82	0.44
4:G:265:LEU:CD1	4:G:287:GLN:HB3	2.45	0.44
5:Q:186:VAL:HG22	5:Q:187:LEU:HD23	2.00	0.44
6:R:133:LYS:HE3	6:R:185:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:34:SER:O	5:Q:35:TRP:HD1	2.00	0.43
4:G:32:GLU:HB2	4:G:33:ASN:H	1.68	0.43
5:Q:47:GLU:HG3	5:Q:48:TRP:H	1.83	0.43
1:B:550:GLN:OE1	1:B:579:ARG:HD3	2.06	0.43
3:E:38:TYR:CE2	3:E:48:LEU:HD22	2.53	0.43
4:G:257:THR:OG1	4:G:375:SER:OG	2.28	0.43
1:B:548:ILE:HG21	4:G:221:ALA:N	2.33	0.43
2:D:6:GLN:NE2	2:D:92:CYS:H	2.15	0.43
2:D:27:TYR:CD1	2:D:32:TYR:HD1	2.37	0.43
4:G:69:TRP:HA	4:G:111:LEU:HD21	2.01	0.43
4:G:280:ASN:H	4:G:280:ASN:ND2	2.16	0.43
4:G:477:ASP:OD1	4:G:480:ARG:NH1	2.51	0.43
6:R:140:ILE:O	6:R:179:SER:HA	2.19	0.43
2:D:31:PHE:CE1	2:D:98:ARG:HD3	2.53	0.43
3:E:140:ILE:HG12	3:E:178:ALA:O	2.19	0.43
5:Q:163:PHE:H	5:Q:164:PRO:CD	2.32	0.43
5:Q:187:LEU:HA	5:Q:193:TYR:CD1	2.50	0.43
1:B:576:LEU:HD12	1:B:579:ARG:HH21	1.84	0.43
1:B:624:ASP:HB3	2:D:99:ASP:HB2	1.99	0.43
2:D:33:HIS:O	2:D:95:GLY:N	2.50	0.43
2:D:148:GLU:CB	2:D:149:PRO:HD2	2.29	0.43
2:D:108:LEU:H	2:D:108:LEU:HD23	1.84	0.43
2:D:96:LEU:HD13	3:E:51:TYR:CE1	2.54	0.42
2:D:146:PHE:CD1	2:D:146:PHE:C	2.95	0.42
4:G:251:ILE:HG12	4:G:482:GLU:HG2	2.00	0.42
4:G:350:ARG:NH2	4:G:397:SER:H	2.16	0.42
4:G:425:ASN:HB3	4:G:433:ALA:HA	2.01	0.42
1:B:549:VAL:O	1:B:549:VAL:HG22	2.19	0.42
3:E:70:TYR:HB3	3:E:71:TRP:CZ3	2.54	0.42
4:G:265:LEU:HD13	4:G:288:PHE:C	2.44	0.42
6:R:14:VAL:HG12	6:R:107:LEU:HD21	2.01	0.42
15:O:4:MAN:H62	15:O:6:MAN:H2	1.76	0.42
12:K:4:MAN:H3	12:K:5:MAN:H5	2.01	0.42
4:G:265:LEU:HD23	4:G:267:GLU:H	1.85	0.42
5:Q:105:GLY:HA3	5:Q:111:GLU:OE1	2.19	0.42
6:R:199:VAL:O	6:R:205:THR:HB	2.20	0.42
2:D:110:THR:CB	2:D:148:GLU:OE2	2.67	0.42
3:E:144:TYR:CD1	3:E:145:PRO:HA	2.54	0.42
2:D:28:ARG:HG2	2:D:72(H):PHE:O	2.19	0.42
3:E:81:ARG:O	3:E:83:GLU:N	2.51	0.42
4:G:207:LYS:H	4:G:207:LYS:HG2	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:LEU:O	2:D:12:LYS:HD2	2.19	0.42
3:E:49:ILE:HG22	3:E:50:ILE:HG12	2.02	0.42
3:E:81:ARG:C	3:E:83:GLU:H	2.27	0.42
4:G:457:ASP:HB2	4:G:467:THR:O	2.20	0.42
3:E:51:TYR:CE2	3:E:57:ALA:HA	2.55	0.42
4:G:50:THR:OG1	4:G:51:THR:N	2.53	0.42
5:Q:187:LEU:H	5:Q:187:LEU:HD23	1.83	0.42
6:R:164:GLU:O	6:R:181:TYR:O	2.37	0.42
3:E:189:TRP:NE1	3:E:212:PRO:HB2	2.35	0.42
4:G:105:HIS:HD2	4:G:476:ARG:HE	1.68	0.42
4:G:424:ILE:HD12	4:G:424:ILE:HA	1.88	0.42
6:R:20:ALA:HB3	6:R:76:ILE:HG12	2.00	0.42
3:E:132:ASN:HB3	3:E:186:PRO:HB3	2.02	0.41
5:Q:139:PHE:HZ	6:R:128:GLU:HB3	1.86	0.41
4:G:86:LEU:HG	4:G:244:THR:HG22	2.03	0.41
4:G:233:PHE:CE1	4:G:239:CYS:HB2	2.55	0.41
6:R:125:SER:O	6:R:126:SER:HB3	2.21	0.41
6:R:170:LYS:HG3	6:R:176:TYR:CE1	2.55	0.41
1:B:618:ASN:OD1	19:B:701:NAG:N2	2.53	0.41
4:G:172:VAL:HG21	4:G:309:ILE:HG21	2.02	0.41
4:G:456:ARG:HH21	4:G:458:GLY:HA2	1.84	0.41
5:Q:24:VAL:HG11	5:Q:35:TRP:HH2	1.84	0.41
10:H:2:NAG:O4	10:H:2:NAG:O6	2.32	0.41
11:I:1:NAG:H61	11:I:2:NAG:H83	2.02	0.41
13:L:1:NAG:H62	13:L:2:NAG:H82	2.02	0.41
4:G:69:TRP:O	4:G:111:LEU:HD21	2.21	0.41
5:Q:107:VAL:C	5:Q:109:LEU:H	2.27	0.41
6:R:124:PRO:HB3	6:R:135:THR:O	2.20	0.41
6:R:174:ASN:N	6:R:174:ASN:HD22	2.18	0.41
4:G:136:ASN:O	4:G:139:THR:HG22	2.21	0.41
4:G:207:LYS:HE2	4:G:207:LYS:HB3	1.96	0.41
5:Q:35:TRP:HE3	5:Q:79:PHE:CE2	2.38	0.41
6:R:121:LEU:HG	6:R:197:CYS:SG	2.61	0.41
1:B:537:LEU:HD21	1:B:603:ILE:HD11	2.02	0.41
2:D:49:GLY:HA3	2:D:59:LEU:HG	2.02	0.41
4:G:359:ILE:HG23	4:G:467:THR:HG21	2.02	0.41
4:G:348:GLN:O	4:G:352:HIS:ND1	2.54	0.41
5:Q:89:ALA:C	5:Q:91:THR:H	2.28	0.41
4:G:158:SER:OG	4:G:159:PHE:N	2.54	0.41
5:Q:95:TYR:OH	6:R:39:GLN:NE2	2.53	0.41
2:D:51:ILE:HD11	2:D:69:MET:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:HIS:HB2	2:D:203:SER:O	2.21	0.41
3:E:117:PRO:HG3	3:E:143:PHE:HB3	2.03	0.41
3:E:142:ASP:OD1	3:E:175:LYS:HG3	2.21	0.41
4:G:174:SER:C	4:G:175:LEU:HD12	2.46	0.41
4:G:233:PHE:HE2	4:G:236:THR:HG22	1.86	0.41
2:D:47:TRP:HB2	3:E:101:PHE:CE2	2.53	0.41
2:D:4:LEU:HD11	2:D:22:CYS:HB3	2.03	0.40
2:D:29:PHE:HB3	2:D:72(B):GLU:OE1	2.21	0.40
3:E:154:ALA:HB2	3:E:195:TYR:CZ	2.56	0.40
4:G:288:PHE:CZ	4:G:452:LEU:HG	2.56	0.40
5:Q:34:SER:C	5:Q:35:TRP:CD1	2.99	0.40
6:R:206:VAL:HG12	6:R:207:GLU:N	2.35	0.40
3:E:95:HIS:NE2	8:C:5:NAG:O6	2.48	0.40
6:R:173:ASN:C	6:R:174:ASN:HD22	2.25	0.40
15:O:4:MAN:O4	15:O:6:MAN:H3	2.21	0.40
2:D:154:TRP:HE1	2:D:158:ALA:H	1.69	0.40
4:G:152:THR:C	4:G:154:LEU:H	2.28	0.40
3:E:138:CYS:O	3:E:179:SER:OG	2.27	0.40
5:Q:184:PRO:HA	5:Q:195:LEU:HG	2.04	0.40
1:B:575:GLN:O	1:B:579:ARG:HG3	2.22	0.40
3:E:6:GLN:HB3	3:E:105:THR:CG2	2.50	0.40
3:E:119:VAL:HG22	3:E:140:ILE:HG22	2.03	0.40
6:R:143:PHE:CE2	6:R:176:TYR:HB2	2.56	0.40
14:N:1:NAG:O3	14:N:2:NAG:N2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	130/153 (85%)	118 (91%)	11 (8%)	1 (1%)	16 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	222/243 (91%)	192 (86%)	26 (12%)	4 (2%)	6	33
3	E	211/216 (98%)	182 (86%)	26 (12%)	3 (1%)	9	37
4	G	444/479 (93%)	377 (85%)	62 (14%)	5 (1%)	11	41
5	Q	229/241 (95%)	194 (85%)	34 (15%)	1 (0%)	30	62
6	R	209/215 (97%)	156 (75%)	46 (22%)	7 (3%)	3	24
All	All	1445/1547 (93%)	1219 (84%)	205 (14%)	21 (2%)	8	36

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	548	ILE
2	D	147	PRO
3	E	52	GLU
4	G	61	TYR
2	D	148	GLU
4	G	501	CYS
3	E	193	ARG
4	G	364	SER
4	G	465	THR
6	R	10	PRO
6	R	98	TYR
6	R	127	GLU
5	Q	216	ASN
6	R	88	TYR
2	D	149	PRO
2	D	201	LYS
3	E	71	TRP
4	G	356	ASN
6	R	53	SER
6	R	195	TYR
6	R	212	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	116/129 (90%)	111 (96%)	5 (4%)	26	50
2	D	190/206 (92%)	188 (99%)	2 (1%)	65	73
3	E	186/189 (98%)	180 (97%)	6 (3%)	34	56
4	G	401/427 (94%)	389 (97%)	12 (3%)	36	57
5	Q	187/208 (90%)	181 (97%)	6 (3%)	34	56
6	R	163/182 (90%)	156 (96%)	7 (4%)	26	50
All	All	1243/1341 (93%)	1205 (97%)	38 (3%)	35	57

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	542	ARG
1	B	565	LEU
1	B	583	VAL
1	B	618	ASN
1	B	638	TYR
2	D	59	LEU
2	D	166	PHE
3	E	48	LEU
3	E	52	GLU
3	E	74	TYR
3	E	99	CYS
3	E	110	LEU
3	E	195	TYR
4	G	32	GLU
4	G	74	CYS
4	G	122	LEU
4	G	131	CYS
4	G	160	ASN
4	G	217	TYR
4	G	234	ASN
4	G	280	ASN
4	G	284	ILE
4	G	353	PHE
4	G	414	ILE
4	G	449	ILE
5	Q	60	TYR
5	Q	81	LEU
5	Q	106	VAL
5	Q	117	MET
5	Q	139	PHE

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Mol	Chain	Res	Type
5	Q	181	HIS
6	R	76	ILE
6	R	86	ASP
6	R	99	LYS
6	R	107	LEU
6	R	174	ASN
6	R	195	TYR
6	R	200	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	551	GLN
1	B	552	GLN
1	B	575	GLN
1	B	652	GLN
2	D	192	GLN
2	D	199	ASN
2	D	200	HIS
3	E	112	GLN
4	G	80	ASN
4	G	105	HIS
4	G	293	GLN
4	G	398	ASN
5	Q	55	ASN
6	R	174	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

78 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	1	7,1	14,14,15	0.37	0	17,19,21	0.60	0
7	NAG	A	2	7	14,14,15	0.42	0	17,19,21	0.74	0
7	BMA	A	3	7	11,11,12	0.33	0	15,15,17	0.79	0
7	MAN	A	4	7	11,11,12	0.28	0	15,15,17	0.71	0
7	FUC	A	5	7	10,10,11	0.73	0	14,14,16	0.81	0
8	NAG	C	1	8,4	14,14,15	0.33	0	17,19,21	1.60	4 (23%)
8	NAG	C	2	8	14,14,15	0.30	0	17,19,21	1.22	2 (11%)
8	BMA	C	3	8	11,11,12	0.45	0	15,15,17	1.55	3 (20%)
8	MAN	C	4	8	11,11,12	0.68	0	15,15,17	1.89	4 (26%)
8	NAG	C	5	8	14,14,15	0.40	0	17,19,21	1.33	1 (5%)
8	GAL	C	6	8	11,11,12	0.53	0	15,15,17	0.99	1 (6%)
8	MAN	C	7	8	11,11,12	0.22	0	15,15,17	0.69	0
8	FUC	C	8	8	10,10,11	1.05	0	14,14,16	1.12	3 (21%)
9	NAG	F	1	4,9	14,14,15	0.31	0	17,19,21	0.62	0
9	NAG	F	2	9	14,14,15	0.36	0	17,19,21	0.95	1 (5%)
9	BMA	F	3	9	11,11,12	0.39	0	15,15,17	1.51	1 (6%)
9	MAN	F	4	9	11,11,12	0.57	0	15,15,17	0.99	0
9	NAG	F	5	9	14,14,15	0.33	0	17,19,21	0.59	0
9	MAN	F	6	9	11,11,12	0.29	0	15,15,17	0.75	0
9	MAN	F	7	9	11,11,12	0.28	0	15,15,17	0.68	0
9	FUC	F	8	9	10,10,11	0.95	0	14,14,16	1.00	1 (7%)
10	NAG	H	1	4,10	14,14,15	0.40	0	17,19,21	0.90	0
10	NAG	H	2	10	14,14,15	0.44	0	17,19,21	1.13	3 (17%)
10	BMA	H	3	10	11,11,12	0.26	0	15,15,17	0.64	0
11	NAG	I	1	11,4	14,14,15	0.51	0	17,19,21	1.08	3 (17%)
11	NAG	I	2	11	14,14,15	0.68	1 (7%)	17,19,21	0.73	0
11	BMA	I	3	11	11,11,12	0.29	0	15,15,17	0.62	0
11	MAN	I	4	11	11,11,12	0.26	0	15,15,17	0.66	0
10	NAG	J	1	4,10	14,14,15	0.30	0	17,19,21	0.81	1 (5%)
10	NAG	J	2	10	14,14,15	0.37	0	17,19,21	0.99	1 (5%)
10	BMA	J	3	10	11,11,12	0.28	0	15,15,17	0.69	0
12	NAG	K	1	12,4	14,14,15	0.29	0	17,19,21	1.16	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	K	2	12	14,14,15	0.61	0	17,19,21	1.32	2 (11%)
12	BMA	K	3	12	11,11,12	0.35	0	15,15,17	1.28	2 (13%)
12	MAN	K	4	12	11,11,12	0.37	0	15,15,17	0.77	0
12	MAN	K	5	12	11,11,12	0.88	1 (9%)	15,15,17	1.65	3 (20%)
12	MAN	K	6	12	11,11,12	0.27	0	15,15,17	0.65	0
12	MAN	K	7	12	11,11,12	0.23	0	15,15,17	0.73	0
13	NAG	L	1	4,13	14,14,15	0.38	0	17,19,21	1.32	3 (17%)
13	NAG	L	2	13	14,14,15	0.36	0	17,19,21	0.93	1 (5%)
13	BMA	L	3	13	11,11,12	0.22	0	15,15,17	0.69	0
13	MAN	L	4	13	11,11,12	0.27	0	15,15,17	0.64	0
13	MAN	L	5	13	11,11,12	0.88	1 (9%)	15,15,17	1.61	3 (20%)
13	MAN	L	6	13	11,11,12	0.24	0	15,15,17	0.67	0
10	NAG	M	1	4,10	14,14,15	0.25	0	17,19,21	0.71	0
10	NAG	M	2	10	14,14,15	0.45	0	17,19,21	1.16	1 (5%)
10	BMA	M	3	10	11,11,12	0.56	0	15,15,17	0.90	0
14	NAG	N	1	4,14	14,14,15	0.34	0	17,19,21	1.17	1 (5%)
14	NAG	N	2	14	14,14,15	0.52	0	17,19,21	0.70	0
15	NAG	O	1	4,15	14,14,15	0.35	0	17,19,21	0.45	0
15	NAG	O	2	15	14,14,15	0.37	0	17,19,21	1.00	2 (11%)
15	BMA	O	3	15	11,11,12	0.69	0	15,15,17	1.47	3 (20%)
15	MAN	O	4	15	11,11,12	0.68	0	15,15,17	2.31	7 (46%)
15	MAN	O	5	15	11,11,12	0.33	0	15,15,17	0.77	0
15	MAN	O	6	15	11,11,12	0.49	0	15,15,17	1.12	1 (6%)
15	MAN	O	7	15	11,11,12	0.26	0	15,15,17	0.74	0
16	NAG	P	1	4,16	14,14,15	0.39	0	17,19,21	0.77	0
16	NAG	P	2	16	14,14,15	0.44	0	17,19,21	1.45	3 (17%)
16	BMA	P	3	16	11,11,12	0.49	0	15,15,17	1.79	4 (26%)
16	MAN	P	4	16	11,11,12	0.28	0	15,15,17	0.90	0
16	MAN	P	5	16	11,11,12	0.26	0	15,15,17	0.53	0
16	MAN	P	6	16	11,11,12	0.19	0	15,15,17	0.71	0
16	MAN	P	7	16	11,11,12	0.24	0	15,15,17	0.66	0
17	NAG	S	1	17,4	14,14,15	0.35	0	17,19,21	1.17	2 (11%)
17	NAG	S	2	17	14,14,15	0.52	0	17,19,21	0.75	0
17	BMA	S	3	17	11,11,12	0.33	0	15,15,17	1.18	2 (13%)
17	MAN	S	4	17	11,11,12	0.24	0	15,15,17	0.80	1 (6%)
17	MAN	S	5	17	11,11,12	0.26	0	15,15,17	0.58	0
17	MAN	S	6	17	11,11,12	0.28	0	15,15,17	0.65	0
18	NAG	T	1	18,4	14,14,15	0.32	0	17,19,21	1.78	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	NAG	T	2	18	14,14,15	0.89	1 (7%)	17,19,21	1.71	4 (23%)
18	BMA	T	3	18	11,11,12	0.29	0	15,15,17	0.85	1 (6%)
18	MAN	T	4	18	11,11,12	0.31	0	15,15,17	0.64	0
18	MAN	T	5	18	11,11,12	0.44	0	15,15,17	1.19	2 (13%)
18	MAN	T	6	18	11,11,12	0.26	0	15,15,17	0.68	0
18	MAN	T	7	18	11,11,12	0.33	0	15,15,17	0.75	0
18	MAN	T	8	18	11,11,12	0.71	0	15,15,17	1.67	3 (20%)
18	MAN	T	9	18	11,11,12	0.33	0	15,15,17	0.94	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	3/6/23/26	0/1/1/1
7	BMA	A	3	7	-	0/2/19/22	0/1/1/1
7	MAN	A	4	7	-	0/2/19/22	0/1/1/1
7	FUC	A	5	7	-	-	0/1/1/1
8	NAG	C	1	8,4	-	6/6/23/26	0/1/1/1
8	NAG	C	2	8	-	3/6/23/26	0/1/1/1
8	BMA	C	3	8	-	0/2/19/22	0/1/1/1
8	MAN	C	4	8	-	0/2/19/22	0/1/1/1
8	NAG	C	5	8	-	3/6/23/26	0/1/1/1
8	GAL	C	6	8	-	0/2/19/22	0/1/1/1
8	MAN	C	7	8	-	0/2/19/22	0/1/1/1
8	FUC	C	8	8	-	-	0/1/1/1
9	NAG	F	1	4,9	-	4/6/23/26	0/1/1/1
9	NAG	F	2	9	-	4/6/23/26	0/1/1/1
9	BMA	F	3	9	-	2/2/19/22	0/1/1/1
9	MAN	F	4	9	-	0/2/19/22	0/1/1/1
9	NAG	F	5	9	-	3/6/23/26	0/1/1/1
9	MAN	F	6	9	-	1/2/19/22	0/1/1/1
9	MAN	F	7	9	-	0/2/19/22	0/1/1/1
9	FUC	F	8	9	-	-	0/1/1/1
10	NAG	H	1	4,10	-	3/6/23/26	0/1/1/1
10	NAG	H	2	10	-	4/6/23/26	0/1/1/1
10	BMA	H	3	10	-	2/2/19/22	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	MAN	P	6	16	-	0/2/19/22	0/1/1/1
16	MAN	P	7	16	-	0/2/19/22	0/1/1/1
17	NAG	S	1	17,4	-	0/6/23/26	0/1/1/1
17	NAG	S	2	17	-	3/6/23/26	0/1/1/1
17	BMA	S	3	17	-	1/2/19/22	0/1/1/1
17	MAN	S	4	17	-	1/2/19/22	0/1/1/1
17	MAN	S	5	17	-	0/2/19/22	0/1/1/1
17	MAN	S	6	17	-	1/2/19/22	0/1/1/1
18	NAG	T	1	18,4	-	2/6/23/26	0/1/1/1
18	NAG	T	2	18	-	1/6/23/26	0/1/1/1
18	BMA	T	3	18	-	2/2/19/22	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	-	0/2/19/22	0/1/1/1
18	MAN	T	7	18	-	1/2/19/22	0/1/1/1
18	MAN	T	8	18	-	2/2/19/22	0/1/1/1
18	MAN	T	9	18	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	2	NAG	C1-C2	2.70	1.56	1.52
13	L	5	MAN	O5-C1	2.03	1.47	1.43
11	I	2	NAG	C1-C2	2.03	1.55	1.52
12	K	5	MAN	O5-C1	2.02	1.47	1.43

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	3	BMA	O3-C3-C2	-5.23	99.38	110.05
18	T	1	NAG	O4-C4-C3	-5.10	98.34	110.38
8	C	4	MAN	O2-C2-C1	4.83	120.29	109.22
18	T	8	MAN	O2-C2-C3	4.59	119.66	110.15
13	L	5	MAN	C1-C2-C3	4.17	115.72	109.64
15	O	4	MAN	O5-C5-C6	4.08	115.61	107.66
12	K	5	MAN	C1-C2-C3	4.08	115.58	109.64
18	T	1	NAG	O4-C4-C5	-3.95	99.60	109.32
13	L	1	NAG	O4-C4-C5	-3.90	99.73	109.32
8	C	5	NAG	C2-N2-C7	3.84	128.05	122.90
8	C	1	NAG	O4-C4-C5	-3.76	100.08	109.32
8	C	4	MAN	O3-C3-C4	3.60	118.87	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	T	2	NAG	O5-C1-C2	-3.60	105.72	111.29
16	P	3	BMA	O3-C3-C2	-3.55	102.81	110.05
12	K	2	NAG	O5-C1-C2	-3.51	105.87	111.29
16	P	2	NAG	O4-C4-C3	3.47	118.56	110.38
8	C	3	BMA	C1-O5-C5	-3.44	107.57	112.19
10	M	2	NAG	O4-C4-C3	3.43	118.47	110.38
12	K	5	MAN	C1-O5-C5	3.42	116.77	112.19
16	P	3	BMA	O3-C3-C4	3.41	118.41	110.38
15	O	4	MAN	C1-C2-C3	3.35	114.52	109.64
18	T	2	NAG	O4-C4-C3	-3.30	102.59	110.38
15	O	4	MAN	O6-C6-C5	-3.26	100.25	111.33
18	T	2	NAG	O4-C4-C5	-3.23	101.37	109.32
17	S	1	NAG	O4-C4-C3	-3.22	102.79	110.38
8	C	1	NAG	O4-C4-C3	-3.19	102.85	110.38
15	O	4	MAN	C1-O5-C5	-3.17	107.94	112.19
8	C	2	NAG	O4-C4-C5	-3.13	101.62	109.32
12	K	1	NAG	O4-C4-C3	-3.11	103.04	110.38
13	L	5	MAN	C1-O5-C5	3.08	116.32	112.19
17	S	3	BMA	O5-C5-C6	3.08	113.67	107.66
15	O	3	BMA	O3-C3-C4	3.08	117.64	110.38
8	C	2	NAG	O5-C1-C2	-3.08	106.53	111.29
15	O	4	MAN	O3-C3-C4	3.00	117.46	110.38
15	O	6	MAN	C1-C2-C3	2.85	113.80	109.64
12	K	2	NAG	O4-C4-C5	-2.85	102.31	109.32
12	K	5	MAN	O5-C1-C2	-2.73	104.28	110.79
14	N	1	NAG	C1-O5-C5	2.72	115.83	112.19
18	T	8	MAN	O3-C3-C2	2.68	115.53	110.05
18	T	5	MAN	O3-C3-C4	2.67	116.67	110.38
18	T	8	MAN	C1-C2-C3	-2.67	105.75	109.64
15	O	4	MAN	C3-C4-C5	-2.64	105.45	110.23
12	K	3	BMA	O3-C3-C2	2.61	115.37	110.05
15	O	2	NAG	O4-C4-C5	-2.59	102.95	109.32
13	L	5	MAN	O5-C1-C2	-2.58	104.63	110.79
8	C	3	BMA	O5-C5-C6	2.55	112.62	107.66
18	T	2	NAG	C1-O5-C5	-2.54	108.79	112.19
15	O	4	MAN	O4-C4-C3	2.52	116.33	110.38
17	S	1	NAG	O5-C1-C2	-2.46	107.49	111.29
16	P	2	NAG	C4-C3-C2	-2.44	107.44	111.02
16	P	3	BMA	C1-O5-C5	-2.44	108.92	112.19
15	O	2	NAG	O5-C1-C2	-2.40	107.57	111.29
11	I	1	NAG	C1-O5-C5	-2.38	109.00	112.19
8	C	4	MAN	C1-C2-C3	-2.38	106.18	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1	NAG	C6-C5-C4	-2.36	107.22	113.02
16	P	2	NAG	C1-O5-C5	2.35	115.34	112.19
18	T	3	BMA	C1-O5-C5	-2.32	109.08	112.19
16	P	3	BMA	O5-C1-C2	-2.32	105.26	110.79
8	C	4	MAN	C3-C4-C5	-2.30	106.06	110.23
13	L	2	NAG	C1-O5-C5	2.30	115.26	112.19
9	F	2	NAG	O4-C4-C5	-2.29	103.68	109.32
9	F	8	FUC	O2-C2-C1	2.28	114.44	109.22
10	J	2	NAG	C2-N2-C7	2.25	125.92	122.90
10	J	1	NAG	C2-N2-C7	2.24	125.91	122.90
11	I	1	NAG	O4-C4-C3	2.22	115.61	110.38
8	C	6	GAL	C1-O5-C5	2.18	115.11	112.19
18	T	1	NAG	O5-C1-C2	-2.18	107.92	111.29
8	C	8	FUC	O5-C5-C4	2.17	113.47	109.55
13	L	1	NAG	C2-N2-C7	2.11	125.73	122.90
12	K	1	NAG	C1-C2-N2	-2.10	107.12	110.43
10	H	2	NAG	O4-C4-C5	-2.08	104.19	109.32
8	C	1	NAG	C1-O5-C5	-2.07	109.41	112.19
18	T	5	MAN	O3-C3-C2	-2.07	105.83	110.05
12	K	3	BMA	O3-C3-C4	-2.07	105.50	110.38
11	I	1	NAG	C1-C2-N2	-2.06	107.18	110.43
8	C	8	FUC	C1-C2-C3	2.05	112.63	109.64
15	O	3	BMA	C6-C5-C4	2.05	118.05	113.02
8	C	3	BMA	O2-C2-C3	-2.04	105.93	110.15
17	S	3	BMA	C1-O5-C5	-2.04	109.45	112.19
10	H	2	NAG	O4-C4-C3	2.02	115.14	110.38
8	C	8	FUC	C1-O5-C5	2.02	117.73	112.97
17	S	4	MAN	O5-C1-C2	-2.02	105.98	110.79
13	L	1	NAG	C1-O5-C5	-2.01	109.49	112.19
15	O	3	BMA	C1-O5-C5	-2.01	109.49	112.19
10	H	2	NAG	O3-C3-C2	-2.00	105.24	109.40

There are no chirality outliers.

All (137) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1	NAG	C1-C2-N2-C7
8	C	1	NAG	C8-C7-N2-C2
8	C	1	NAG	O7-C7-N2-C2
8	C	2	NAG	C3-C2-N2-C7
8	C	2	NAG	C8-C7-N2-C2
8	C	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
8	C	5	NAG	C1-C2-N2-C7
8	C	5	NAG	C8-C7-N2-C2
8	C	5	NAG	O7-C7-N2-C2
9	F	2	NAG	C3-C2-N2-C7
9	F	2	NAG	C8-C7-N2-C2
9	F	2	NAG	O7-C7-N2-C2
9	F	5	NAG	C8-C7-N2-C2
9	F	5	NAG	O7-C7-N2-C2
10	H	1	NAG	C3-C2-N2-C7
10	H	1	NAG	C8-C7-N2-C2
10	H	1	NAG	O7-C7-N2-C2
10	J	1	NAG	C1-C2-N2-C7
10	J	1	NAG	C8-C7-N2-C2
10	J	1	NAG	O7-C7-N2-C2
10	M	1	NAG	C3-C2-N2-C7
10	M	1	NAG	C8-C7-N2-C2
10	M	1	NAG	O7-C7-N2-C2
11	I	1	NAG	C3-C2-N2-C7
11	I	1	NAG	C8-C7-N2-C2
11	I	1	NAG	O7-C7-N2-C2
11	I	2	NAG	C1-C2-N2-C7
12	K	1	NAG	C3-C2-N2-C7
12	K	1	NAG	C8-C7-N2-C2
12	K	1	NAG	O7-C7-N2-C2
12	K	2	NAG	C1-C2-N2-C7
12	K	2	NAG	C8-C7-N2-C2
12	K	2	NAG	O7-C7-N2-C2
13	L	1	NAG	C3-C2-N2-C7
13	L	1	NAG	C8-C7-N2-C2
13	L	1	NAG	O7-C7-N2-C2
14	N	1	NAG	C8-C7-N2-C2
14	N	1	NAG	O7-C7-N2-C2
15	O	2	NAG	C3-C2-N2-C7
15	O	2	NAG	C8-C7-N2-C2
15	O	2	NAG	O7-C7-N2-C2
16	P	2	NAG	C1-C2-N2-C7
16	P	2	NAG	C8-C7-N2-C2
16	P	2	NAG	O7-C7-N2-C2
17	S	2	NAG	C3-C2-N2-C7
17	S	2	NAG	C8-C7-N2-C2
17	S	2	NAG	O7-C7-N2-C2
15	O	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	F	1	NAG	C8-C7-N2-C2
9	F	1	NAG	O7-C7-N2-C2
14	N	1	NAG	O5-C5-C6-O6
18	T	9	MAN	C4-C5-C6-O6
16	P	5	MAN	O5-C5-C6-O6
14	N	1	NAG	C4-C5-C6-O6
7	A	2	NAG	C8-C7-N2-C2
14	N	2	NAG	C8-C7-N2-C2
13	L	3	BMA	O5-C5-C6-O6
15	O	3	BMA	O5-C5-C6-O6
7	A	1	NAG	O5-C5-C6-O6
7	A	1	NAG	C4-C5-C6-O6
15	O	4	MAN	C4-C5-C6-O6
7	A	2	NAG	O7-C7-N2-C2
14	N	2	NAG	O7-C7-N2-C2
15	O	1	NAG	C8-C7-N2-C2
18	T	1	NAG	C8-C7-N2-C2
18	T	4	MAN	O5-C5-C6-O6
15	O	1	NAG	O7-C7-N2-C2
18	T	1	NAG	O7-C7-N2-C2
8	C	1	NAG	C4-C5-C6-O6
15	O	2	NAG	C4-C5-C6-O6
15	O	2	NAG	O5-C5-C6-O6
18	T	3	BMA	O5-C5-C6-O6
18	T	9	MAN	O5-C5-C6-O6
11	I	2	NAG	C8-C7-N2-C2
11	I	2	NAG	O7-C7-N2-C2
11	I	3	BMA	O5-C5-C6-O6
12	K	1	NAG	O5-C5-C6-O6
10	H	3	BMA	O5-C5-C6-O6
10	H	3	BMA	C4-C5-C6-O6
12	K	6	MAN	O5-C5-C6-O6
13	L	4	MAN	O5-C5-C6-O6
10	M	2	NAG	C8-C7-N2-C2
16	P	5	MAN	C4-C5-C6-O6
8	C	1	NAG	O5-C5-C6-O6
15	O	6	MAN	C4-C5-C6-O6
12	K	6	MAN	C4-C5-C6-O6
13	L	1	NAG	O5-C5-C6-O6
13	L	4	MAN	C4-C5-C6-O6
18	T	4	MAN	C4-C5-C6-O6
10	M	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
13	L	2	NAG	O5-C5-C6-O6
11	I	2	NAG	O5-C5-C6-O6
16	P	2	NAG	O5-C5-C6-O6
17	S	3	BMA	O5-C5-C6-O6
12	K	3	BMA	O5-C5-C6-O6
13	L	5	MAN	O5-C5-C6-O6
15	O	1	NAG	O5-C5-C6-O6
18	T	5	MAN	O5-C5-C6-O6
10	H	2	NAG	O5-C5-C6-O6
9	F	2	NAG	O5-C5-C6-O6
15	O	4	MAN	O5-C5-C6-O6
17	S	4	MAN	O5-C5-C6-O6
12	K	2	NAG	O5-C5-C6-O6
16	P	1	NAG	O5-C5-C6-O6
13	L	2	NAG	C8-C7-N2-C2
10	H	2	NAG	C3-C2-N2-C7
10	M	2	NAG	C3-C2-N2-C7
14	N	1	NAG	C3-C2-N2-C7
9	F	5	NAG	O5-C5-C6-O6
15	O	6	MAN	O5-C5-C6-O6
10	M	2	NAG	O5-C5-C6-O6
17	S	6	MAN	O5-C5-C6-O6
13	L	3	BMA	C4-C5-C6-O6
10	J	2	NAG	C1-C2-N2-C7
13	L	2	NAG	O7-C7-N2-C2
10	J	2	NAG	C4-C5-C6-O6
10	H	2	NAG	C8-C7-N2-C2
18	T	3	BMA	C4-C5-C6-O6
18	T	8	MAN	C4-C5-C6-O6
10	J	2	NAG	O5-C5-C6-O6
10	H	2	NAG	O7-C7-N2-C2
7	A	2	NAG	C3-C2-N2-C7
8	C	1	NAG	C3-C2-N2-C7
14	N	2	NAG	C3-C2-N2-C7
9	F	6	MAN	O5-C5-C6-O6
9	F	3	BMA	O5-C5-C6-O6
18	T	8	MAN	O5-C5-C6-O6
12	K	7	MAN	C4-C5-C6-O6
18	T	7	MAN	O5-C5-C6-O6
9	F	1	NAG	C3-C2-N2-C7
10	J	2	NAG	C3-C2-N2-C7
18	T	2	NAG	C3-C2-N2-C7

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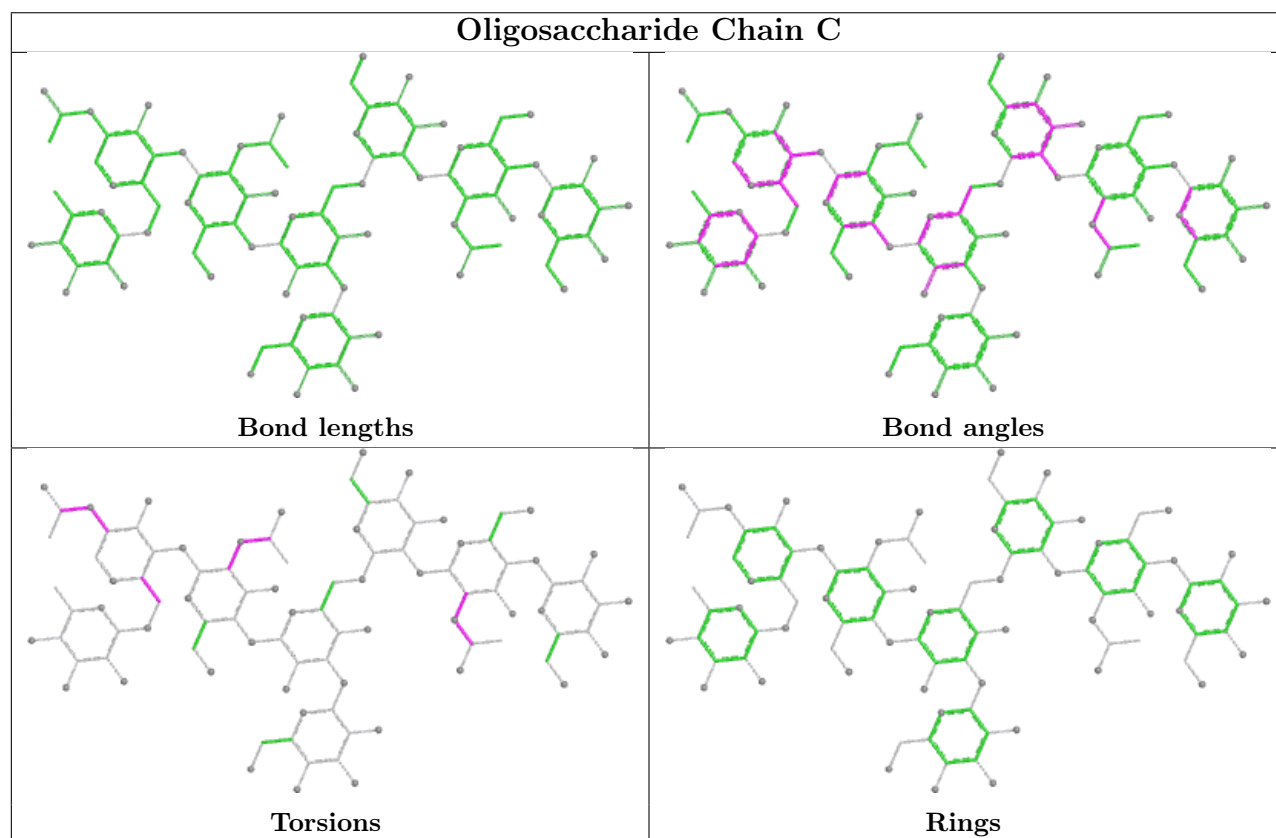
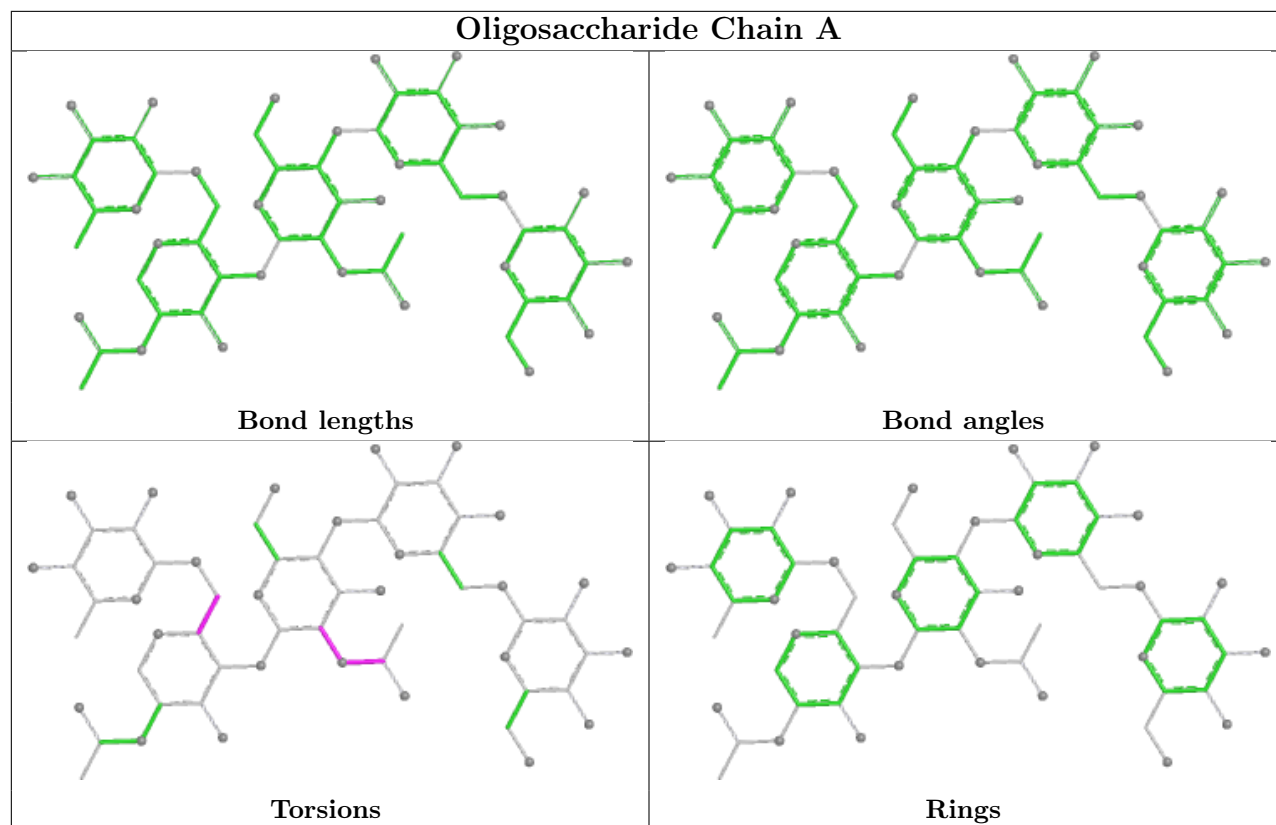
Mol	Chain	Res	Type	Atoms
9	F	3	BMA	C4-C5-C6-O6
9	F	1	NAG	C4-C5-C6-O6
12	K	1	NAG	C4-C5-C6-O6
14	N	2	NAG	C4-C5-C6-O6
12	K	7	MAN	O5-C5-C6-O6

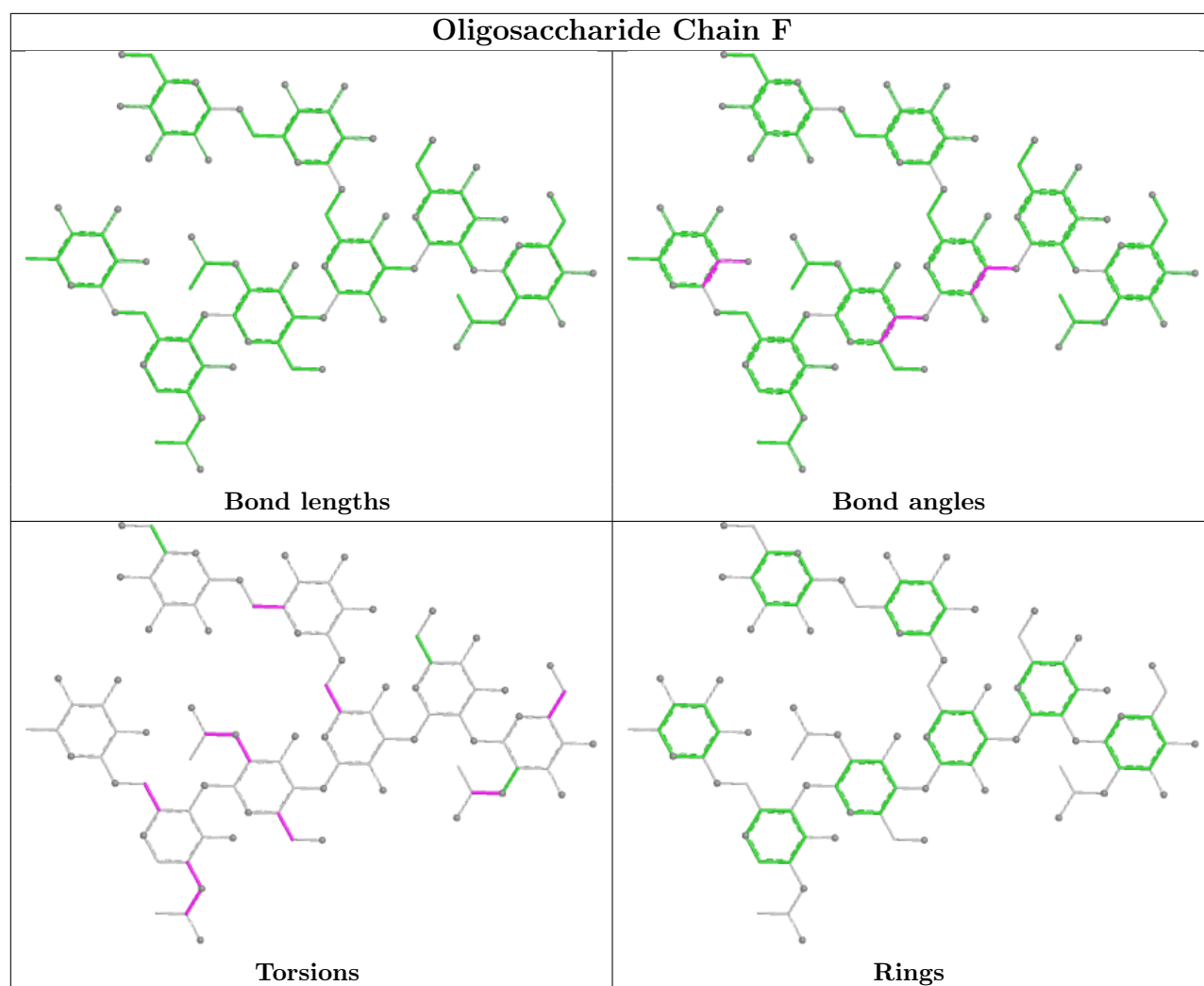
There are no ring outliers.

29 monomers are involved in 29 short contacts:

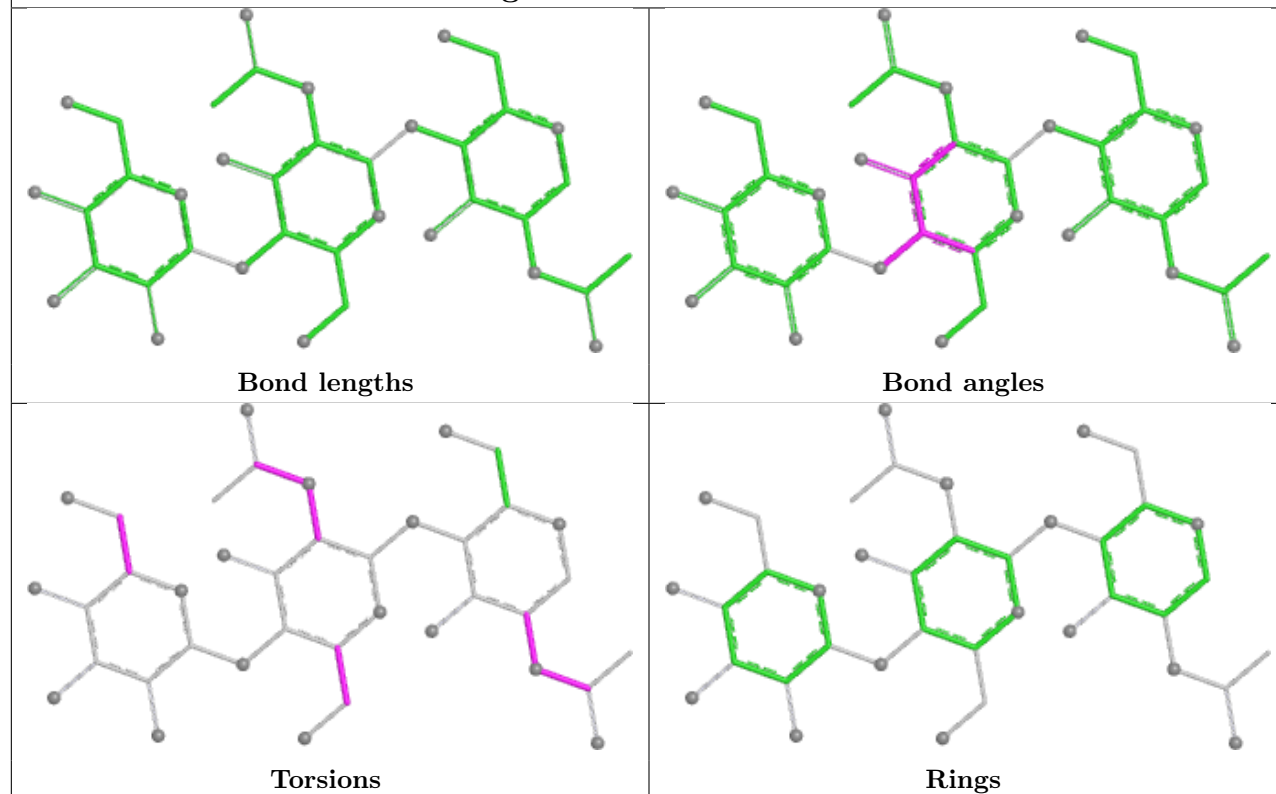
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	O	4	MAN	2	0
13	L	1	NAG	2	0
15	O	2	NAG	2	0
13	L	4	MAN	1	0
16	P	6	MAN	2	0
10	H	1	NAG	1	0
11	I	1	NAG	3	0
12	K	4	MAN	1	0
13	L	5	MAN	1	0
13	L	2	NAG	1	0
17	S	6	MAN	1	0
18	T	3	BMA	1	0
17	S	3	BMA	1	0
9	F	5	NAG	1	0
18	T	9	MAN	1	0
10	J	3	BMA	1	0
10	J	1	NAG	2	0
15	O	1	NAG	2	0
15	O	6	MAN	2	0
12	K	5	MAN	1	0
14	N	1	NAG	3	0
9	F	1	NAG	1	0
18	T	7	MAN	1	0
9	F	4	MAN	1	0
8	C	5	NAG	1	0
11	I	2	NAG	2	0
14	N	2	NAG	3	0
8	C	1	NAG	2	0
10	H	2	NAG	1	0

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

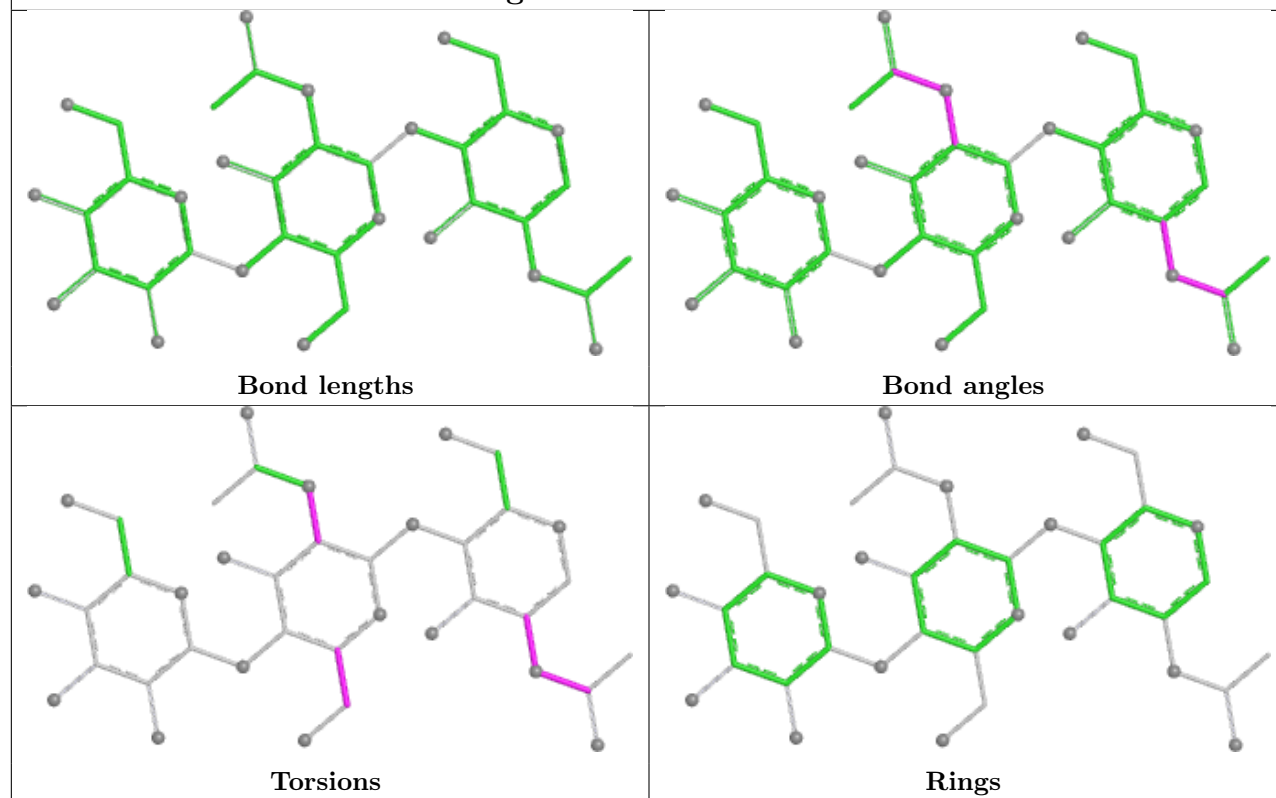




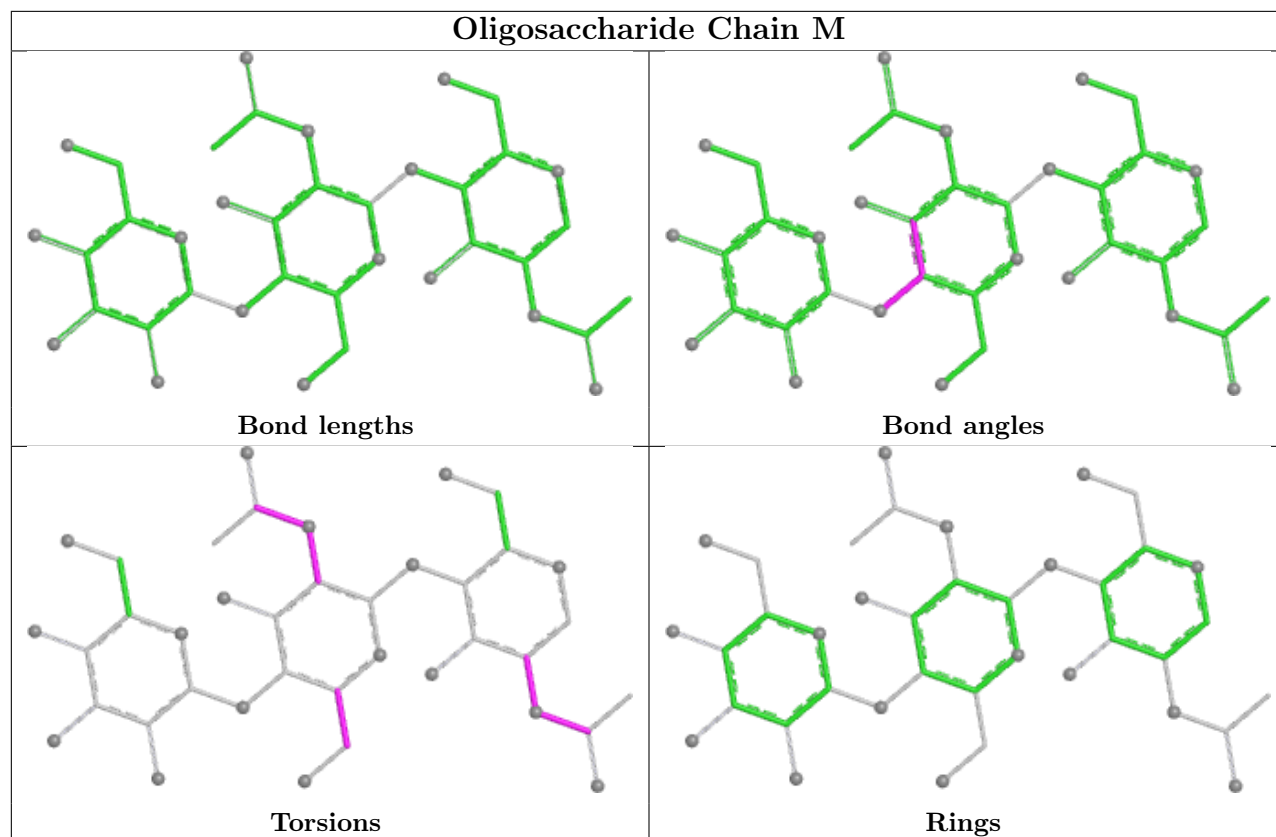
Oligosaccharide Chain H



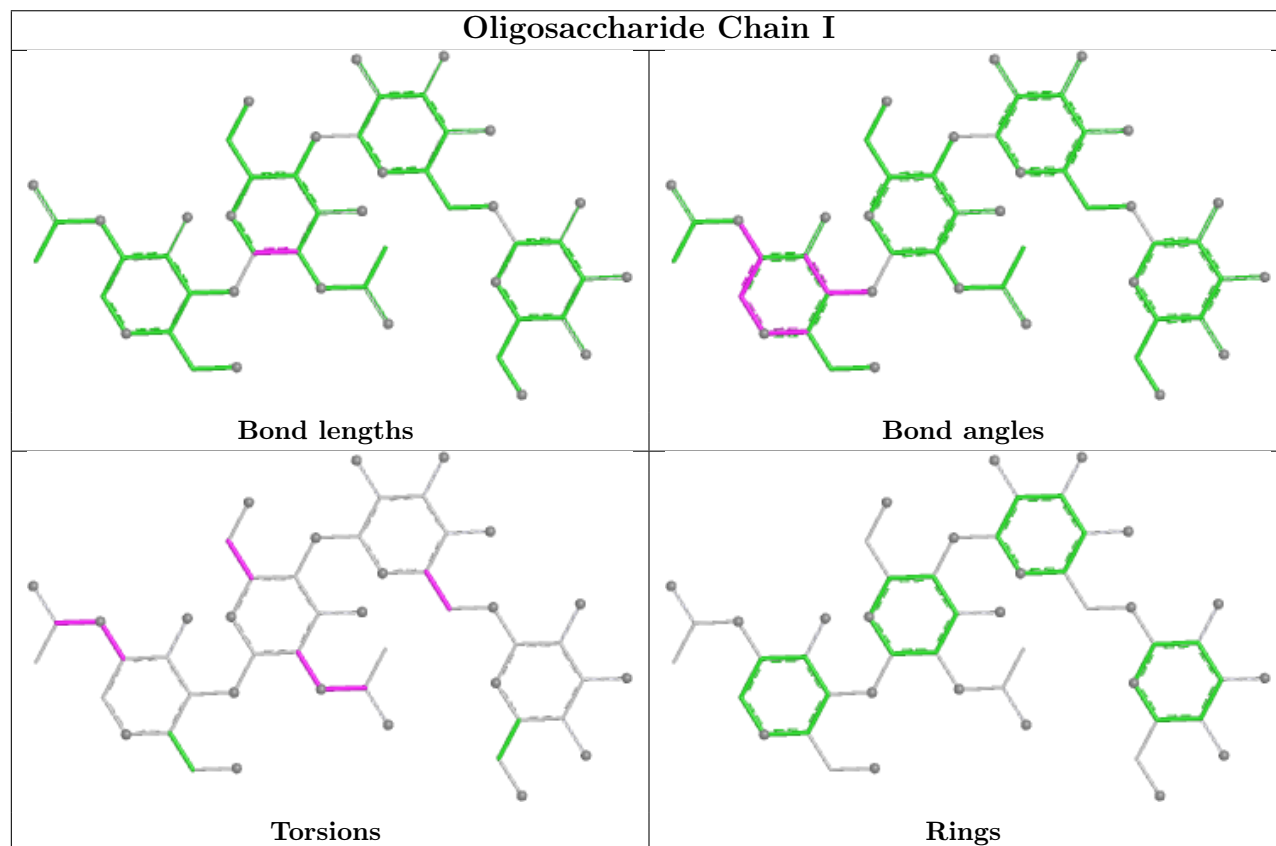
Oligosaccharide Chain J

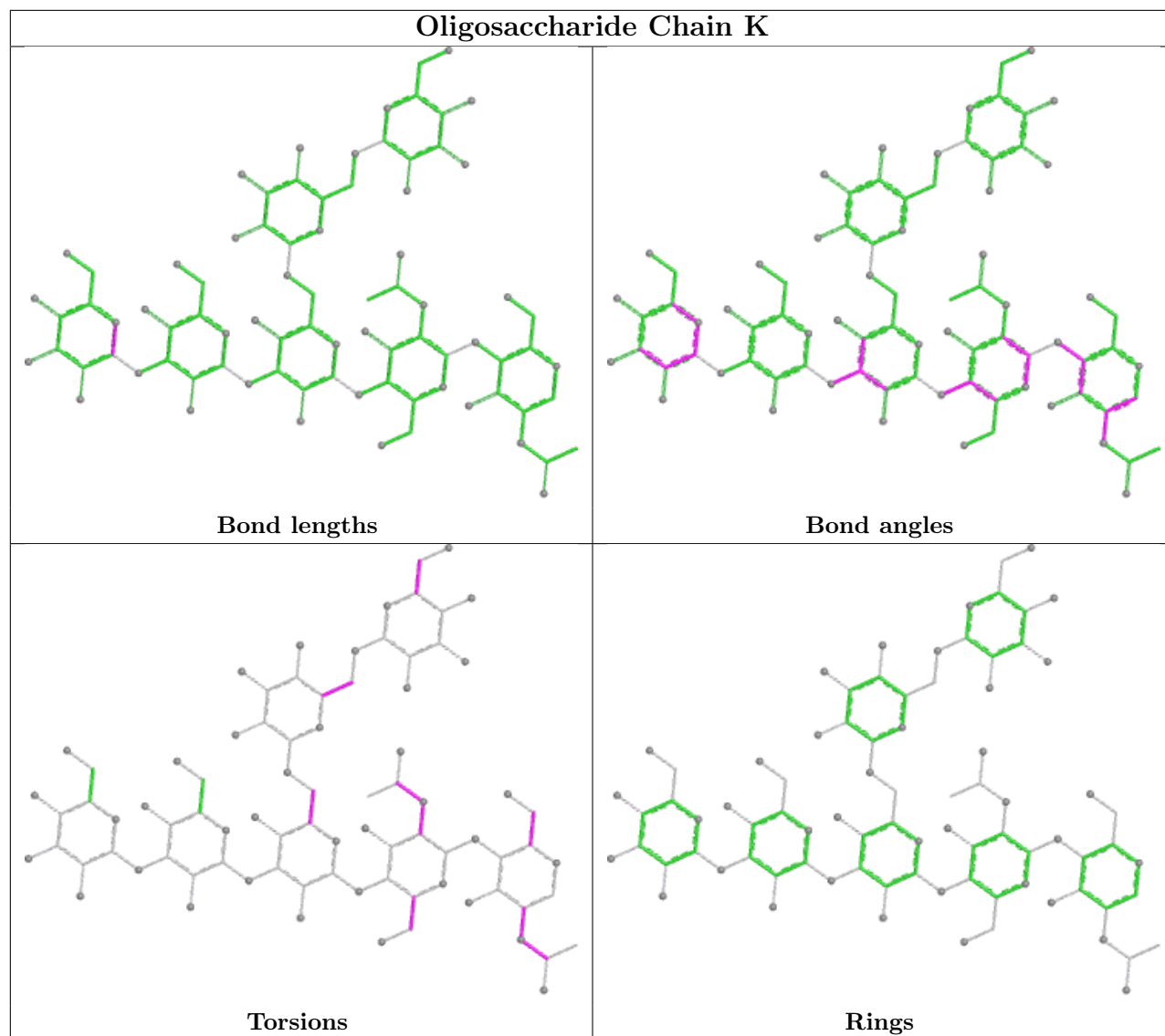


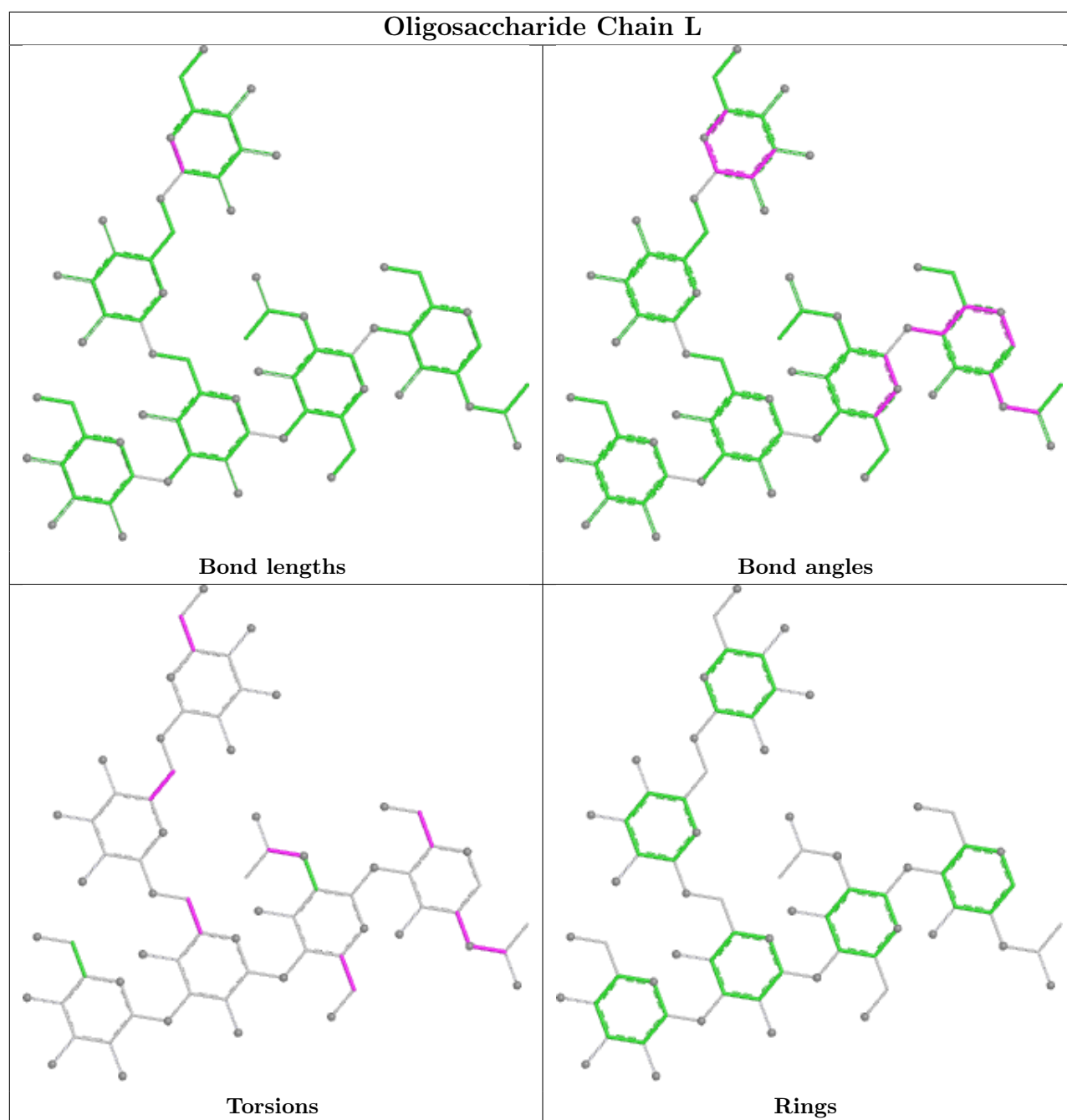
Oligosaccharide Chain M

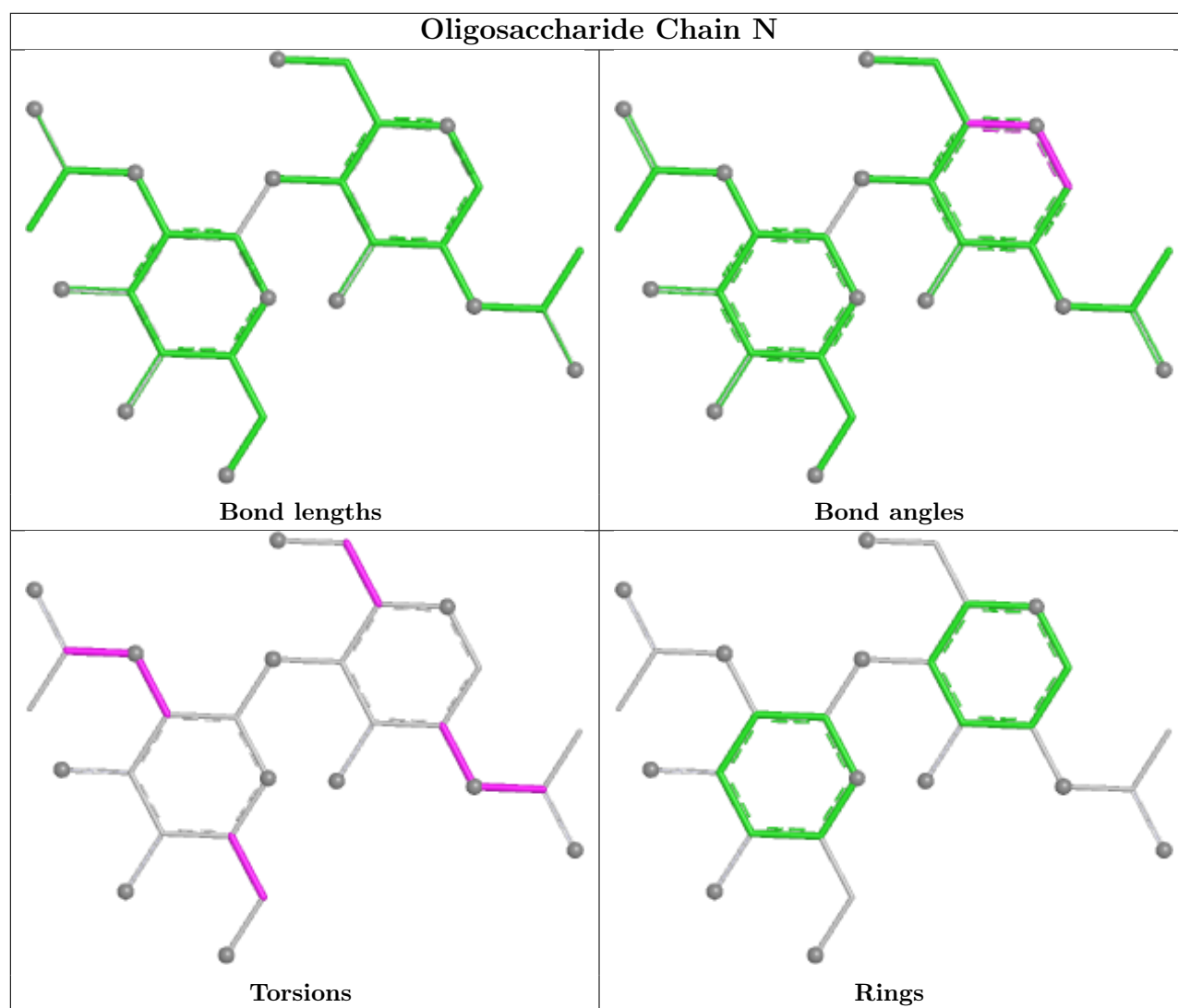


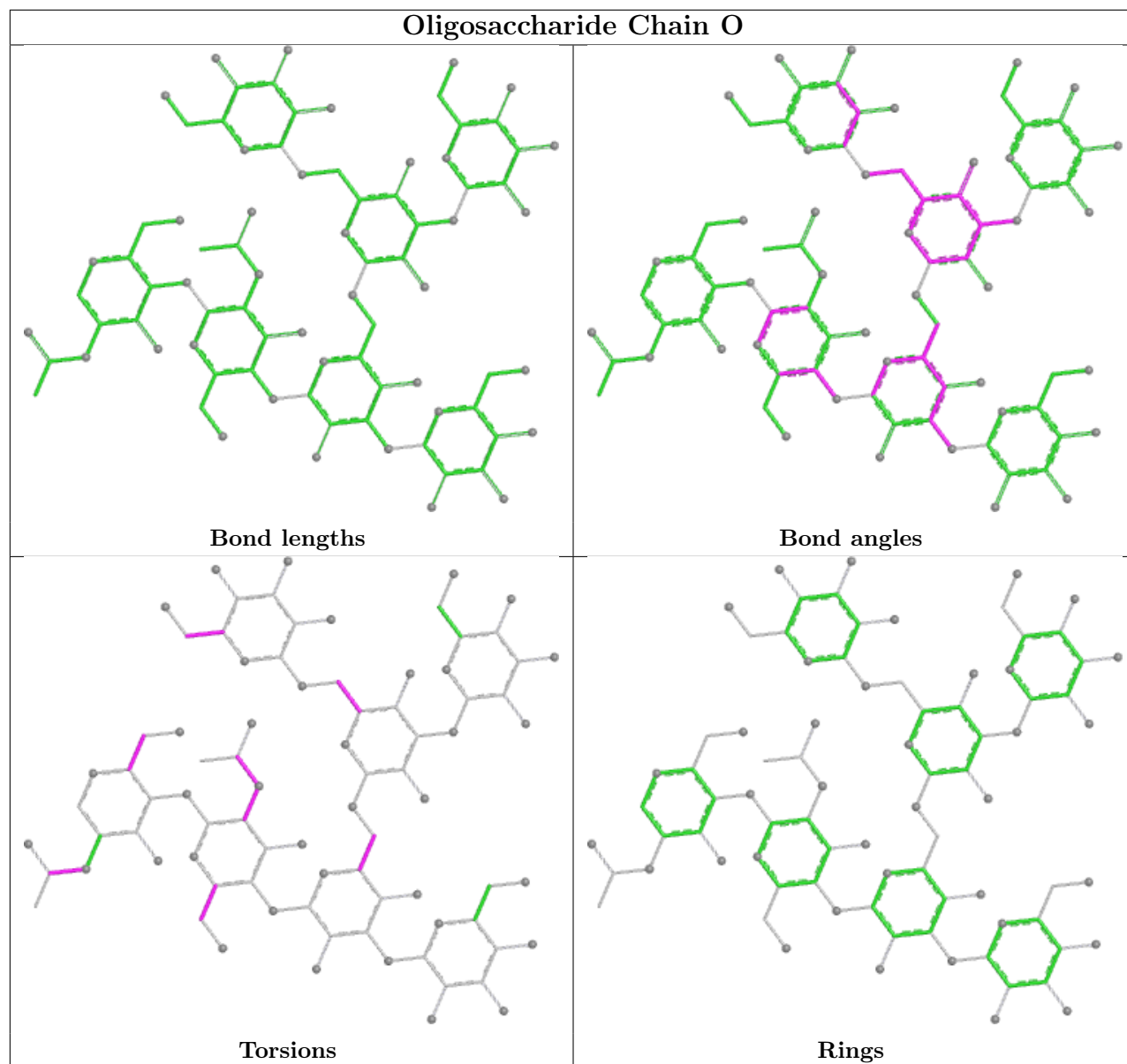
Oligosaccharide Chain I

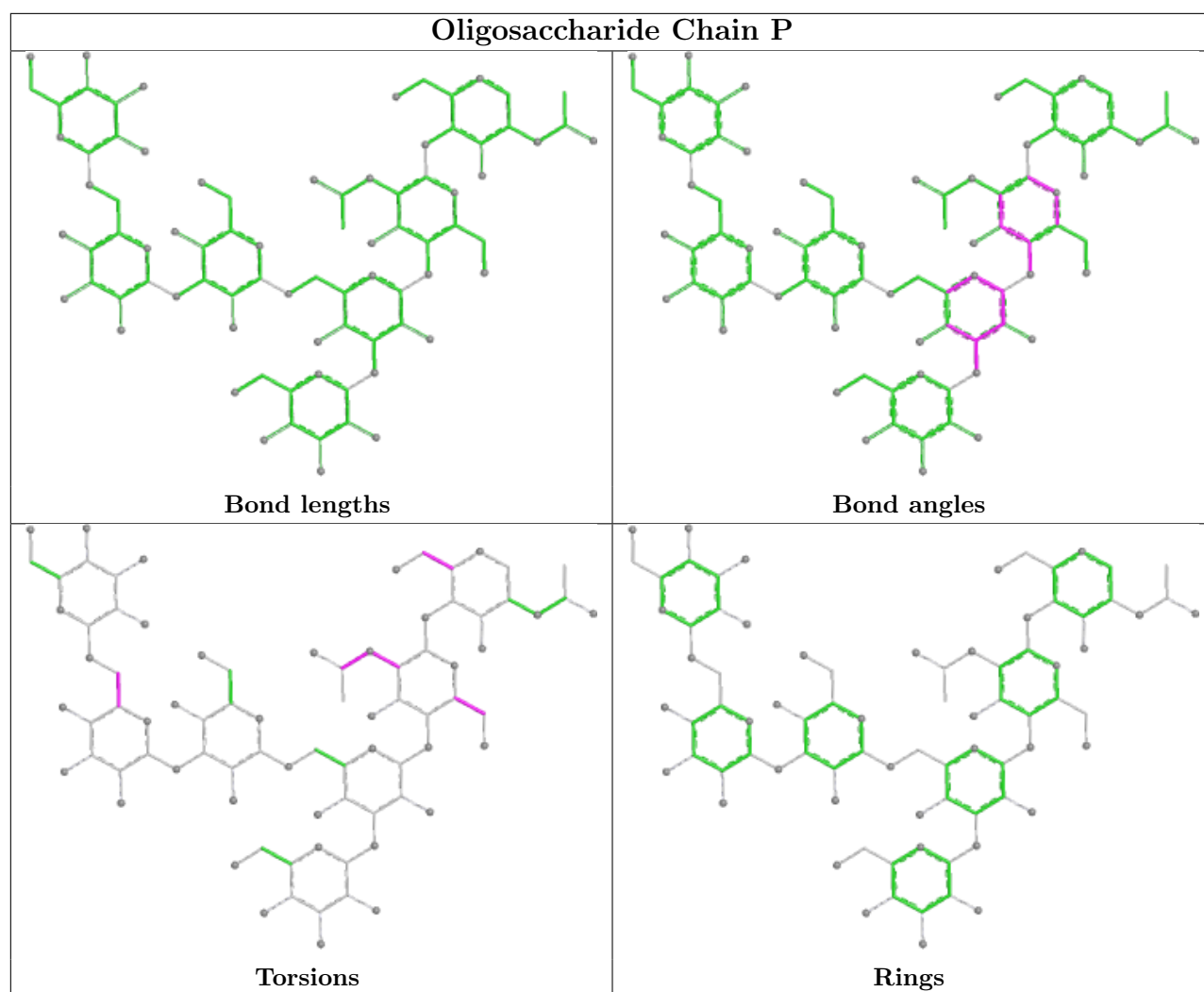


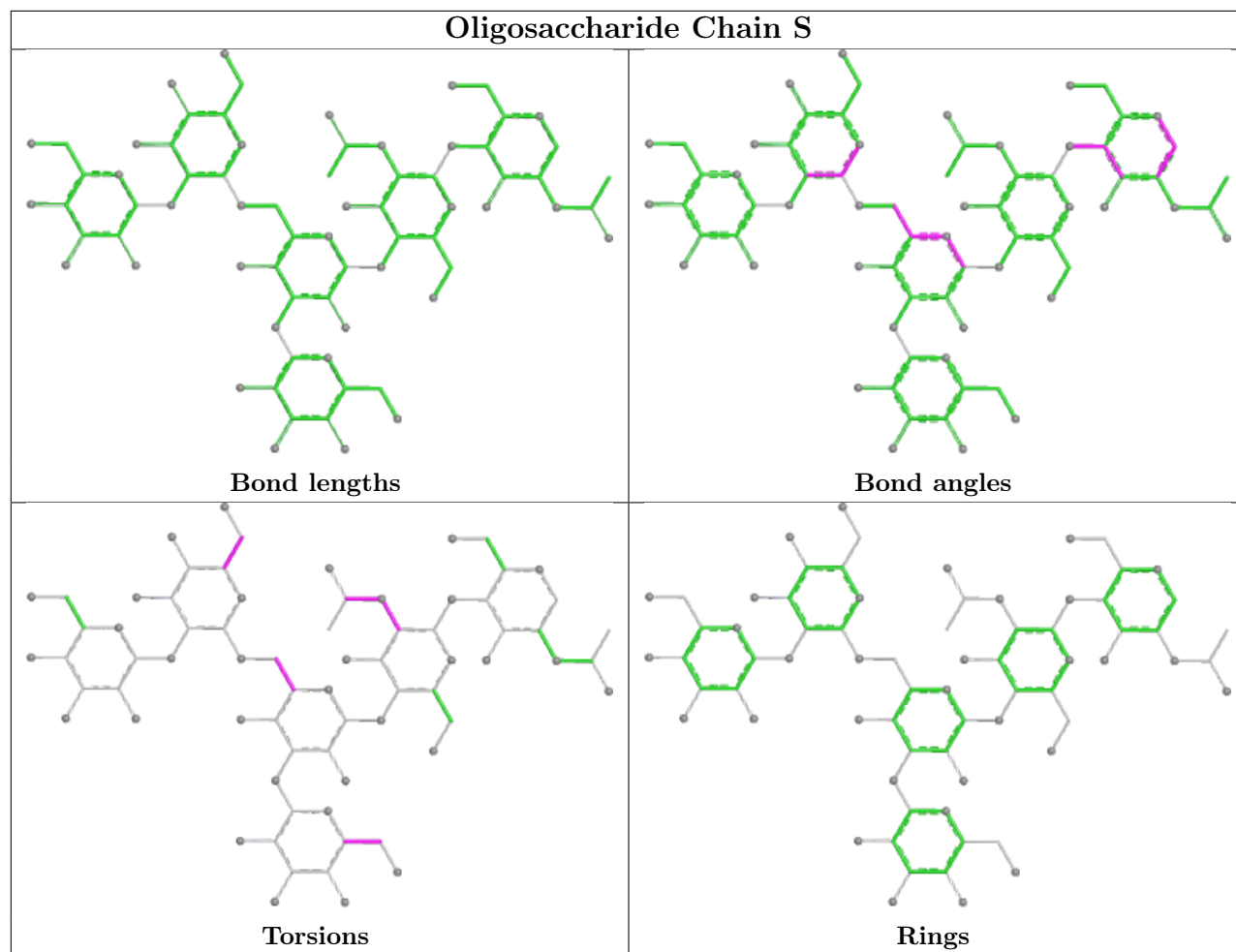


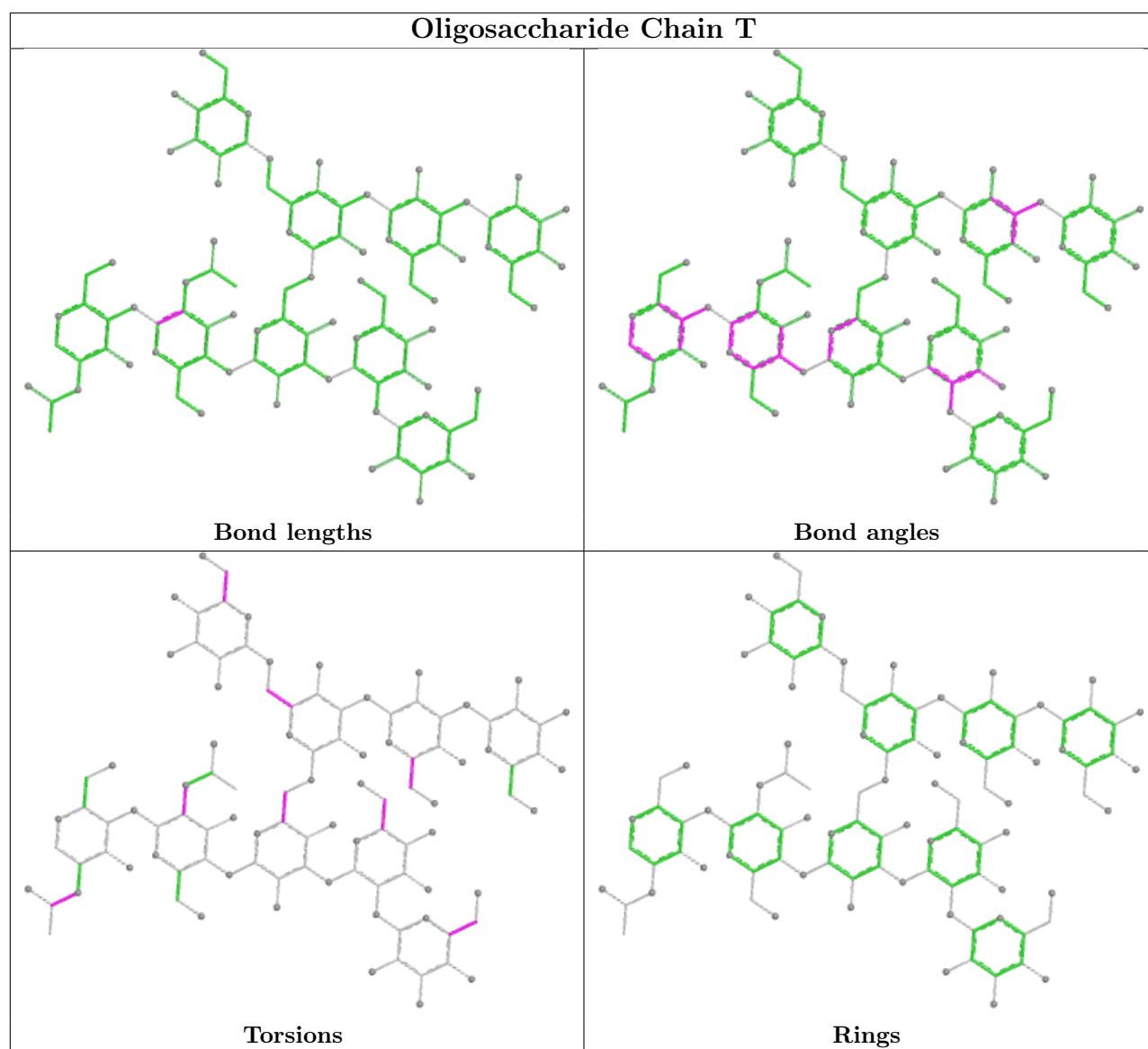












5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
19	NAG	G	601	4	14,14,15	0.30	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	NAG	B	701	1	14,14,15	0.40	0	17,19,21	0.74	0
19	NAG	G	602	4	14,14,15	0.30	0	17,19,21	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	NAG	G	601	4	-	2/6/23/26	0/1/1/1
19	NAG	B	701	1	-	2/6/23/26	0/1/1/1
19	NAG	G	602	4	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	G	602	NAG	C8-C7-N2-C2
19	G	602	NAG	O7-C7-N2-C2
19	B	701	NAG	C8-C7-N2-C2
19	B	701	NAG	O7-C7-N2-C2
19	G	601	NAG	O5-C5-C6-O6
19	G	602	NAG	O5-C5-C6-O6
19	G	602	NAG	C1-C2-N2-C7
19	G	601	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	701	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	134/153 (87%)	-0.40	0	100 100	81, 167, 236, 280	0
2	D	226/243 (93%)	-0.45	1 (0%)	88 74	106, 235, 309, 337	0
3	E	213/216 (98%)	-0.48	2 (0%)	81 60	101, 219, 319, 361	0
4	G	452/479 (94%)	-0.41	1 (0%)	91 81	75, 172, 258, 336	0
5	Q	231/241 (95%)	-0.47	1 (0%)	88 74	120, 224, 305, 346	0
6	R	211/215 (98%)	-0.38	4 (1%)	66 45	129, 241, 304, 358	0
All	All	1467/1547 (94%)	-0.43	9 (0%)	85 68	75, 204, 303, 361	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	122	PHE	3.4
6	R	117	PRO	2.4
5	Q	35	TRP	2.4
2	D	153	SER	2.2
6	R	21	ARG	2.1
6	R	56	SER	2.1
6	R	118	SER	2.1
3	E	51	TYR	2.0
4	G	496	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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	A	1	14/15	-	-	264,264,264,264	0
7	NAG	A	2	14/15	-	-	292,292,292,292	0
7	BMA	A	3	11/12	-	-	336,336,336,336	0
7	MAN	A	4	11/12	-	-	290,290,290,290	0
7	FUC	A	5	10/11	-	-	282,282,282,282	0
8	NAG	C	1	14/15	-	-	222,222,222,222	0
8	NAG	C	2	14/15	-	-	261,261,261,261	0
8	BMA	C	3	11/12	-	-	262,262,262,262	0
8	MAN	C	4	11/12	-	-	242,242,242,242	0
8	NAG	C	5	14/15	-	-	281,281,281,281	0
8	GAL	C	6	11/12	-	-	306,306,306,306	0
8	MAN	C	7	11/12	-	-	242,242,242,242	0
8	FUC	C	8	10/11	-	-	274,274,274,274	0
9	NAG	F	1	14/15	-	-	204,204,204,204	0
9	NAG	F	2	14/15	-	-	285,285,285,285	0
9	BMA	F	3	11/12	-	-	341,341,341,341	0
9	MAN	F	4	11/12	-	-	353,353,353,353	0
9	NAG	F	5	14/15	-	-	326,326,326,326	0
9	MAN	F	6	11/12	-	-	335,335,335,335	0
9	MAN	F	7	11/12	-	-	330,330,330,330	0
9	FUC	F	8	10/11	-	-	294,294,294,294	0
11	MAN	I	4	11/12	0.31	0.09	328,328,328,328	0
10	BMA	M	3	11/12	0.41	0.10	351,351,351,351	0
14	NAG	N	2	14/15	0.41	0.12	298,298,298,298	0
10	NAG	H	2	14/15	0.42	0.15	249,249,249,249	0
15	BMA	O	3	11/12	0.42	0.07	317,317,317,317	0
18	MAN	T	7	11/12	0.42	0.12	207,207,207,207	0
16	NAG	P	2	14/15	0.43	0.07	302,302,302,302	0
10	BMA	J	3	11/12	0.49	0.07	303,303,303,303	0
18	MAN	T	5	11/12	0.53	0.07	246,246,246,246	0
18	MAN	T	6	11/12	0.57	0.09	280,280,280,280	0
17	MAN	S	6	11/12	0.59	0.04	321,321,321,321	0
18	MAN	T	8	11/12	0.65	0.13	230,230,230,230	0
17	MAN	S	4	11/12	0.68	0.05	319,319,319,319	0
10	NAG	H	1	14/15	0.68	0.10	206,206,206,206	0
10	NAG	J	2	14/15	0.70	0.06	291,291,291,291	0
13	NAG	L	1	14/15	0.72	0.09	261,261,261,261	0

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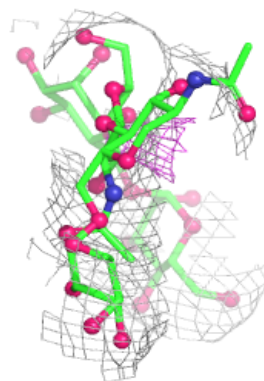
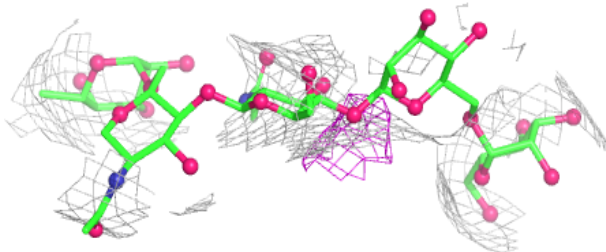
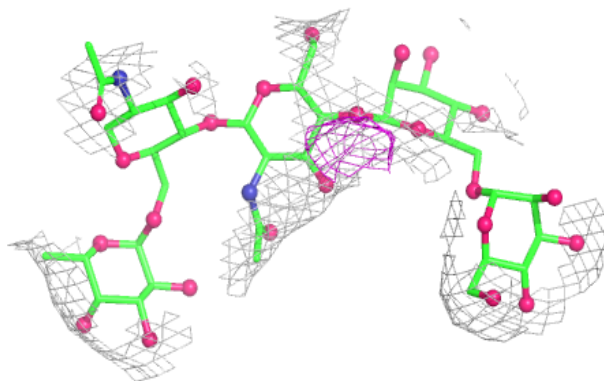
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	NAG	S	2	14/15	0.72	0.07	276,276,276,276	0
12	MAN	K	5	11/12	-	-	334,334,334,334	0
12	MAN	K	6	11/12	-	-	332,332,332,332	0
12	MAN	K	7	11/12	-	-	296,296,296,296	0
12	MAN	K	4	11/12	0.73	0.05	340,340,340,340	0
11	NAG	I	2	14/15	0.73	0.05	290,290,290,290	0
16	NAG	P	1	14/15	0.74	0.07	283,283,283,283	0
13	MAN	L	4	11/12	-	-	325,325,325,325	0
13	MAN	L	5	11/12	-	-	314,314,314,314	0
13	MAN	L	6	11/12	-	-	301,301,301,301	0
18	BMA	T	3	11/12	0.74	0.06	240,240,240,240	0
15	NAG	O	2	14/15	0.76	0.06	263,263,263,263	0
13	BMA	L	3	11/12	0.77	0.07	327,327,327,327	0
18	MAN	T	4	11/12	0.77	0.06	241,241,241,241	0
14	NAG	N	1	14/15	0.78	0.09	293,293,293,293	0
15	MAN	O	4	11/12	-	-	355,355,355,355	0
15	MAN	O	5	11/12	-	-	357,357,357,357	0
15	MAN	O	6	11/12	-	-	343,343,343,343	0
15	MAN	O	7	11/12	-	-	284,284,284,284	0
17	MAN	S	5	11/12	0.79	0.08	309,309,309,309	0
18	MAN	T	9	11/12	0.79	0.06	220,220,220,220	0
16	BMA	P	3	11/12	-	-	318,318,318,318	0
16	MAN	P	4	11/12	-	-	297,297,297,297	0
16	MAN	P	5	11/12	-	-	204,204,204,204	0
16	MAN	P	6	11/12	-	-	223,223,223,223	0
16	MAN	P	7	11/12	-	-	312,312,312,312	0
12	BMA	K	3	11/12	0.80	0.04	303,303,303,303	0
17	NAG	S	1	14/15	0.81	0.06	233,233,233,233	0
13	NAG	L	2	14/15	0.82	0.08	287,287,287,287	0
17	BMA	S	3	11/12	0.82	0.05	337,337,337,337	0
11	NAG	I	1	14/15	0.82	0.10	236,236,236,236	0
10	NAG	J	1	14/15	0.82	0.07	237,237,237,237	0
10	NAG	M	2	14/15	0.84	0.07	319,319,319,319	0
18	NAG	T	2	14/15	0.85	0.17	248,248,248,248	0
11	BMA	I	3	11/12	0.86	0.05	315,315,315,315	0
18	NAG	T	1	14/15	0.86	0.13	210,210,210,210	0
12	NAG	K	2	14/15	0.89	0.06	223,223,223,223	0
10	BMA	H	3	11/12	0.89	0.10	289,289,289,289	0
12	NAG	K	1	14/15	0.89	0.06	193,193,193,193	0
15	NAG	O	1	14/15	0.90	0.10	235,235,235,235	0
10	NAG	M	1	14/15	0.96	0.07	235,235,235,235	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

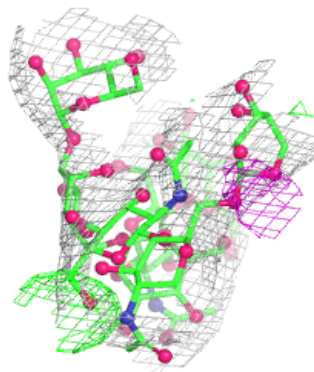
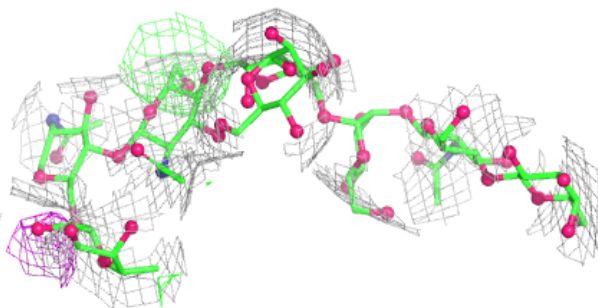
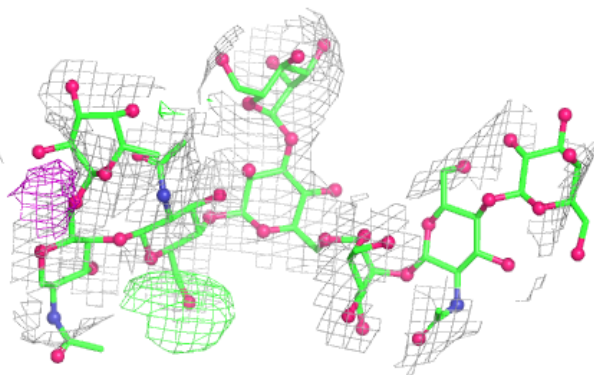
Electron density around Chain A:

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



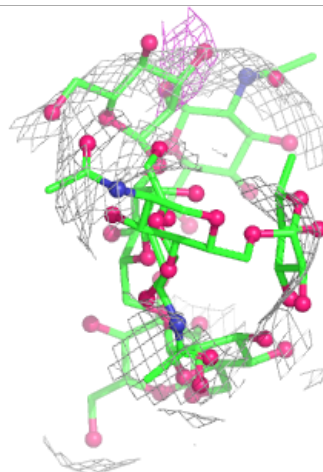
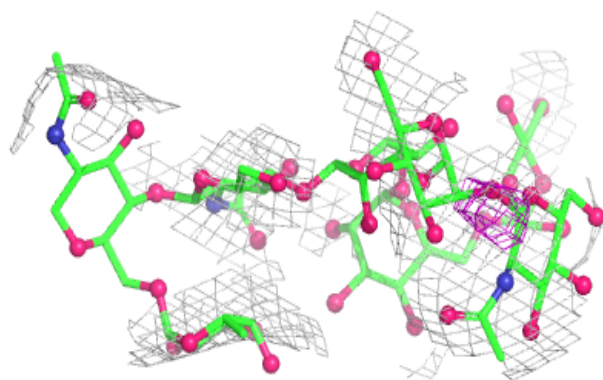
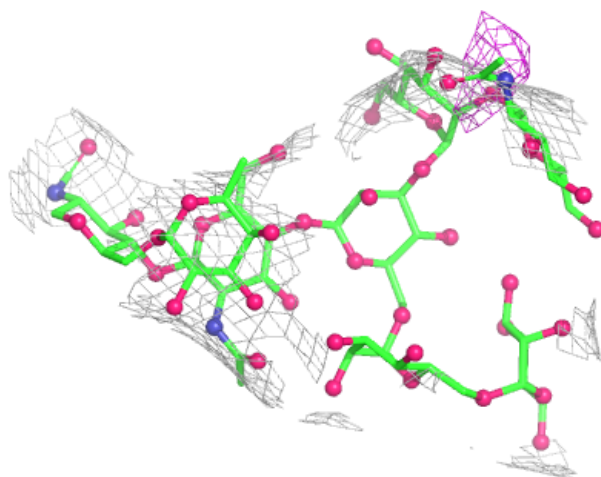
Electron density around Chain C:

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



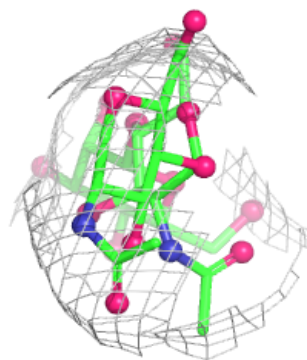
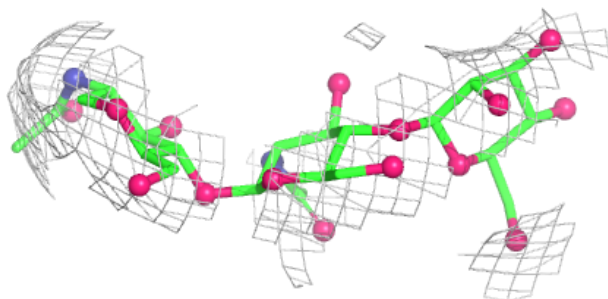
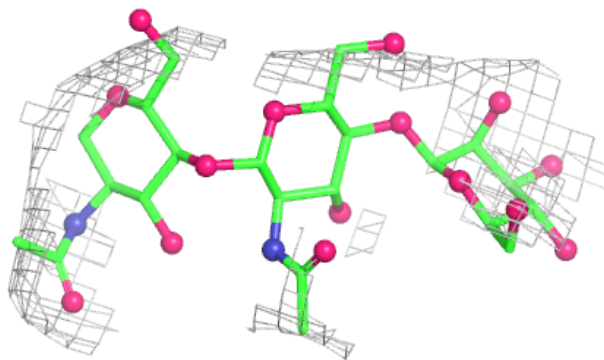
Electron density around Chain F:

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

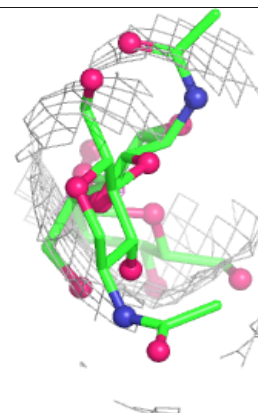
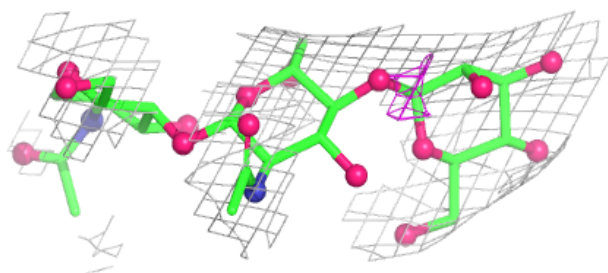
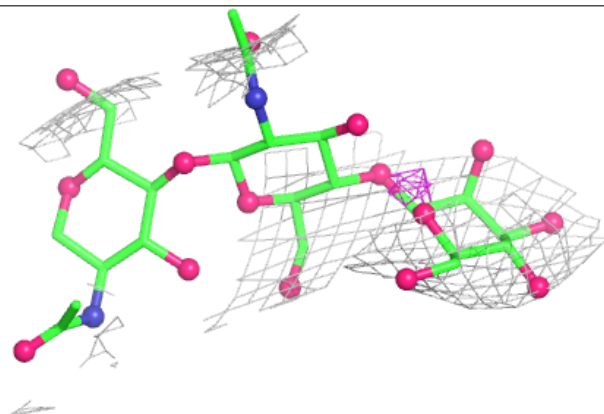


Electron density around Chain H:

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

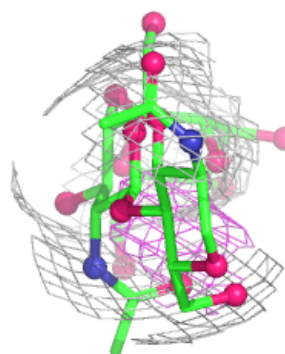
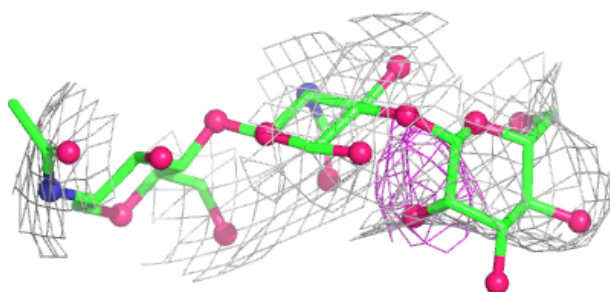
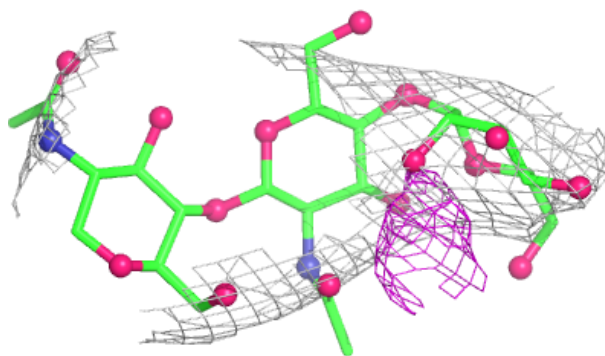
**Electron density around Chain J:**

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and green (positive)

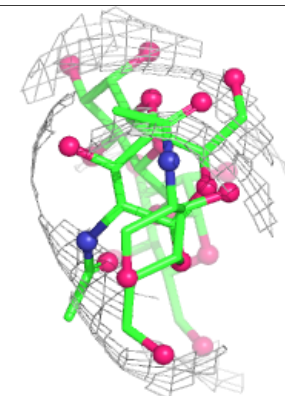
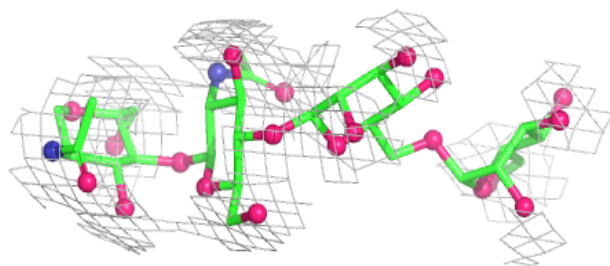
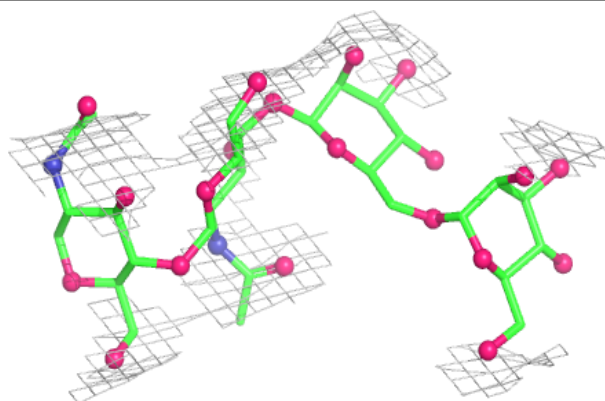


Electron density around Chain M:

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

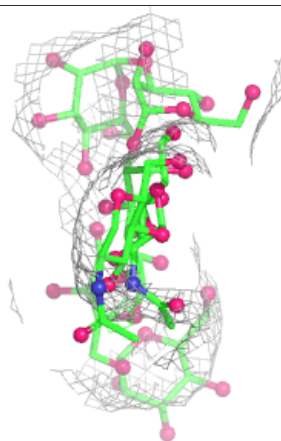
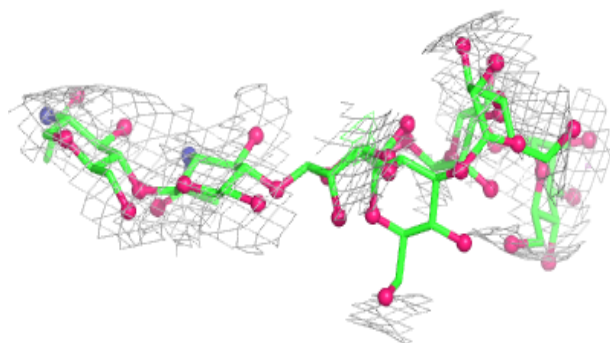
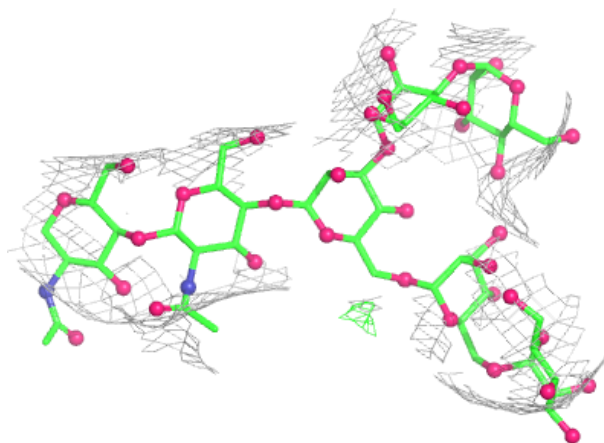
**Electron density around Chain I:**

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



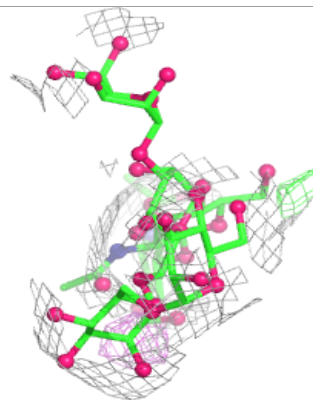
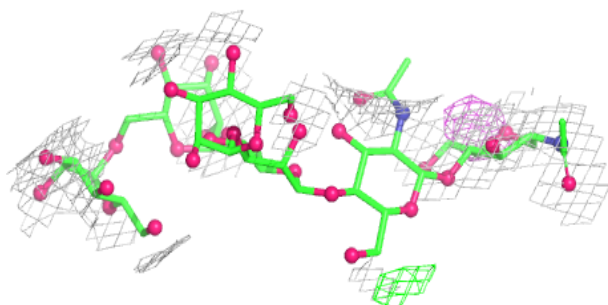
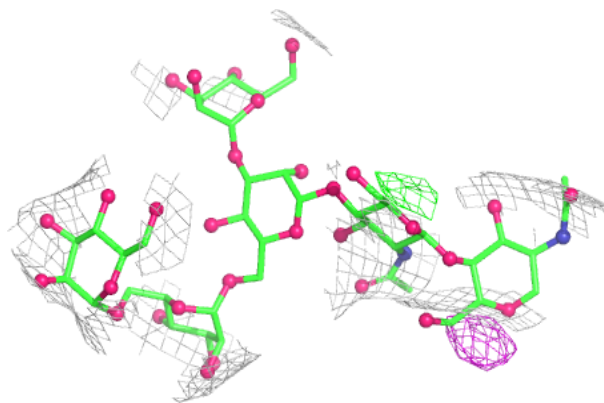
Electron density around Chain K:

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



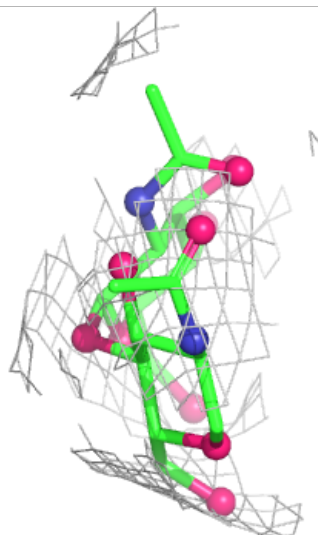
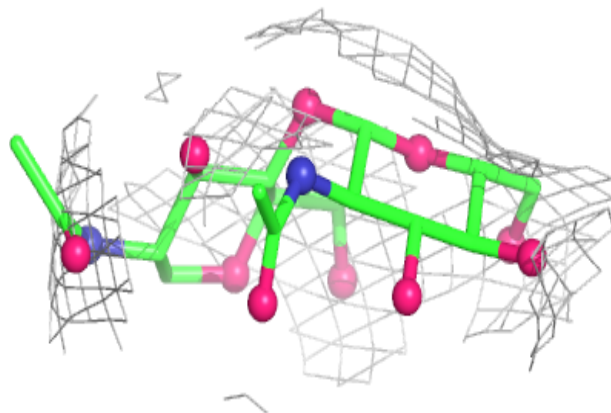
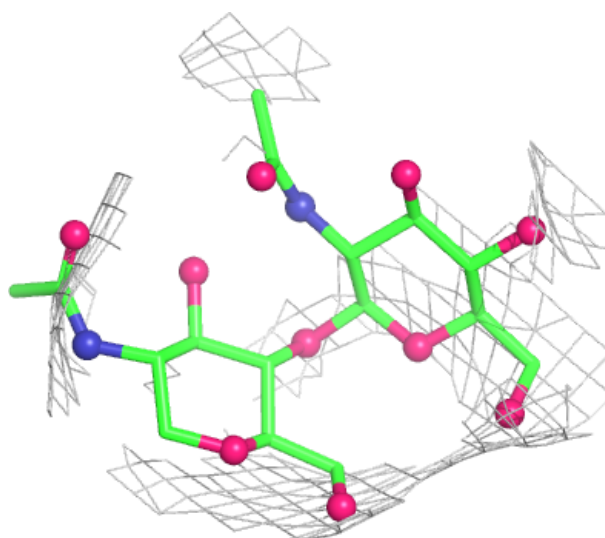
Electron density around Chain L:

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



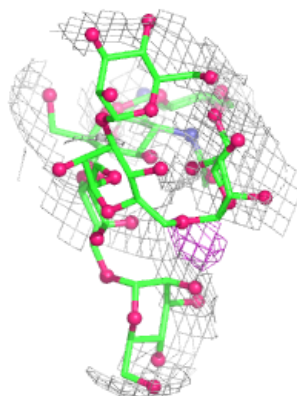
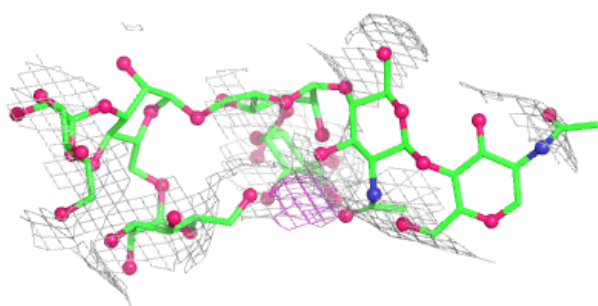
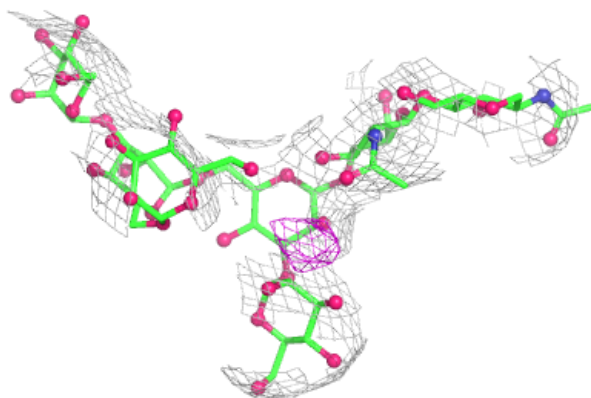
Electron density around Chain N:

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



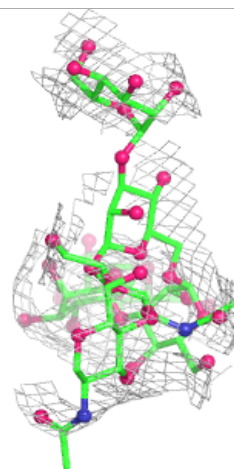
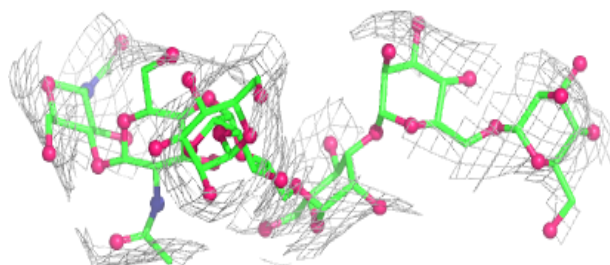
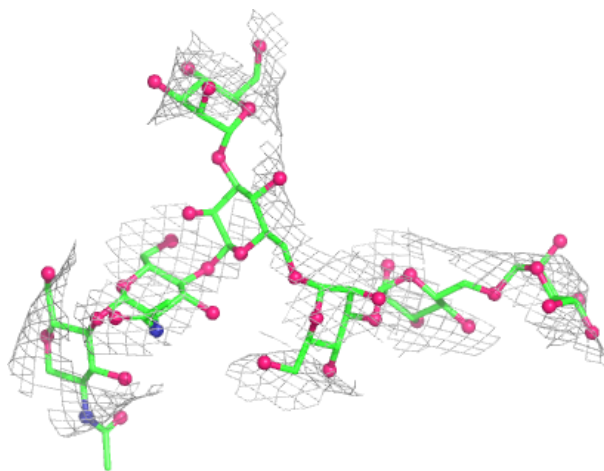
Electron density around Chain O:

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



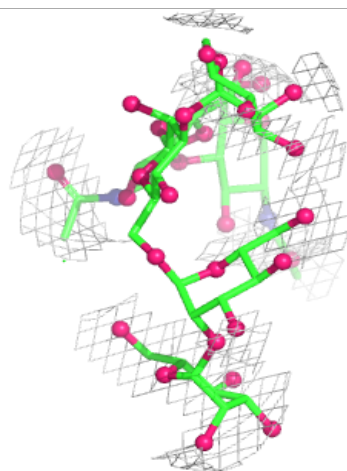
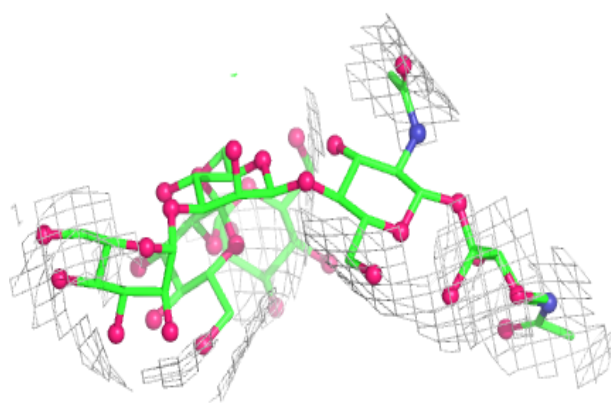
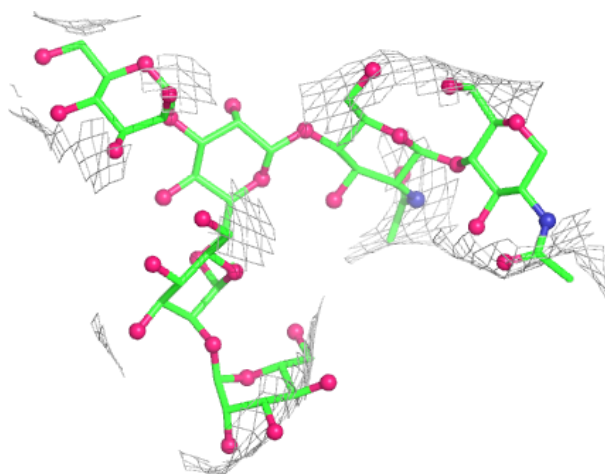
Electron density around Chain P:

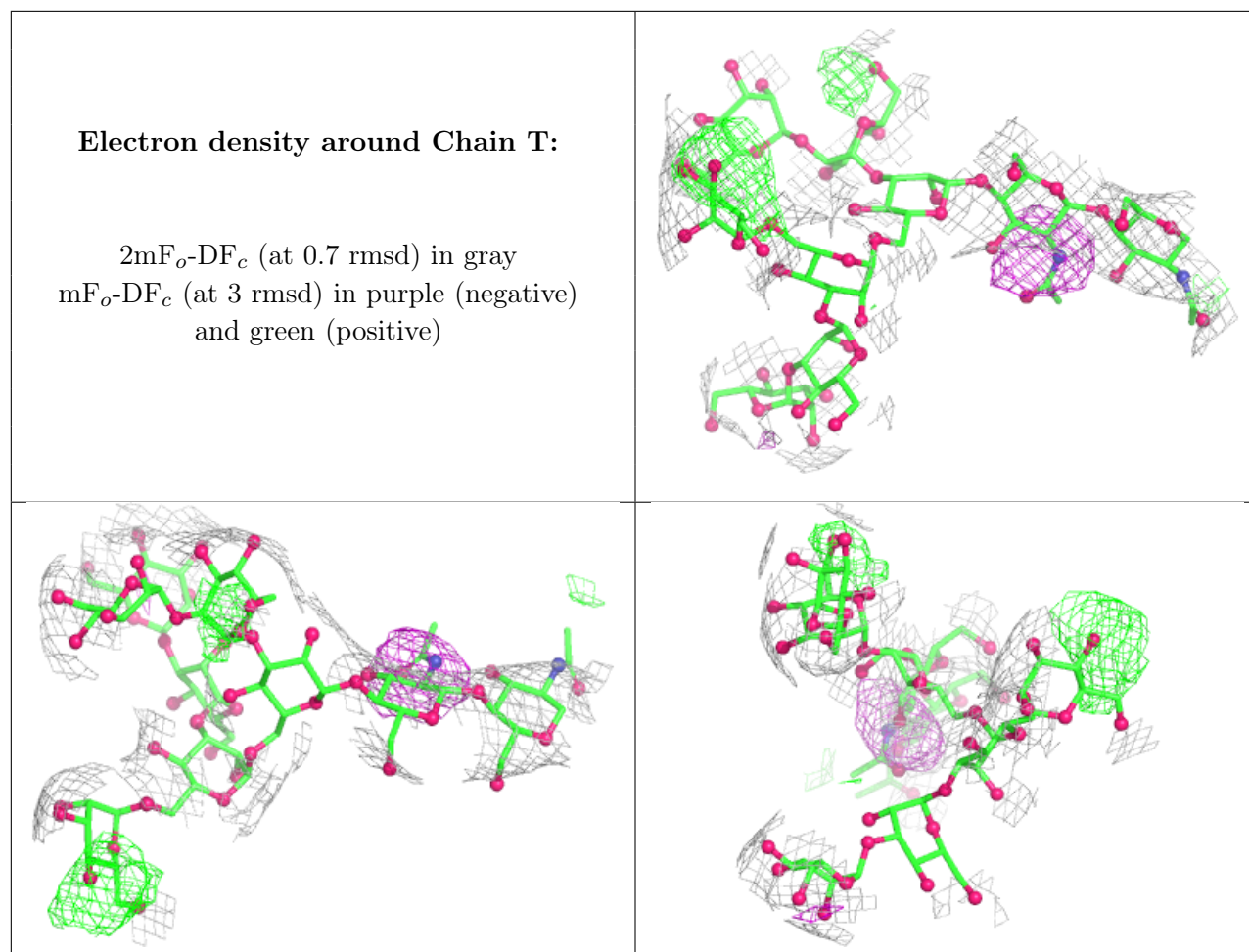
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain S:

$2mF_o-DF_c$ (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
19	NAG	G	601	14/15	0.60	0.08	266,266,266,266	0
19	NAG	B	701	14/15	0.77	0.07	189,189,189,189	0
19	NAG	G	602	14/15	0.83	0.05	171,171,171,171	0

6.5 Other polymers [i](#)

There are no such residues in this entry.