



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:19 AM EDT

PDB ID : 6CH9 / pdb_00006ch9
Title : Crystal structure of a natively-glycosylated B41 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 : 4.85 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:

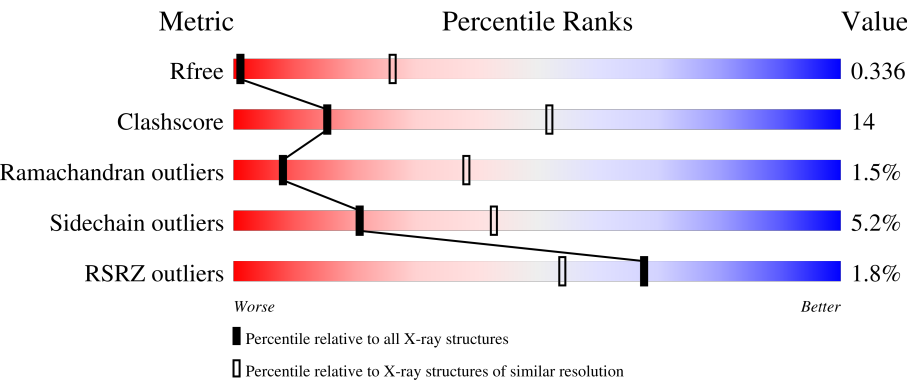
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 4.85 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	1024 (5.74-3.94)
Clashscore	190562	1007 (5.70-3.98)
Ramachandran outliers	187476	1110 (5.78-3.90)
Sidechain outliers	187428	1091 (5.78-3.90)
RSRZ outliers	180081	1019 (5.74-3.94)

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	65%21%11%
2	D	243	86%10%
3	E	216	88%10%
4	G	518	2% 59%21%5%14%
5	Q	240	3% 71%22%

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Mol	Chain	Length	Quality of chain
6	R	215	
7	A	3	
7	C	3	
7	H	3	
7	J	3	
7	O	3	
7	P	3	
7	T	3	
8	F	4	
9	I	2	
9	K	2	
9	N	2	
10	L	6	
11	M	4	
12	S	5	
13	U	6	

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
10	NAG	L	1	-	-	X	-
13	NAG	U	1	-	-	X	-
8	MAN	F	4	-	-	X	-
9	NAG	K	1	-	-	X	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 11974 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	136	Total	C	N	O	S	0	0	0
			1094	692	188	206	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP B3UEZ6
B	605	CYS	THR	engineered mutation	UNP B3UEZ6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	236	Total	C	N	O	S	0	0	0
			1777	1129	296	344	8			

- 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	448	Total	C	N	O	S	0	0	0
			3499	2198	617	658	26			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	MET	-	initiating methionine	UNP B3UES2
G	-3	ASP	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	ALA	-	expression tag	UNP B3UES2
G	-1	MET	-	expression tag	UNP B3UES2
G	0	LYS	-	expression tag	UNP B3UES2
G	1	ARG	-	expression tag	UNP B3UES2
G	2	GLY	-	expression tag	UNP B3UES2
G	3	LEU	-	expression tag	UNP B3UES2
G	4	CYS	-	expression tag	UNP B3UES2
G	5	CYS	-	expression tag	UNP B3UES2
G	6	VAL	-	expression tag	UNP B3UES2
G	7	LEU	-	expression tag	UNP B3UES2
G	8	LEU	-	expression tag	UNP B3UES2
G	9	LEU	-	expression tag	UNP B3UES2
G	10	CYS	-	expression tag	UNP B3UES2
G	11	GLY	-	expression tag	UNP B3UES2
G	12	ALA	-	expression tag	UNP B3UES2
G	13	VAL	-	expression tag	UNP B3UES2
G	14	PHE	-	expression tag	UNP B3UES2
G	15	VAL	-	expression tag	UNP B3UES2
G	16	SER	-	expression tag	UNP B3UES2
G	17	PRO	-	expression tag	UNP B3UES2
G	18	SER	-	expression tag	UNP B3UES2
G	19	GLN	-	expression tag	UNP B3UES2
G	20	GLU	-	expression tag	UNP B3UES2
G	21	ILE	-	expression tag	UNP B3UES2
G	22	HIS	-	expression tag	UNP B3UES2
G	23	ALA	-	expression tag	UNP B3UES2
G	24	ARG	-	expression tag	UNP B3UES2
G	25	PHE	-	expression tag	UNP B3UES2
G	26	ARG	-	expression tag	UNP B3UES2
G	27	ARG	-	expression tag	UNP B3UES2
G	28	GLY	-	expression tag	UNP B3UES2
G	29	ALA	-	expression tag	UNP B3UES2
G	30	ARG	-	expression tag	UNP B3UES2
G	501	CYS	ALA	engineered mutation	UNP B3UES2

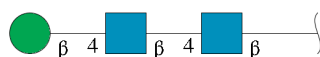
- Molecule 5 is a protein called BG18 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Q	231	Total	C	N	O	S	0	0	0
			1731	1089	298	336	8			

- Molecule 6 is a protein called BG18 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	R	205	Total	C	N	O	S	0	0	0
			1540	963	257	314	6			

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



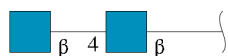
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	A	3	Total	C	N	O		0	0	0
			39	22	2	15				
7	C	3	Total	C	N	O		0	0	0
			39	22	2	15				
7	H	3	Total	C	N	O		0	0	0
			39	22	2	15				
7	J	3	Total	C	N	O		0	0	0
			39	22	2	15				
7	O	3	Total	C	N	O		0	0	0
			39	22	2	15				
7	P	3	Total	C	N	O		0	0	0
			39	22	2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

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



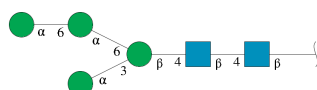
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	4	Total	C	N	O		0	0	0
			50	28	2	20				

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



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

- Molecule 10 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.



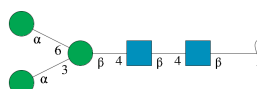
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	L	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 11 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.



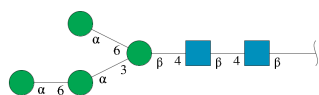
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	M	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



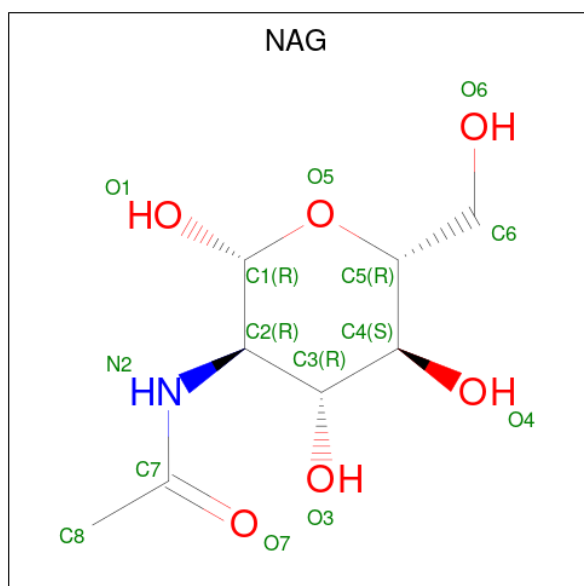
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	S	5	Total	C	N	O	0	0	0
			61	34	2	25			

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

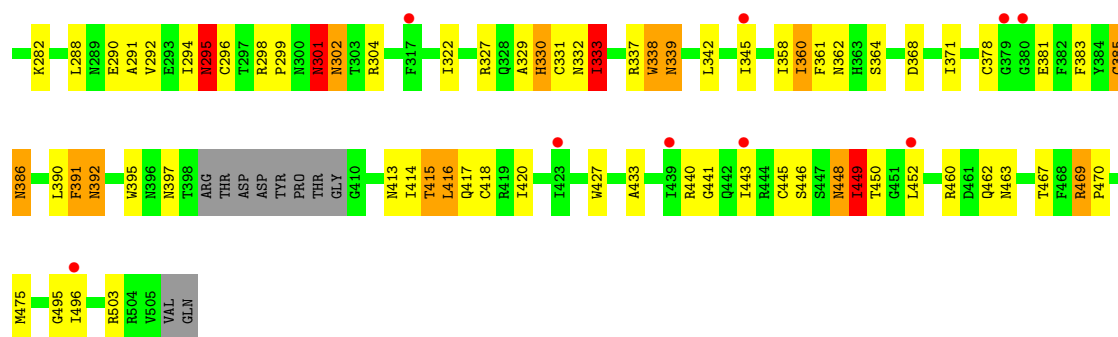


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	U	6	Total	C	N	O	0	0	0
			72	40	2	30			

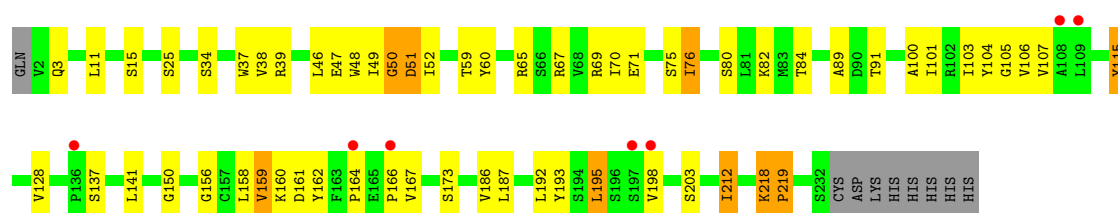
- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



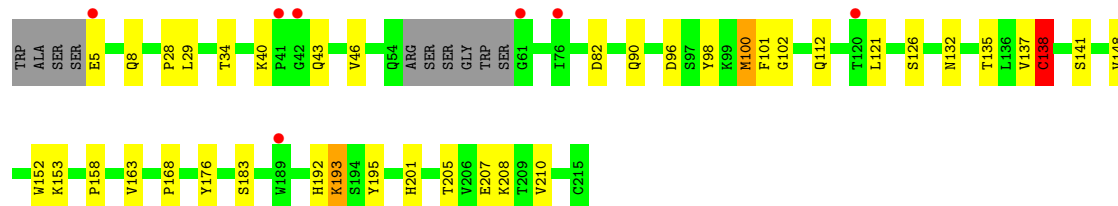
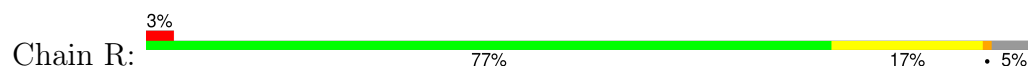
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		
14	G	1	Total	C	N	O	0	0
			14	8	1	5		



• Molecule 5: BG18 Heavy Chain



• Molecule 6: BG18 Light Chain



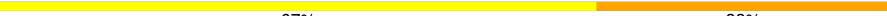
• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

Chain H:  67% 33%

MAG1
MAG2
BMA3

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

Chain J:  100%

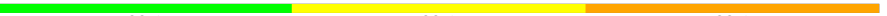
MAG1
MAG2
BMA3

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

Chain O:  33% 67%

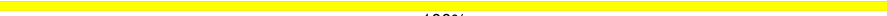
MAG1
MAG2
BMA3

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

Chain P:  33% 33% 33%

MAG1
MAG2
BMA3

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

Chain T:  100%

MAG1
MAG2
BMA3

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

Chain F:  25% 75%

MAG1
MAG2
BMA3
MAN4

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

Chain I:  100%

MAG1
MAG2

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

Chain K:  50% 50%

MAG1
MAG2

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

Chain N:  50% 50%

MAG1
MAG2

- Molecule 10: 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:  50% 50%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

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

Chain M:  75% 25%

MAG1
MAG2
BMA3
MAN4

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

Chain S:  60% 40%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain U:  33% 67%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	241.08Å 241.08Å 345.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.90 – 4.85 39.90 – 4.85	Depositor EDS
% Data completeness (in resolution range)	95.3 (39.90-4.85) 95.1 (39.90-4.85)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 4.84Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.285 , 0.292 0.302 , 0.336	Depositor DCC
R_{free} test set	838 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	275.7	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 366.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11974	wwPDB-VP
Average B, all atoms (Å ²)	300.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.75	0/1113	1.39	2/1509 (0.1%)
2	D	0.77	0/1822	1.15	6/2481 (0.2%)
3	E	0.73	0/1659	1.11	3/2269 (0.1%)
4	G	0.82	5/3572 (0.1%)	1.54	36/4857 (0.7%)
5	Q	0.73	0/1776	1.18	4/2423 (0.2%)
6	R	0.82	0/1577	1.24	6/2153 (0.3%)
All	All	0.78	5/11519 (0.0%)	1.32	57/15692 (0.4%)

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
4	G	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	392	ASN	C-N	11.37	1.49	1.33
4	G	295	ASN	C-N	7.55	1.43	1.33
4	G	385	CYS	C-N	6.87	1.42	1.33
4	G	361	PHE	C-N	6.40	1.42	1.33
4	G	160	ASN	C-N	5.38	1.40	1.33

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	234	ASN	O-C-N	-21.08	95.02	122.43
4	G	295	ASN	CA-C-N	17.03	147.28	121.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	295	ASN	C-N-CA	17.03	147.28	121.40
4	G	275	GLU	O-C-N	16.17	140.59	122.15
4	G	295	ASN	O-C-N	-15.20	105.46	122.79
1	B	648	VAL	N-CA-C	15.05	124.67	110.53
4	G	233	PHE	O-C-N	14.90	143.75	123.34
4	G	198	THR	N-CA-C	14.83	126.94	111.07
4	G	391	PHE	CA-C-N	14.12	146.51	121.66
4	G	391	PHE	C-N-CA	14.12	146.51	121.66
4	G	233	PHE	CA-C-N	-13.83	100.21	122.34
4	G	233	PHE	C-N-CA	-13.83	100.21	122.34
4	G	301	ASN	O-C-N	-10.68	109.74	122.87
4	G	301	ASN	CA-C-N	9.56	136.79	122.93
4	G	301	ASN	C-N-CA	9.56	136.79	122.93
5	Q	50	GLY	N-CA-C	9.55	128.78	111.02
4	G	263	GLY	N-CA-C	9.45	125.27	111.76
1	B	621	GLU	N-CA-C	8.81	120.50	111.07
4	G	267	GLU	N-CA-C	8.81	122.44	110.55
4	G	234	ASN	CA-C-N	8.26	137.59	121.41
4	G	234	ASN	C-N-CA	8.26	137.59	121.41
4	G	159	PHE	N-CA-C	7.47	119.50	108.14
4	G	261	LEU	N-CA-C	7.40	122.74	112.45
4	G	275	GLU	CA-C-N	-7.36	108.08	121.69
4	G	275	GLU	C-N-CA	-7.36	108.08	121.69
2	D	203	SER	N-CA-C	-7.35	96.28	108.34
4	G	386	ASN	O-C-N	-7.00	115.04	122.96
4	G	132	ASN	N-CA-C	-6.45	99.77	108.86
2	D	146	PHE	C-N-CD	-6.33	106.68	120.60
2	D	146	PHE	CA-C-N	6.33	142.18	127.00
2	D	146	PHE	C-N-CA	6.33	142.18	127.00
4	G	277	ILE	N-CA-C	6.33	122.50	109.34
4	G	449	ILE	N-CA-C	-6.18	98.72	107.75
4	G	138	ASN	N-CA-C	6.02	119.55	111.24
3	E	97	SER	N-CA-C	5.94	118.73	109.52
5	Q	115	TYR	N-CA-C	-5.93	106.21	113.50
6	R	126	SER	CA-C-N	5.61	128.07	120.38
6	R	126	SER	C-N-CA	5.61	128.07	120.38
4	G	275	GLU	N-CA-C	-5.56	105.30	111.36
2	D	31	PHE	CA-CB-CG	5.52	119.32	113.80
3	E	99	CYS	N-CA-C	5.36	118.00	110.23
2	D	204	ASN	N-CA-C	-5.32	100.06	108.73
4	G	54	CYS	CA-C-N	5.25	128.68	121.33
4	G	54	CYS	C-N-CA	5.25	128.68	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	186	VAL	CA-C-N	5.23	129.06	120.63
5	Q	186	VAL	C-N-CA	5.23	129.06	120.63
4	G	302	ASN	CA-CB-CG	5.21	117.81	112.60
4	G	441	GLY	CA-C-N	5.19	128.22	120.90
4	G	441	GLY	C-N-CA	5.19	128.22	120.90
4	G	441	GLY	N-CA-C	5.13	118.88	111.24
6	R	46	VAL	CA-C-N	5.11	127.96	120.71
6	R	46	VAL	C-N-CA	5.11	127.96	120.71
4	G	191	TYR	N-CA-C	5.08	114.99	108.34
3	E	79	ASP	CA-CB-CG	5.06	117.66	112.60
4	G	333	ILE	CB-CA-C	-5.05	104.28	111.40
6	R	193	LYS	CA-C-N	5.02	127.46	120.63
6	R	193	LYS	C-N-CA	5.02	127.46	120.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	234	ASN	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	1094	0	1075	35	0
2	D	1777	0	1755	20	0
3	E	1615	0	1550	10	0
4	G	3499	0	3441	204	0
5	Q	1731	0	1685	45	0
6	R	1540	0	1496	15	0
7	A	39	0	34	1	0
7	C	39	0	34	1	0
7	H	39	0	34	5	0
7	J	39	0	34	0	0
7	O	39	0	34	1	0
7	P	39	0	34	1	0
7	T	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	50	0	43	11	0
9	I	28	0	25	0	0
9	K	28	0	25	10	0
9	N	28	0	25	1	0
10	L	72	0	61	11	0
11	M	50	0	43	5	0
12	S	61	0	52	5	0
13	U	72	0	61	18	0
14	B	14	0	13	4	0
14	G	42	0	39	0	0
All	All	11974	0	11627	319	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 14.

All (319) 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:333:ILE:CD1	4:G:414:ILE:HB	1.30	1.60
4:G:338:TRP:CZ3	4:G:390:LEU:HD22	1.37	1.57
4:G:292:VAL:HB	4:G:449:ILE:CD1	1.30	1.55
4:G:292:VAL:CB	4:G:449:ILE:HD12	1.46	1.44
4:G:292:VAL:O	4:G:449:ILE:CD1	1.68	1.41
4:G:332:ASN:HD21	13:U:1:NAG:C1	1.31	1.41
4:G:292:VAL:CB	4:G:449:ILE:CD1	1.97	1.39
5:Q:158:LEU:O	5:Q:159:VAL:HG12	1.21	1.29
4:G:338:TRP:CZ3	4:G:390:LEU:CD2	2.15	1.28
4:G:333:ILE:CD1	4:G:414:ILE:CB	2.09	1.27
4:G:115:SER:O	4:G:116:LEU:HG	1.17	1.25
5:Q:75:SER:O	5:Q:76:ILE:HG12	1.07	1.24
4:G:292:VAL:O	4:G:449:ILE:CG1	1.88	1.20
4:G:115:SER:O	4:G:116:LEU:CG	1.91	1.18
4:G:292:VAL:CA	4:G:449:ILE:HD12	1.73	1.18
4:G:332:ASN:ND2	13:U:1:NAG:C1	2.08	1.15
4:G:292:VAL:HB	4:G:449:ILE:HD13	1.27	1.15
4:G:292:VAL:O	4:G:449:ILE:HD11	1.38	1.13
4:G:338:TRP:HH2	4:G:390:LEU:HB3	1.09	1.13
4:G:229:ASN:H	9:K:1:NAG:H83	1.16	1.11
4:G:338:TRP:CH2	4:G:390:LEU:HB3	1.86	1.10
5:Q:75:SER:O	5:Q:76:ILE:CG1	2.00	1.10
4:G:133:ASN:OD1	4:G:134:VAL:HG23	1.48	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:106:VAL:H	13:U:2:NAG:H3	1.15	1.09
4:G:292:VAL:C	4:G:449:ILE:CD1	2.25	1.08
4:G:333:ILE:HD11	4:G:414:ILE:C	1.78	1.08
4:G:333:ILE:HD13	4:G:414:ILE:CB	1.78	1.07
5:Q:141:LEU:HD21	5:Q:158:LEU:HD13	1.15	1.07
4:G:333:ILE:CD1	4:G:414:ILE:O	2.03	1.06
4:G:292:VAL:O	4:G:449:ILE:HG13	1.52	1.05
4:G:292:VAL:C	4:G:449:ILE:HD11	1.81	1.05
4:G:333:ILE:HD11	4:G:414:ILE:CB	1.80	1.04
5:Q:106:VAL:CB	13:U:2:NAG:H5	1.90	1.01
4:G:338:TRP:CH2	4:G:390:LEU:HD22	1.97	0.97
4:G:333:ILE:HD12	4:G:414:ILE:O	1.63	0.97
4:G:199:SER:OG	4:G:433:ALA:HB2	1.63	0.97
2:D:200:HIS:HB3	2:D:203:SER:O	1.66	0.95
4:G:338:TRP:CH2	4:G:390:LEU:CD2	2.48	0.94
5:Q:158:LEU:O	5:Q:159:VAL:CG1	2.12	0.94
4:G:292:VAL:HG22	4:G:337:ARG:NE	1.83	0.92
4:G:338:TRP:HZ3	4:G:390:LEU:HD22	1.14	0.92
4:G:133:ASN:OD1	4:G:134:VAL:N	2.02	0.91
4:G:333:ILE:CD1	4:G:414:ILE:C	2.42	0.91
4:G:292:VAL:HB	4:G:449:ILE:HD12	0.91	0.90
2:D:100(D):TRP:HZ2	8:F:4:MAN:H2	1.36	0.89
4:G:252:ARG:CD	4:G:262:ASN:ND2	2.35	0.89
5:Q:106:VAL:N	13:U:2:NAG:H3	1.88	0.89
4:G:252:ARG:HD2	4:G:262:ASN:CG	1.96	0.89
4:G:292:VAL:CG1	4:G:449:ILE:CD1	2.51	0.89
4:G:332:ASN:ND2	13:U:1:NAG:HN2	1.72	0.88
2:D:100(D):TRP:CZ2	8:F:4:MAN:H2	2.09	0.87
4:G:332:ASN:ND2	13:U:1:NAG:N2	2.24	0.86
4:G:133:ASN:OD1	4:G:134:VAL:CG2	2.22	0.86
4:G:252:ARG:HD3	4:G:262:ASN:ND2	1.93	0.83
4:G:333:ILE:HD13	4:G:414:ILE:HB	0.83	0.83
4:G:173:TYR:HB3	7:H:1:NAG:HN2	1.43	0.82
4:G:333:ILE:HD11	4:G:414:ILE:CA	2.09	0.81
4:G:115:SER:C	4:G:116:LEU:HG	2.06	0.81
4:G:448:ASN:HB2	10:L:1:NAG:H81	1.63	0.80
4:G:338:TRP:CH2	4:G:390:LEU:CB	2.62	0.80
4:G:333:ILE:CD1	4:G:414:ILE:CA	2.60	0.80
5:Q:75:SER:C	5:Q:76:ILE:HG12	2.04	0.79
5:Q:3:GLN:HB2	5:Q:25:SER:HB3	1.65	0.78
4:G:292:VAL:CA	4:G:449:ILE:CD1	2.44	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:229:ASN:N	9:K:1:NAG:H83	1.98	0.78
1:B:617:LYS:HD2	1:B:617:LYS:N	1.97	0.77
4:G:292:VAL:HG22	4:G:337:ARG:CZ	2.13	0.77
4:G:292:VAL:HG22	4:G:337:ARG:HE	1.50	0.77
4:G:333:ILE:HD11	4:G:414:ILE:CG2	2.14	0.77
4:G:252:ARG:HD2	4:G:262:ASN:ND2	1.99	0.77
5:Q:158:LEU:C	5:Q:159:VAL:HG12	2.10	0.76
4:G:252:ARG:NE	10:L:1:NAG:O5	2.20	0.75
4:G:115:SER:O	4:G:116:LEU:CD1	2.34	0.75
4:G:292:VAL:C	4:G:449:ILE:HD12	2.03	0.75
5:Q:69:ARG:HB2	5:Q:82:LYS:HB3	1.68	0.74
1:B:621:GLU:HG3	14:B:704:NAG:O7	1.87	0.74
4:G:292:VAL:HG12	4:G:449:ILE:HD11	1.68	0.74
1:B:618:THR:OG1	1:B:621:GLU:HB3	1.88	0.73
4:G:278:THR:HG23	11:M:1:NAG:HN2	1.52	0.73
6:R:96:ASP:HB2	12:S:4:MAN:O4	1.87	0.73
4:G:332:ASN:HD22	13:U:1:NAG:HN2	1.37	0.73
4:G:386:ASN:ND2	4:G:417:GLN:OE1	2.22	0.72
4:G:338:TRP:CZ3	4:G:390:LEU:HD23	2.23	0.72
4:G:173:TYR:HB3	7:H:1:NAG:N2	2.05	0.72
4:G:395:TRP:NE1	4:G:397:ASN:O	2.23	0.71
2:D:100(D):TRP:HZ2	8:F:4:MAN:C2	2.03	0.71
4:G:252:ARG:HD3	10:L:1:NAG:C1	2.21	0.71
2:D:33:HIS:NE2	8:F:2:NAG:O7	2.23	0.71
4:G:332:ASN:ND2	13:U:1:NAG:C2	2.53	0.70
4:G:292:VAL:CB	4:G:449:ILE:HD11	2.19	0.69
4:G:291:ALA:HB1	4:G:448:ASN:OD1	1.92	0.69
1:B:530:MET:HB3	1:B:623:TRP:HA	1.75	0.69
4:G:88:ASN:ND2	8:F:1:NAG:H83	2.08	0.69
5:Q:141:LEU:CD2	5:Q:158:LEU:HD13	2.10	0.69
4:G:252:ARG:CD	10:L:1:NAG:C1	2.71	0.68
4:G:333:ILE:HD12	4:G:333:ILE:H	1.56	0.68
4:G:333:ILE:HD12	4:G:333:ILE:N	2.09	0.68
4:G:333:ILE:HD11	4:G:414:ILE:HG22	1.76	0.68
2:D:200:HIS:ND1	2:D:203:SER:OG	2.27	0.67
4:G:133:ASN:CG	4:G:134:VAL:H	1.97	0.67
4:G:122:LEU:HB2	4:G:201:ILE:HG23	1.77	0.67
5:Q:150:GLY:HA2	5:Q:203:SER:O	1.95	0.67
1:B:604:CYS:SG	4:G:503:ARG:NH2	2.67	0.66
6:R:168:PRO:HB3	6:R:176:TYR:HB3	1.76	0.66
1:B:618:THR:OG1	1:B:621:GLU:CB	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:119:PRO:HD2	2:D:205:THR:HG21	1.78	0.65
4:G:117:LYS:O	4:G:117:LYS:NZ	2.24	0.65
1:B:582:ALA:HB1	4:G:221:ALA:HB3	1.79	0.65
4:G:292:VAL:HG12	4:G:449:ILE:CD1	2.25	0.65
1:B:621:GLU:OE2	14:B:704:NAG:H81	1.97	0.64
4:G:291:ALA:C	4:G:337:ARG:HH21	2.04	0.64
2:D:100(D):TRP:CZ2	8:F:4:MAN:C2	2.80	0.63
4:G:229:ASN:HB3	9:K:1:NAG:C7	2.28	0.63
4:G:261:LEU:N	4:G:261:LEU:HD12	2.13	0.63
4:G:333:ILE:CD1	4:G:414:ILE:CG2	2.74	0.63
4:G:262:ASN:C	4:G:450:THR:HG21	2.22	0.63
4:G:332:ASN:H	4:G:415:THR:HG22	1.64	0.63
4:G:329:ALA:HB3	4:G:418:CYS:HB3	1.81	0.62
1:B:621:GLU:OE2	14:B:704:NAG:C8	2.48	0.61
4:G:290:GLU:O	4:G:337:ARG:NH2	2.33	0.61
4:G:116:LEU:HD12	4:G:116:LEU:C	2.26	0.60
5:Q:141:LEU:HD21	5:Q:158:LEU:CD1	2.10	0.60
4:G:243:SER:HB3	9:K:1:NAG:H81	1.83	0.60
4:G:229:ASN:HB3	9:K:1:NAG:N2	2.16	0.60
5:Q:160:LYS:O	5:Q:160:LYS:HG2	2.02	0.60
4:G:252:ARG:CD	10:L:1:NAG:O5	2.50	0.59
4:G:386:ASN:HD22	4:G:417:GLN:CD	2.10	0.59
4:G:292:VAL:HG22	4:G:337:ARG:NH2	2.17	0.59
4:G:243:SER:CB	9:K:1:NAG:H81	2.33	0.58
4:G:278:THR:OG1	11:M:1:NAG:H3	2.02	0.58
1:B:604:CYS:HA	4:G:503:ARG:HH21	1.68	0.58
2:D:100(D):TRP:HZ2	8:F:4:MAN:C3	2.17	0.58
5:Q:103:ILE:O	13:U:3:BMA:H3	2.03	0.58
4:G:252:ARG:HD3	10:L:1:NAG:O5	2.04	0.58
4:G:291:ALA:O	4:G:337:ARG:NH2	2.37	0.58
4:G:462:GLN:HA	4:G:462:GLN:OE1	2.03	0.57
2:D:1:GLU:OE2	7:A:3:BMA:O4	2.23	0.57
4:G:338:TRP:CD1	4:G:339:ASN:N	2.72	0.57
4:G:338:TRP:CH2	4:G:390:LEU:HD23	2.34	0.57
4:G:330:HIS:NE2	13:U:1:NAG:H5	2.20	0.56
10:L:6:MAN:O4	10:L:6:MAN:O6	2.22	0.56
5:Q:48:TRP:CH2	5:Q:50:GLY:O	2.58	0.56
5:Q:106:VAL:H	13:U:2:NAG:C3	2.05	0.56
4:G:292:VAL:CG1	4:G:449:ILE:HD13	2.31	0.56
4:G:296:CYS:H	4:G:445:CYS:HB2	1.70	0.56
4:G:55:ALA:HB3	4:G:216:HIS:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:338:TRP:CD1	4:G:338:TRP:C	2.85	0.55
4:G:268:GLU:OE1	4:G:268:GLU:HA	2.06	0.55
7:O:1:NAG:H62	7:O:2:NAG:O7	2.07	0.55
2:D:97:LEU:HD12	2:D:100(C):THR:HG22	1.88	0.55
4:G:69:TRP:HA	4:G:111:LEU:HD21	1.89	0.54
4:G:261:LEU:O	10:L:1:NAG:O7	2.25	0.54
4:G:292:VAL:O	4:G:449:ILE:HD12	1.87	0.54
2:D:31:PHE:HA	8:F:1:NAG:H62	1.90	0.53
4:G:360:ILE:HA	4:G:467:THR:HA	1.90	0.53
4:G:278:THR:OG1	11:M:1:NAG:H5	2.08	0.53
4:G:261:LEU:HB3	10:L:1:NAG:O7	2.08	0.53
5:Q:218:LYS:HB3	5:Q:219:PRO:HD3	1.91	0.53
1:B:636:ASP:O	1:B:639:THR:HG22	2.09	0.53
1:B:621:GLU:CG	14:B:704:NAG:O7	2.55	0.53
1:B:621:GLU:O	1:B:625:ASN:HB3	2.07	0.53
4:G:241:ASN:O	9:K:1:NAG:H82	2.08	0.53
5:Q:67:ARG:HG3	5:Q:84:THR:O	2.09	0.53
1:B:616:ASN:C	1:B:617:LYS:HD2	2.34	0.53
3:E:20:ILE:HG21	3:E:105:THR:HG21	1.91	0.53
4:G:117:LYS:N	4:G:118:PRO:CD	2.72	0.53
6:R:135:THR:HA	6:R:183:SER:HA	1.91	0.53
5:Q:107:VAL:HG22	13:U:1:NAG:H62	1.91	0.52
4:G:440:ARG:HG2	9:N:1:NAG:H81	1.90	0.52
4:G:196:CYS:SG	4:G:197:ASN:N	2.82	0.52
5:Q:37:TRP:HB2	5:Q:49:ILE:HB	1.91	0.52
6:R:40:LYS:HB3	6:R:43:GLN:HB2	1.91	0.52
2:D:6:GLN:HE21	2:D:107:THR:HG23	1.75	0.52
3:E:91:CYS:SG	3:E:99:CYS:HB3	2.50	0.52
4:G:298:ARG:HB3	4:G:443:ILE:HG13	1.92	0.52
4:G:278:THR:CG2	11:M:1:NAG:HN2	2.20	0.51
4:G:295:ASN:O	4:G:331:CYS:O	2.28	0.51
4:G:292:VAL:CB	4:G:449:ILE:HD13	2.03	0.51
4:G:292:VAL:CG2	4:G:337:ARG:NH2	2.73	0.51
6:R:8:GLN:HB2	6:R:102:GLY:HA3	1.93	0.51
1:B:566:LEU:HD21	1:B:568:LEU:HD12	1.93	0.51
4:G:229:ASN:CB	9:K:1:NAG:C7	2.88	0.51
4:G:117:LYS:O	4:G:117:LYS:HD2	2.11	0.51
4:G:368:ASP:HB2	4:G:371:ILE:HD12	1.92	0.51
5:Q:91:THR:HG21	5:Q:128:VAL:HB	1.93	0.51
4:G:153:GLU:HB3	4:G:178:LYS:HB2	1.93	0.50
4:G:299:PRO:HD3	4:G:329:ALA:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:6:GLN:HB3	3:E:105:THR:HB	1.93	0.50
2:D:100(D):TRP:CZ2	8:F:4:MAN:C3	2.95	0.50
1:B:617:LYS:N	1:B:617:LYS:CD	2.73	0.50
4:G:195:ASN:OD1	4:G:199:SER:O	2.29	0.50
2:D:87:THR:HG23	2:D:110:THR:HA	1.93	0.50
4:G:261:LEU:N	4:G:261:LEU:CD1	2.73	0.50
4:G:292:VAL:N	4:G:449:ILE:HD12	2.25	0.50
4:G:95:MET:H	4:G:236:SER:HB2	1.77	0.50
4:G:460:ARG:NE	4:G:463:ASN:HD22	2.09	0.50
1:B:594:GLY:HA2	1:B:599:SER:HB3	1.94	0.49
4:G:173:TYR:HB3	7:H:1:NAG:C7	2.41	0.49
4:G:332:ASN:HA	4:G:415:THR:HG23	1.94	0.49
4:G:291:ALA:C	4:G:337:ARG:NH2	2.70	0.49
5:Q:50:GLY:O	5:Q:51:ASP:CB	2.60	0.49
3:E:33:LYS:HG2	3:E:94:THR:HG23	1.93	0.49
4:G:116:LEU:CD1	4:G:116:LEU:C	2.86	0.49
1:B:608:VAL:HG21	1:B:646:LEU:HA	1.94	0.49
1:B:551:GLN:HE22	4:G:78:ASP:HB2	1.76	0.49
4:G:42:VAL:HG21	4:G:495:GLY:HA3	1.95	0.49
5:Q:34:SER:HB2	5:Q:101:ILE:HD11	1.94	0.48
5:Q:104:TYR:O	13:U:3:BMA:H2	2.13	0.48
4:G:262:ASN:CG	10:L:1:NAG:H82	2.38	0.48
4:G:462:GLN:O	4:G:463:ASN:HB2	2.13	0.48
6:R:163:VAL:HG21	6:R:183:SER:H	1.77	0.48
4:G:299:PRO:HB2	4:G:327:ARG:HD3	1.95	0.48
2:D:100(C):THR:HG21	8:F:2:NAG:O6	2.14	0.48
4:G:195:ASN:ND2	4:G:199:SER:O	2.46	0.48
4:G:292:VAL:CG2	4:G:337:ARG:HH21	2.27	0.48
4:G:392:ASN:OD1	12:S:1:NAG:N2	2.43	0.48
6:R:163:VAL:HG11	6:R:183:SER:HB2	1.95	0.48
4:G:117:LYS:N	4:G:118:PRO:HD2	2.29	0.47
1:B:648:VAL:HA	1:B:652:GLN:HB3	1.95	0.47
13:U:6:MAN:O6	13:U:6:MAN:O4	2.16	0.47
1:B:642:ILE:HG21	4:G:496:ILE:HG21	1.95	0.47
1:B:651:ILE:HD13	1:B:655:LYS:HG3	1.96	0.47
4:G:185:GLU:HB3	4:G:190:ASN:HB3	1.96	0.47
1:B:578:ALA:HB1	4:G:220:PRO:HB3	1.96	0.47
5:Q:173:SER:HB2	5:Q:212:ILE:HD11	1.96	0.47
4:G:337:ARG:HD2	4:G:337:ARG:O	2.14	0.47
4:G:115:SER:O	4:G:116:LEU:HD12	2.14	0.47
4:G:243:SER:HB2	9:K:1:NAG:C8	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:TRP:CD2	4:G:54:CYS:HB2	2.50	0.47
2:D:116:THR:HG21	2:D:202:PRO:HB2	1.97	0.47
4:G:392:ASN:CG	12:S:1:NAG:N2	2.73	0.47
2:D:100(D):TRP:CZ2	8:F:4:MAN:O3	2.65	0.46
1:B:540:GLN:HG2	4:G:43:PRO:HB3	1.97	0.46
4:G:183:PRO:HA	4:G:191:TYR:HB3	1.96	0.46
5:Q:100:ALA:HB3	5:Q:115:TYR:HB3	1.95	0.46
6:R:121:LEU:HG	6:R:208:LYS:HB2	1.96	0.46
4:G:154:MET:HE3	4:G:175:LEU:HD22	1.97	0.46
4:G:290:GLU:C	4:G:337:ARG:HH22	2.22	0.46
4:G:385:CYS:HB2	4:G:416:LEU:HB2	1.97	0.46
4:G:276:ASN:HB3	4:G:282:LYS:HB2	1.97	0.46
5:Q:60:TYR:HE1	5:Q:65:ARG:HA	1.82	0.45
1:B:648:VAL:O	1:B:653:GLN:N	2.49	0.45
4:G:195:ASN:CG	4:G:199:SER:O	2.60	0.45
4:G:196:CYS:O	4:G:197:ASN:C	2.56	0.45
4:G:329:ALA:HB2	4:G:420:ILE:HD11	1.99	0.45
1:B:604:CYS:HA	4:G:503:ARG:NH2	2.32	0.45
4:G:157:CYS:HB2	4:G:176:PHE:HE2	1.82	0.45
5:Q:48:TRP:CZ2	5:Q:50:GLY:O	2.70	0.45
5:Q:160:LYS:O	5:Q:161:ASP:HB3	2.17	0.45
5:Q:161:ASP:HB2	5:Q:192:LEU:HD22	1.98	0.45
5:Q:162:TYR:CZ	5:Q:193:TYR:HB2	2.52	0.45
3:E:196:SER:HA	3:E:209:THR:HG23	1.99	0.45
4:G:260:LEU:C	4:G:261:LEU:HD12	2.42	0.45
4:G:262:ASN:CA	4:G:450:THR:HG21	2.47	0.44
4:G:278:THR:HG23	11:M:1:NAG:N2	2.27	0.44
5:Q:39:ARG:HB3	5:Q:47:GLU:HB2	1.99	0.44
1:B:637:ASN:HB2	7:C:1:NAG:C2	2.47	0.44
4:G:117:LYS:HD2	4:G:117:LYS:C	2.42	0.44
4:G:333:ILE:HD12	4:G:414:ILE:C	2.28	0.44
4:G:329:ALA:O	4:G:330:HIS:HB3	2.18	0.44
4:G:333:ILE:HD11	4:G:414:ILE:O	1.83	0.44
4:G:446:SER:HB3	10:L:2:NAG:H5	1.99	0.44
4:G:270:ILE:HG22	4:G:288:LEU:HA	1.99	0.44
5:Q:71:GLU:HB3	5:Q:80:SER:HB3	2.00	0.44
4:G:96:TRP:HB2	4:G:275:GLU:HG3	2.00	0.44
4:G:332:ASN:HA	4:G:414:ILE:O	2.17	0.43
4:G:59:LYS:HE3	4:G:214:PRO:HD2	2.00	0.43
4:G:338:TRP:CE3	4:G:390:LEU:CD2	2.92	0.43
4:G:469:ARG:HH21	7:P:1:NAG:C7	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:292:VAL:HG13	4:G:337:ARG:HG3	2.00	0.43
4:G:299:PRO:HB2	4:G:327:ARG:CD	2.49	0.43
1:B:635:ILE:O	1:B:636:ASP:C	2.61	0.43
6:R:138:CYS:O	6:R:138:CYS:SG	2.76	0.43
4:G:296:CYS:N	4:G:445:CYS:HB2	2.33	0.43
5:Q:48:TRP:HB2	6:R:101:PHE:HE1	1.83	0.43
6:R:98:TYR:CE1	6:R:100:MET:HB3	2.54	0.43
6:R:153:LYS:HA	6:R:158:PRO:HA	2.01	0.43
1:B:616:ASN:OD1	1:B:616:ASN:N	2.50	0.42
4:G:173:TYR:CB	7:H:1:NAG:HN2	2.22	0.42
4:G:392:ASN:CG	12:S:1:NAG:HN2	2.27	0.42
4:G:70:ALA:O	4:G:74:CYS:HB3	2.19	0.42
5:Q:105:GLY:HA2	13:U:2:NAG:C3	2.49	0.42
4:G:304:ARG:HG3	4:G:440:ARG:HD2	2.02	0.42
1:B:608:VAL:HG22	1:B:649:SER:HB3	2.01	0.42
1:B:610:TRP:HE3	4:G:36:VAL:HG22	1.85	0.42
4:G:240:THR:OG1	4:G:241:ASN:OD1	2.37	0.42
5:Q:39:ARG:HB2	5:Q:49:ILE:HD11	1.99	0.42
4:G:301:ASN:O	4:G:322:ILE:HA	2.19	0.42
3:E:10:VAL:HG21	3:E:20:ILE:HG12	2.01	0.42
4:G:294:ILE:HG23	4:G:294:ILE:O	2.19	0.42
4:G:330:HIS:CE1	13:U:1:NAG:H3	2.55	0.42
5:Q:59:THR:HB	12:S:4:MAN:H4	2.02	0.42
4:G:117:LYS:C	4:G:117:LYS:CD	2.91	0.42
1:B:534:SER:HA	1:B:537:LEU:HD23	2.01	0.42
1:B:604:CYS:CA	4:G:503:ARG:HH21	2.31	0.42
4:G:333:ILE:HD12	4:G:333:ILE:O	2.20	0.42
4:G:427:TRP:CD1	4:G:475:MET:HG3	2.54	0.42
5:Q:137:SER:O	5:Q:159:VAL:HA	2.19	0.42
1:B:525:ALA:HB1	1:B:533:ALA:HA	2.02	0.41
5:Q:156:GLY:HA2	5:Q:198:VAL:HG12	2.02	0.41
6:R:5:GLU:HB3	6:R:100:MET:HB2	2.02	0.41
4:G:386:ASN:HB2	4:G:417:GLN:HB2	2.02	0.41
2:D:143:LYS:HE3	3:E:133:LYS:HD2	2.02	0.41
3:E:85:GLU:HB3	3:E:109:VAL:H	1.85	0.41
3:E:92:SER:HB2	3:E:100:VAL:HB	2.03	0.41
5:Q:167:VAL:HG11	5:Q:195:LEU:HD22	2.02	0.41
6:R:148:VAL:HG22	6:R:201:HIS:HB2	2.02	0.41
2:D:169:VAL:HG21	3:E:166:THR:HB	2.01	0.41
4:G:156:ASN:ND2	7:H:1:NAG:C7	2.83	0.41
6:R:192:HIS:CD2	6:R:193:LYS:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:378:CYS:HB3	4:G:383:PHE:CE1	2.56	0.41
13:U:1:NAG:H83	13:U:1:NAG:H2	1.84	0.40
4:G:241:ASN:OD1	4:G:241:ASN:N	2.53	0.40
4:G:243:SER:HB2	9:K:1:NAG:H81	2.02	0.40
4:G:342:LEU:HA	4:G:345:ILE:HD12	2.03	0.40
5:Q:164:PRO:HB2	5:Q:166:PRO:HD2	2.02	0.40
4:G:391:PHE:CE1	4:G:470:PRO:HG3	2.56	0.40
4:G:277:ILE:O	4:G:277:ILE:HG12	2.19	0.40
5:Q:51:ASP:HB3	5:Q:59:THR:HG23	2.03	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	132/153 (86%)	119 (90%)	13 (10%)	0	100	100
2	D	232/243 (96%)	205 (88%)	26 (11%)	1 (0%)	30	67
3	E	211/216 (98%)	192 (91%)	17 (8%)	2 (1%)	14	49
4	G	440/518 (85%)	366 (83%)	69 (16%)	5 (1%)	11	45
5	Q	229/240 (95%)	178 (78%)	44 (19%)	7 (3%)	3	21
6	R	201/215 (94%)	140 (70%)	54 (27%)	7 (4%)	3	20
All	All	1445/1585 (91%)	1200 (83%)	223 (15%)	22 (2%)	8	38

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	53	ASP
4	G	197	ASN
5	Q	51	ASP

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Mol	Chain	Res	Type
5	Q	159	VAL
6	R	29	LEU
6	R	100	MET
4	G	156	ASN
6	R	28	PRO
3	E	71	TRP
5	Q	218	LYS
6	R	195	TYR
2	D	147	PRO
4	G	235	GLY
4	G	236	SER
5	Q	219	PRO
6	R	132	ASN
4	G	330	HIS
5	Q	15	SER
5	Q	89	ALA
6	R	138	CYS
5	Q	76	ILE
6	R	112	GLN

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	119/130 (92%)	116 (98%)	3 (2%)	42	62
2	D	199/206 (97%)	192 (96%)	7 (4%)	32	54
3	E	186/189 (98%)	181 (97%)	5 (3%)	39	60
4	G	393/455 (86%)	360 (92%)	33 (8%)	10	30
5	Q	193/207 (93%)	185 (96%)	8 (4%)	27	49
6	R	174/182 (96%)	164 (94%)	10 (6%)	18	41
All	All	1264/1369 (92%)	1198 (95%)	66 (5%)	21	43

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	616	ASN
1	B	619	ILE
1	B	635	ILE
2	D	11	LEU
2	D	51	ILE
2	D	89	THR
2	D	97	LEU
2	D	138	LEU
2	D	170	LEU
2	D	191	THR
3	E	53	ASP
3	E	74	TYR
3	E	139	LEU
3	E	149	THR
3	E	179	SER
4	G	63	THR
4	G	116	LEU
4	G	123	THR
4	G	134	VAL
4	G	156	ASN
4	G	157	CYS
4	G	201	ILE
4	G	225	ILE
4	G	231	LYS
4	G	233	PHE
4	G	262	ASN
4	G	270	ILE
4	G	273	ARG
4	G	276	ASN
4	G	277	ILE
4	G	295	ASN
4	G	301	ASN
4	G	302	ASN
4	G	333	ILE
4	G	338	TRP
4	G	339	ASN
4	G	358	ILE
4	G	360	ILE
4	G	362	ASN
4	G	364	SER
4	G	381	GLU
4	G	413	ASN
4	G	415	THR

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Mol	Chain	Res	Type
4	G	416	LEU
4	G	448	ASN
4	G	449	ILE
4	G	452	LEU
4	G	469	ARG
5	Q	11	LEU
5	Q	38	VAL
5	Q	46	LEU
5	Q	52	ILE
5	Q	70	ILE
5	Q	187	LEU
5	Q	195	LEU
5	Q	212	ILE
6	R	34	THR
6	R	82	ASP
6	R	90	GLN
6	R	137	VAL
6	R	138	CYS
6	R	141	SER
6	R	152	TRP
6	R	205	THR
6	R	207	GLU
6	R	210	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	551	GLN
1	B	590	GLN
1	B	607	ASN
2	D	6	GLN
2	D	30	ASN
2	D	171	GLN
2	D	197	ASN
3	E	6	GLN
3	E	192	HIS
3	E	201	HIS
4	G	105	HIS
4	G	130	ASN
4	G	203	GLN
4	G	302	ASN
4	G	332	ASN

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Mol	Chain	Res	Type
4	G	355	ASN
4	G	363	HIS
4	G	463	ASN
4	G	478	ASN
5	Q	61	ASN
5	Q	99	ASN
5	Q	188	GLN
6	R	188	GLN
6	R	192	HIS

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 ⓘ

52 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	1	1,7	14,14,15	0.94	0	17,19,21	2.24	4 (23%)
7	NAG	A	2	7	14,14,15	0.85	1 (7%)	17,19,21	1.23	2 (11%)
7	BMA	A	3	7	11,11,12	0.39	0	15,15,17	0.86	0
7	NAG	C	1	1,7	14,14,15	0.78	0	17,19,21	1.95	3 (17%)
7	NAG	C	2	7	14,14,15	0.67	0	17,19,21	2.21	4 (23%)
7	BMA	C	3	7	11,11,12	0.43	0	15,15,17	0.75	0
8	NAG	F	1	8	14,14,15	0.93	0	17,19,21	2.26	6 (35%)
8	NAG	F	2	8	14,14,15	1.11	2 (14%)	17,19,21	2.73	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BMA	F	3	8	11,11,12	1.50	2 (18%)	15,15,17	1.95	5 (33%)
8	MAN	F	4	8	11,11,12	2.08	2 (18%)	15,15,17	2.12	6 (40%)
7	NAG	H	1	4,7	14,14,15	0.93	1 (7%)	17,19,21	1.89	7 (41%)
7	NAG	H	2	7	14,14,15	1.24	2 (14%)	17,19,21	2.32	5 (29%)
7	BMA	H	3	7	11,11,12	0.82	0	15,15,17	1.34	2 (13%)
9	NAG	I	1	4,9	14,14,15	1.02	1 (7%)	17,19,21	1.20	1 (5%)
9	NAG	I	2	9	14,14,15	1.18	1 (7%)	17,19,21	1.61	4 (23%)
7	NAG	J	1	4,7	14,14,15	0.80	0	17,19,21	1.71	5 (29%)
7	NAG	J	2	7	14,14,15	1.41	1 (7%)	17,19,21	1.54	3 (17%)
7	BMA	J	3	7	11,11,12	0.74	0	15,15,17	0.96	1 (6%)
9	NAG	K	1	4,9	14,14,15	0.93	1 (7%)	17,19,21	2.31	6 (35%)
9	NAG	K	2	9	14,14,15	0.69	1 (7%)	17,19,21	0.97	0
10	NAG	L	1	4,10	14,14,15	1.15	1 (7%)	17,19,21	3.06	7 (41%)
10	NAG	L	2	10	14,14,15	0.74	0	17,19,21	2.44	7 (41%)
10	BMA	L	3	10	11,11,12	0.74	0	15,15,17	2.42	5 (33%)
10	MAN	L	4	10	11,11,12	0.42	0	15,15,17	1.75	3 (20%)
10	MAN	L	5	10	11,11,12	0.75	0	15,15,17	1.25	1 (6%)
10	MAN	L	6	10	11,11,12	0.99	1 (9%)	15,15,17	1.41	2 (13%)
11	NAG	M	1	4,11	14,14,15	1.42	2 (14%)	17,19,21	2.55	5 (29%)
11	NAG	M	2	11	14,14,15	0.59	0	17,19,21	1.52	2 (11%)
11	BMA	M	3	11	11,11,12	0.88	0	15,15,17	1.65	4 (26%)
11	MAN	M	4	11	11,11,12	0.65	0	15,15,17	1.33	2 (13%)
9	NAG	N	1	4,9	14,14,15	0.86	1 (7%)	17,19,21	2.34	3 (17%)
9	NAG	N	2	9	14,14,15	0.48	0	17,19,21	1.26	2 (11%)
7	NAG	O	1	4,7	14,14,15	0.38	0	17,19,21	1.26	3 (17%)
7	NAG	O	2	7	14,14,15	0.73	0	17,19,21	1.66	2 (11%)
7	BMA	O	3	7	11,11,12	0.38	0	15,15,17	0.97	0
7	NAG	P	1	4,7	14,14,15	0.62	0	17,19,21	1.38	2 (11%)
7	NAG	P	2	7	14,14,15	0.85	1 (7%)	17,19,21	1.19	1 (5%)
7	BMA	P	3	7	11,11,12	0.46	0	15,15,17	0.86	0
12	NAG	S	1	4,12	14,14,15	1.28	1 (7%)	17,19,21	1.55	4 (23%)
12	NAG	S	2	12	14,14,15	1.38	2 (14%)	17,19,21	2.70	7 (41%)
12	BMA	S	3	12	11,11,12	1.31	1 (9%)	15,15,17	2.21	5 (33%)
12	MAN	S	4	12	11,11,12	0.83	1 (9%)	15,15,17	2.62	7 (46%)
12	MAN	S	5	12	11,11,12	0.72	0	15,15,17	1.14	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	T	1	4,7	14,14,15	0.67	0	17,19,21	1.66	3 (17%)
7	NAG	T	2	7	14,14,15	0.82	0	17,19,21	1.44	4 (23%)
7	BMA	T	3	7	11,11,12	0.64	0	15,15,17	1.44	2 (13%)
13	NAG	U	1	13	14,14,15	1.47	3 (21%)	17,19,21	2.20	5 (29%)
13	NAG	U	2	13	14,14,15	0.87	0	17,19,21	2.82	8 (47%)
13	BMA	U	3	13	11,11,12	0.77	0	15,15,17	2.17	5 (33%)
13	MAN	U	4	13	11,11,12	0.63	0	15,15,17	1.85	5 (33%)
13	MAN	U	5	13	11,11,12	0.52	0	15,15,17	1.27	1 (6%)
13	MAN	U	6	13	11,11,12	0.83	1 (9%)	15,15,17	2.65	9 (60%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	L	1	4,10	-	5/6/23/26	0/1/1/1
10	NAG	L	2	10	-	1/6/23/26	0/1/1/1
10	BMA	L	3	10	-	2/2/19/22	0/1/1/1
10	MAN	L	4	10	-	2/2/19/22	0/1/1/1
10	MAN	L	5	10	-	1/2/19/22	0/1/1/1
10	MAN	L	6	10	-	1/2/19/22	0/1/1/1
11	NAG	M	1	4,11	-	4/6/23/26	0/1/1/1
11	NAG	M	2	11	-	3/6/23/26	0/1/1/1
11	BMA	M	3	11	-	0/2/19/22	0/1/1/1
11	MAN	M	4	11	-	0/2/19/22	0/1/1/1
9	NAG	N	1	4,9	-	5/6/23/26	0/1/1/1
9	NAG	N	2	9	-	4/6/23/26	0/1/1/1
7	NAG	O	1	4,7	-	3/6/23/26	0/1/1/1
7	NAG	O	2	7	-	5/6/23/26	0/1/1/1
7	BMA	O	3	7	-	1/2/19/22	0/1/1/1
7	NAG	P	1	4,7	-	3/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
7	BMA	P	3	7	-	1/2/19/22	0/1/1/1
12	NAG	S	1	4,12	-	2/6/23/26	0/1/1/1
12	NAG	S	2	12	-	2/6/23/26	0/1/1/1
12	BMA	S	3	12	-	2/2/19/22	0/1/1/1
12	MAN	S	4	12	-	2/2/19/22	0/1/1/1
12	MAN	S	5	12	-	1/2/19/22	0/1/1/1
7	NAG	T	1	4,7	-	4/6/23/26	0/1/1/1
7	NAG	T	2	7	-	2/6/23/26	0/1/1/1
7	BMA	T	3	7	-	2/2/19/22	0/1/1/1
13	NAG	U	1	13	-	4/6/23/26	0/1/1/1
13	NAG	U	2	13	-	3/6/23/26	0/1/1/1
13	BMA	U	3	13	-	0/2/19/22	0/1/1/1
13	MAN	U	4	13	-	1/2/19/22	0/1/1/1
13	MAN	U	5	13	-	0/2/19/22	0/1/1/1
13	MAN	U	6	13	-	2/2/19/22	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	4	MAN	O5-C1	5.56	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	1	NAG	C1-C2	3.75	1.57	1.52
7	J	2	NAG	C1-C2	3.64	1.57	1.52
9	I	2	NAG	C1-C2	3.32	1.56	1.52
12	S	3	BMA	C2-C3	3.28	1.57	1.52
8	F	4	MAN	C1-C2	3.28	1.60	1.52
13	U	1	NAG	O4-C4	3.13	1.50	1.43
12	S	2	NAG	C1-C2	2.89	1.56	1.52
12	S	2	NAG	O4-C4	2.83	1.50	1.43
7	H	2	NAG	C1-C2	2.78	1.56	1.52
8	F	3	BMA	C1-C2	2.64	1.58	1.52
7	H	1	NAG	O4-C4	2.63	1.49	1.43
7	H	2	NAG	O4-C4	2.50	1.49	1.43
9	K	1	NAG	C1-C2	2.49	1.55	1.52
7	A	2	NAG	C1-C2	2.47	1.55	1.52
7	P	2	NAG	C1-C2	2.42	1.55	1.52
12	S	1	NAG	C4-C5	2.41	1.58	1.53
8	F	2	NAG	C4-C5	2.35	1.58	1.53
13	U	1	NAG	C1-C2	-2.31	1.49	1.52
13	U	1	NAG	O5-C1	-2.27	1.39	1.43
9	K	2	NAG	C1-C2	2.24	1.55	1.52
9	N	1	NAG	C1-C2	2.24	1.55	1.52
10	L	1	NAG	C1-C2	2.20	1.55	1.52
8	F	2	NAG	O4-C4	2.17	1.48	1.43
10	L	6	MAN	C2-C3	2.16	1.55	1.52
11	M	1	NAG	O5-C1	2.08	1.47	1.43
13	U	6	MAN	C1-C2	2.05	1.57	1.52
9	I	1	NAG	O5-C5	2.04	1.47	1.43
12	S	4	MAN	C1-C2	2.04	1.57	1.52
8	F	3	BMA	O6-C6	2.02	1.50	1.42

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	1	NAG	C2-N2-C7	8.07	133.71	122.90
9	N	1	NAG	C2-N2-C7	7.90	133.49	122.90
12	S	2	NAG	C2-N2-C7	7.16	132.49	122.90
11	M	1	NAG	C2-N2-C7	6.89	132.14	122.90
13	U	2	NAG	O4-C4-C5	-6.75	92.71	109.32
13	U	6	MAN	C1-C2-C3	6.24	118.73	109.64
8	F	2	NAG	C1-O5-C5	6.08	120.34	112.19
7	A	1	NAG	C1-O5-C5	-5.76	104.47	112.19
8	F	2	NAG	O4-C4-C5	5.74	123.46	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	2	NAG	C2-N2-C7	5.47	130.24	122.90
7	H	2	NAG	O5-C1-C2	-5.39	102.95	111.29
13	U	1	NAG	C1-C2-N2	-5.38	101.95	110.43
9	K	1	NAG	C2-N2-C7	5.38	130.11	122.90
8	F	1	NAG	O5-C1-C2	-5.34	103.03	111.29
7	C	2	NAG	C2-N2-C7	5.24	129.93	122.90
12	S	2	NAG	O5-C1-C2	-5.24	103.19	111.29
13	U	2	NAG	O5-C1-C2	-5.13	103.35	111.29
7	O	2	NAG	C2-N2-C7	5.11	129.74	122.90
7	C	2	NAG	C1-O5-C5	5.10	119.02	112.19
12	S	3	BMA	O5-C5-C6	4.92	117.24	107.66
7	H	2	NAG	C3-C4-C5	-4.90	101.35	110.23
12	S	4	MAN	O4-C4-C3	-4.83	99.00	110.38
11	M	1	NAG	C4-C3-C2	4.82	118.08	111.02
8	F	1	NAG	C2-N2-C7	-4.80	116.46	122.90
12	S	4	MAN	C1-O5-C5	-4.74	105.83	112.19
10	L	1	NAG	C1-C2-N2	4.74	117.90	110.43
10	L	2	NAG	C1-O5-C5	4.71	118.50	112.19
13	U	3	BMA	O6-C6-C5	4.69	127.30	111.33
9	K	1	NAG	C1-O5-C5	-4.52	106.13	112.19
10	L	3	BMA	O5-C5-C6	4.46	116.34	107.66
7	C	1	NAG	C1-C2-N2	4.43	117.42	110.43
7	A	1	NAG	C2-N2-C7	4.42	128.82	122.90
10	L	1	NAG	O5-C1-C2	-4.41	104.47	111.29
7	T	1	NAG	C2-N2-C7	4.37	128.76	122.90
12	S	3	BMA	O3-C3-C2	4.35	118.94	110.05
13	U	3	BMA	O3-C3-C2	-4.29	101.30	110.05
10	L	3	BMA	O3-C3-C4	-4.28	100.28	110.38
13	U	2	NAG	C4-C3-C2	4.22	117.20	111.02
13	U	1	NAG	O4-C4-C3	4.21	120.31	110.38
10	L	2	NAG	C1-C2-N2	4.21	117.06	110.43
10	L	1	NAG	C8-C7-N2	4.06	122.85	116.12
7	H	2	NAG	C1-O5-C5	4.06	117.62	112.19
8	F	3	BMA	O5-C5-C6	4.03	115.50	107.66
10	L	4	MAN	O5-C5-C6	4.03	115.50	107.66
7	C	1	NAG	C2-N2-C7	3.93	128.17	122.90
9	I	2	NAG	O5-C1-C2	-3.92	105.23	111.29
11	M	2	NAG	O5-C1-C2	-3.88	105.29	111.29
13	U	2	NAG	O5-C5-C6	3.86	115.17	107.66
7	C	1	NAG	O3-C3-C2	-3.85	101.41	109.40
8	F	4	MAN	C2-C3-C4	3.84	117.62	110.86
10	L	3	BMA	C6-C5-C4	-3.81	103.67	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	1	NAG	O5-C5-C6	-3.77	100.32	107.66
7	J	2	NAG	C2-N2-C7	3.76	127.93	122.90
10	L	4	MAN	C3-C4-C5	-3.72	103.49	110.23
12	S	4	MAN	C3-C4-C5	3.71	116.97	110.23
7	J	1	NAG	C4-C3-C2	-3.70	105.60	111.02
12	S	2	NAG	C1-C2-N2	3.68	116.23	110.43
13	U	6	MAN	O4-C4-C3	3.68	119.05	110.38
9	K	1	NAG	O4-C4-C3	-3.62	101.83	110.38
12	S	4	MAN	O2-C2-C1	3.58	117.43	109.22
13	U	4	MAN	C2-C3-C4	-3.52	104.67	110.86
13	U	1	NAG	C3-C4-C5	-3.42	104.04	110.23
11	M	1	NAG	O4-C4-C3	-3.42	102.33	110.38
13	U	6	MAN	C1-O5-C5	3.41	116.76	112.19
7	H	1	NAG	O5-C1-C2	-3.41	106.01	111.29
7	J	1	NAG	C1-O5-C5	3.39	116.73	112.19
11	M	2	NAG	C1-O5-C5	3.32	116.63	112.19
10	L	3	BMA	O4-C4-C3	-3.30	102.60	110.38
8	F	4	MAN	C3-C4-C5	-3.29	104.27	110.23
7	O	1	NAG	O4-C4-C5	-3.26	101.29	109.32
7	P	2	NAG	O5-C1-C2	-3.26	106.25	111.29
10	L	1	NAG	C1-O5-C5	3.25	116.54	112.19
8	F	2	NAG	O3-C3-C2	3.20	116.05	109.40
8	F	3	BMA	O6-C6-C5	3.17	122.13	111.33
9	I	2	NAG	C1-O5-C5	3.16	116.43	112.19
9	N	2	NAG	C1-O5-C5	3.15	116.41	112.19
7	H	1	NAG	O4-C4-C5	3.14	117.05	109.32
7	P	1	NAG	O4-C4-C3	-3.13	103.00	110.38
11	M	3	BMA	O3-C3-C4	3.10	117.69	110.38
9	I	1	NAG	O4-C4-C5	3.09	116.93	109.32
8	F	3	BMA	O4-C4-C5	3.09	116.92	109.32
8	F	2	NAG	C6-C5-C4	3.08	120.57	113.02
11	M	4	MAN	O5-C1-C2	-3.05	103.53	110.79
7	T	2	NAG	C1-O5-C5	3.03	116.25	112.19
8	F	2	NAG	O6-C6-C5	3.01	121.57	111.33
13	U	3	BMA	O5-C5-C6	3.00	113.50	107.66
7	H	3	BMA	O5-C5-C6	2.97	113.44	107.66
9	I	2	NAG	C1-C2-N2	2.94	115.06	110.43
13	U	6	MAN	O3-C3-C2	-2.93	104.06	110.05
7	A	1	NAG	O4-C4-C3	-2.93	103.46	110.38
7	T	3	BMA	O5-C5-C6	2.93	113.37	107.66
7	H	2	NAG	O4-C4-C5	2.93	116.55	109.32
8	F	2	NAG	O5-C5-C6	-2.93	101.96	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	U	6	MAN	O5-C1-C2	-2.92	103.83	110.79
12	S	4	MAN	O2-C2-C3	-2.90	104.15	110.15
9	N	1	NAG	O7-C7-N2	2.89	127.09	121.98
7	T	3	BMA	O2-C2-C1	2.88	115.82	109.22
7	C	2	NAG	O4-C4-C3	2.86	117.12	110.38
7	H	1	NAG	C1-C2-N2	2.85	114.93	110.43
12	S	1	NAG	O5-C5-C6	2.85	113.20	107.66
7	A	2	NAG	C2-N2-C7	2.84	126.70	122.90
13	U	4	MAN	O4-C4-C3	2.84	117.06	110.38
7	O	2	NAG	C8-C7-N2	2.83	120.81	116.12
10	L	1	NAG	O7-C7-C8	-2.83	117.02	122.05
10	L	5	MAN	O5-C1-C2	-2.82	104.06	110.79
8	F	3	BMA	O2-C2-C1	2.82	115.68	109.22
13	U	3	BMA	O3-C3-C4	2.82	117.01	110.38
13	U	6	MAN	O5-C5-C4	-2.81	103.98	110.83
12	S	2	NAG	C4-C3-C2	2.81	115.13	111.02
13	U	4	MAN	O5-C5-C4	-2.77	104.09	110.83
12	S	2	NAG	O3-C3-C2	-2.73	103.73	109.40
8	F	4	MAN	O4-C4-C5	2.72	116.02	109.32
7	A	1	NAG	O5-C1-C2	2.72	115.50	111.29
11	M	3	BMA	C2-C3-C4	-2.70	106.11	110.86
13	U	4	MAN	O4-C4-C5	2.70	115.97	109.32
12	S	1	NAG	O4-C4-C3	-2.69	104.04	110.38
10	L	6	MAN	O2-C2-C3	2.68	115.70	110.15
12	S	4	MAN	O4-C4-C5	-2.67	102.75	109.32
8	F	4	MAN	O2-C2-C3	2.66	115.66	110.15
10	L	3	BMA	O3-C3-C2	-2.66	104.63	110.05
8	F	2	NAG	C3-C4-C5	-2.66	105.42	110.23
8	F	1	NAG	C3-C4-C5	-2.65	105.42	110.23
11	M	1	NAG	C1-C2-N2	2.64	114.59	110.43
12	S	3	BMA	O5-C1-C2	-2.62	104.54	110.79
7	J	2	NAG	C1-O5-C5	2.61	115.68	112.19
8	F	4	MAN	O3-C3-C4	-2.60	104.24	110.38
7	T	1	NAG	C8-C7-N2	2.59	120.41	116.12
8	F	1	NAG	C1-O5-C5	2.56	115.62	112.19
8	F	1	NAG	O3-C3-C4	2.55	116.39	110.38
9	K	1	NAG	O3-C3-C2	2.55	114.70	109.40
7	H	1	NAG	O4-C4-C3	-2.55	104.37	110.38
7	H	1	NAG	O5-C5-C6	-2.53	102.74	107.66
13	U	4	MAN	C1-C2-C3	2.53	113.33	109.64
7	H	3	BMA	O5-C1-C2	-2.52	104.77	110.79
11	M	4	MAN	C1-O5-C5	2.50	115.54	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	1	NAG	C4-C3-C2	-2.49	107.37	111.02
13	U	2	NAG	C1-O5-C5	2.46	115.49	112.19
13	U	5	MAN	C6-C5-C4	2.45	119.04	113.02
7	C	2	NAG	C1-C2-N2	2.44	114.27	110.43
7	T	2	NAG	C1-C2-N2	2.43	114.26	110.43
7	T	2	NAG	O5-C1-C2	-2.43	107.53	111.29
7	O	1	NAG	O4-C4-C3	-2.42	104.68	110.38
7	J	2	NAG	C1-C2-N2	2.42	114.24	110.43
7	H	2	NAG	C4-C3-C2	2.40	114.54	111.02
9	N	2	NAG	O5-C1-C2	-2.39	107.59	111.29
10	L	2	NAG	C6-C5-C4	2.38	118.87	113.02
8	F	4	MAN	C6-C5-C4	-2.38	107.17	113.02
13	U	1	NAG	C1-O5-C5	2.37	115.36	112.19
11	M	3	BMA	C1-C2-C3	2.37	113.09	109.64
11	M	1	NAG	O7-C7-C8	-2.37	117.84	122.05
7	J	1	NAG	O3-C3-C4	2.36	115.94	110.38
10	L	6	MAN	O5-C5-C6	2.36	112.25	107.66
12	S	1	NAG	O6-C6-C5	2.35	119.34	111.33
10	L	2	NAG	O4-C4-C5	2.35	115.11	109.32
12	S	1	NAG	O4-C4-C5	2.35	115.10	109.32
12	S	3	BMA	C1-C2-C3	2.32	113.03	109.64
10	L	2	NAG	O5-C5-C6	2.31	112.16	107.66
7	T	1	NAG	O5-C1-C2	-2.31	107.72	111.29
12	S	3	BMA	O4-C4-C3	2.27	115.73	110.38
10	L	2	NAG	C3-C4-C5	-2.27	106.12	110.23
9	K	1	NAG	C8-C7-N2	-2.26	112.36	116.12
12	S	2	NAG	O5-C5-C6	-2.26	103.27	107.66
7	J	1	NAG	O4-C4-C3	2.25	115.69	110.38
9	N	1	NAG	O4-C4-C5	-2.25	103.77	109.32
13	U	6	MAN	O2-C2-C1	2.25	114.38	109.22
7	T	2	NAG	C3-C4-C5	-2.22	106.21	110.23
10	L	1	NAG	O4-C4-C5	2.22	114.78	109.32
9	K	1	NAG	O7-C7-N2	2.21	125.89	121.98
7	J	3	BMA	O5-C5-C6	2.21	111.96	107.66
13	U	1	NAG	O4-C4-C5	2.20	114.75	109.32
11	M	3	BMA	O5-C1-C2	-2.20	105.55	110.79
10	L	4	MAN	O5-C1-C2	-2.19	105.57	110.79
13	U	3	BMA	O5-C1-C2	-2.18	105.60	110.79
7	H	1	NAG	C4-C3-C2	2.18	114.21	111.02
7	H	1	NAG	C2-N2-C7	2.14	125.76	122.90
7	O	1	NAG	C6-C5-C4	-2.12	107.81	113.02
8	F	3	BMA	C1-C2-C3	2.11	112.72	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	U	2	NAG	O3-C3-C2	-2.10	105.03	109.40
12	S	4	MAN	O5-C5-C6	2.08	111.71	107.66
7	J	1	NAG	C2-N2-C7	-2.06	120.14	122.90
7	A	2	NAG	C1-O5-C5	2.05	114.94	112.19
13	U	6	MAN	O2-C2-C3	-2.04	105.92	110.15
12	S	5	MAN	O2-C2-C1	2.03	113.87	109.22
9	I	2	NAG	O5-C5-C6	2.02	111.59	107.66
12	S	2	NAG	O7-C7-N2	2.02	125.55	121.98
13	U	2	NAG	O4-C4-C3	2.01	115.11	110.38
13	U	2	NAG	C2-N2-C7	2.01	125.59	122.90
13	U	6	MAN	C6-C5-C4	-2.01	108.10	113.02

There are no chirality outliers.

All (130) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1	NAG	C3-C2-N2-C7
7	A	1	NAG	C8-C7-N2-C2
7	A	1	NAG	O7-C7-N2-C2
7	A	2	NAG	C8-C7-N2-C2
7	A	2	NAG	O7-C7-N2-C2
7	C	1	NAG	C1-C2-N2-C7
7	H	1	NAG	C1-C2-N2-C7
7	H	1	NAG	C8-C7-N2-C2
7	H	1	NAG	O7-C7-N2-C2
7	J	1	NAG	C8-C7-N2-C2
7	J	1	NAG	O7-C7-N2-C2
7	J	2	NAG	C3-C2-N2-C7
7	J	2	NAG	C8-C7-N2-C2
7	J	2	NAG	O7-C7-N2-C2
7	O	1	NAG	C8-C7-N2-C2
7	O	1	NAG	O7-C7-N2-C2
7	O	2	NAG	C1-C2-N2-C7
7	O	2	NAG	C8-C7-N2-C2
7	O	2	NAG	O7-C7-N2-C2
7	P	1	NAG	C8-C7-N2-C2
7	P	1	NAG	O7-C7-N2-C2
7	P	2	NAG	C8-C7-N2-C2
7	P	2	NAG	O7-C7-N2-C2
7	T	1	NAG	C8-C7-N2-C2
7	T	1	NAG	O7-C7-N2-C2
7	T	2	NAG	C8-C7-N2-C2

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

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

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Mol	Chain	Res	Type	Atoms
9	I	1	NAG	O5-C5-C6-O6
13	U	4	MAN	O5-C5-C6-O6
9	K	2	NAG	O5-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
9	K	1	NAG	O5-C5-C6-O6
7	C	1	NAG	C8-C7-N2-C2
8	F	1	NAG	O5-C5-C6-O6
7	T	3	BMA	C4-C5-C6-O6
7	C	1	NAG	O7-C7-N2-C2
8	F	1	NAG	C4-C5-C6-O6
7	C	2	NAG	C3-C2-N2-C7
7	O	1	NAG	C3-C2-N2-C7
9	K	1	NAG	C3-C2-N2-C7
9	I	2	NAG	O5-C5-C6-O6
10	L	3	BMA	C4-C5-C6-O6
7	C	2	NAG	C1-C2-N2-C7
7	A	1	NAG	C4-C5-C6-O6
7	C	1	NAG	C3-C2-N2-C7
7	T	3	BMA	O5-C5-C6-O6
13	U	2	NAG	O7-C7-N2-C2

There are no ring outliers.

21 monomers are involved in 70 short contacts:

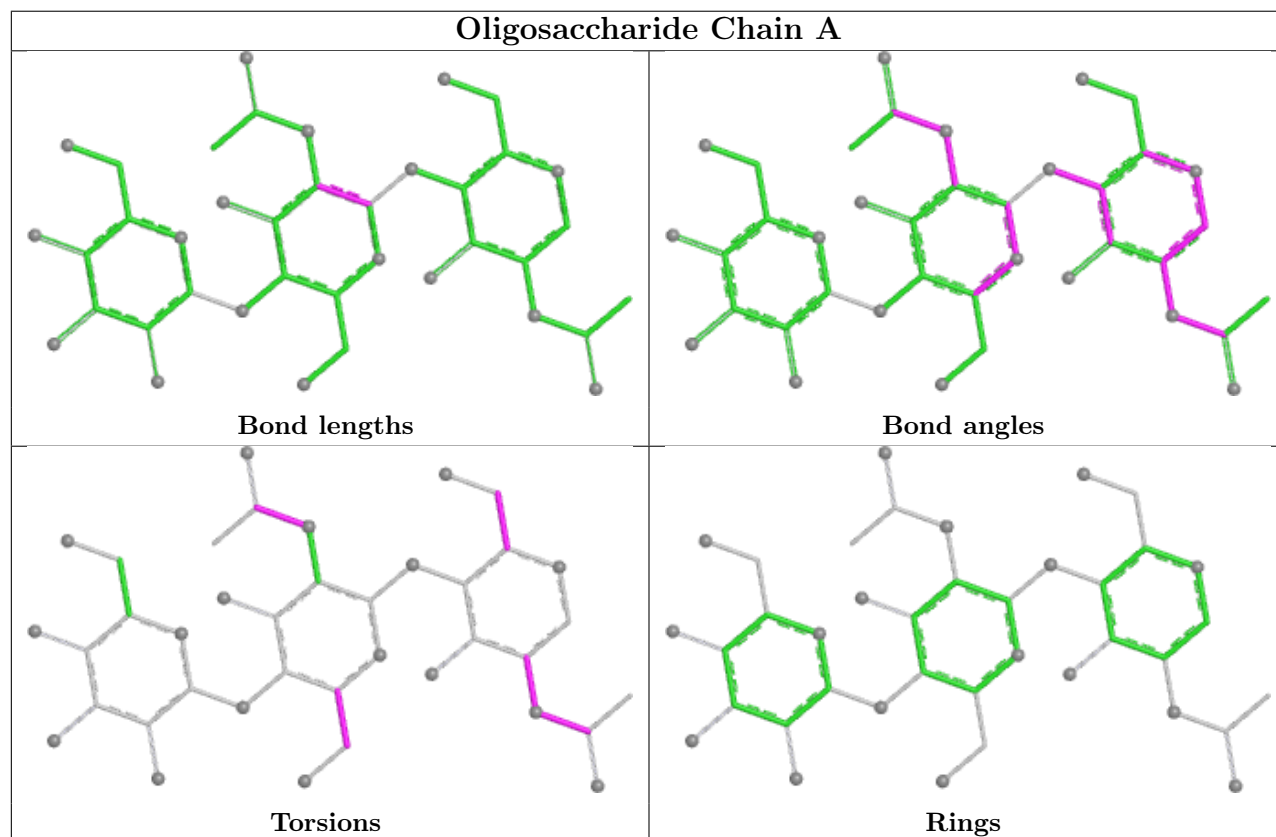
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	U	2	NAG	5	0
13	U	6	MAN	1	0
7	O	2	NAG	1	0
8	F	4	MAN	7	0
12	S	4	MAN	2	0
12	S	1	NAG	3	0
13	U	1	NAG	10	0
7	H	1	NAG	5	0
10	L	2	NAG	1	0
10	L	6	MAN	1	0
11	M	1	NAG	5	0
13	U	3	BMA	2	0
10	L	1	NAG	9	0
7	P	1	NAG	1	0
9	K	1	NAG	10	0
8	F	1	NAG	2	0
7	A	3	BMA	1	0

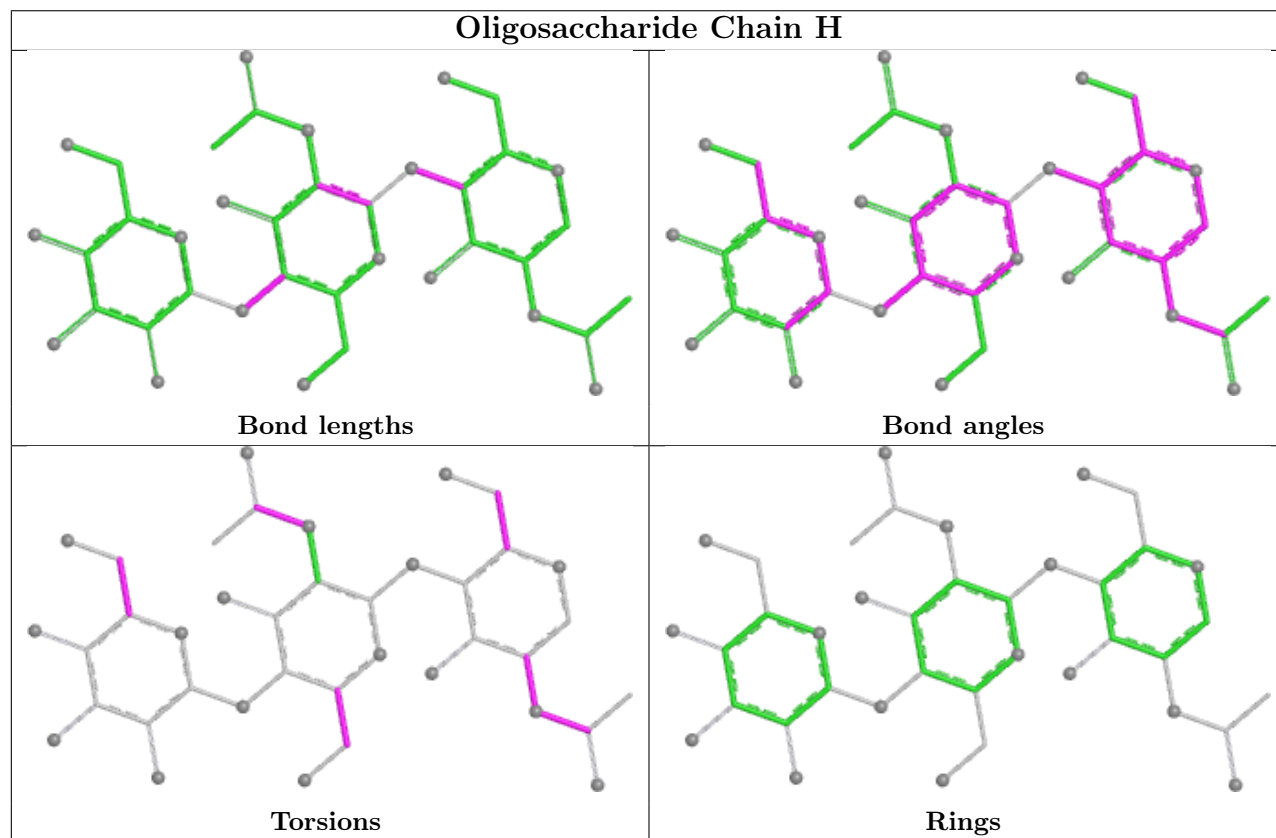
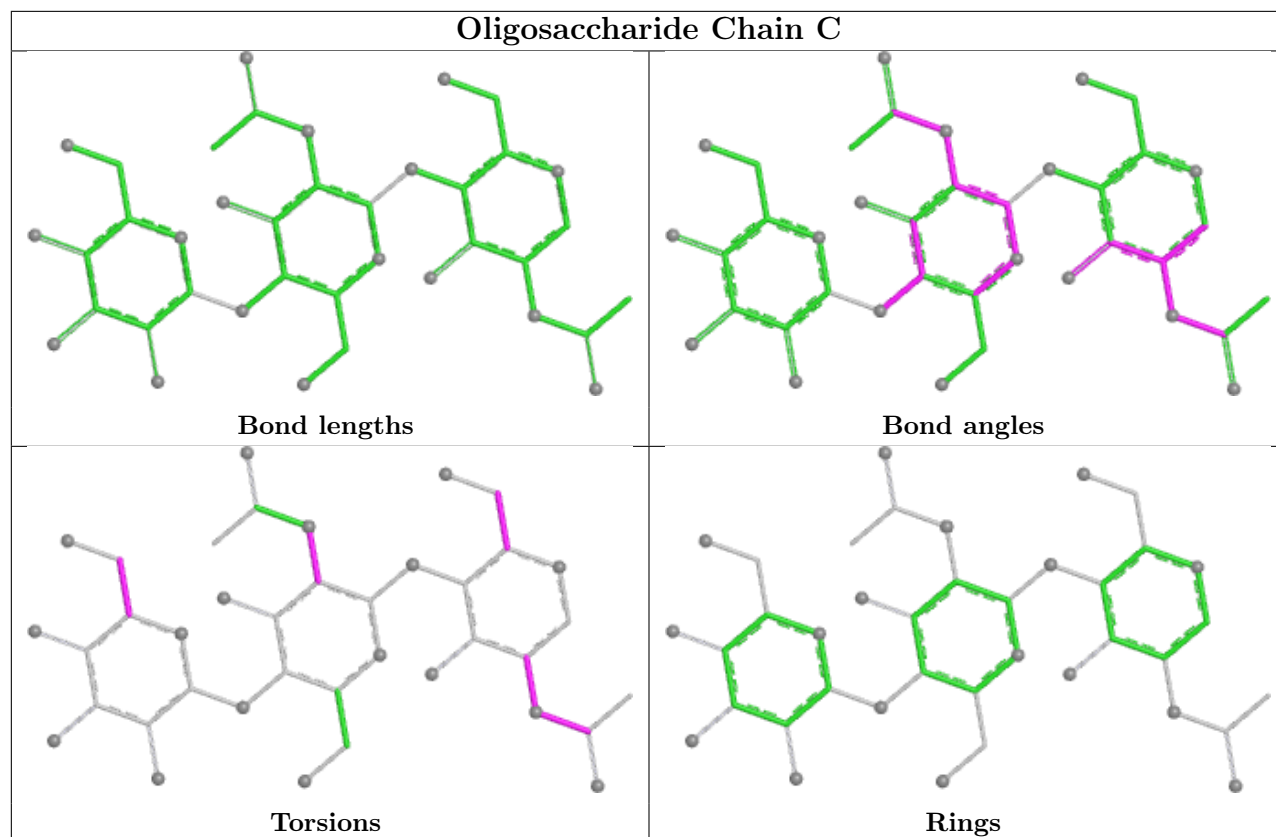
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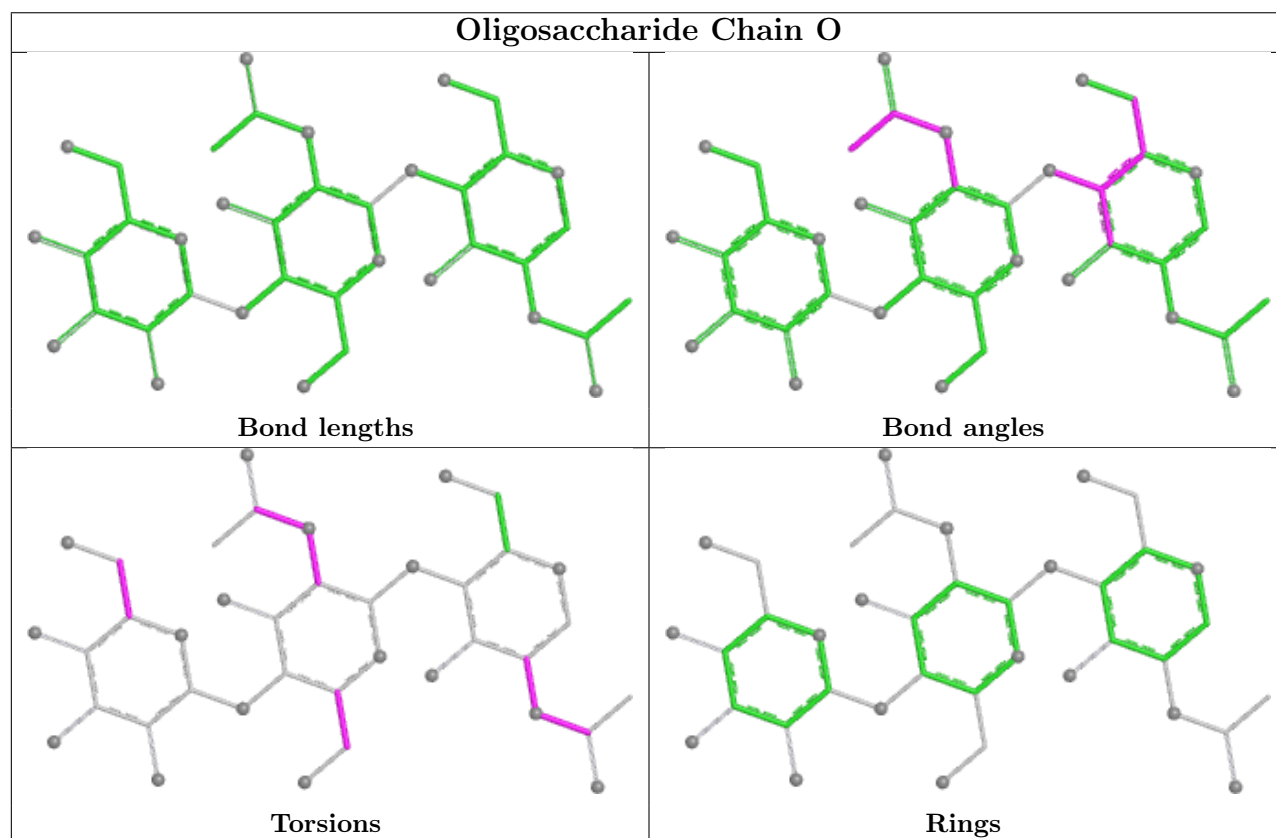
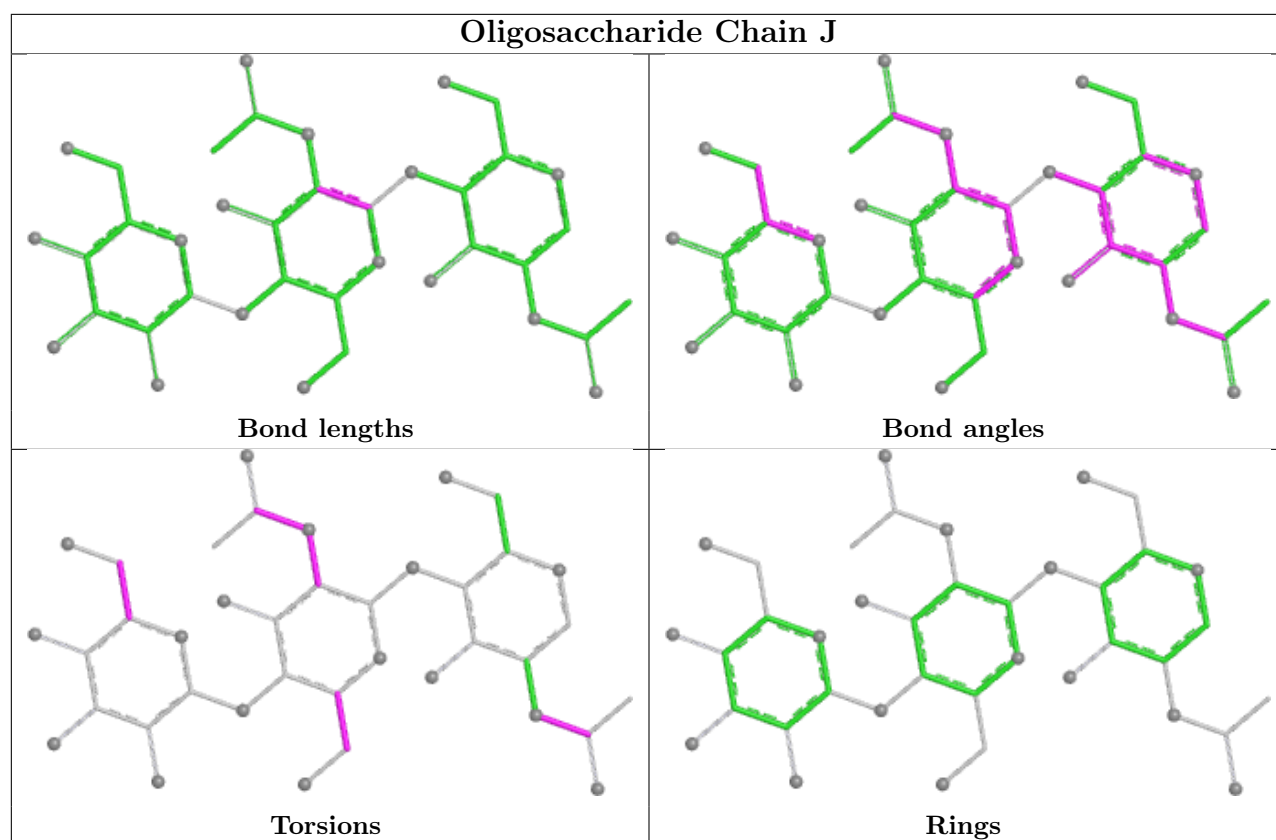
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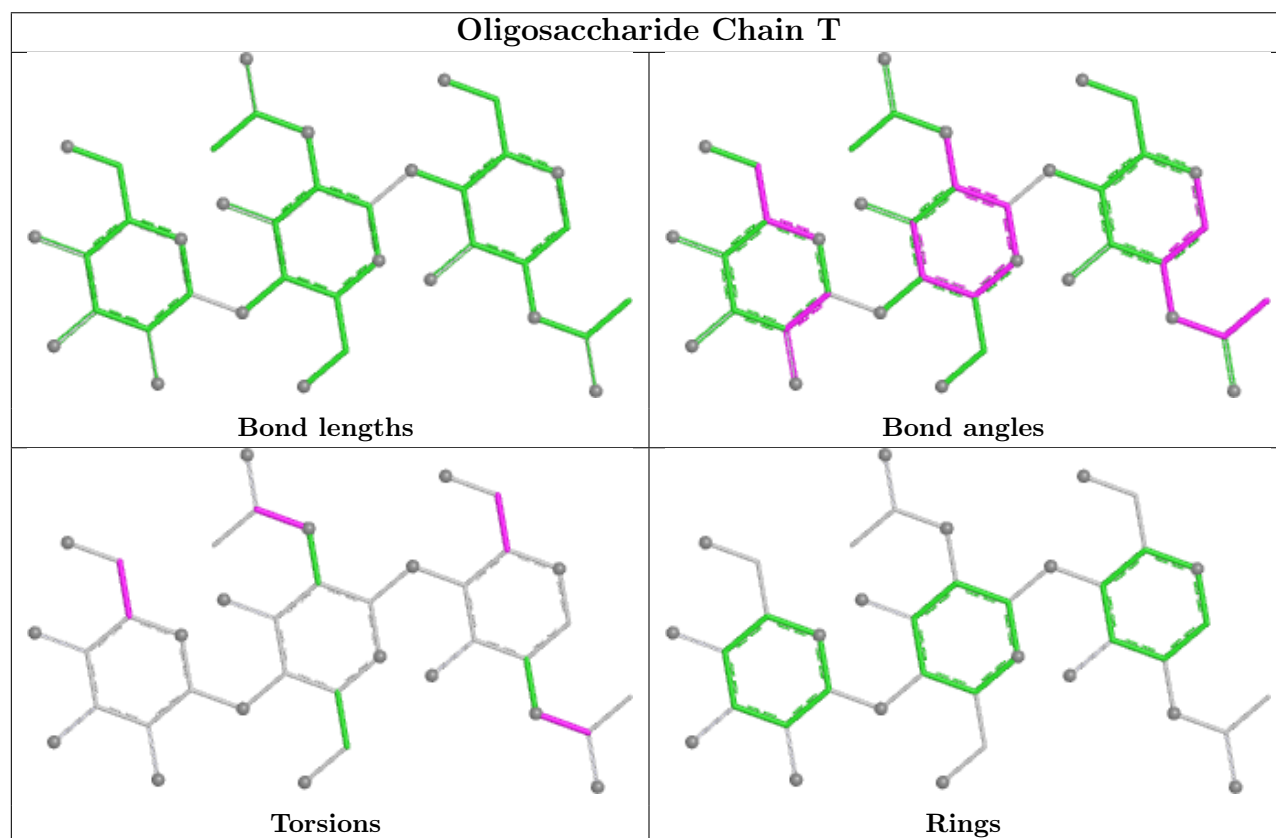
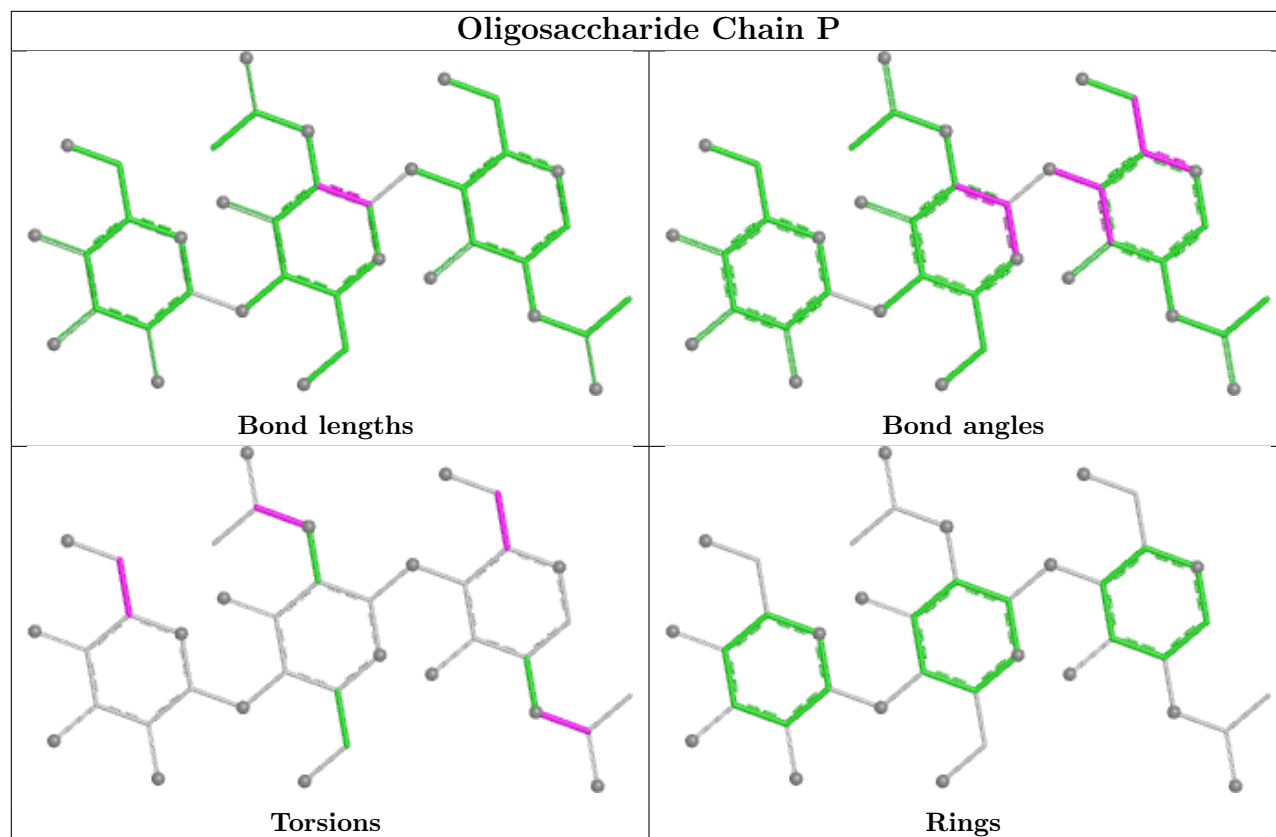
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	2	NAG	2	0
9	N	1	NAG	1	0
7	C	1	NAG	1	0
7	O	1	NAG	1	0

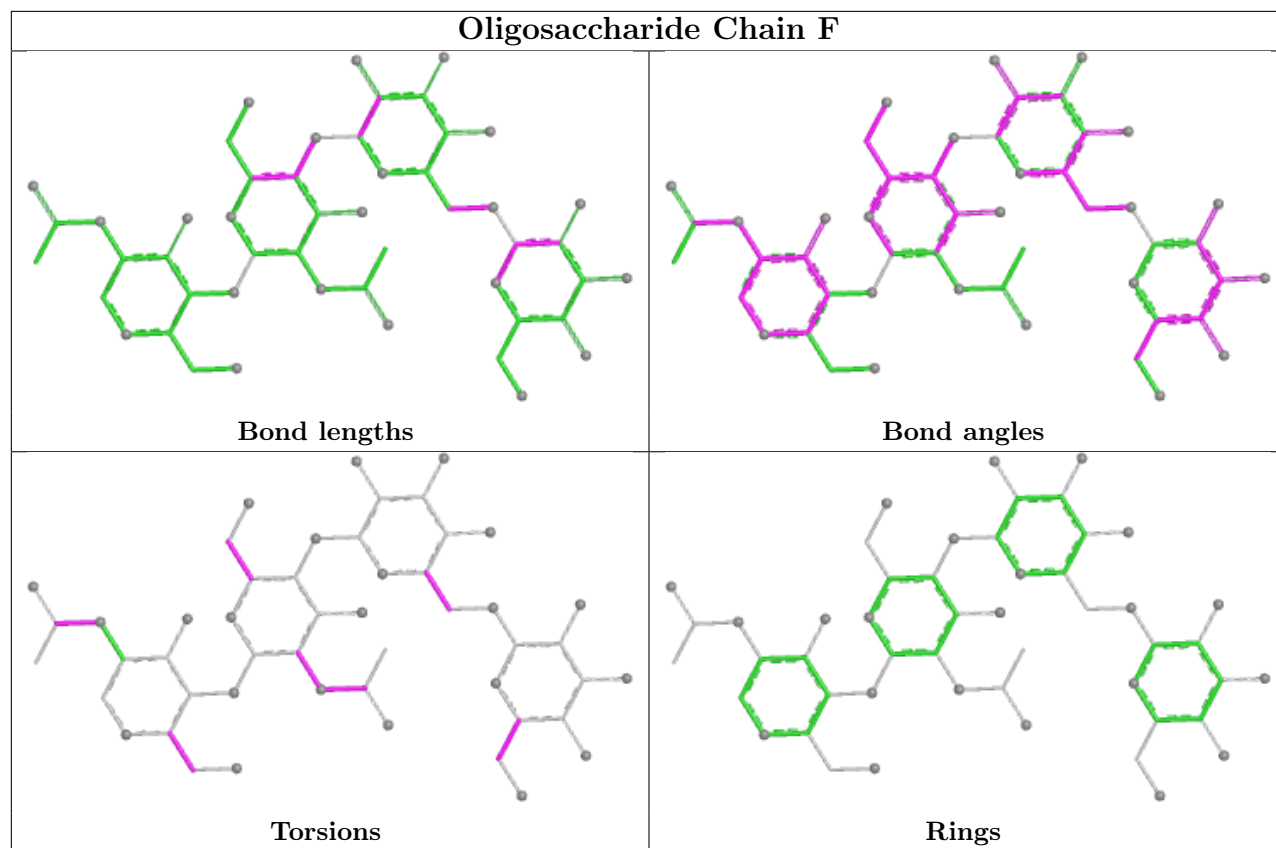
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

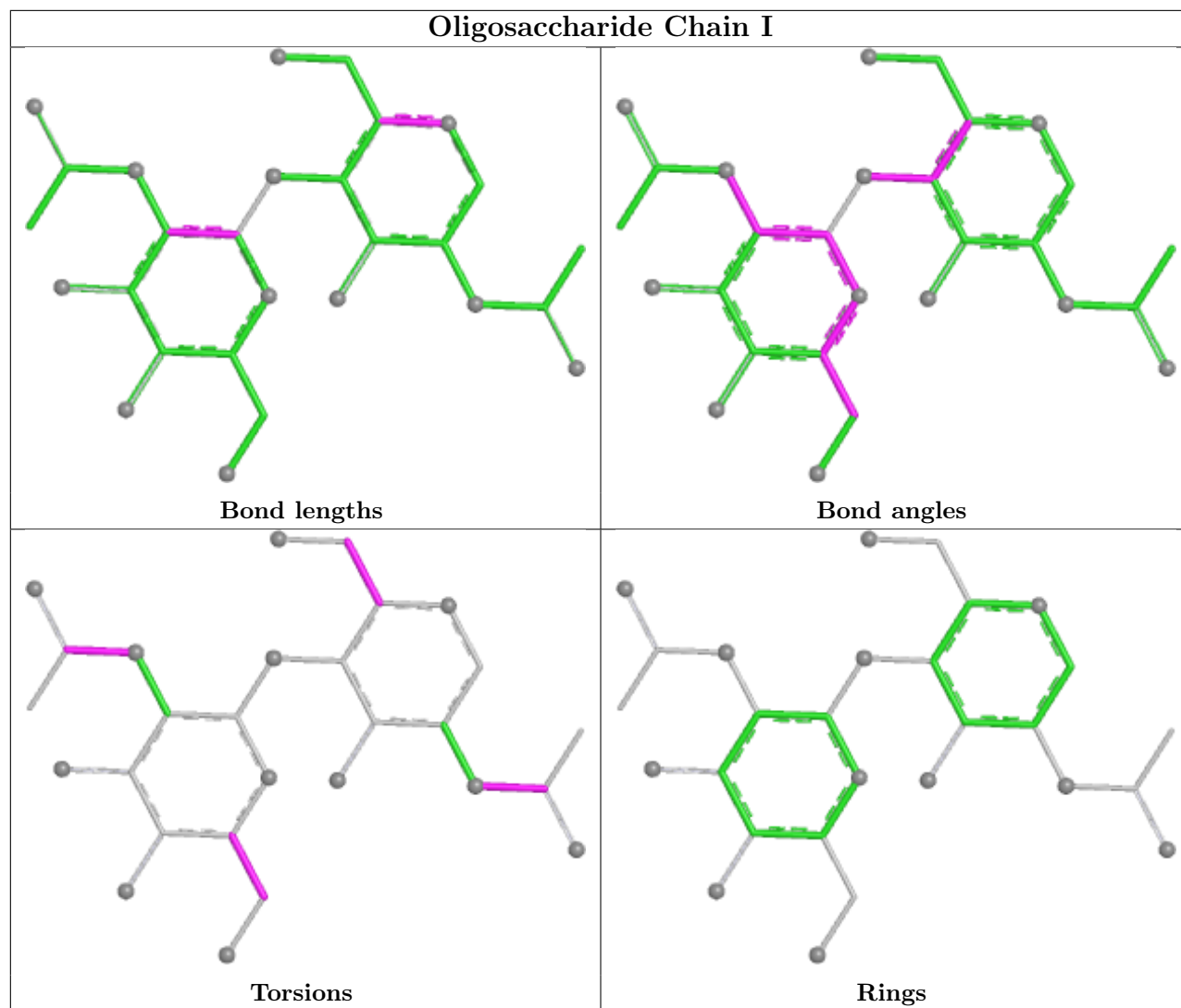


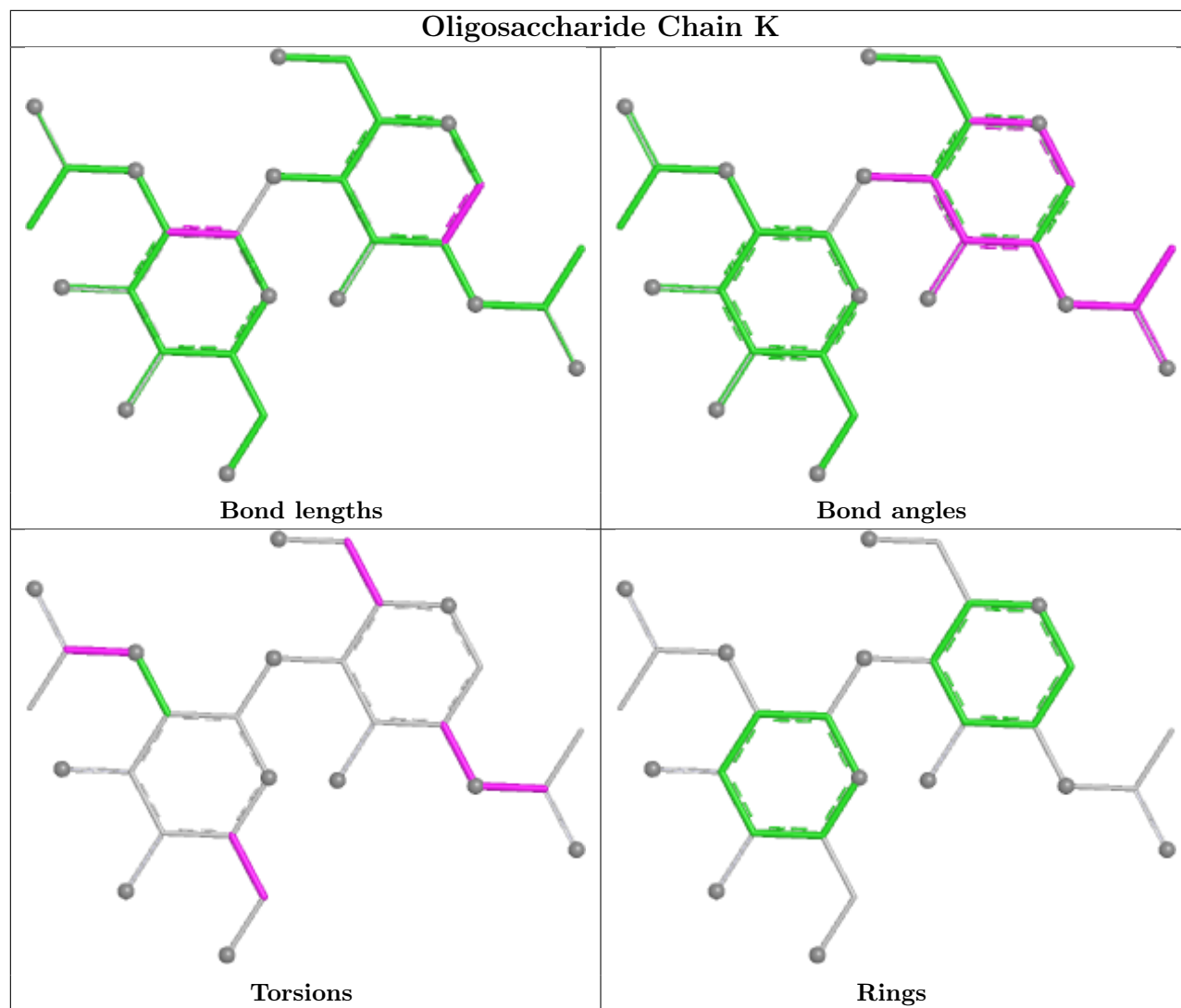


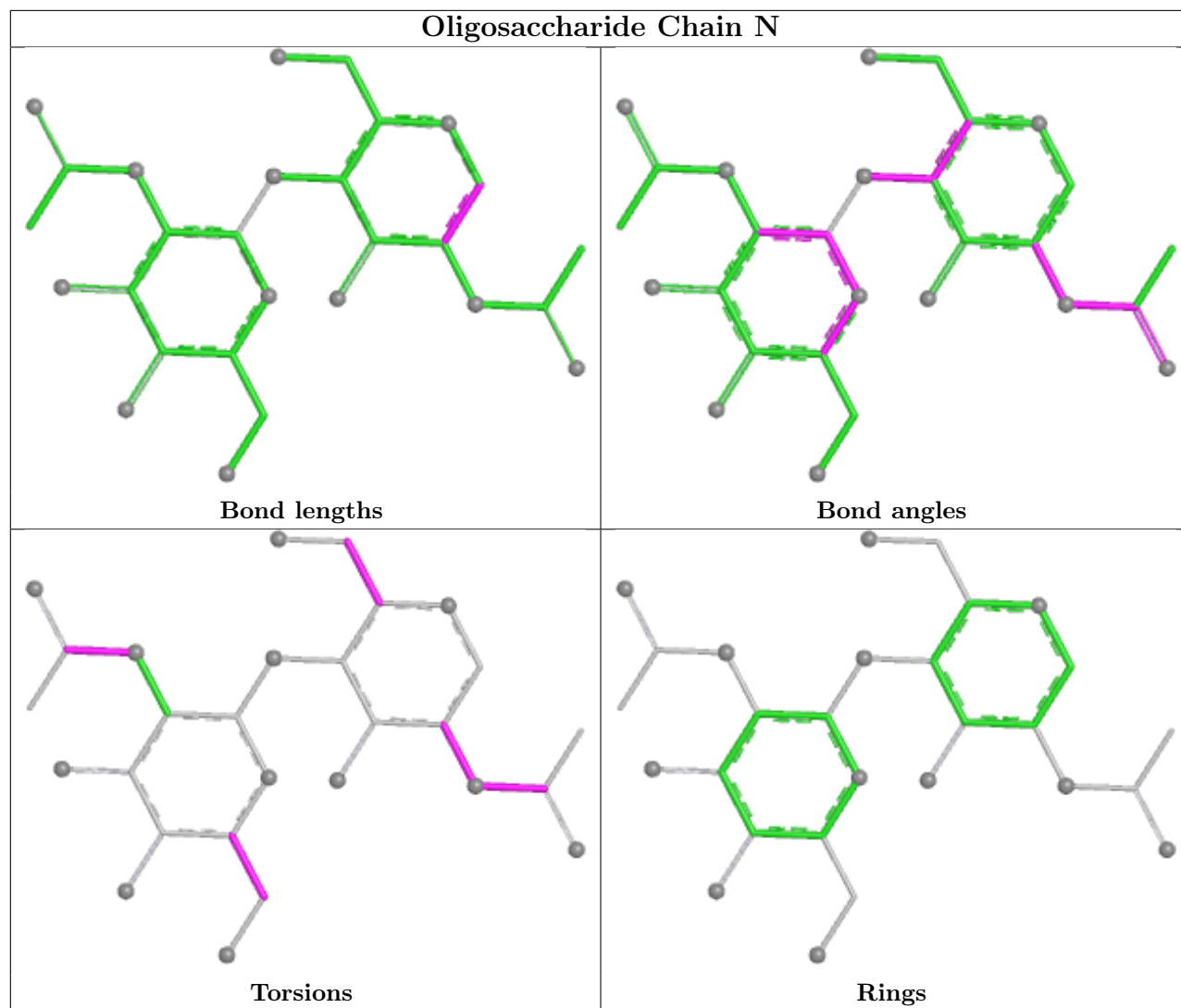


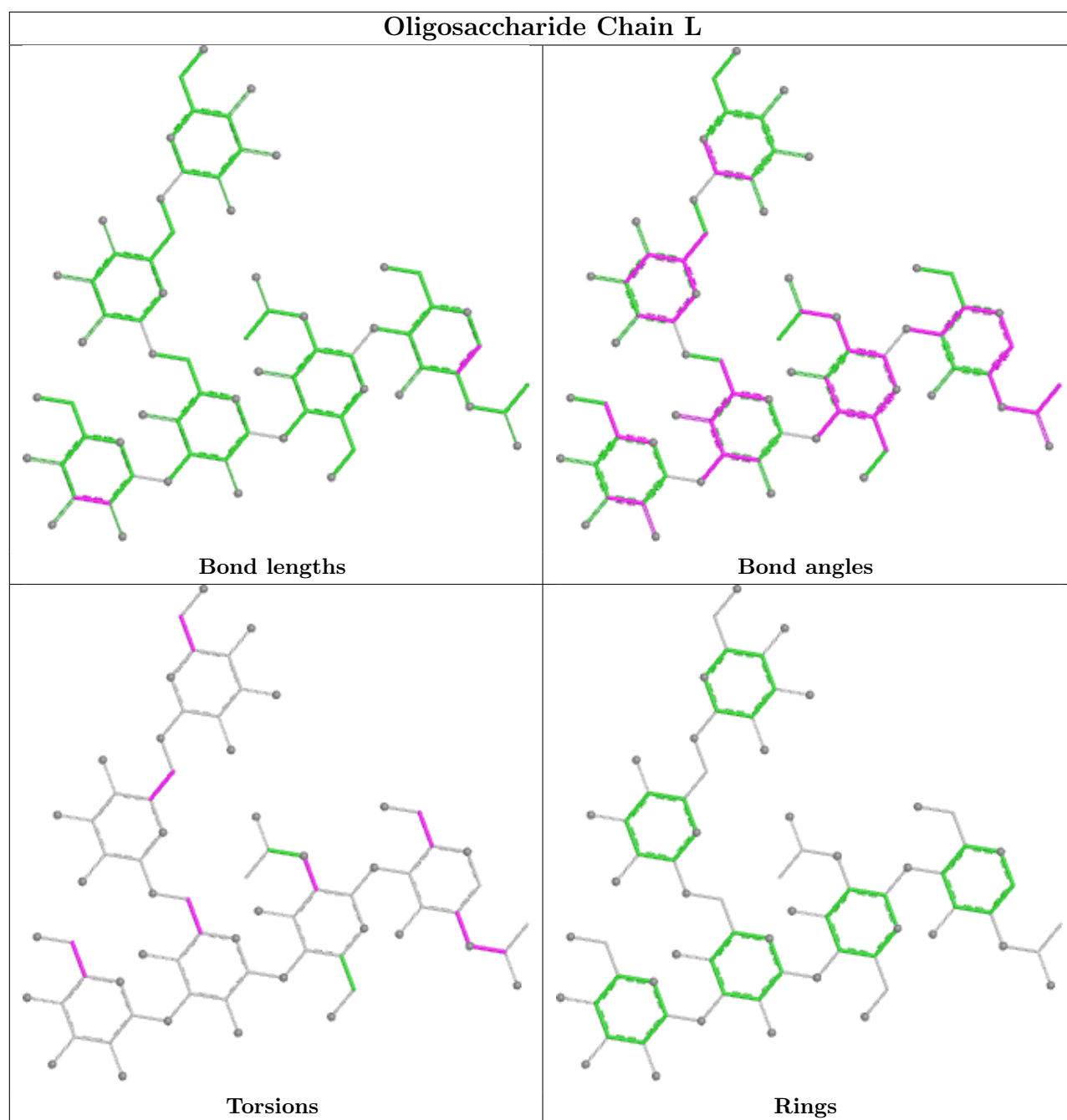




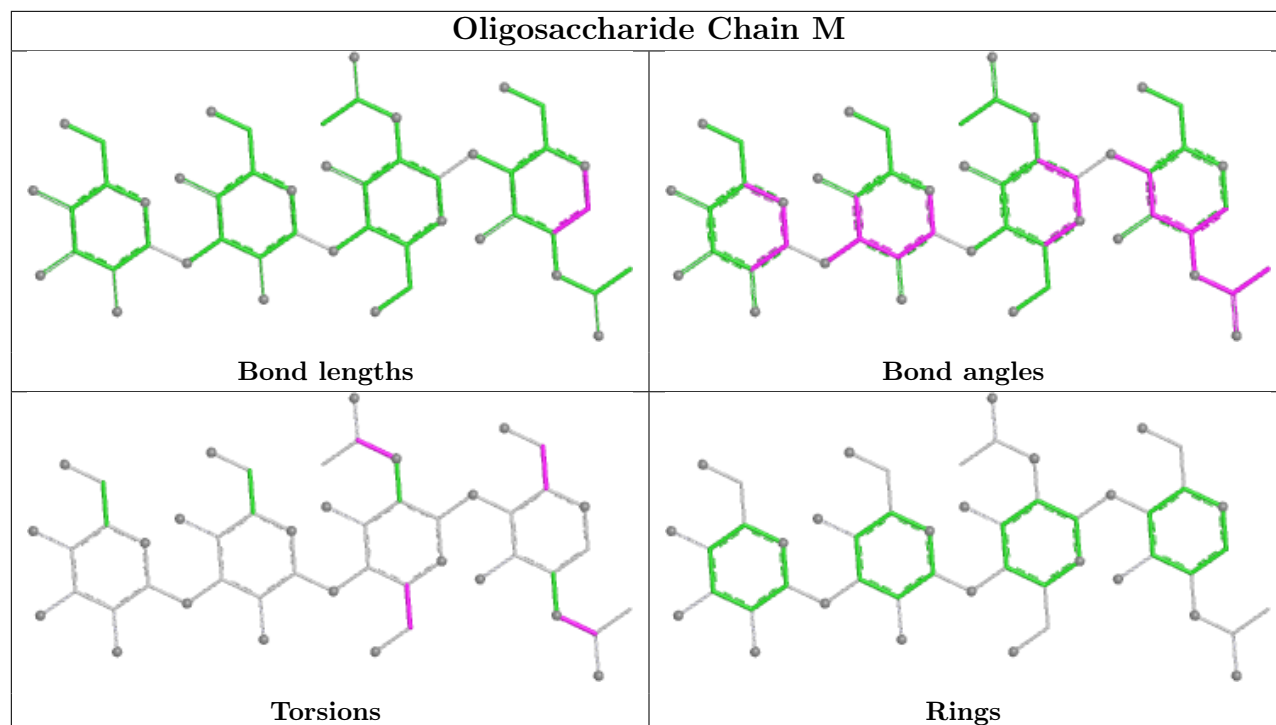




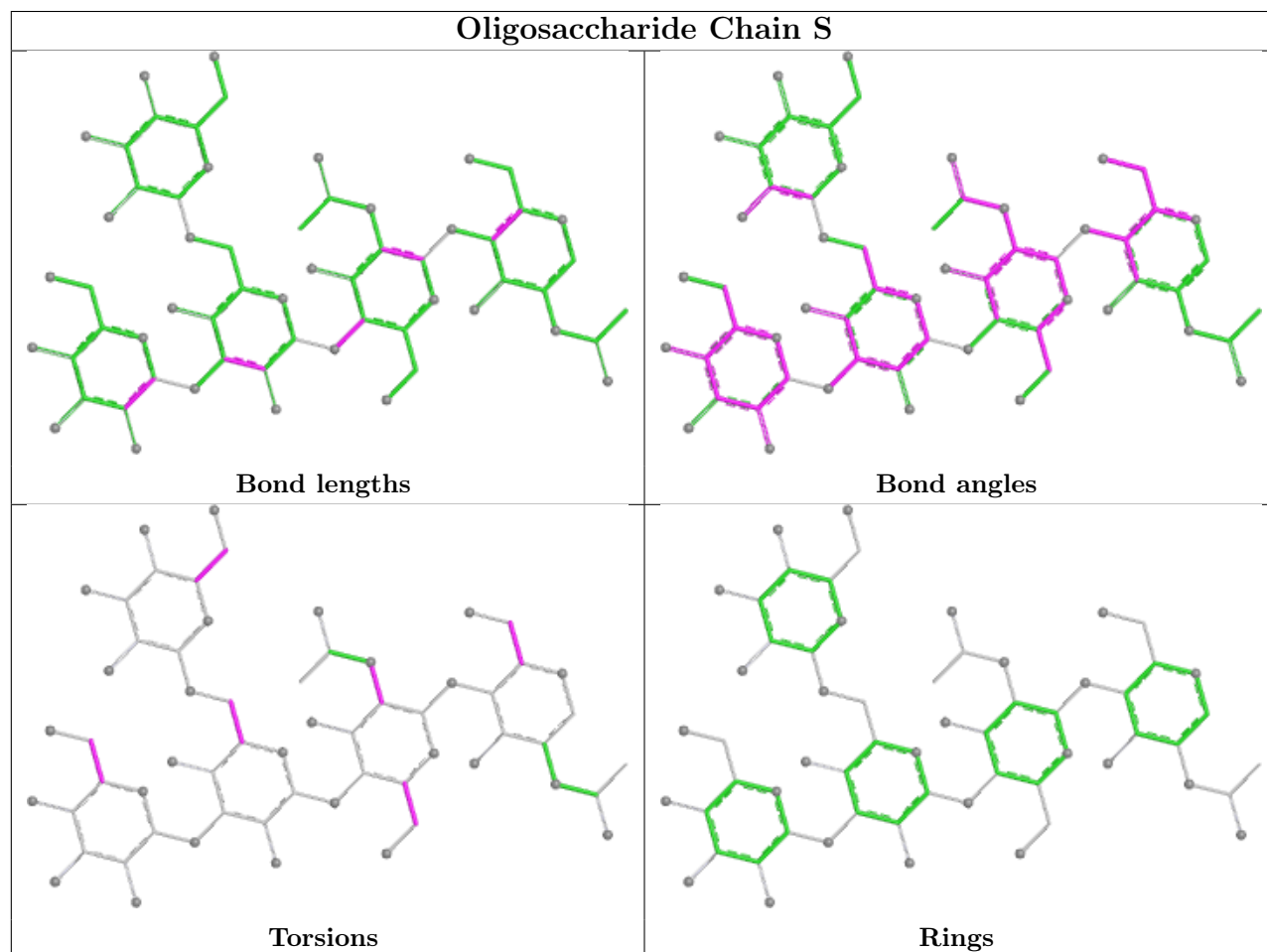


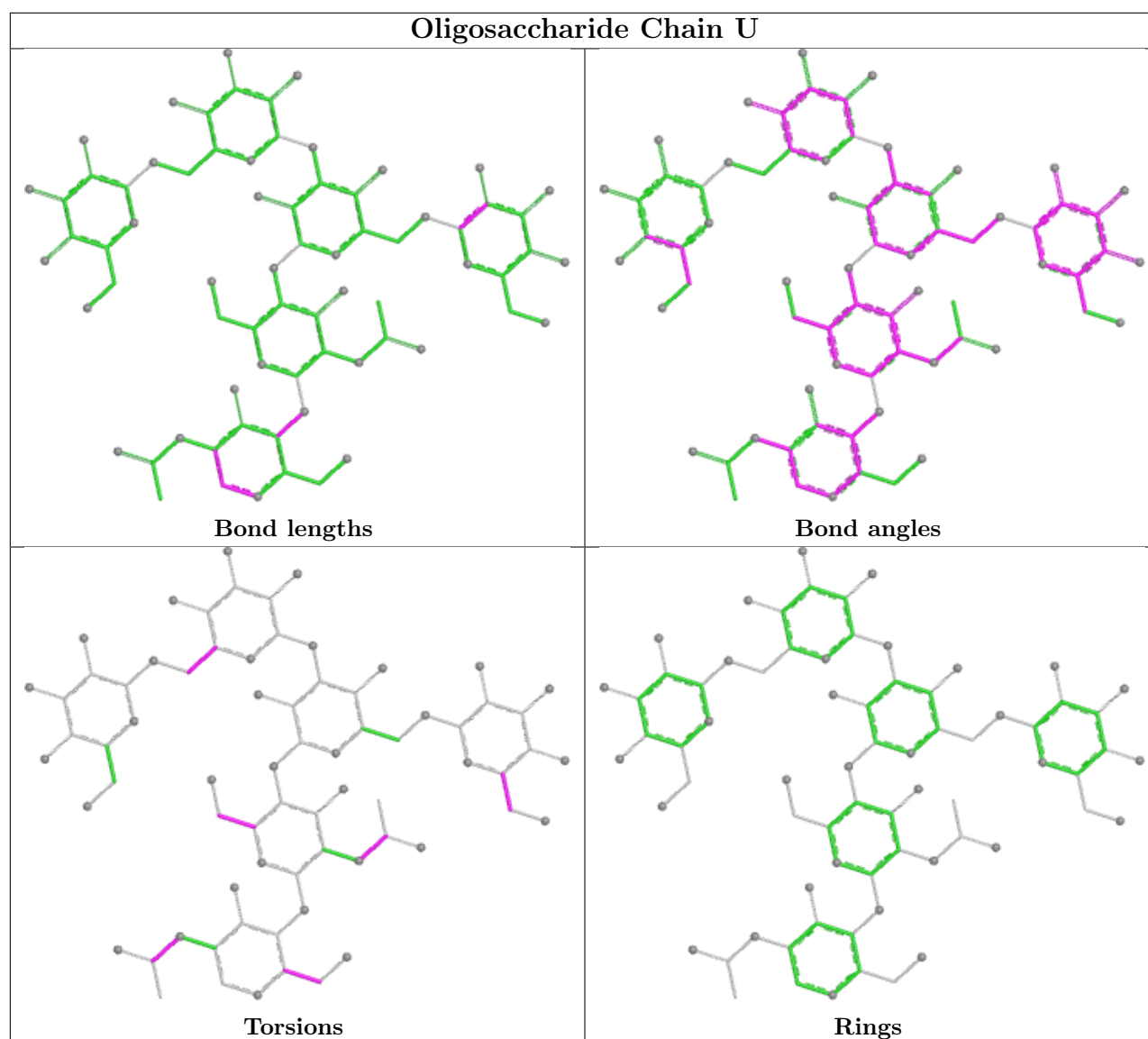


Oligosaccharide Chain M



Oligosaccharide Chain S





5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	NAG	G	606	4	14,14,15	1.27	1 (7%)	17,19,21	1.99	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	NAG	B	704	1	14,14,15	0.30	0	17,19,21	1.12	2 (11%)
14	NAG	G	631	4	14,14,15	0.61	0	17,19,21	1.71	3 (17%)
14	NAG	G	622	4	14,14,15	0.95	1 (7%)	17,19,21	1.93	6 (35%)

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
14	NAG	G	606	4	-	5/6/23/26	0/1/1/1
14	NAG	B	704	1	-	4/6/23/26	0/1/1/1
14	NAG	G	631	4	-	2/6/23/26	0/1/1/1
14	NAG	G	622	4	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	G	606	NAG	C1-C2	3.86	1.57	1.52
14	G	622	NAG	C1-C2	2.58	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	606	NAG	C2-N2-C7	5.77	130.64	122.90
14	G	631	NAG	C2-N2-C7	4.42	128.83	122.90
14	G	622	NAG	C2-N2-C7	3.29	127.31	122.90
14	B	704	NAG	C2-N2-C7	-3.23	118.57	122.90
14	G	622	NAG	C6-C5-C4	-2.93	105.82	113.02
14	G	622	NAG	C1-O5-C5	2.80	115.94	112.19
14	G	631	NAG	O5-C5-C6	2.78	113.07	107.66
14	G	606	NAG	C1-O5-C5	-2.61	108.69	112.19
14	G	606	NAG	C1-C2-N2	2.57	114.48	110.43
14	G	622	NAG	O5-C1-C2	-2.46	107.49	111.29
14	G	622	NAG	O3-C3-C2	2.45	114.49	109.40
14	G	622	NAG	O7-C7-C8	-2.38	117.81	122.05
14	G	606	NAG	C8-C7-N2	2.35	120.02	116.12
14	G	606	NAG	O3-C3-C2	2.32	114.21	109.40
14	B	704	NAG	C4-C3-C2	-2.27	107.69	111.02
14	G	631	NAG	C4-C3-C2	2.05	114.02	111.02

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	B	704	NAG	C8-C7-N2-C2
14	B	704	NAG	O7-C7-N2-C2
14	G	606	NAG	C3-C2-N2-C7
14	G	606	NAG	C8-C7-N2-C2
14	G	606	NAG	O7-C7-N2-C2
14	G	622	NAG	C8-C7-N2-C2
14	G	622	NAG	O7-C7-N2-C2
14	G	606	NAG	C4-C5-C6-O6
14	B	704	NAG	O5-C5-C6-O6
14	G	606	NAG	O5-C5-C6-O6
14	B	704	NAG	C4-C5-C6-O6
14	G	622	NAG	C3-C2-N2-C7
14	G	631	NAG	C3-C2-N2-C7
14	G	631	NAG	C1-C2-N2-C7
14	G	622	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	704	NAG	4	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	136/153 (88%)	0.21	0	100	100	183, 285, 325, 365	0
2	D	236/243 (97%)	-0.05	0	100	100	207, 303, 325, 325	0
3	E	213/216 (98%)	-0.07	1 (0%)	87	75	196, 297, 325, 325	0
4	G	448/518 (86%)	0.10	12 (2%)	56	45	186, 292, 325, 375	0
5	Q	231/240 (96%)	0.13	7 (3%)	52	42	210, 298, 325, 325	0
6	R	205/215 (95%)	-0.01	7 (3%)	48	40	219, 309, 325, 325	0
All	All	1469/1585 (92%)	0.05	27 (1%)	67	54	183, 298, 325, 375	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	439	ILE	5.0
4	G	496	ILE	4.7
4	G	423	ILE	4.1
6	R	76	ILE	3.6
4	G	180	ASP	3.5
4	G	125	LEU	3.4
5	Q	166	PRO	3.3
5	Q	198	VAL	2.8
4	G	452	LEU	2.7
5	Q	109	LEU	2.7
6	R	189	TRP	2.6
4	G	176	PHE	2.5
4	G	345	ILE	2.5
5	Q	136	PRO	2.5
5	Q	108	ALA	2.4
4	G	443	ILE	2.4
4	G	379	GLY	2.2
5	Q	197	SER	2.2
4	G	317	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
6	R	120	THR	2.2
6	R	61	GLY	2.2
5	Q	164	PRO	2.2
4	G	380	GLY	2.1
6	R	42	GLY	2.1
3	E	21	SER	2.1
6	R	5	GLU	2.1
6	R	41	PRO	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($\text{\AA}^2$)	Q<0.9
7	NAG	A	1	14/15	-	-	411,411,411,411	0
7	NAG	A	2	14/15	-	-	430,430,430,430	0
7	BMA	A	3	11/12	-	-	420,420,420,420	0
7	NAG	C	1	14/15	-	-	428,428,428,428	0
7	NAG	C	2	14/15	-	-	449,449,449,449	0
7	BMA	C	3	11/12	-	-	450,450,450,450	0
7	BMA	O	3	11/12	-0.19	0.13	435,435,435,435	0
7	BMA	H	3	11/12	0.22	0.09	478,478,478,478	0
7	NAG	H	2	14/15	0.25	0.12	449,449,449,449	0
7	BMA	J	3	11/12	0.46	0.08	441,441,441,441	0
7	BMA	T	3	11/12	0.54	0.08	415,415,415,415	0
10	BMA	L	3	11/12	0.55	0.11	386,386,386,386	0
12	MAN	S	4	11/12	0.55	0.15	327,327,327,327	0
12	BMA	S	3	11/12	0.59	0.12	415,415,415,415	0
13	BMA	U	3	11/12	0.63	0.11	334,334,334,334	0
7	NAG	J	2	14/15	0.65	0.10	418,418,418,418	0
9	NAG	K	2	14/15	0.67	0.10	333,333,333,333	0
7	BMA	P	3	11/12	-	-	417,417,417,417	0
7	NAG	O	2	14/15	0.68	0.10	428,428,428,428	0
12	MAN	S	5	11/12	0.73	0.12	397,397,397,397	0

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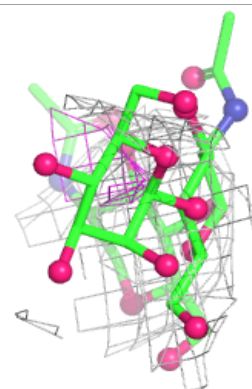
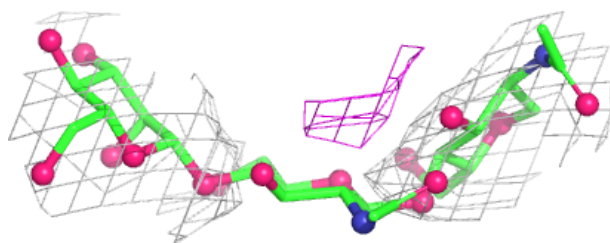
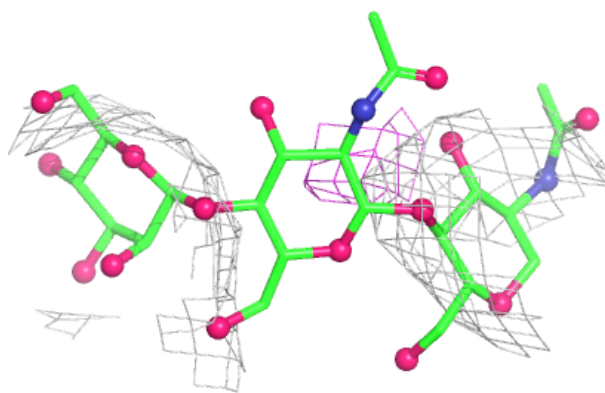
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	NAG	S	2	14/15	0.73	0.10	398,398,398,398	0
8	NAG	F	1	14/15	-	-	343,343,343,343	0
8	NAG	F	2	14/15	-	-	337,337,337,337	0
8	BMA	F	3	11/12	-	-	349,349,349,349	0
8	MAN	F	4	11/12	-	-	360,360,360,360	0
13	MAN	U	6	11/12	0.75	0.09	331,331,331,331	0
13	MAN	U	5	11/12	0.76	0.13	366,366,366,366	0
11	NAG	M	2	14/15	0.77	0.10	405,405,405,405	0
9	NAG	I	1	14/15	0.80	0.13	396,396,396,396	0
7	NAG	T	2	14/15	0.82	0.10	425,425,425,425	0
13	MAN	U	4	11/12	0.82	0.08	373,373,373,373	0
9	NAG	K	1	14/15	0.83	0.11	311,311,311,311	0
7	NAG	P	2	14/15	0.83	0.07	409,409,409,409	0
7	NAG	H	1	14/15	0.84	0.09	383,383,383,383	0
10	MAN	L	4	11/12	-	-	387,387,387,387	0
10	MAN	L	5	11/12	-	-	416,416,416,416	0
10	MAN	L	6	11/12	-	-	369,369,369,369	0
7	NAG	P	1	14/15	0.84	0.11	386,386,386,386	0
9	NAG	I	2	14/15	0.84	0.12	433,433,433,433	0
11	BMA	M	3	11/12	-	-	432,432,432,432	0
11	MAN	M	4	11/12	-	-	456,456,456,456	0
10	NAG	L	2	14/15	0.85	0.10	340,340,340,340	0
11	NAG	M	1	14/15	0.86	0.11	390,390,390,390	0
7	NAG	J	1	14/15	0.86	0.09	384,384,384,384	0
13	NAG	U	1	14/15	0.88	0.11	352,352,352,352	0
9	NAG	N	2	14/15	0.89	0.12	422,422,422,422	0
7	NAG	T	1	14/15	0.90	0.10	380,380,380,380	0
10	NAG	L	1	14/15	0.90	0.13	396,396,396,396	0
12	NAG	S	1	14/15	0.90	0.10	343,343,343,343	0
9	NAG	N	1	14/15	0.92	0.17	391,391,391,391	0
7	NAG	O	1	14/15	0.93	0.13	394,394,394,394	0
13	NAG	U	2	14/15	0.95	0.14	359,359,359,359	0

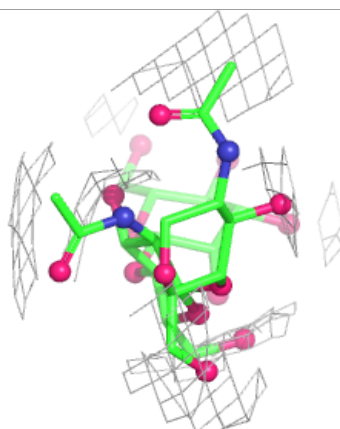
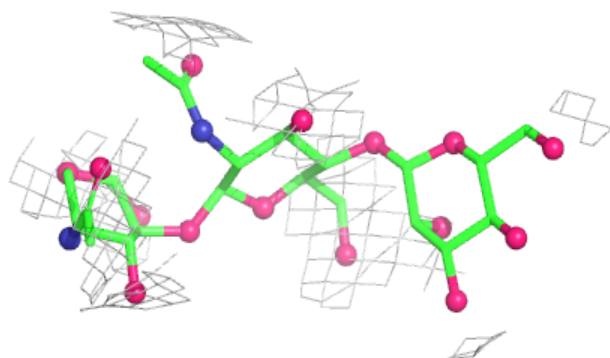
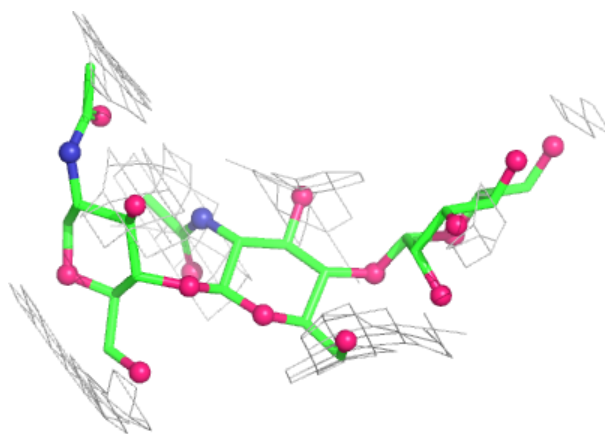
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain A:

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

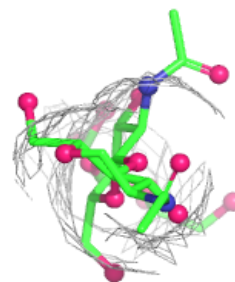
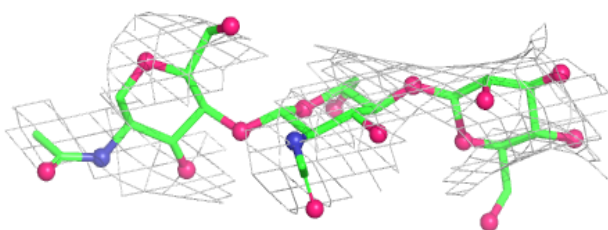
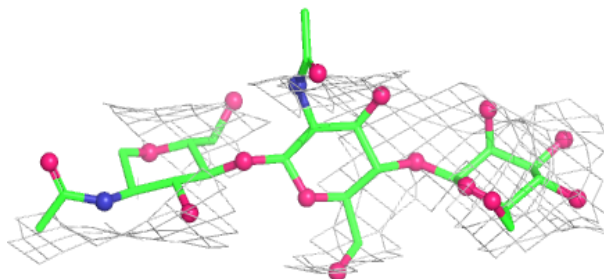
**Electron density around Chain C:**

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

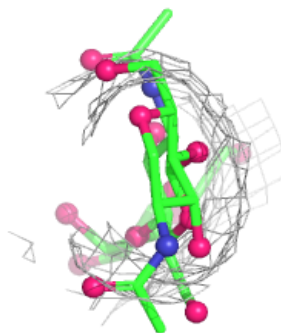
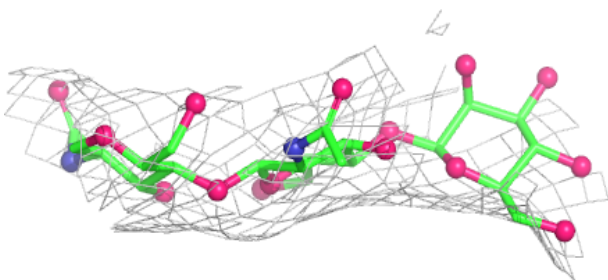
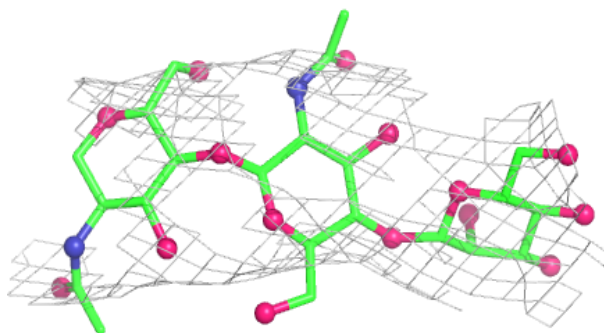


Electron density around Chain H:

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

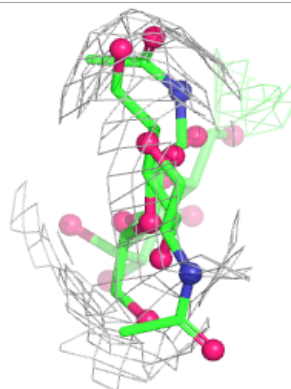
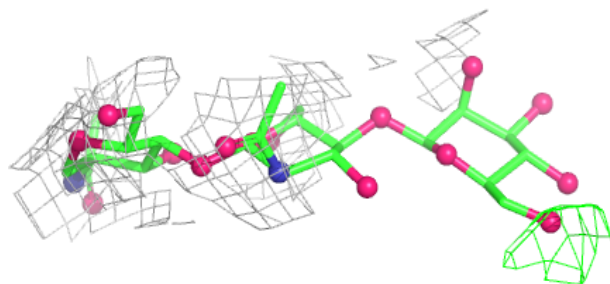
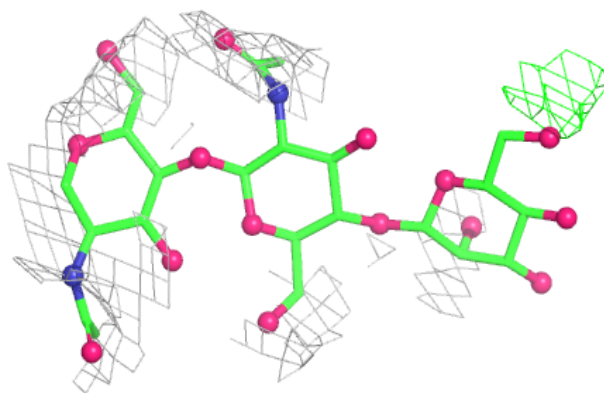
**Electron density around Chain J:**

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

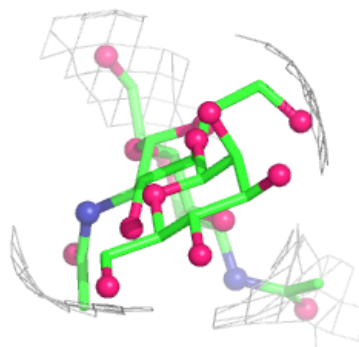
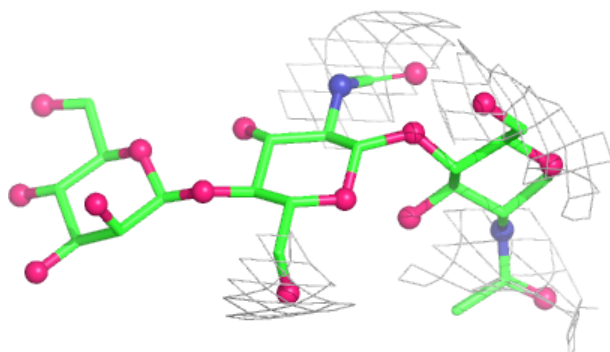
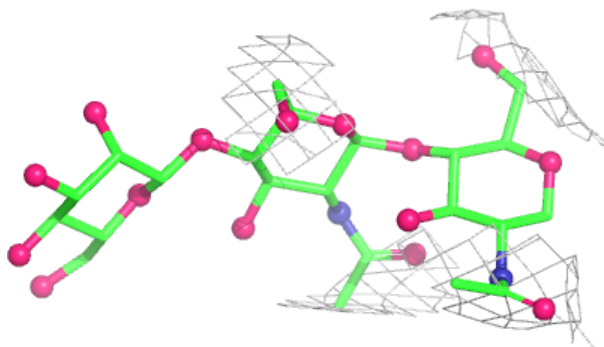


Electron density around Chain O:

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

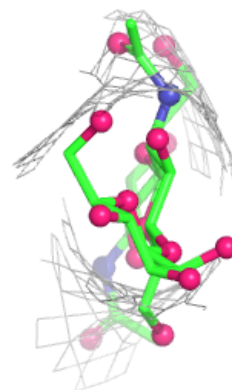
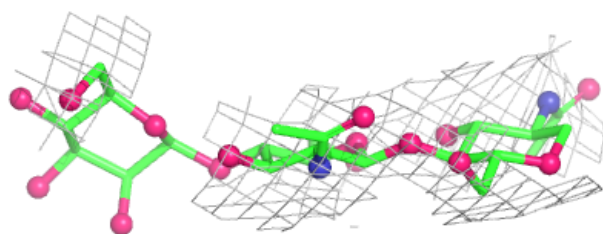
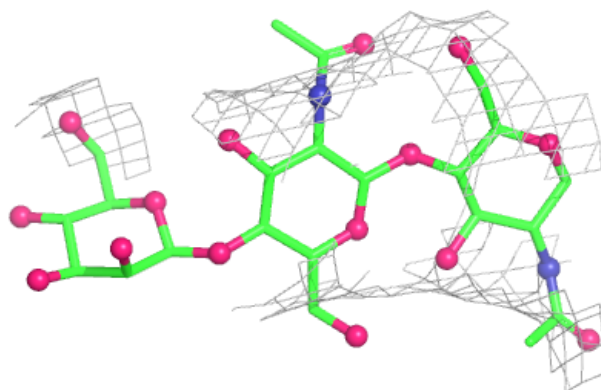
**Electron density around Chain P:**

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

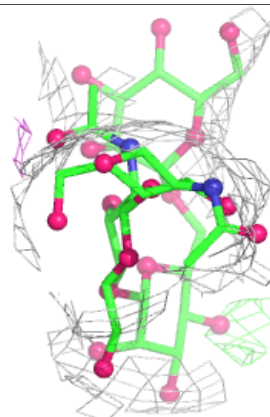
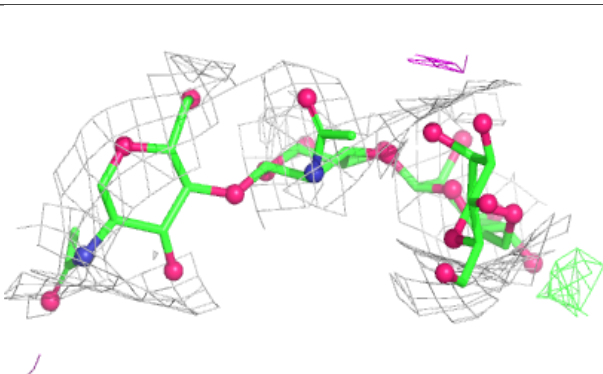
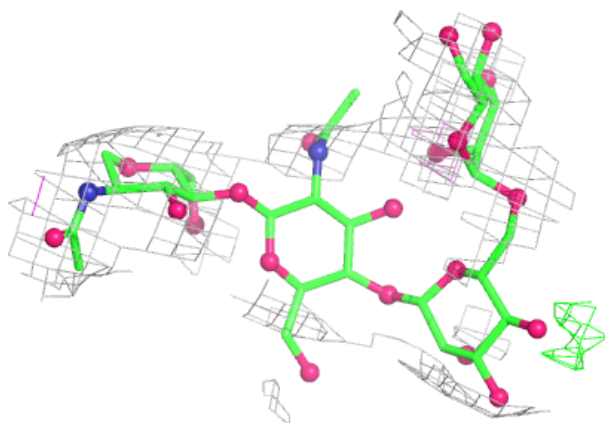


Electron density around Chain T:

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

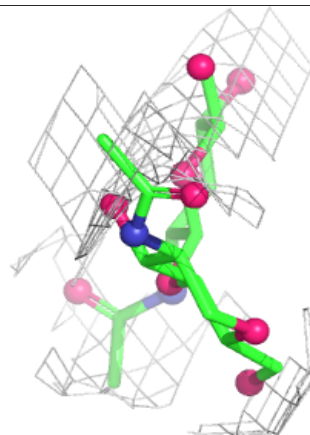
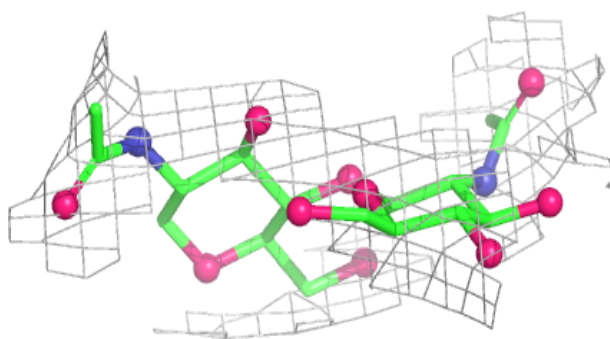
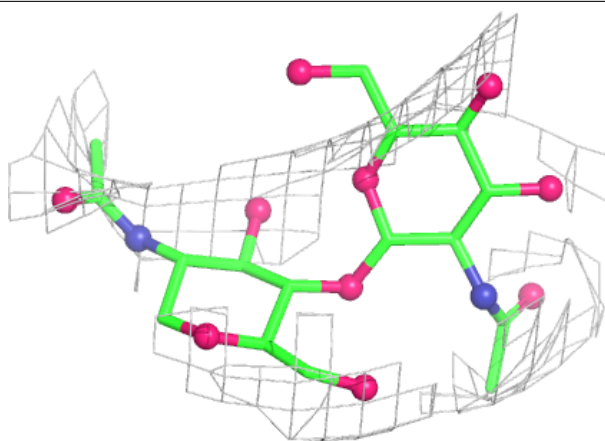
**Electron density around Chain F:**

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



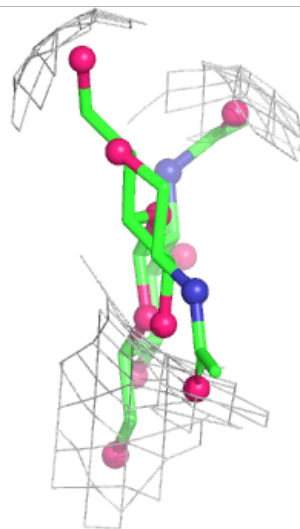
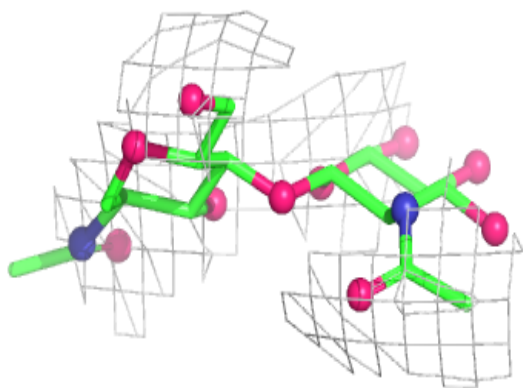
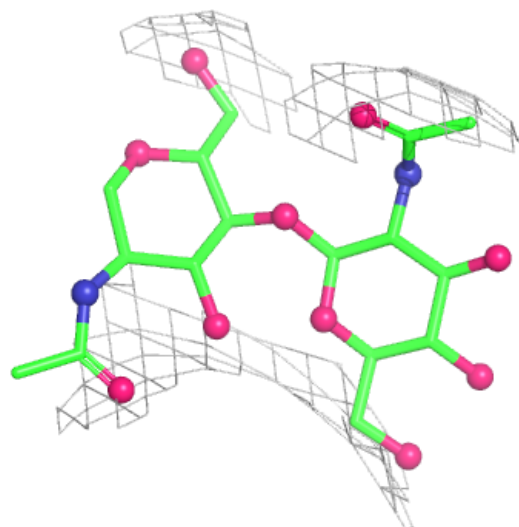
Electron density around Chain I:

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



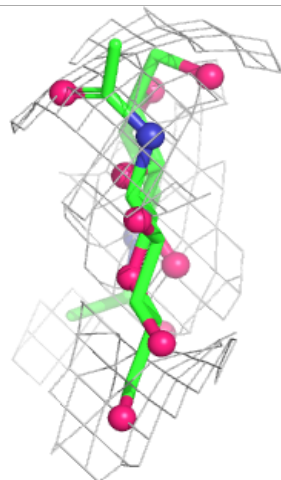
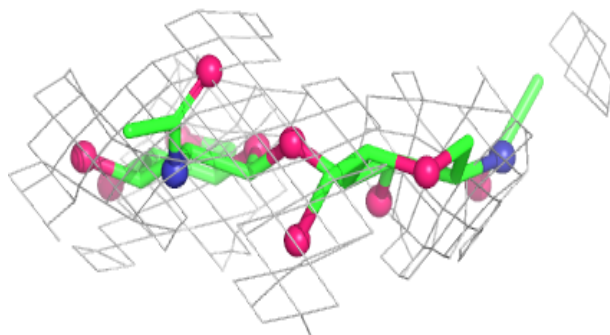
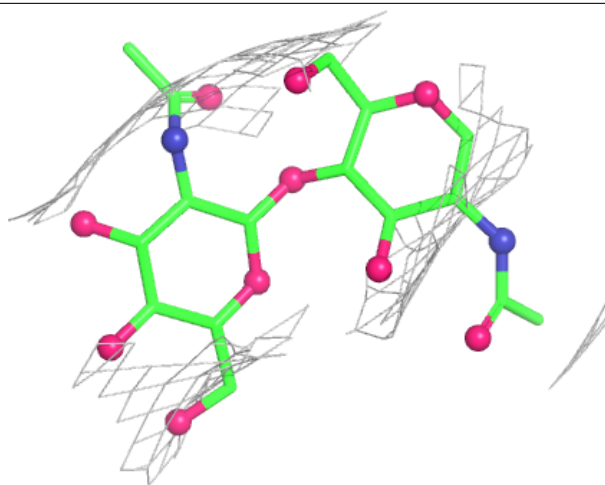
Electron density around Chain K:

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



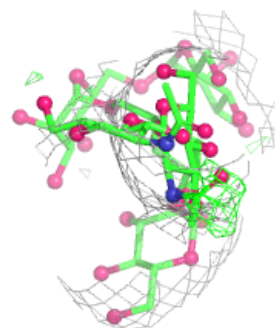
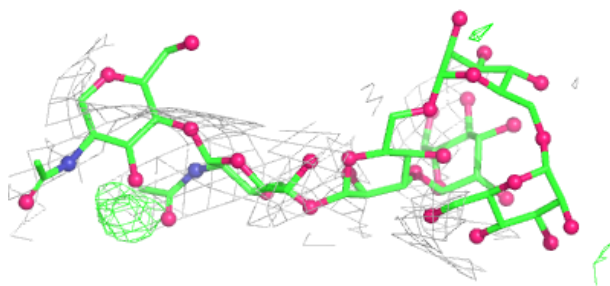
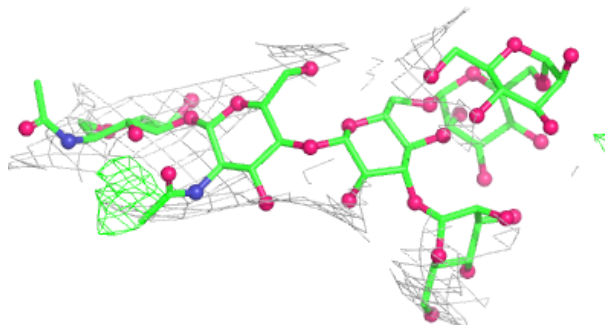
Electron density around Chain N:

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

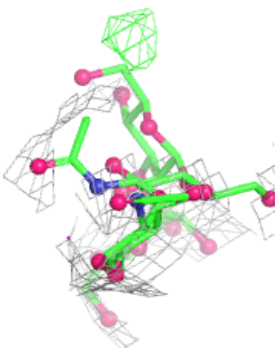
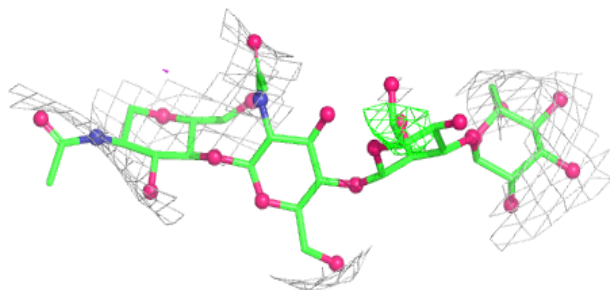
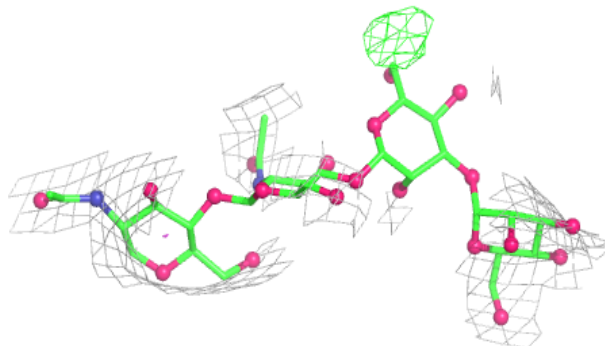


Electron density around Chain L:

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

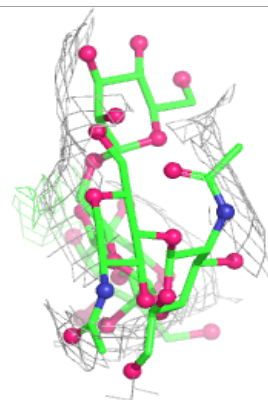
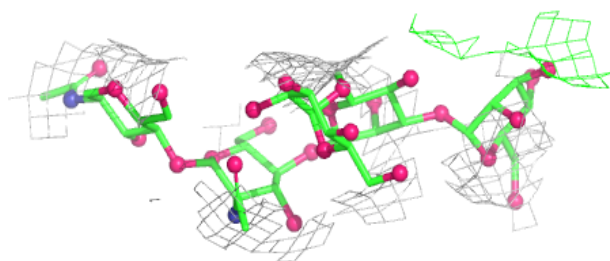
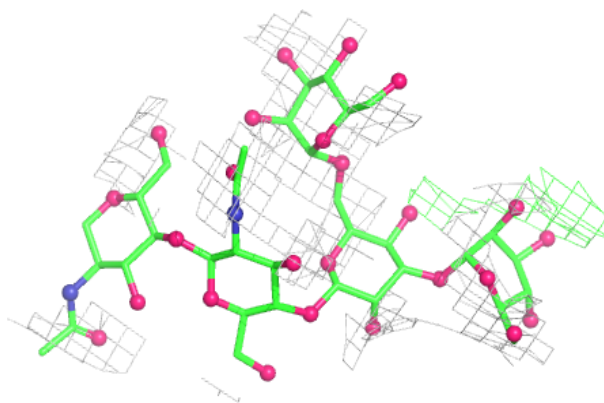
**Electron density around Chain M:**

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

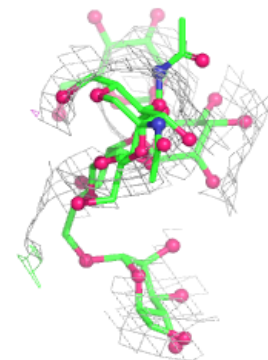
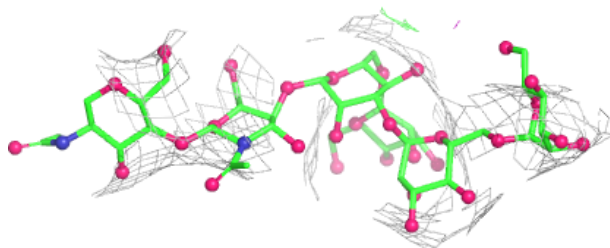
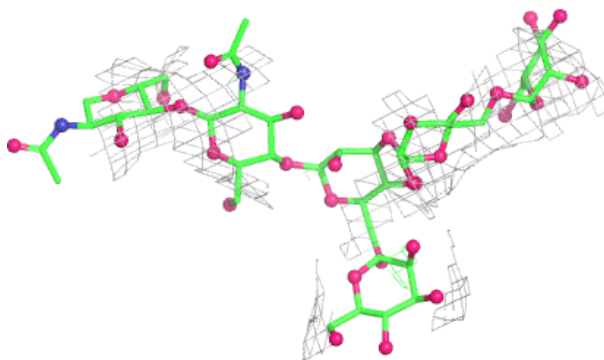


Electron density around Chain S:

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

**Electron density around Chain U:**

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



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
14	NAG	G	606	14/15	0.75	0.14	368,368,368,368	0
14	NAG	G	631	14/15	0.86	0.12	365,365,365,365	0
14	NAG	B	704	14/15	0.90	0.18	326,326,326,326	0
14	NAG	G	622	14/15	0.94	0.10	367,367,367,367	0

6.5 Other polymers [i](#)

There are no such residues in this entry.