



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:16 PM UTC

PDB ID : 6UTK / pdb_00006utk
Title : Crystal structure of 438-B11 Fab in complex with an uncleaved prefusion optimized (UFO) soluble BG505 trimer and Fab 35O22 at 3.80 Angstrom
Authors : Kumar, S.; Wilson, I.A.
Deposited on : 2019-10-29
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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

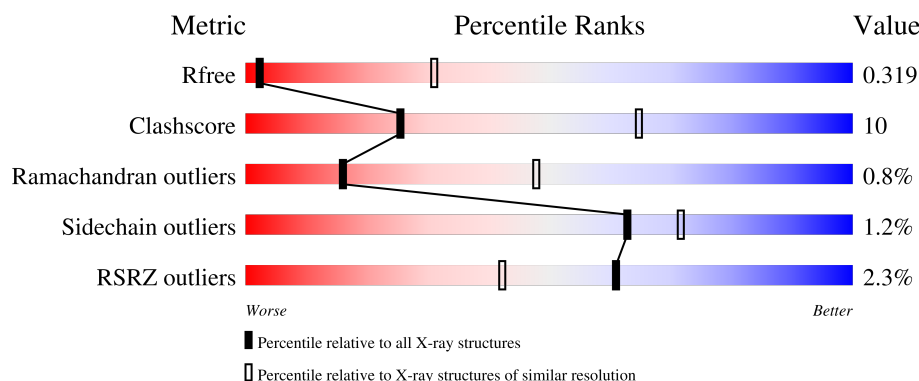
1 Overall quality at a glance

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.



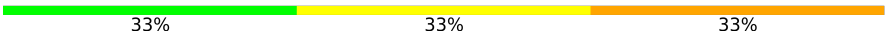
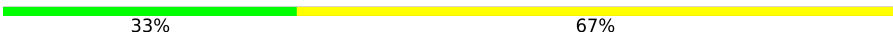
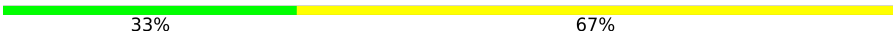
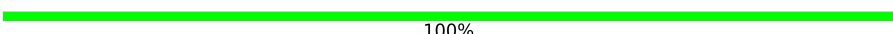
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	D	243	2% 79% 20% .
2	E	216	3% 75% 23% .
3	L	213	2% 84% 16%
4	G	485	2% 67% 26% 7%
5	T	140	5% 74% 22% .

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Mol	Chain	Length	Quality of chain
6	H	233	
7	A	3	
7	I	3	
7	P	3	
7	Q	3	
7	U	3	
8	B	10	
9	C	2	
9	F	2	
9	O	2	
10	J	4	
10	M	4	
11	K	11	
12	N	6	
13	R	7	
14	S	5	
15	V	2	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 12419 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 35O22 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	240	Total	C	N	O	S	0	0	0
			1813	1150	303	352	8			

- Molecule 2 is a protein called 35O22 Fab Light Chain.

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

- Molecule 3 is a protein called B11 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1634	1022	281	327	4			

- Molecule 4 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	453	Total	C	N	O	S	0	0	0
			3563	2234	630	671	28			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	62	ASP	GLU	conflict	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6
G	507	GLY	-	expression tag	UNP Q2N0S6
G	508	GLY	-	expression tag	UNP Q2N0S6
G	509	GLY	-	expression tag	UNP Q2N0S6
G	510	GLY	-	expression tag	UNP Q2N0S6
G	511	GLY	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	512	SER	-	expression tag	UNP Q2N0S6
G	513	GLY	-	expression tag	UNP Q2N0S6
G	514	GLY	-	expression tag	UNP Q2N0S6
G	515	GLY	-	expression tag	UNP Q2N0S6
G	516	GLY	-	expression tag	UNP Q2N0S6
G	517	SER	-	expression tag	UNP Q2N0S6

- Molecule 5 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	T	134	Total	C	N	O	S	0	0	0
			1069	677	182	203	7			

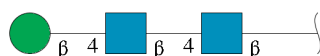
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	547A	ASN	-	linker	UNP Q2N0S9
T	547B	PRO	-	linker	UNP Q2N0S9
T	547C	ASP	-	linker	UNP Q2N0S9
T	547D	TRP	-	linker	UNP Q2N0S9
T	547E	LEU	-	linker	UNP Q2N0S9
T	547F	PRO	-	linker	UNP Q2N0S9
T	547G	ASP	-	linker	UNP Q2N0S9
T	547H	MET	-	linker	UNP Q2N0S9
T	605	CYS	THR	conflict	UNP Q2N0S9

- Molecule 6 is a protein called B11 Fab Heavy chain.

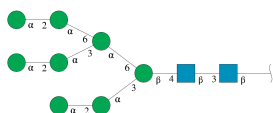
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	231	Total	C	N	O	S	0	0	0
			1747	1109	296	333	9			

- 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	I	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	Q	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	U	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



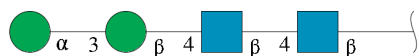
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	B	10	Total	C	N	O	0	0	0
			116	64	2	50			

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



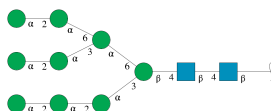
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 10 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.



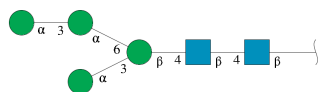
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	4	Total	C	N	O	0	0	0
			50	28	2	20			
10	M	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



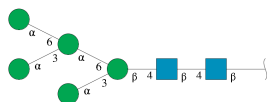
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	K	11	Total	C	N	O	0	0	0
			127	70	2	55			

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



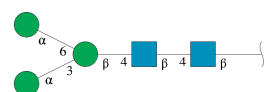
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	N	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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	R	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 14 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
14	S	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 15 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

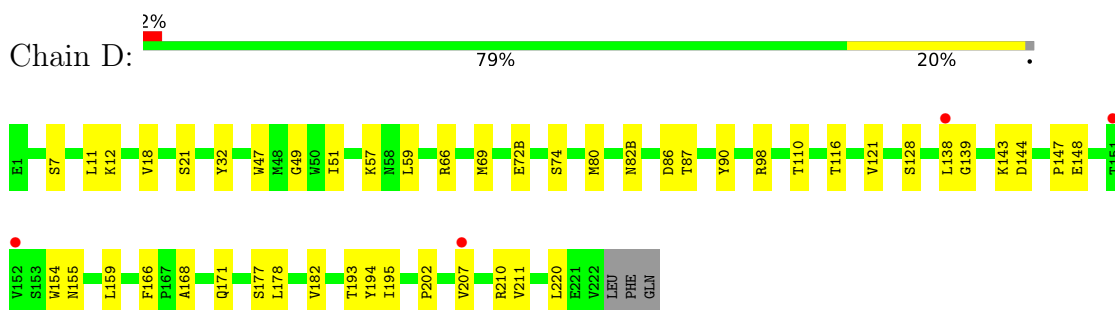


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	T	1	Total	C	N	O	0	0
			14	8	1	5		
16	T	1	Total	C	N	O	0	0
			14	8	1	5		
16	T	1	Total	C	N	O	0	0
			14	8	1	5		

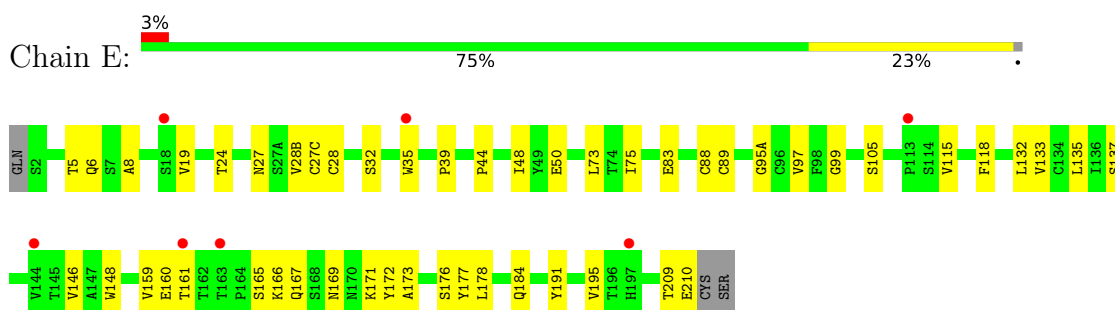
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

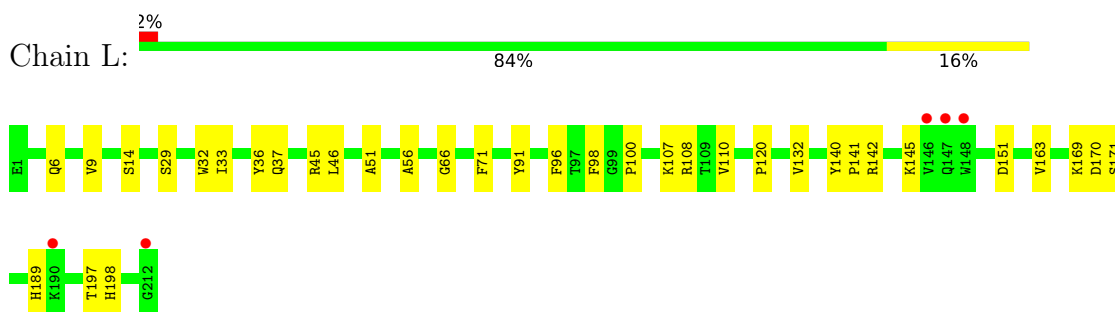
- Molecule 1: 35O22 Fab Heavy Chain



- Molecule 2: 35O22 Fab Light Chain

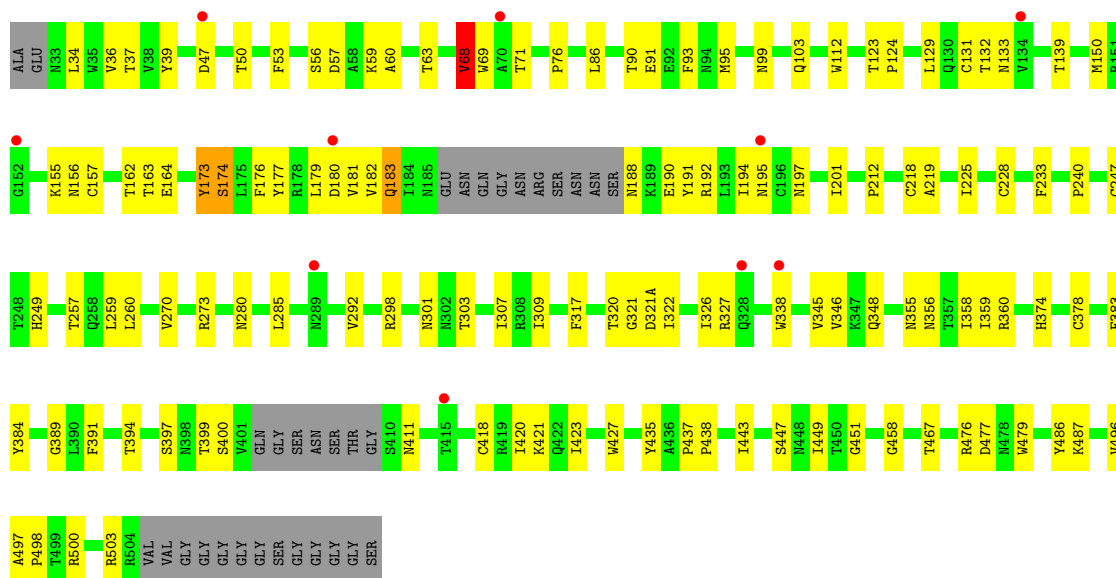


- Molecule 3: B11 Fab Light Chain

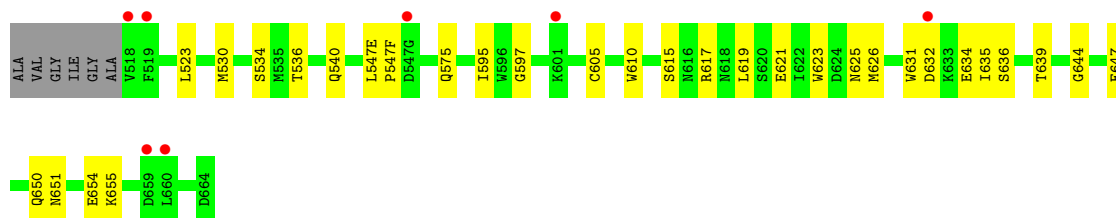
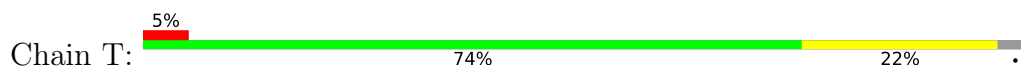


- Molecule 4: Envelope glycoprotein gp120

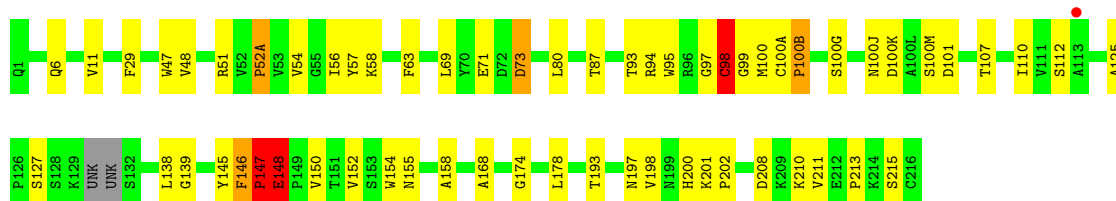




• Molecule 5: Envelope glycoprotein gp41



• Molecule 6: B11 Fab Heavy 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

Chain I:  67% 33%



- 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%



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

Chain Q:  33% 67%



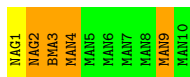
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  33% 67%



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

Chain B:  50% 10% 40%



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

Chain C:  50% 50%



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

Chain F:  50% 50%



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

Chain O: 100%



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

Chain J: 75% 25%



- Molecule 10: 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%



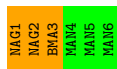
- Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 55% 27% 18%



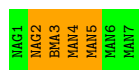
- Molecule 12: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 50% 50%



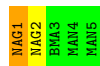
- Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  43% 57%



- Molecule 14: 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% 20% 20%



- Molecule 15: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	247.31Å 247.31Å 257.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.44 – 3.80 49.44 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.44-3.80) 99.5 (49.44-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.299 , 0.317 0.301 , 0.319	Depositor DCC
R_{free} test set	1491 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	131.8	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 89.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12419	wwPDB-VP
Average B, all atoms (Å ²)	166.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	D	0.11	0/1860	0.28	0/2533
2	E	0.08	0/1659	0.29	0/2269
3	L	0.10	0/1669	0.33	0/2267
4	G	0.10	0/3637	0.36	0/4939
5	T	0.10	0/1092	0.33	0/1486
6	H	0.17	0/1793	0.38	2/2442 (0.1%)
All	All	0.11	0/11710	0.33	2/15936 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	147	PRO	N-CA-C	5.20	123.18	112.47
6	H	147	PRO	CA-N-CD	-5.01	104.98	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1813	0	1784	34	0
2	E	1615	0	1544	32	0
3	L	1634	0	1587	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	3563	0	3494	88	0
5	T	1069	0	1033	26	0
6	H	1747	0	1720	40	0
7	A	39	0	34	1	0
7	I	39	0	34	0	0
7	P	39	0	34	1	0
7	Q	39	0	34	0	0
7	U	39	0	34	0	0
8	B	116	0	97	3	0
9	C	28	0	25	0	0
9	F	28	0	25	1	0
9	O	28	0	25	0	0
10	J	50	0	43	1	0
10	M	50	0	43	0	0
11	K	127	0	106	5	0
12	N	72	0	61	2	0
13	R	83	0	70	3	0
14	S	61	0	52	1	0
15	V	28	0	25	0	0
16	G	70	0	65	3	0
16	T	42	0	39	1	0
All	All	12419	0	12008	235	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 10.

All (235) 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)
6:H:98:CYS:SG	6:H:99:GLY:N	2.56	0.78
6:H:146:PHE:HB3	6:H:147:PRO:HD2	1.72	0.71
4:G:292:VAL:HB	4:G:449:ILE:HB	1.74	0.69
4:G:194:ILE:HG23	4:G:197:ASN:HD22	1.56	0.69
3:L:145:LYS:HB3	3:L:197:THR:HB	1.75	0.66
5:T:536:THR:O	5:T:540:GLN:NE2	2.28	0.66
4:G:50:THR:O	4:G:103:GLN:NE2	2.25	0.66
2:E:167:GLN:HG2	2:E:169:ASN:H	1.60	0.66
1:D:7:SER:HB3	1:D:21:SER:H	1.62	0.65
1:D:66:ARG:NH2	1:D:86:ASP:OD2	2.31	0.64
3:L:46:LEU:HD23	6:H:101:ASP:HB3	1.79	0.64
1:D:116:THR:HG23	1:D:147:PRO:HG3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:181:VAL:HG12	4:G:192:ARG:H	1.61	0.64
4:G:397:SER:HB3	16:G:605:NAG:H82	1.78	0.64
1:D:138:LEU:HB2	1:D:211:VAL:HG11	1.81	0.63
2:E:83:GLU:HG3	2:E:105:SER:HA	1.80	0.63
2:E:132:LEU:HD12	2:E:178:LEU:HD23	1.82	0.61
4:G:219:ALA:HB2	4:G:225:ILE:HG13	1.83	0.60
4:G:156:ASN:HA	4:G:176:PHE:HE1	1.66	0.60
1:D:66:ARG:NH2	1:D:82(B):ASN:O	2.35	0.60
1:D:148:GLU:HB2	1:D:202:PRO:HG2	1.84	0.60
1:D:128:SER:HB2	1:D:220:LEU:HB2	1.83	0.60
4:G:447:SER:OG	14:S:1:NAG:O7	2.20	0.59
1:D:143:LYS:NZ	1:D:144:ASP:OD2	2.36	0.58
6:H:56:ILE:HA	8:B:4:MAN:H62	1.84	0.58
5:T:595:ILE:O	5:T:651:ASN:ND2	2.28	0.58
6:H:193:THR:HG23	6:H:210:LYS:HE3	1.86	0.58
4:G:37:THR:HG22	5:T:605:CYS:HA	1.85	0.58
6:H:73:ASP:OD1	6:H:73:ASP:N	2.31	0.58
3:L:141:PRO:HG2	3:L:198:HIS:CE1	2.39	0.58
8:B:3:BMA:H2	8:B:9:MAN:H2	1.86	0.57
2:E:6:GLN:NE2	2:E:88:CYS:SG	2.77	0.57
1:D:11:LEU:HD22	1:D:147:PRO:HB3	1.87	0.57
4:G:179:LEU:HD13	4:G:421:LYS:HG3	1.88	0.56
1:D:12:LYS:HG3	1:D:18:VAL:HB	1.87	0.56
1:D:166:PHE:HE1	2:E:137:SER:HB3	1.70	0.56
3:L:108:ARG:HD2	3:L:171:SER:HB2	1.88	0.56
4:G:346:VAL:HG23	4:G:359:ILE:HD11	1.88	0.56
4:G:356:ASN:H	16:G:604:NAG:H82	1.70	0.56
6:H:200:HIS:CD2	6:H:202:PRO:HD2	2.40	0.56
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.87	0.55
4:G:173:TYR:CD2	10:J:1:NAG:H5	2.41	0.55
6:H:51:ARG:NH2	6:H:71:GLU:OE1	2.39	0.55
6:H:127:SER:HB2	6:H:215:SER:HA	1.89	0.55
4:G:201:ILE:HD11	4:G:435:TYR:HB2	1.89	0.55
1:D:155:ASN:HD21	1:D:194:TYR:HA	1.71	0.55
3:L:110:VAL:HG23	3:L:141:PRO:HG3	1.89	0.55
3:L:142:ARG:HH22	3:L:163:VAL:HG21	1.72	0.55
4:G:181:VAL:CG1	4:G:192:ARG:H	2.20	0.54
4:G:90:THR:HG22	4:G:240:PRO:HA	1.90	0.54
4:G:280:ASN:HD22	4:G:458:GLY:HA3	1.72	0.54
2:E:27:ASN:HA	2:E:27(C):CYS:HB2	1.90	0.54
3:L:96:PHE:HB2	6:H:47:TRP:CG	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:60:ALA:HB1	4:G:71:THR:HG23	1.89	0.54
4:G:181:VAL:HG23	4:G:194:ILE:HD11	1.90	0.54
6:H:94:ARG:NH1	6:H:95:TRP:O	2.41	0.54
6:H:51:ARG:NH2	6:H:52(A):PRO:O	2.41	0.54
3:L:37:GLN:OE1	3:L:45:ARG:NH2	2.40	0.53
13:R:4:MAN:H3	13:R:5:MAN:H3	1.90	0.53
2:E:5:THR:N	2:E:24:THR:O	2.38	0.53
4:G:389:GLY:HA2	12:N:1:NAG:H83	1.90	0.53
6:H:168:ALA:HA	6:H:178:LEU:HB3	1.90	0.53
3:L:29:SER:HB2	3:L:32:TRP:CD1	2.43	0.53
4:G:181:VAL:HG11	4:G:192:ARG:HG2	1.90	0.53
3:L:6:GLN:HG3	3:L:100:PRO:HD2	1.91	0.52
1:D:144:ASP:H	1:D:177:SER:HG	1.54	0.52
1:D:87:THR:HG23	1:D:110:THR:HA	1.91	0.52
4:G:112:TRP:HB3	4:G:427:TRP:HE1	1.73	0.52
4:G:156:ASN:HA	4:G:176:PHE:CE1	2.44	0.52
2:E:118:PHE:HB2	2:E:133:VAL:HB	1.91	0.52
13:R:3:BMA:H61	13:R:4:MAN:H3	1.92	0.52
4:G:129:LEU:O	4:G:191:TYR:N	2.42	0.52
4:G:218:CYS:HA	4:G:247:CYS:HA	1.90	0.52
5:T:617:ARG:HH12	16:T:701:NAG:H83	1.75	0.52
4:G:132:THR:OG1	4:G:188:ASN:OD1	2.28	0.51
4:G:195:ASN:HB2	4:G:423:ILE:HG21	1.93	0.51
4:G:358:ILE:HD11	4:G:394:THR:HB	1.91	0.51
1:D:166:PHE:CE1	2:E:137:SER:HB3	2.46	0.51
1:D:171:GLN:HA	2:E:160:GLU:HG3	1.91	0.51
1:D:210:ARG:NH1	1:D:211:VAL:O	2.44	0.50
4:G:133:ASN:OD1	4:G:155:LYS:NZ	2.41	0.50
4:G:270:VAL:HG11	4:G:345:VAL:HG22	1.93	0.50
4:G:259:LEU:HB2	4:G:374:HIS:CE1	2.46	0.50
6:H:125:ALA:HB1	6:H:213:PRO:HA	1.93	0.50
2:E:167:GLN:N	2:E:171:LYS:O	2.41	0.50
3:L:36:TYR:HE1	3:L:46:LEU:HD13	1.77	0.50
2:E:166:LYS:HA	2:E:172:TYR:HD1	1.77	0.50
8:B:1:NAG:O4	8:B:2:NAG:N2	2.44	0.50
4:G:34:LEU:HD12	4:G:498:PRO:HB2	1.93	0.49
2:E:133:VAL:HG13	2:E:177:TYR:HE1	1.77	0.49
4:G:260:LEU:HD12	4:G:451:GLY:HA3	1.94	0.49
5:T:632:ASP:O	5:T:636:SER:OG	2.27	0.49
4:G:181:VAL:HG13	4:G:183:GLN:N	2.28	0.49
6:H:97:GLY:O	6:H:99:GLY:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:635:ILE:HG22	5:T:639:THR:HB	1.93	0.49
4:G:503:ARG:HH12	5:T:597:GLY:HA3	1.77	0.49
4:G:496:VAL:O	5:T:631:TRP:NE1	2.41	0.48
1:D:51:ILE:HG13	1:D:57:LYS:HB3	1.96	0.48
4:G:322:ILE:HG21	4:G:326:ILE:HG22	1.95	0.48
6:H:155:ASN:HB2	6:H:158:ALA:HB3	1.95	0.48
5:T:651:ASN:HB3	5:T:655:LYS:HD3	1.96	0.48
1:D:121:VAL:HB	1:D:207:VAL:HG11	1.95	0.48
3:L:169:LYS:HG2	3:L:170:ASP:N	2.27	0.48
1:D:139:GLY:HA2	1:D:154:TRP:HH2	1.79	0.48
4:G:53:PHE:HB2	4:G:218:CYS:HB3	1.96	0.48
4:G:360:ARG:O	4:G:467:THR:HA	2.14	0.48
6:H:98:CYS:SG	6:H:100(A):CYS:N	2.81	0.47
2:E:89:CYS:SG	2:E:97:VAL:N	2.86	0.47
4:G:355:ASN:HB3	16:G:604:NAG:HN2	1.79	0.47
4:G:68:VAL:HG12	4:G:69:TRP:H	1.79	0.47
4:G:383:PHE:HB3	4:G:418:CYS:SG	2.54	0.47
4:G:384:TYR:CE2	4:G:421:LYS:HD3	2.50	0.47
5:T:617:ARG:NH1	5:T:626:MET:SD	2.88	0.47
2:E:165:SER:O	2:E:173:ALA:N	2.46	0.47
6:H:48:VAL:HA	6:H:63:PHE:HE2	1.79	0.47
4:G:384:TYR:HE2	4:G:421:LYS:HD3	1.80	0.47
6:H:112:SER:OG	6:H:174:GLY:O	2.26	0.47
6:H:152:VAL:HG22	6:H:198:VAL:HG22	1.97	0.47
6:H:51:ARG:HG3	6:H:57:TYR:HB3	1.97	0.47
4:G:249:HIS:ND1	4:G:486:TYR:OH	2.35	0.46
1:D:193:THR:HG23	1:D:210:ARG:NE	2.30	0.46
2:E:115:VAL:HA	2:E:135:LEU:O	2.15	0.46
3:L:66:GLY:HA3	3:L:71:PHE:HA	1.96	0.46
4:G:47:ASP:N	4:G:47:ASP:OD1	2.48	0.46
4:G:163:THR:OG1	4:G:164:GLU:N	2.47	0.46
4:G:270:VAL:HB	4:G:348:GLN:HG3	1.95	0.46
2:E:35:TRP:HB2	2:E:48:ILE:HB	1.97	0.46
2:E:148:TRP:HD1	2:E:159:VAL:HG13	1.79	0.46
4:G:476:ARG:HA	4:G:479:TRP:HD1	1.80	0.46
4:G:307:ILE:HD11	4:G:317:PHE:HD2	1.81	0.46
4:G:338:TRP:HZ2	4:G:391:PHE:HE1	1.64	0.46
5:T:617:ARG:NH2	5:T:634:GLU:OE2	2.49	0.46
2:E:32:SER:HB3	2:E:50:GLU:HA	1.98	0.46
4:G:257:THR:C	4:G:259:LEU:H	2.24	0.46
6:H:69:LEU:HD23	6:H:80:LEU:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:ALA:HA	1:D:178:LEU:HB3	1.98	0.45
12:N:2:NAG:H4	12:N:3:BMA:H2	1.76	0.45
4:G:93:PHE:HB2	4:G:233:PHE:HZ	1.80	0.45
6:H:139:GLY:HA2	6:H:154:TRP:CH2	2.51	0.45
4:G:56:SER:HB3	4:G:76:PRO:HA	1.98	0.45
6:H:54:VAL:HG21	6:H:100(G):SER:OG	2.16	0.45
1:D:194:TYR:O	1:D:210:ARG:NH1	2.49	0.45
3:L:107:LYS:HA	3:L:140:TYR:OH	2.15	0.45
3:L:108:ARG:NE	3:L:170:ASP:O	2.50	0.45
4:G:194:ILE:O	4:G:197:ASN:HB3	2.17	0.45
6:H:11:VAL:HG22	6:H:110:ILE:HB	1.99	0.45
9:F:1:NAG:H4	9:F:2:NAG:H2	1.62	0.45
2:E:146:VAL:HG22	2:E:195:VAL:HG22	1.99	0.45
4:G:298:ARG:HB3	4:G:443:ILE:HB	1.98	0.45
5:T:644:GLY:HA2	5:T:647:GLU:HG2	1.98	0.45
6:H:93:THR:HB	6:H:100(M):SER:HB3	1.99	0.45
2:E:209:THR:HG23	2:E:210:GLU:HG3	1.99	0.44
4:G:139:THR:O	4:G:150:MET:HG2	2.17	0.44
4:G:174:SER:HB3	4:G:320:THR:O	2.17	0.44
6:H:148:GLU:C	6:H:150:VAL:H	2.25	0.44
2:E:35:TRP:CE2	2:E:73:LEU:HB2	2.52	0.44
2:E:19:VAL:HG12	2:E:75:ILE:HB	1.99	0.44
5:T:651:ASN:O	5:T:655:LYS:HD3	2.17	0.44
5:T:650:GLN:O	5:T:654:GLU:N	2.27	0.44
1:D:49:GLY:HA3	1:D:59:LEU:HD23	1.99	0.44
2:E:148:TRP:HB3	2:E:178:LEU:HD22	1.98	0.44
11:K:7:MAN:H4	11:K:10:MAN:H3	2.00	0.44
1:D:159:LEU:HD21	1:D:182:VAL:HG21	1.99	0.44
4:G:69:TRP:CD1	4:G:212:PRO:HA	2.53	0.44
4:G:177:TYR:CE1	4:G:420:ILE:HB	2.53	0.44
4:G:399:THR:OG1	4:G:400:SER:N	2.51	0.44
4:G:303:THR:HG23	4:G:321:GLY:HA3	1.99	0.44
4:G:93:PHE:CE2	4:G:228:CYS:HB2	2.53	0.43
3:L:14:SER:OG	3:L:107:LYS:HB3	2.18	0.43
4:G:181:VAL:HG13	4:G:183:GLN:H	1.81	0.43
1:D:69:MET:HG2	1:D:80:MET:HG3	2.00	0.43
4:G:36:VAL:HG12	5:T:610:TRP:HE3	1.83	0.43
4:G:285:LEU:HD21	4:G:477:ASP:HB3	2.01	0.43
4:G:321(A):ASP:OD1	4:G:321(A):ASP:N	2.50	0.43
6:H:58:LYS:HD2	6:H:58:LYS:HA	1.67	0.43
7:P:1:NAG:H61	7:P:2:NAG:N2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:139:GLY:HA2	6:H:154:TRP:HH2	1.83	0.43
4:G:34:LEU:HG	5:T:610:TRP:HB3	1.99	0.43
4:G:195:ASN:OD1	4:G:201:ILE:HB	2.18	0.43
7:A:1:NAG:H61	7:A:2:NAG:N2	2.33	0.43
2:E:161:THR:HG23	2:E:176:SER:HB2	1.99	0.43
4:G:60:ALA:O	4:G:63:THR:OG1	2.33	0.43
3:L:33:ILE:HB	3:L:51:ALA:HB2	2.00	0.43
4:G:179:LEU:HD13	4:G:421:LYS:HE3	2.00	0.43
4:G:183:GLN:HB3	4:G:190:GLU:O	2.19	0.43
2:E:184:GLN:O	2:E:191:TYR:OH	2.36	0.43
4:G:131:CYS:HA	4:G:157:CYS:HA	2.01	0.43
5:T:619:LEU:C	5:T:621:GLU:H	2.27	0.43
4:G:162:THR:HG23	4:G:309:ILE:HG23	2.00	0.42
6:H:100:MET:O	6:H:100(B):PRO:HD3	2.19	0.42
6:H:145:TYR:HE2	6:H:148:GLU:HA	1.83	0.42
5:T:547(E):LEU:N	5:T:547(F):PRO:HD2	2.34	0.42
2:E:39:PRO:HD2	2:E:44:PRO:HA	2.02	0.42
3:L:36:TYR:HE2	3:L:98:PHE:HE1	1.68	0.42
3:L:56:ALA:HB2	11:K:11:MAN:H4	2.01	0.42
6:H:87:THR:HG23	6:H:110:ILE:HA	2.00	0.42
1:D:32:TYR:OH	5:T:625:ASN:ND2	2.51	0.42
1:D:86:ASP:O	1:D:90:TYR:OH	2.37	0.42
4:G:123:THR:N	4:G:124:PRO:HD2	2.35	0.42
6:H:6:GLN:NE2	6:H:107:THR:OG1	2.52	0.42
3:L:151:ASP:OD2	3:L:189:HIS:ND1	2.44	0.42
4:G:93:PHE:HE2	4:G:228:CYS:HB2	1.85	0.42
6:H:29:PHE:O	6:H:52(A):PRO:HG2	2.19	0.42
3:L:91:TYR:OH	11:K:6:MAN:O3	2.32	0.42
6:H:100(K):ASP:OD2	11:K:5:MAN:O6	2.36	0.42
1:D:47:TRP:CH2	2:E:95(A):GLY:HA3	2.55	0.41
6:H:197:ASN:ND2	6:H:208:ASP:OD1	2.47	0.41
1:D:155:ASN:OD1	1:D:195:ILE:N	2.49	0.41
4:G:131:CYS:SG	4:G:191:TYR:HB2	2.60	0.41
4:G:179:LEU:O	4:G:179:LEU:HG	2.20	0.41
5:T:610:TRP:HZ2	5:T:615:SER:HB2	1.85	0.41
4:G:53:PHE:CE1	5:T:575:GLN:HB2	2.55	0.41
2:E:6:GLN:HE21	2:E:99:GLY:HA3	1.85	0.41
2:E:6:GLN:HE22	2:E:88:CYS:H	1.68	0.41
6:H:138:LEU:HB2	6:H:211:VAL:HG11	2.02	0.41
5:T:530:MET:O	5:T:534:SER:OG	2.32	0.41
1:D:177:SER:HB2	2:E:177:TYR:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:91:GLU:OE2	4:G:487:LYS:NZ	2.49	0.41
6:H:146:PHE:CB	6:H:147:PRO:HD2	2.47	0.41
1:D:51:ILE:HA	1:D:57:LYS:HA	2.03	0.41
1:D:72(B):GLU:HB2	1:D:74:SER:HB2	2.02	0.41
4:G:37:THR:OG1	4:G:497:ALA:O	2.34	0.41
4:G:39:TYR:CZ	5:T:623:TRP:HH2	2.38	0.41
4:G:86:LEU:HD22	5:T:523:LEU:O	2.21	0.41
4:G:95:MET:SD	4:G:273:ARG:HD3	2.60	0.41
4:G:194:ILE:HD13	4:G:194:ILE:HA	1.89	0.41
4:G:59:LYS:O	4:G:63:THR:HG23	2.21	0.41
6:H:201:LYS:HB3	6:H:202:PRO:HD3	2.01	0.41
5:T:635:ILE:O	5:T:639:THR:N	2.54	0.40
6:H:100(J):ASN:O	11:K:5:MAN:H61	2.21	0.40
1:D:98:ARG:O	13:R:2:NAG:H5	2.20	0.40
5:T:615:SER:O	5:T:617:ARG:N	2.54	0.40
2:E:35:TRP:CZ3	2:E:88:CYS:HB3	2.56	0.40
4:G:259:LEU:HD12	4:G:374:HIS:CD2	2.57	0.40
4:G:437:PRO:HA	4:G:438:PRO:HD3	1.95	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	D	238/243 (98%)	223 (94%)	15 (6%)	0	100	100
2	E	211/216 (98%)	191 (90%)	19 (9%)	1 (0%)	24	57
3	L	211/213 (99%)	189 (90%)	21 (10%)	1 (0%)	24	57
4	G	447/485 (92%)	402 (90%)	40 (9%)	5 (1%)	11	41
5	T	132/140 (94%)	114 (86%)	18 (14%)	0	100	100
6	H	227/233 (97%)	205 (90%)	17 (8%)	5 (2%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1466/1530 (96%)	1324 (90%)	130 (9%)	12 (1%)	16	48

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	183	GLN
6	H	147	PRO
4	G	301	ASN
6	H	98	CYS
4	G	174	SER
4	G	411	ASN
6	H	100(B)	PRO
6	H	148	GLU
2	E	8	ALA
3	L	9	VAL
6	H	52(A)	PRO
4	G	68	VAL

5.3.2 Protein sidechains [i](#)

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	D	203/206 (98%)	203 (100%)	0	100	100
2	E	186/189 (98%)	184 (99%)	2 (1%)	65	73
3	L	183/183 (100%)	183 (100%)	0	100	100
4	G	405/424 (96%)	396 (98%)	9 (2%)	45	63
5	T	116/118 (98%)	116 (100%)	0	100	100
6	H	197/197 (100%)	192 (98%)	5 (2%)	42	61
All	All	1290/1317 (98%)	1274 (99%)	16 (1%)	63	72

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	28(B)	VAL
2	E	28	CYS
4	G	57	ASP
4	G	68	VAL
4	G	99	ASN
4	G	173	TYR
4	G	180	ASP
4	G	182	VAL
4	G	327	ARG
4	G	378	CYS
4	G	500	ARG
6	H	73	ASP
6	H	98	CYS
6	H	146	PHE
6	H	147	PRO
6	H	148	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	164	HIS
1	D	171	GLN
2	E	6	GLN
3	L	198	HIS
4	G	293	GLN
4	G	300	ASN
4	G	432	GLN
6	H	1	GLN
6	H	39	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

70 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	A	1	7,3	14,14,15	0.29	0	17,19,21	0.62	0
7	NAG	A	2	7	14,14,15	0.30	0	17,19,21	0.65	0
7	BMA	A	3	7	11,11,12	0.57	0	15,15,17	0.70	0
8	NAG	B	1	4,8	14,14,15	0.45	0	17,19,21	1.02	0
8	MAN	B	10	8	11,11,12	0.27	0	15,15,17	0.73	0
8	NAG	B	2	8	14,14,15	0.44	0	17,19,21	2.18	3 (17%)
8	BMA	B	3	8	11,11,12	1.14	0	15,15,17	1.02	1 (6%)
8	MAN	B	4	8	11,11,12	0.63	0	15,15,17	1.47	2 (13%)
8	MAN	B	5	8	11,11,12	0.36	0	15,15,17	0.79	0
8	MAN	B	6	8	11,11,12	0.26	0	15,15,17	0.68	0
8	MAN	B	7	8	11,11,12	0.43	0	15,15,17	0.88	0
8	MAN	B	8	8	11,11,12	0.29	0	15,15,17	0.62	0
8	MAN	B	9	8	11,11,12	1.00	1 (9%)	15,15,17	1.64	3 (20%)
9	NAG	C	1	4,9	14,14,15	0.46	0	17,19,21	1.28	4 (23%)
9	NAG	C	2	9	14,14,15	0.29	0	17,19,21	0.65	0
9	NAG	F	1	4,9	14,14,15	0.27	0	17,19,21	1.09	1 (5%)
9	NAG	F	2	9	14,14,15	0.44	0	17,19,21	0.69	0
7	NAG	I	1	4,7	14,14,15	0.29	0	17,19,21	0.80	0
7	NAG	I	2	7	14,14,15	0.27	0	17,19,21	0.85	1 (5%)
7	BMA	I	3	7	11,11,12	0.61	0	15,15,17	0.69	0
10	NAG	J	1	4,10	14,14,15	0.35	0	17,19,21	0.60	0
10	NAG	J	2	10	14,14,15	0.32	0	17,19,21	0.68	0
10	BMA	J	3	10	11,11,12	0.66	0	15,15,17	0.64	0
10	MAN	J	4	10	11,11,12	0.27	0	15,15,17	0.62	0
11	NAG	K	1	4,11	14,14,15	0.26	0	17,19,21	0.62	0
11	MAN	K	10	11	11,11,12	0.29	0	15,15,17	0.97	1 (6%)
11	MAN	K	11	11	11,11,12	0.28	0	15,15,17	0.80	1 (6%)
11	NAG	K	2	11	14,14,15	0.33	0	17,19,21	0.81	0
11	BMA	K	3	11	11,11,12	0.53	0	15,15,17	0.84	0
11	MAN	K	4	11	11,11,12	0.25	0	15,15,17	0.79	0
11	MAN	K	5	11	11,11,12	0.35	0	15,15,17	0.95	0
11	MAN	K	6	11	11,11,12	0.22	0	15,15,17	0.56	0
11	MAN	K	7	11	11,11,12	0.26	0	15,15,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MAN	K	8	11	11,11,12	0.34	0	15,15,17	0.98	0
11	MAN	K	9	11	11,11,12	0.32	0	15,15,17	0.73	0
10	NAG	M	1	4,10	14,14,15	0.28	0	17,19,21	0.85	0
10	NAG	M	2	10	14,14,15	0.31	0	17,19,21	0.91	1 (5%)
10	BMA	M	3	10	11,11,12	0.68	0	15,15,17	0.70	0
10	MAN	M	4	10	11,11,12	0.26	0	15,15,17	0.63	0
12	NAG	N	1	4,12	14,14,15	0.34	0	17,19,21	1.47	3 (17%)
12	NAG	N	2	12	14,14,15	0.31	0	17,19,21	0.90	1 (5%)
12	BMA	N	3	12	11,11,12	0.85	0	15,15,17	0.85	1 (6%)
12	MAN	N	4	12	11,11,12	0.58	0	15,15,17	0.94	0
12	MAN	N	5	12	11,11,12	0.30	0	15,15,17	0.67	0
12	MAN	N	6	12	11,11,12	0.31	0	15,15,17	0.72	0
9	NAG	O	1	4,9	14,14,15	0.30	0	17,19,21	0.62	0
9	NAG	O	2	9	14,14,15	0.29	0	17,19,21	0.70	0
7	NAG	P	1	4,7	14,14,15	0.29	0	17,19,21	0.93	1 (5%)
7	NAG	P	2	7	14,14,15	0.31	0	17,19,21	0.68	0
7	BMA	P	3	7	11,11,12	0.61	0	15,15,17	0.80	0
7	NAG	Q	1	4,7	14,14,15	0.32	0	17,19,21	0.88	1 (5%)
7	NAG	Q	2	7	14,14,15	0.34	0	17,19,21	0.89	1 (5%)
7	BMA	Q	3	7	11,11,12	0.60	0	15,15,17	0.79	0
13	NAG	R	1	4,13	14,14,15	0.30	0	17,19,21	0.59	0
13	NAG	R	2	13	14,14,15	0.36	0	17,19,21	2.02	3 (17%)
13	BMA	R	3	13	11,11,12	0.93	0	15,15,17	1.18	1 (6%)
13	MAN	R	4	13	11,11,12	0.66	0	15,15,17	1.78	4 (26%)
13	MAN	R	5	13	11,11,12	0.63	0	15,15,17	1.33	2 (13%)
13	MAN	R	6	13	11,11,12	0.35	0	15,15,17	0.78	0
13	MAN	R	7	13	11,11,12	0.26	0	15,15,17	0.65	0
14	NAG	S	1	4,14	14,14,15	0.31	0	17,19,21	1.10	2 (11%)
14	NAG	S	2	14	14,14,15	0.40	0	17,19,21	2.13	4 (23%)
14	BMA	S	3	14	11,11,12	0.61	0	15,15,17	0.76	0
14	MAN	S	4	14	11,11,12	0.24	0	15,15,17	0.65	0
14	MAN	S	5	14	11,11,12	0.25	0	15,15,17	0.67	0
7	NAG	U	1	7	14,14,15	0.27	0	17,19,21	0.62	0
7	NAG	U	2	7	14,14,15	0.33	0	17,19,21	1.26	3 (17%)
7	BMA	U	3	7	11,11,12	1.05	1 (9%)	15,15,17	1.10	2 (13%)
15	NAG	V	1	5,15	14,14,15	0.32	0	17,19,21	0.70	0
15	NAG	V	2	15	14,14,15	0.28	0	17,19,21	0.53	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	7,3	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	0/6/23/26	0/1/1/1
7	BMA	A	3	7	-	0/2/19/22	0/1/1/1
8	NAG	B	1	4,8	-	1/6/23/26	0/1/1/1
8	MAN	B	10	8	-	1/2/19/22	0/1/1/1
8	NAG	B	2	8	-	5/6/23/26	0/1/1/1
8	BMA	B	3	8	-	2/2/19/22	0/1/1/1
8	MAN	B	4	8	-	2/2/19/22	0/1/1/1
8	MAN	B	5	8	-	0/2/19/22	0/1/1/1
8	MAN	B	6	8	-	0/2/19/22	0/1/1/1
8	MAN	B	7	8	-	1/2/19/22	0/1/1/1
8	MAN	B	8	8	-	1/2/19/22	0/1/1/1
8	MAN	B	9	8	-	0/2/19/22	0/1/1/1
9	NAG	C	1	4,9	-	2/6/23/26	0/1/1/1
9	NAG	C	2	9	-	2/6/23/26	0/1/1/1
9	NAG	F	1	4,9	-	3/6/23/26	0/1/1/1
9	NAG	F	2	9	-	0/6/23/26	0/1/1/1
7	NAG	I	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	I	2	7	-	4/6/23/26	0/1/1/1
7	BMA	I	3	7	-	1/2/19/22	0/1/1/1
10	NAG	J	1	4,10	-	0/6/23/26	0/1/1/1
10	NAG	J	2	10	-	1/6/23/26	0/1/1/1
10	BMA	J	3	10	-	0/2/19/22	0/1/1/1
10	MAN	J	4	10	-	2/2/19/22	0/1/1/1
11	NAG	K	1	4,11	-	2/6/23/26	0/1/1/1
11	MAN	K	10	11	-	0/2/19/22	0/1/1/1
11	MAN	K	11	11	-	1/2/19/22	0/1/1/1
11	NAG	K	2	11	-	2/6/23/26	0/1/1/1
11	BMA	K	3	11	-	2/2/19/22	0/1/1/1
11	MAN	K	4	11	-	0/2/19/22	0/1/1/1
11	MAN	K	5	11	-	2/2/19/22	0/1/1/1
11	MAN	K	6	11	-	0/2/19/22	0/1/1/1
11	MAN	K	7	11	-	2/2/19/22	0/1/1/1
11	MAN	K	8	11	-	1/2/19/22	0/1/1/1
11	MAN	K	9	11	-	2/2/19/22	0/1/1/1
10	NAG	M	1	4,10	-	2/6/23/26	0/1/1/1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	3	BMA	C1-C2	2.48	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	9	MAN	C1-C2	2.17	1.57	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	2	NAG	C2-N2-C7	7.19	132.53	122.90
14	S	2	NAG	C2-N2-C7	6.54	131.67	122.90
13	R	2	NAG	C2-N2-C7	6.38	131.45	122.90
12	N	1	NAG	O4-C4-C3	-4.07	100.78	110.38
8	B	9	MAN	C1-C2-C3	3.79	115.16	109.64
13	R	4	MAN	C6-C5-C4	-3.77	103.75	113.02
13	R	5	MAN	C1-C2-C3	3.75	115.11	109.64
8	B	2	NAG	C8-C7-N2	3.59	122.06	116.12
8	B	4	MAN	O3-C3-C2	3.48	117.15	110.05
13	R	4	MAN	C1-C2-C3	3.25	114.38	109.64
13	R	2	NAG	C1-C2-N2	3.20	115.48	110.43
14	S	2	NAG	C1-C2-N2	3.13	115.36	110.43
14	S	2	NAG	C8-C7-N2	3.09	121.24	116.12
13	R	4	MAN	O3-C3-C4	-2.88	103.58	110.38
13	R	2	NAG	C8-C7-N2	2.73	120.65	116.12
7	U	2	NAG	O5-C1-C2	-2.65	107.19	111.29
13	R	3	BMA	C6-C5-C4	2.61	119.43	113.02
7	U	2	NAG	O4-C4-C3	-2.58	104.30	110.38
9	C	1	NAG	O4-C4-C5	-2.47	103.24	109.32
8	B	9	MAN	O2-C2-C3	2.45	115.23	110.15
8	B	9	MAN	O2-C2-C1	2.44	114.82	109.22
8	B	4	MAN	O5-C1-C2	-2.38	105.11	110.79
7	U	3	BMA	O2-C2-C3	-2.35	105.28	110.15
14	S	1	NAG	O5-C1-C2	-2.35	107.65	111.29
14	S	1	NAG	C2-N2-C7	2.33	126.03	122.90
8	B	3	BMA	O3-C3-C2	2.33	114.80	110.05
12	N	1	NAG	C1-O5-C5	-2.29	109.12	112.19
7	U	3	BMA	C1-C2-C3	-2.24	106.38	109.64
13	R	4	MAN	O5-C1-C2	-2.17	105.61	110.79
8	B	2	NAG	C1-C2-N2	2.16	113.84	110.43
7	Q	1	NAG	C1-O5-C5	2.15	115.07	112.19
12	N	2	NAG	O5-C1-C2	-2.14	107.99	111.29
14	S	2	NAG	O5-C1-C2	-2.13	108.00	111.29
11	K	10	MAN	O2-C2-C1	2.12	114.08	109.22
11	K	11	MAN	C1-O5-C5	-2.12	109.34	112.19
12	N	1	NAG	O4-C4-C5	-2.10	104.14	109.32
10	M	2	NAG	O5-C1-C2	-2.10	108.05	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	2	NAG	C2-N2-C7	2.08	125.69	122.90
9	F	1	NAG	C2-N2-C7	2.08	125.69	122.90
12	N	3	BMA	O2-C2-C3	-2.08	105.85	110.15
7	P	1	NAG	C2-N2-C7	2.08	125.68	122.90
7	I	2	NAG	C2-N2-C7	2.07	125.67	122.90
9	C	1	NAG	O4-C4-C3	-2.06	105.51	110.38
7	Q	2	NAG	C2-N2-C7	2.06	125.66	122.90
13	R	5	MAN	O5-C1-C2	-2.05	105.90	110.79
9	C	1	NAG	C1-C2-N2	2.03	113.63	110.43
9	C	1	NAG	C2-N2-C7	2.01	125.60	122.90

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	M	2	NAG	C1-C2-N2-C7
13	R	2	NAG	C1-C2-N2-C7
13	R	2	NAG	C8-C7-N2-C2
13	R	2	NAG	O7-C7-N2-C2
14	S	2	NAG	C1-C2-N2-C7
14	S	2	NAG	C8-C7-N2-C2
14	S	2	NAG	O7-C7-N2-C2
12	N	6	MAN	O5-C5-C6-O6
14	S	1	NAG	O5-C5-C6-O6
13	R	3	BMA	C4-C5-C6-O6
11	K	7	MAN	C4-C5-C6-O6
10	M	4	MAN	O5-C5-C6-O6
8	B	3	BMA	C4-C5-C6-O6
7	I	2	NAG	O5-C5-C6-O6
7	P	1	NAG	O5-C5-C6-O6
10	J	4	MAN	O5-C5-C6-O6
8	B	4	MAN	O5-C5-C6-O6
12	N	6	MAN	C4-C5-C6-O6
14	S	1	NAG	C4-C5-C6-O6
11	K	1	NAG	C8-C7-N2-C2
11	K	1	NAG	O7-C7-N2-C2
13	R	3	BMA	O5-C5-C6-O6
9	C	2	NAG	O5-C5-C6-O6
8	B	4	MAN	C4-C5-C6-O6
7	I	2	NAG	C4-C5-C6-O6
9	C	2	NAG	C4-C5-C6-O6
7	P	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	B	3	BMA	O5-C5-C6-O6
11	K	7	MAN	O5-C5-C6-O6
11	K	5	MAN	O5-C5-C6-O6
11	K	9	MAN	O5-C5-C6-O6
7	I	1	NAG	C8-C7-N2-C2
7	I	1	NAG	O7-C7-N2-C2
8	B	2	NAG	C8-C7-N2-C2
8	B	2	NAG	O7-C7-N2-C2
10	M	2	NAG	C8-C7-N2-C2
7	U	2	NAG	O5-C5-C6-O6
8	B	8	MAN	O5-C5-C6-O6
7	U	2	NAG	C4-C5-C6-O6
10	M	4	MAN	C4-C5-C6-O6
12	N	1	NAG	C4-C5-C6-O6
12	N	1	NAG	O5-C5-C6-O6
10	M	2	NAG	O7-C7-N2-C2
11	K	2	NAG	C8-C7-N2-C2
9	O	1	NAG	O5-C5-C6-O6
11	K	5	MAN	C4-C5-C6-O6
12	N	5	MAN	O5-C5-C6-O6
9	O	1	NAG	C4-C5-C6-O6
10	J	4	MAN	C4-C5-C6-O6
13	R	7	MAN	O5-C5-C6-O6
13	R	5	MAN	O5-C5-C6-O6
8	B	7	MAN	O5-C5-C6-O6
13	R	4	MAN	O5-C5-C6-O6
7	Q	2	NAG	O5-C5-C6-O6
8	B	10	MAN	O5-C5-C6-O6
13	R	2	NAG	O5-C5-C6-O6
11	K	3	BMA	C4-C5-C6-O6
7	U	1	NAG	O5-C5-C6-O6
13	R	6	MAN	O5-C5-C6-O6
7	I	3	BMA	O5-C5-C6-O6
9	F	1	NAG	O5-C5-C6-O6
10	J	2	NAG	O5-C5-C6-O6
15	V	2	NAG	O5-C5-C6-O6
11	K	11	MAN	O5-C5-C6-O6
12	N	4	MAN	O5-C5-C6-O6
8	B	2	NAG	O5-C5-C6-O6
11	K	8	MAN	O5-C5-C6-O6
14	S	4	MAN	O5-C5-C6-O6
11	K	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	U	3	BMA	C4-C5-C6-O6
8	B	1	NAG	C4-C5-C6-O6
13	R	4	MAN	C4-C5-C6-O6
7	I	2	NAG	C1-C2-N2-C7
7	P	1	NAG	C1-C2-N2-C7
7	Q	2	NAG	C1-C2-N2-C7
7	U	2	NAG	C1-C2-N2-C7
9	F	1	NAG	C1-C2-N2-C7
14	S	1	NAG	C1-C2-N2-C7
13	R	1	NAG	C4-C5-C6-O6
7	P	1	NAG	C3-C2-N2-C7
7	Q	2	NAG	C3-C2-N2-C7
7	U	2	NAG	C3-C2-N2-C7
9	C	1	NAG	C3-C2-N2-C7
9	F	1	NAG	C3-C2-N2-C7
10	M	1	NAG	C3-C2-N2-C7
12	N	1	NAG	C3-C2-N2-C7
14	S	1	NAG	C3-C2-N2-C7
13	R	1	NAG	O5-C5-C6-O6
11	K	3	BMA	O5-C5-C6-O6
7	A	1	NAG	C4-C5-C6-O6
7	U	3	BMA	O5-C5-C6-O6
8	B	2	NAG	C1-C2-N2-C7
9	C	1	NAG	C1-C2-N2-C7
10	M	1	NAG	C1-C2-N2-C7
12	N	1	NAG	C1-C2-N2-C7
7	I	2	NAG	C3-C2-N2-C7
8	B	2	NAG	C3-C2-N2-C7
12	N	4	MAN	C4-C5-C6-O6
7	A	1	NAG	O5-C5-C6-O6
11	K	9	MAN	C4-C5-C6-O6

There are no ring outliers.

25 monomers are involved in 18 short contacts:

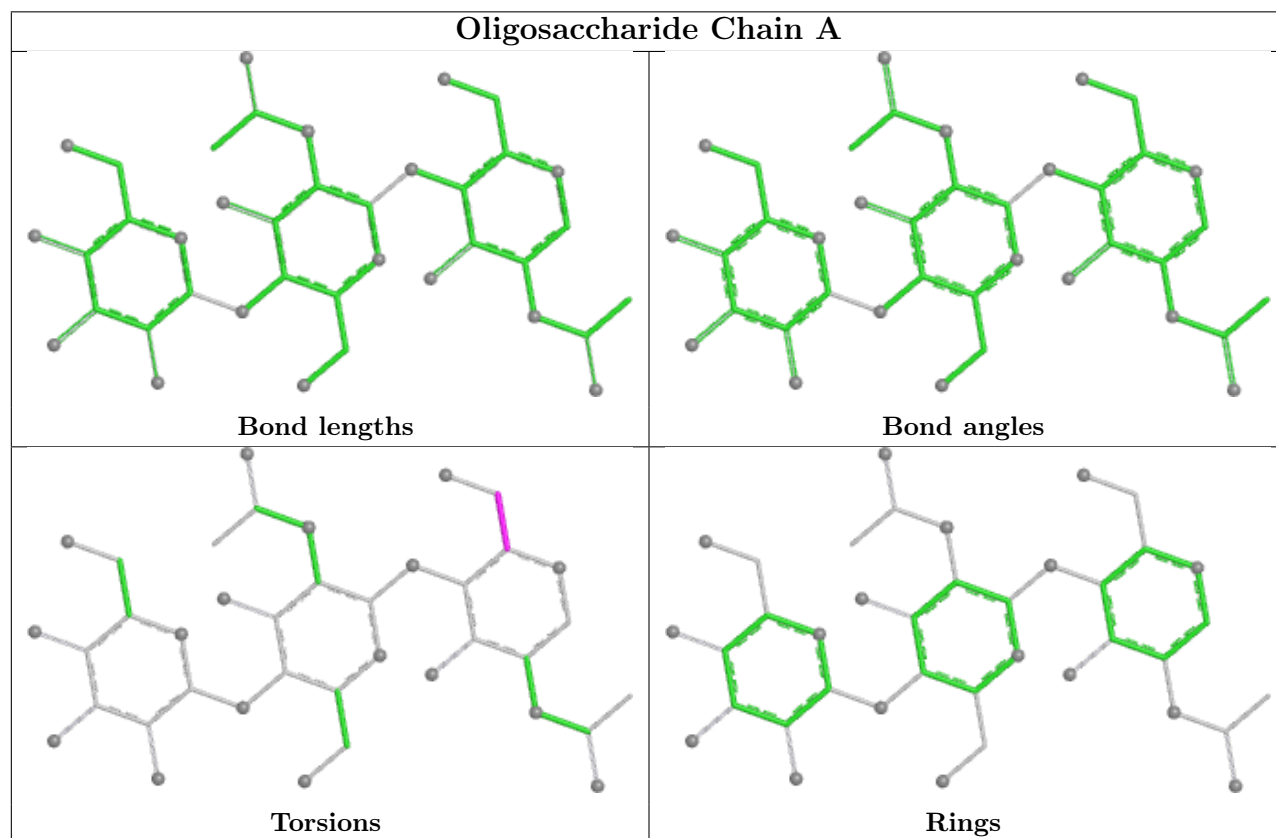
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2	NAG	1	0
12	N	1	NAG	1	0
8	B	9	MAN	1	0
7	P	2	NAG	1	0
7	P	1	NAG	1	0
8	B	4	MAN	1	0

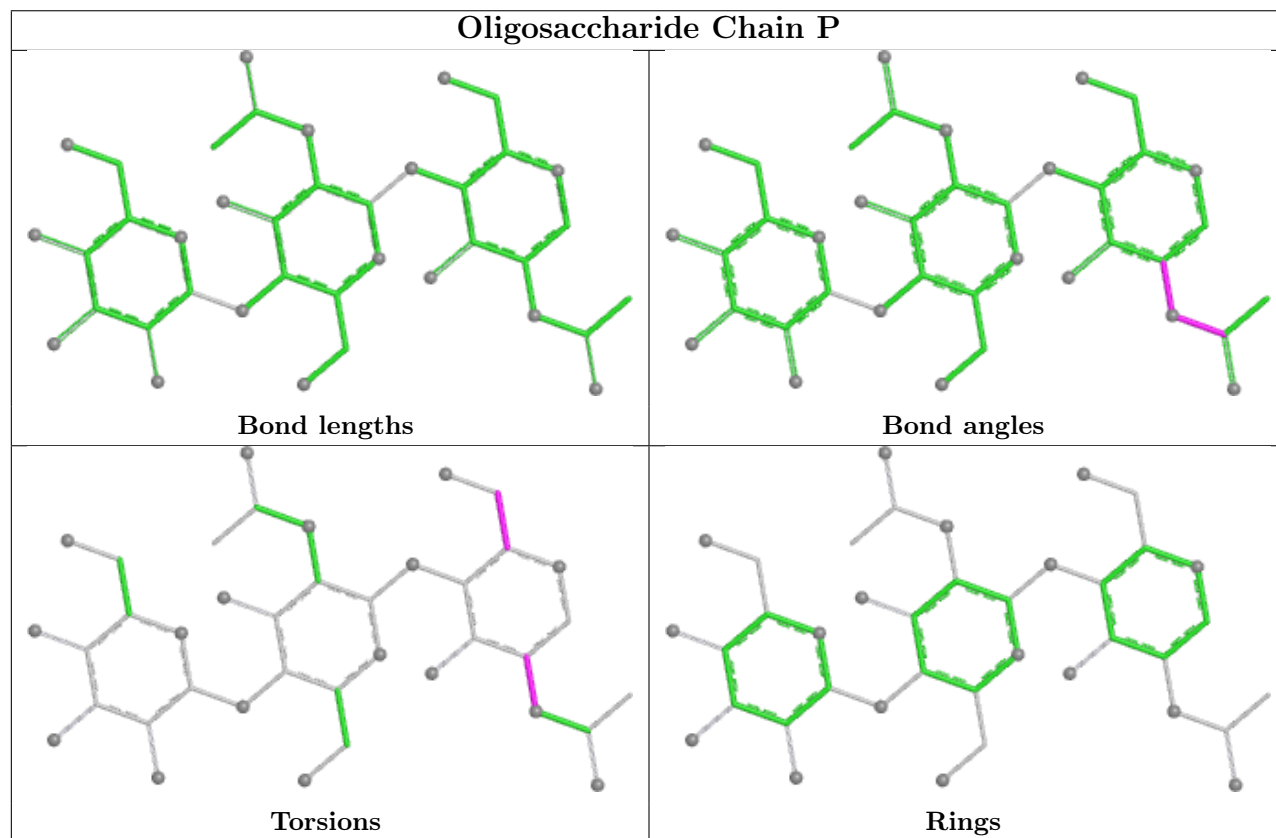
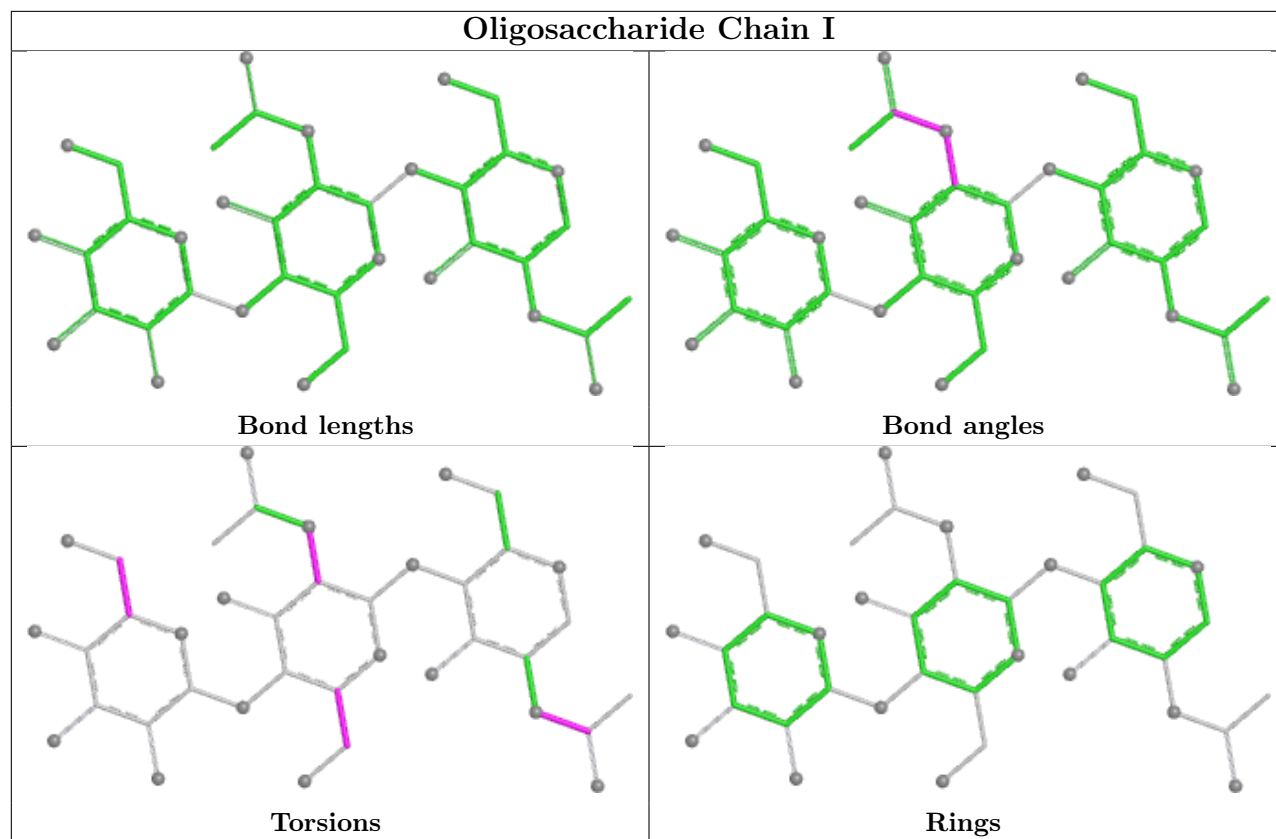
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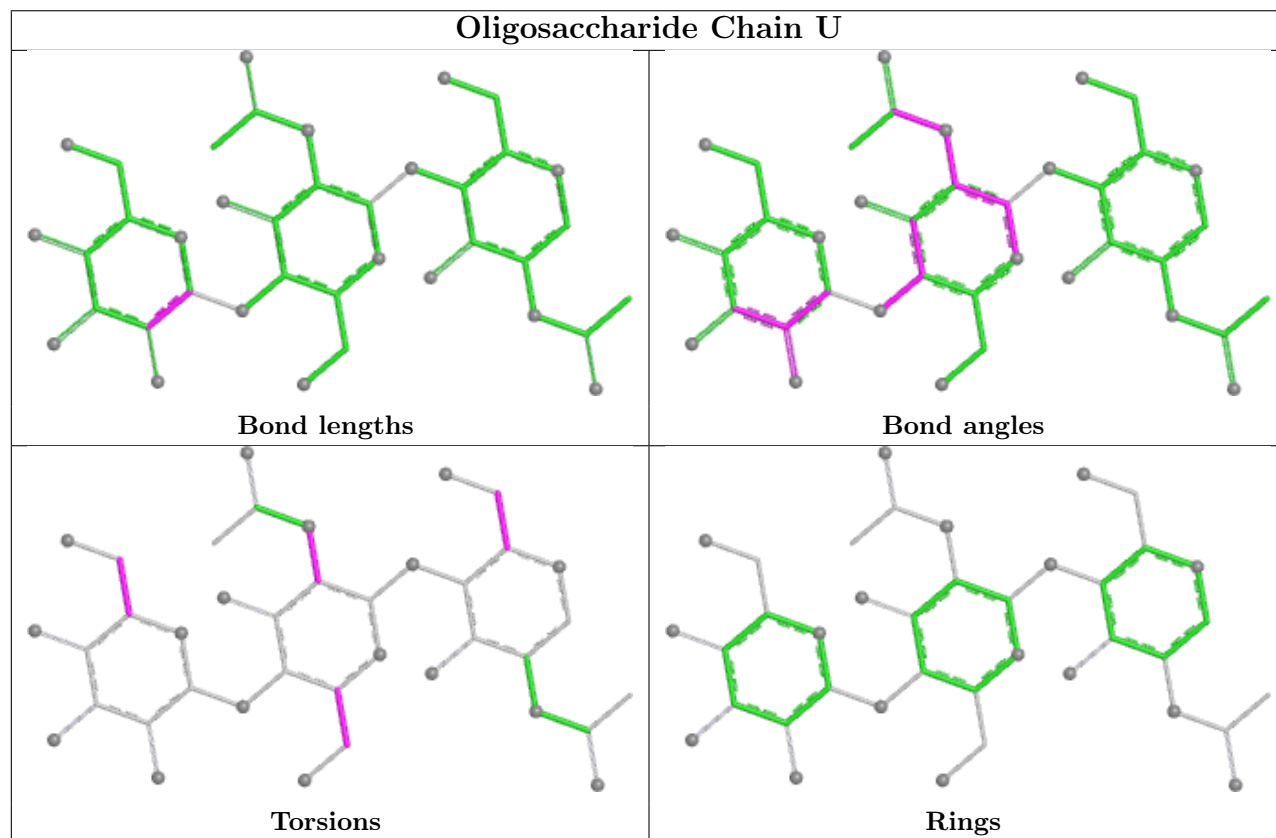
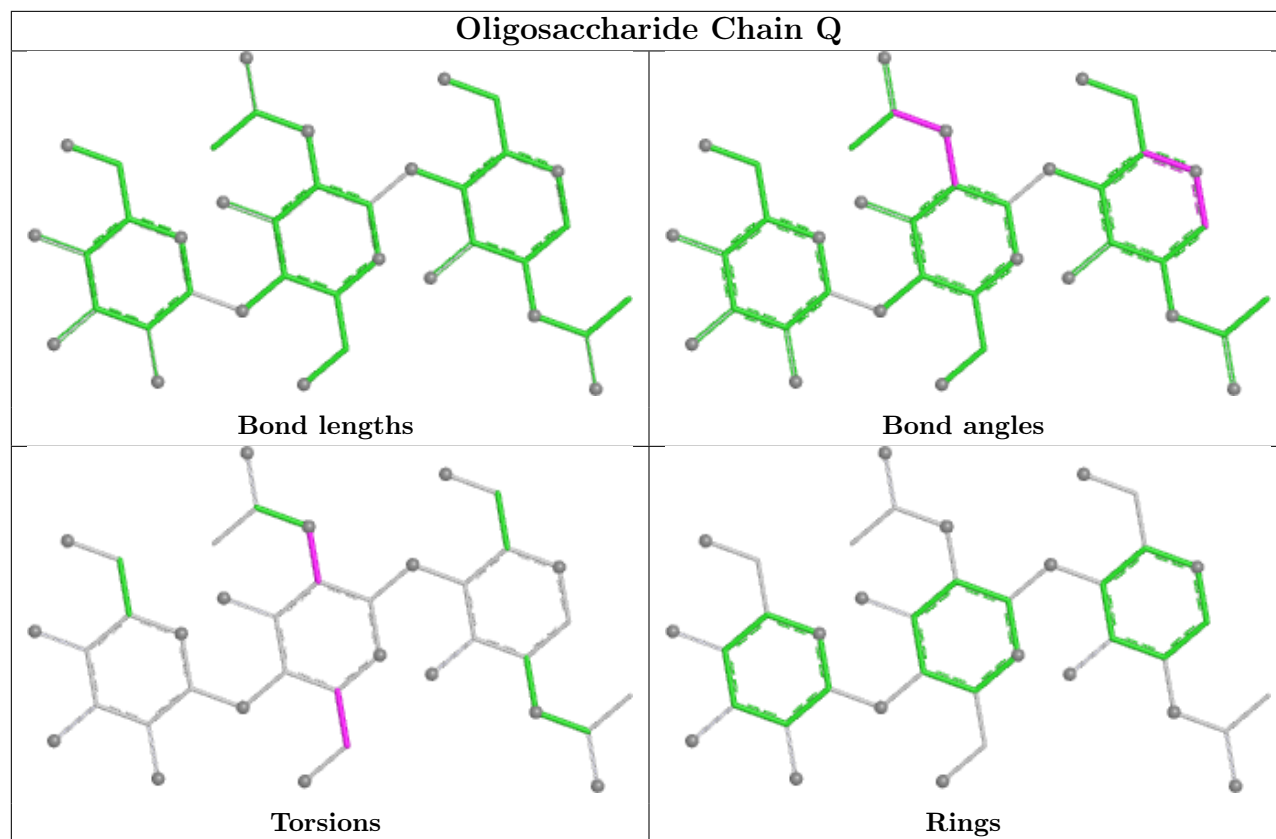
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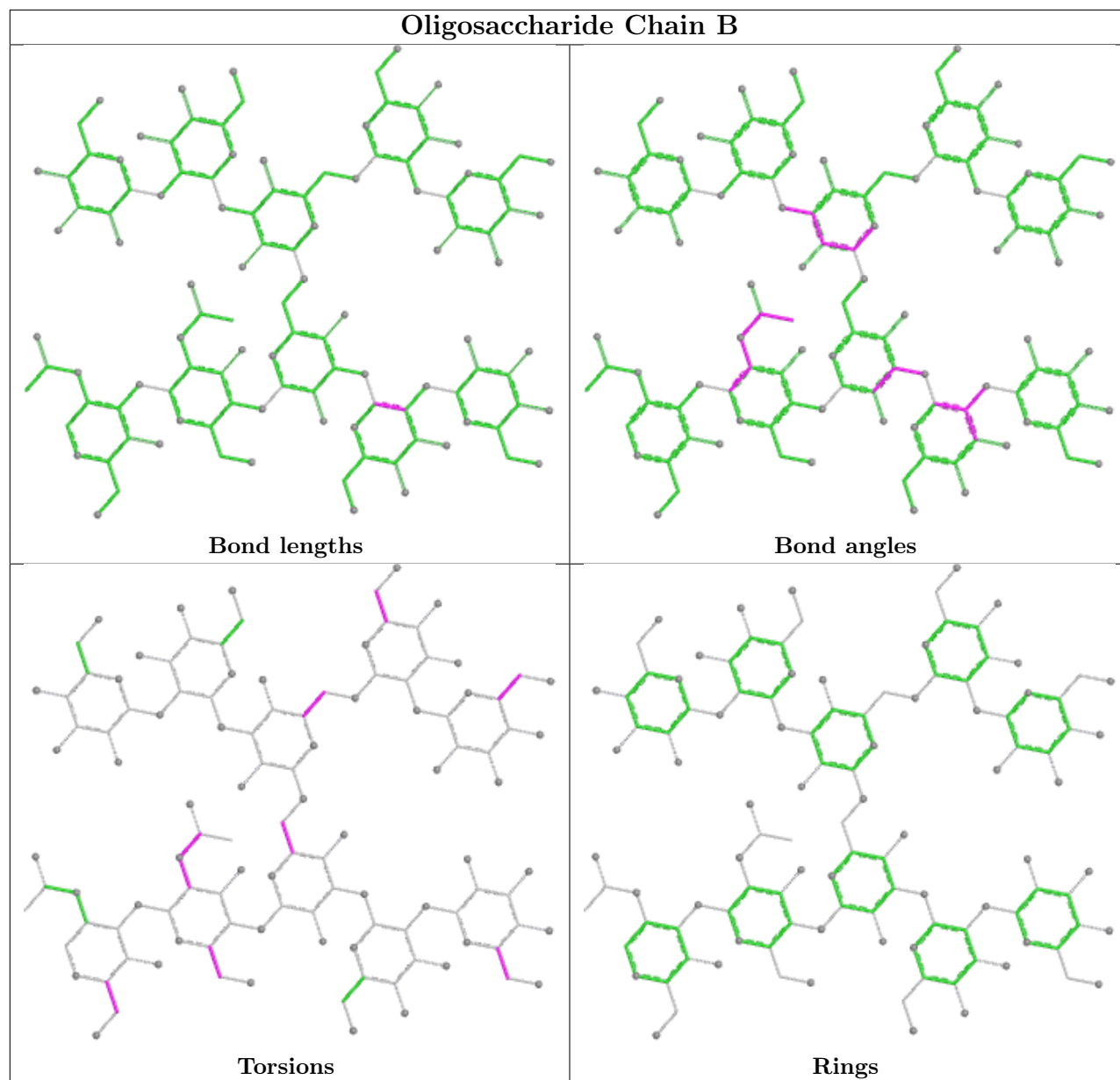
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	3	BMA	1	0
10	J	1	NAG	1	0
13	R	5	MAN	1	0
8	B	1	NAG	1	0
7	A	1	NAG	1	0
11	K	7	MAN	1	0
12	N	2	NAG	1	0
14	S	1	NAG	1	0
12	N	3	BMA	1	0
13	R	3	BMA	1	0
8	B	2	NAG	1	0
13	R	4	MAN	2	0
11	K	5	MAN	2	0
11	K	10	MAN	1	0
9	F	2	NAG	1	0
11	K	11	MAN	1	0
11	K	6	MAN	1	0
13	R	2	NAG	1	0
9	F	1	NAG	1	0

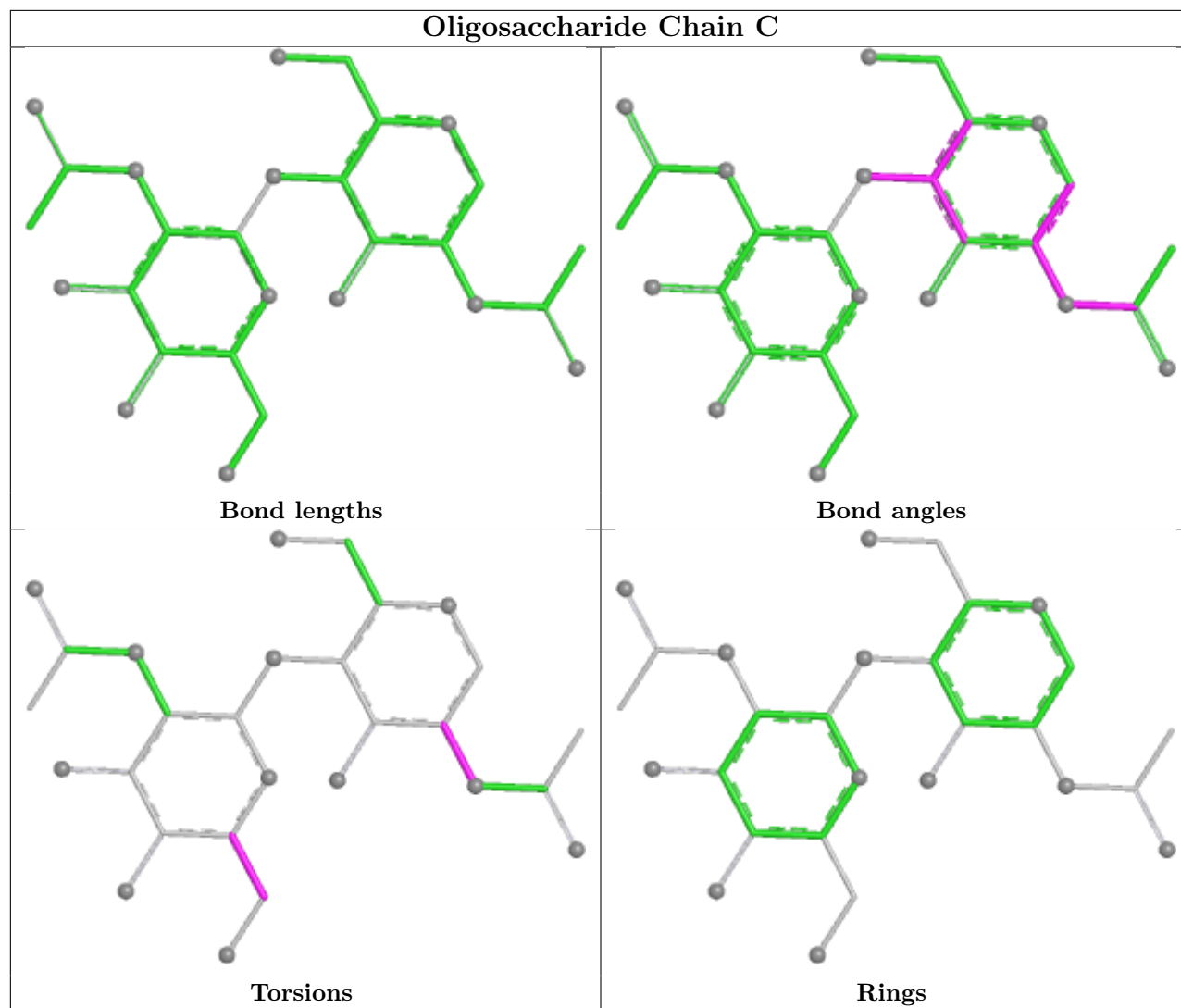
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

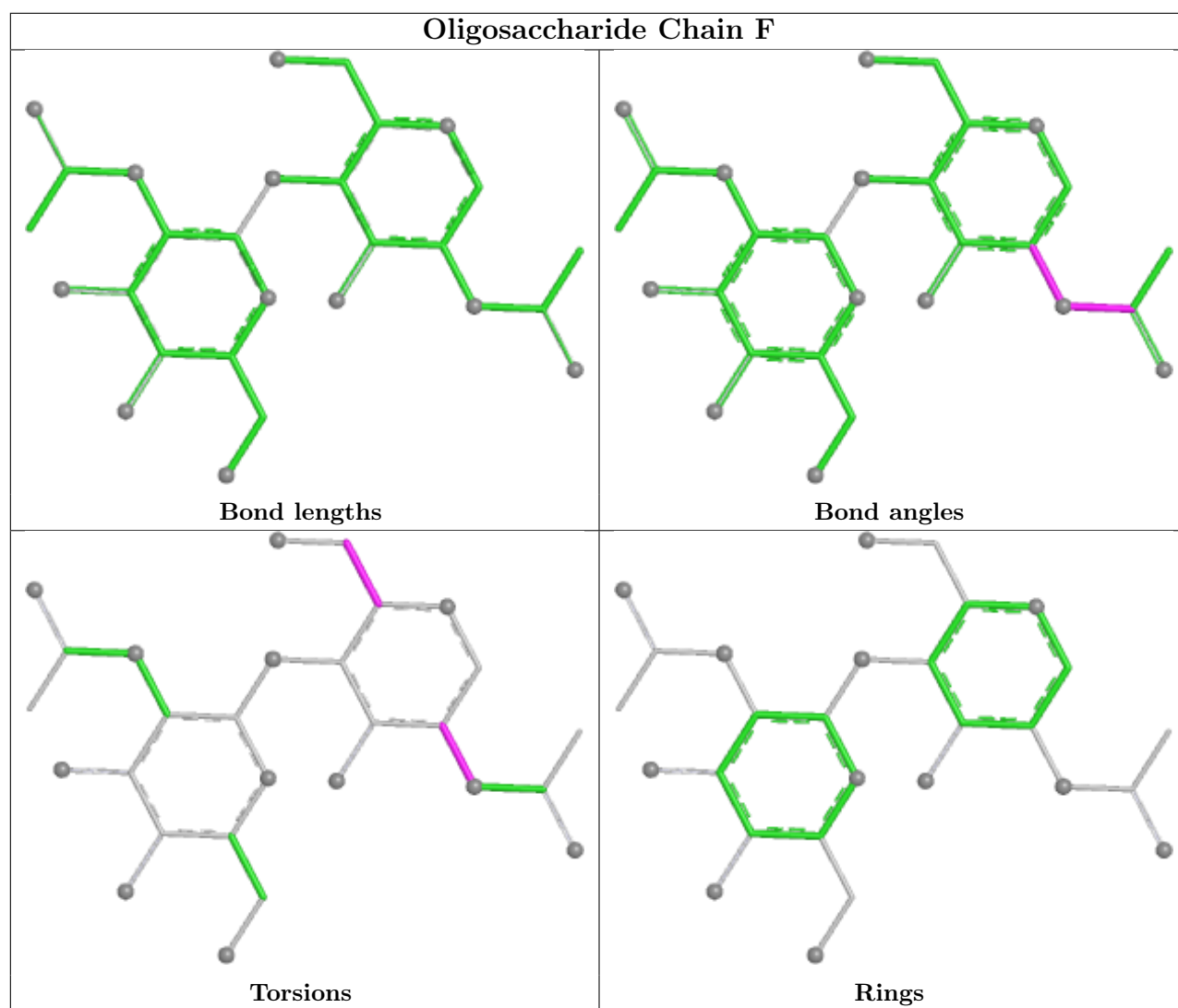


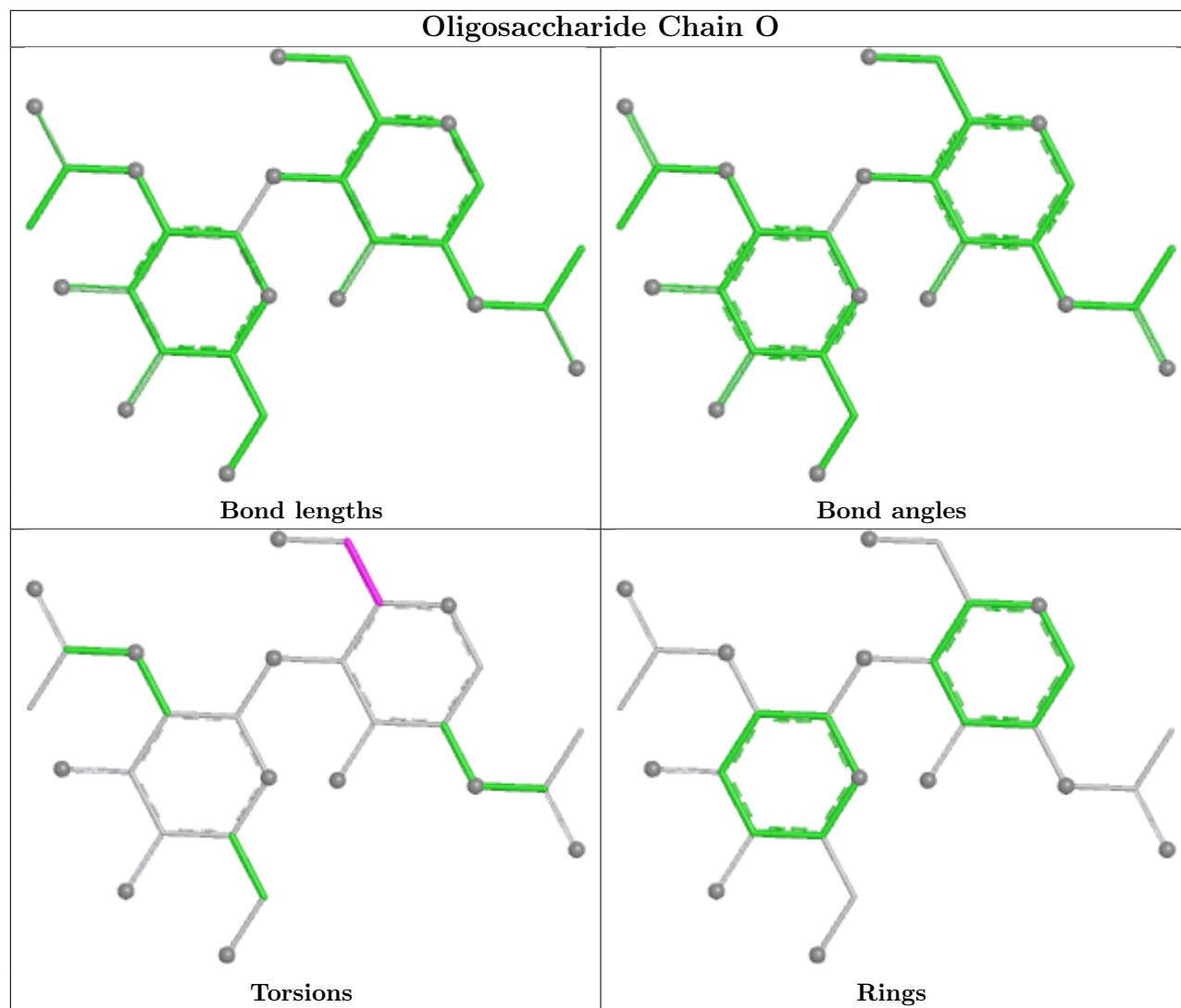


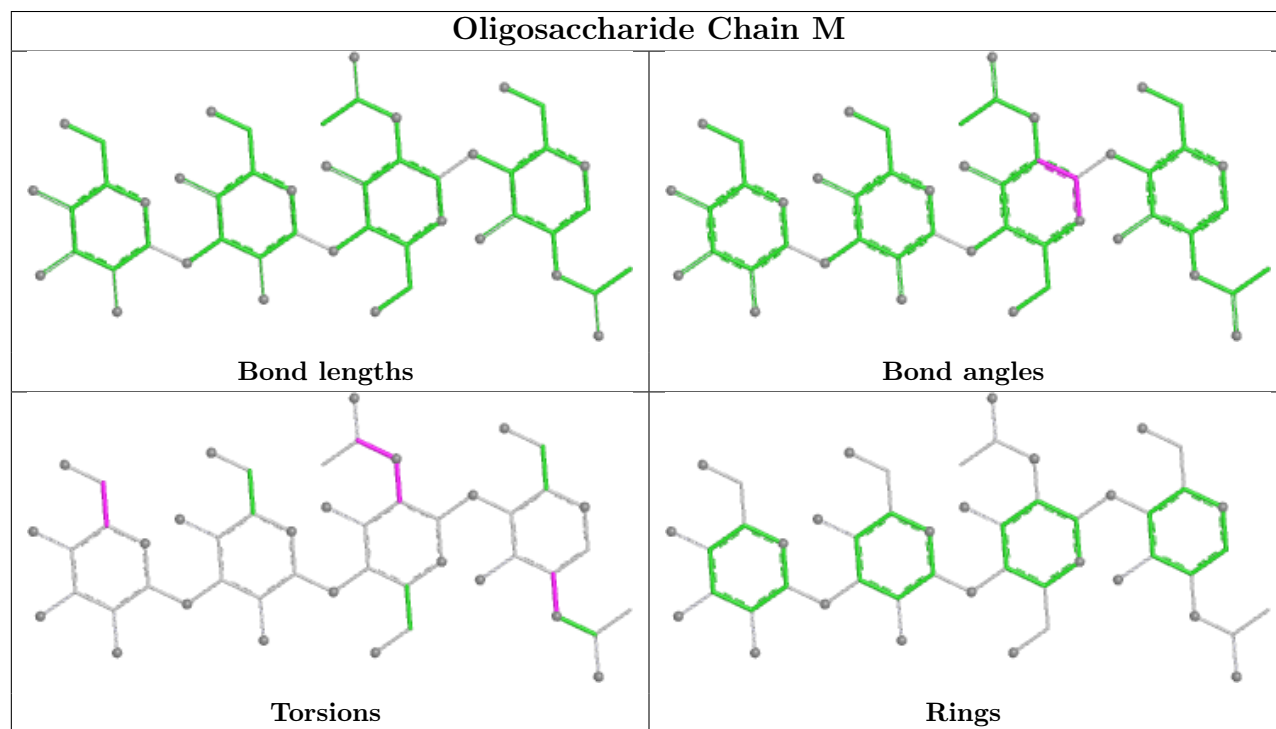
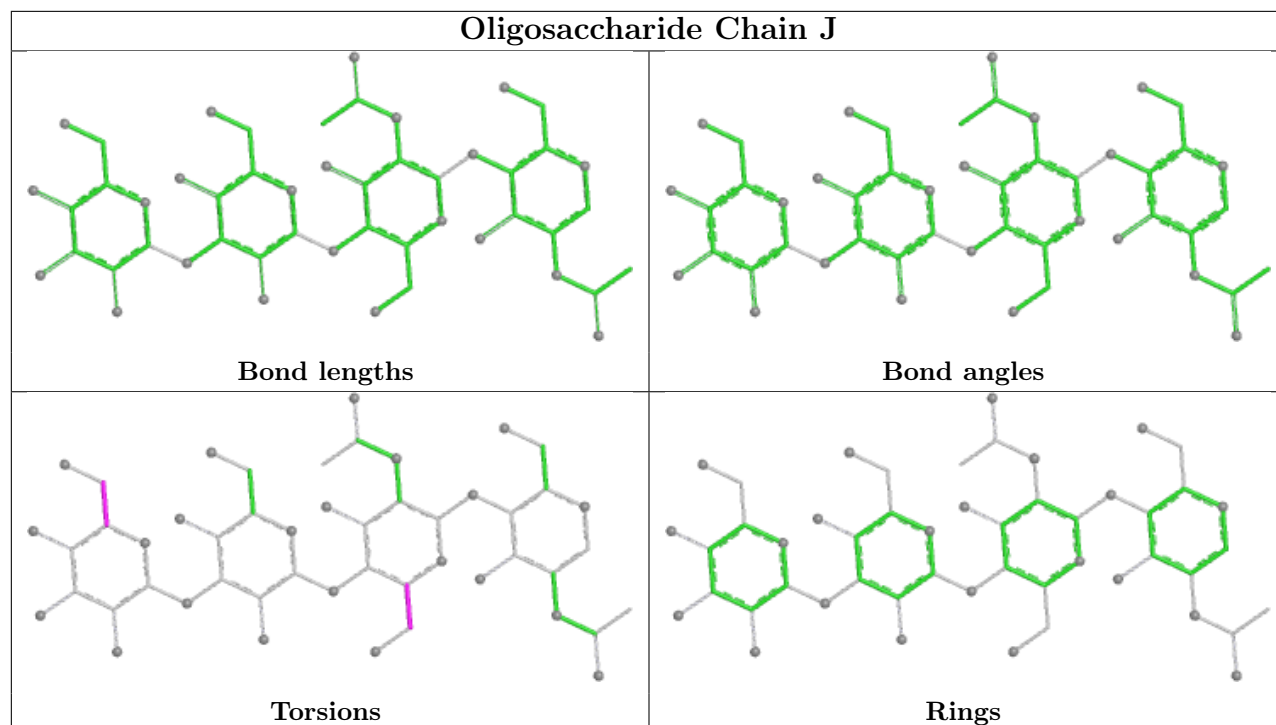


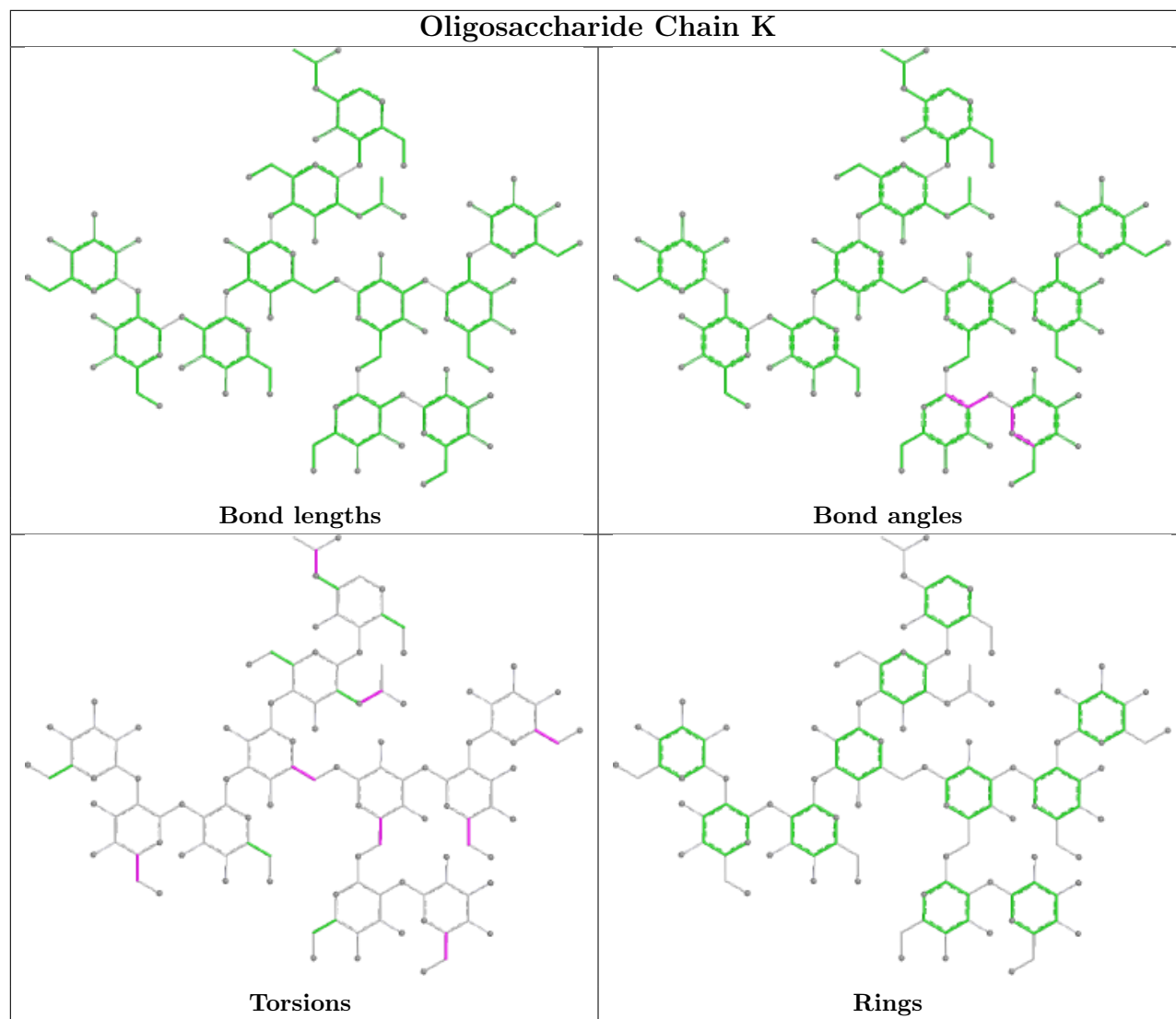


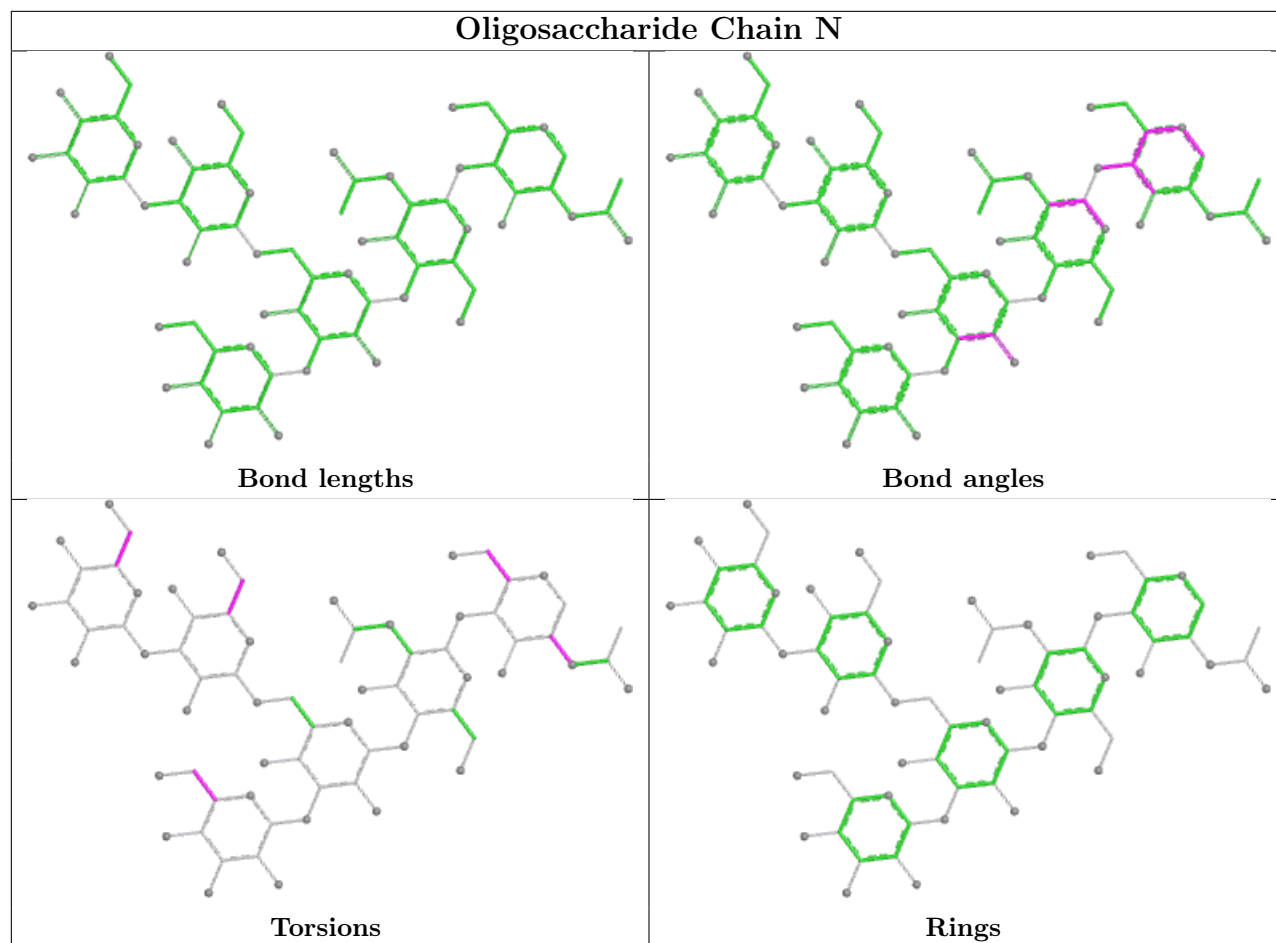


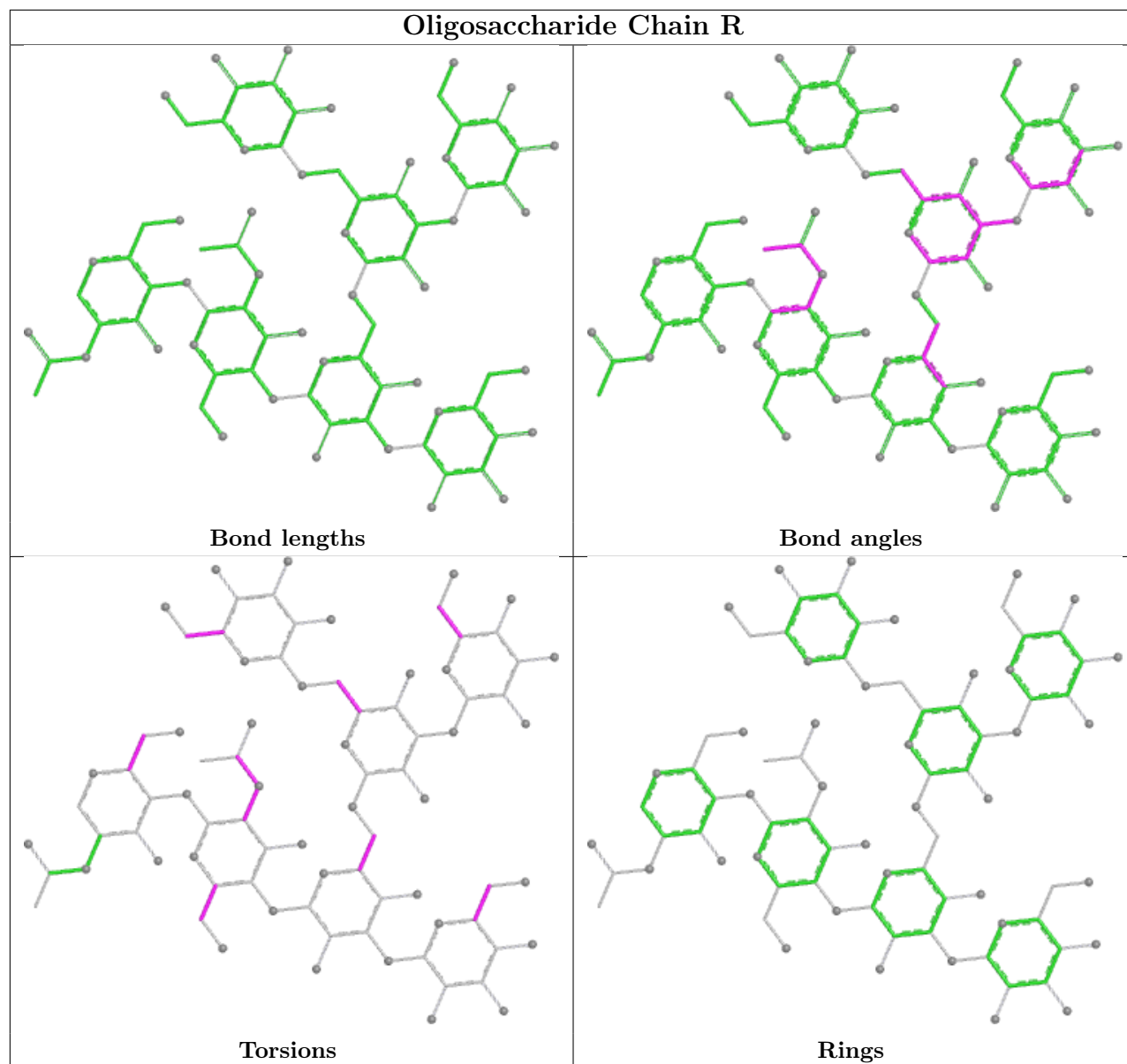


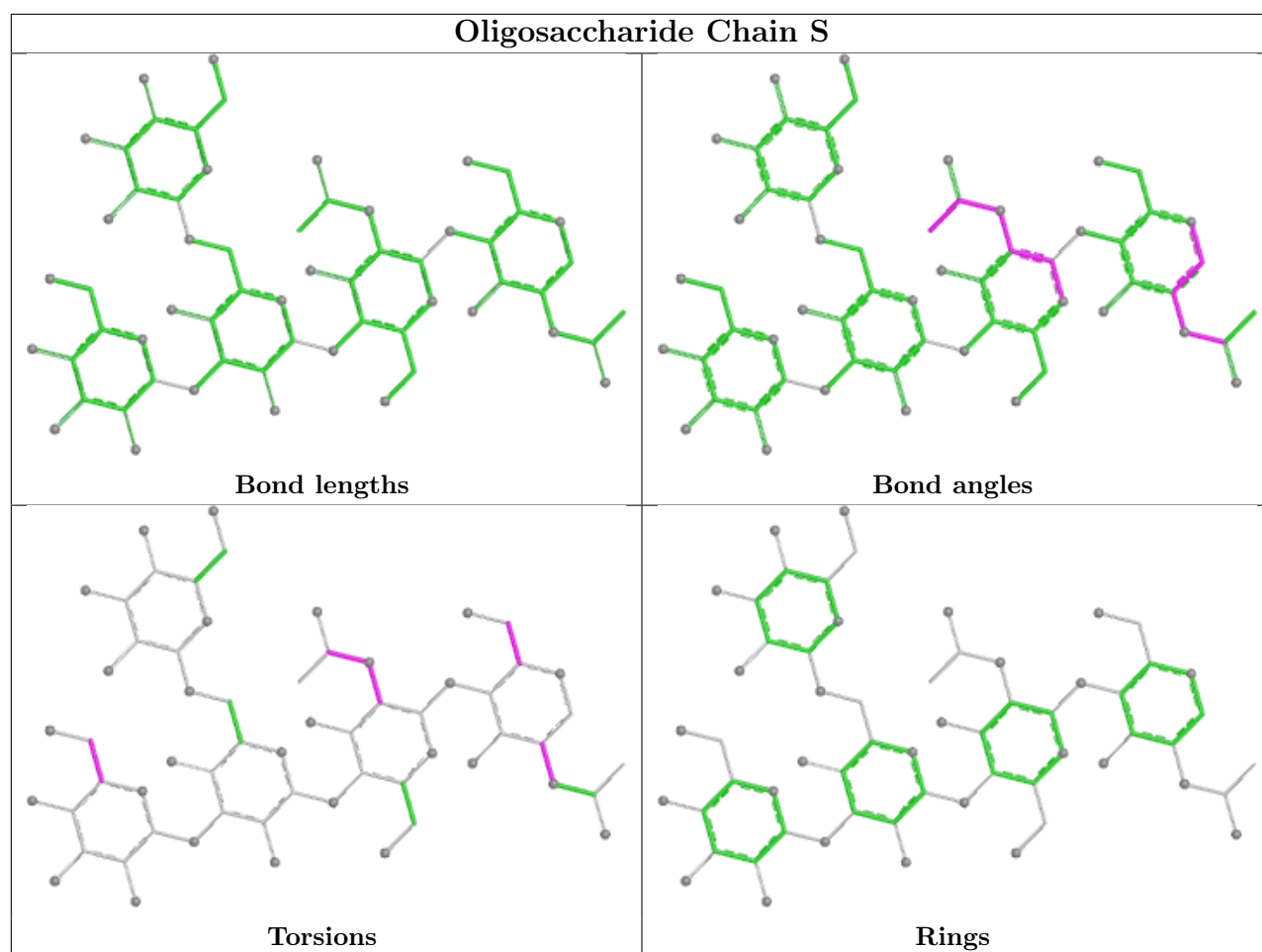


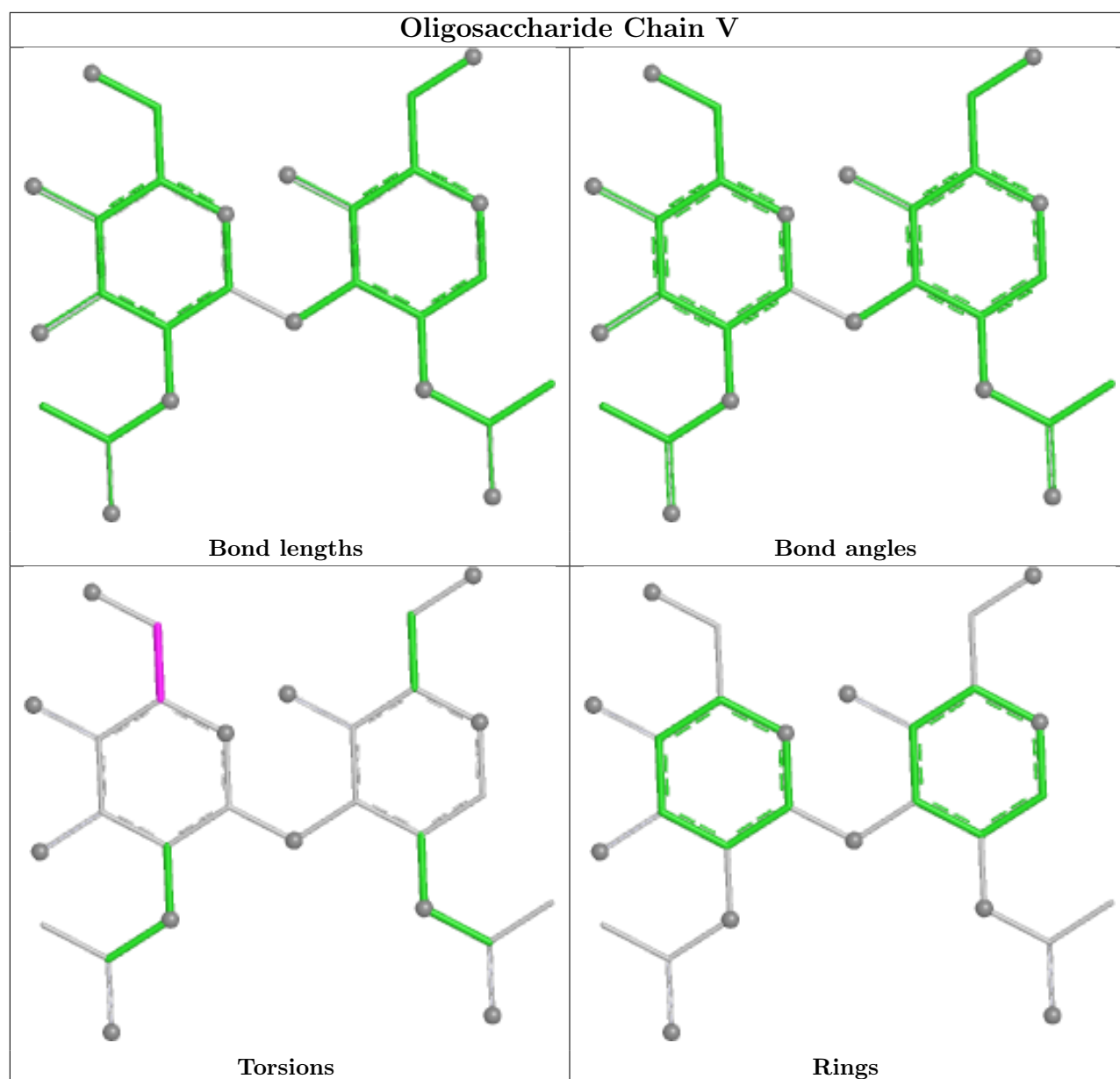












5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	NAG	G	604	4	14,14,15	0.34	0	17,19,21	0.90	1 (5%)
16	NAG	G	602	4	14,14,15	0.31	0	17,19,21	0.86	0
16	NAG	G	601	4	14,14,15	0.32	0	17,19,21	0.54	0
16	NAG	T	702	5	14,14,15	0.31	0	17,19,21	0.67	0
16	NAG	T	701	5	14,14,15	0.30	0	17,19,21	0.86	1 (5%)
16	NAG	T	703	5	14,14,15	0.28	0	17,19,21	0.57	0
16	NAG	G	605	4	14,14,15	0.29	0	17,19,21	0.64	0
16	NAG	G	603	4	14,14,15	0.30	0	17,19,21	0.59	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
16	NAG	G	604	4	-	5/6/23/26	0/1/1/1
16	NAG	G	602	4	-	2/6/23/26	0/1/1/1
16	NAG	G	601	4	-	4/6/23/26	0/1/1/1
16	NAG	T	702	5	-	2/6/23/26	0/1/1/1
16	NAG	T	701	5	-	2/6/23/26	0/1/1/1
16	NAG	T	703	5	-	2/6/23/26	0/1/1/1
16	NAG	G	605	4	-	0/6/23/26	0/1/1/1
16	NAG	G	603	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	701	NAG	C1-O5-C5	2.29	115.26	112.19
16	G	604	NAG	C1-O5-C5	2.13	115.05	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	G	604	NAG	O7-C7-N2-C2
16	G	602	NAG	C4-C5-C6-O6
16	T	702	NAG	O5-C5-C6-O6
16	G	604	NAG	C8-C7-N2-C2

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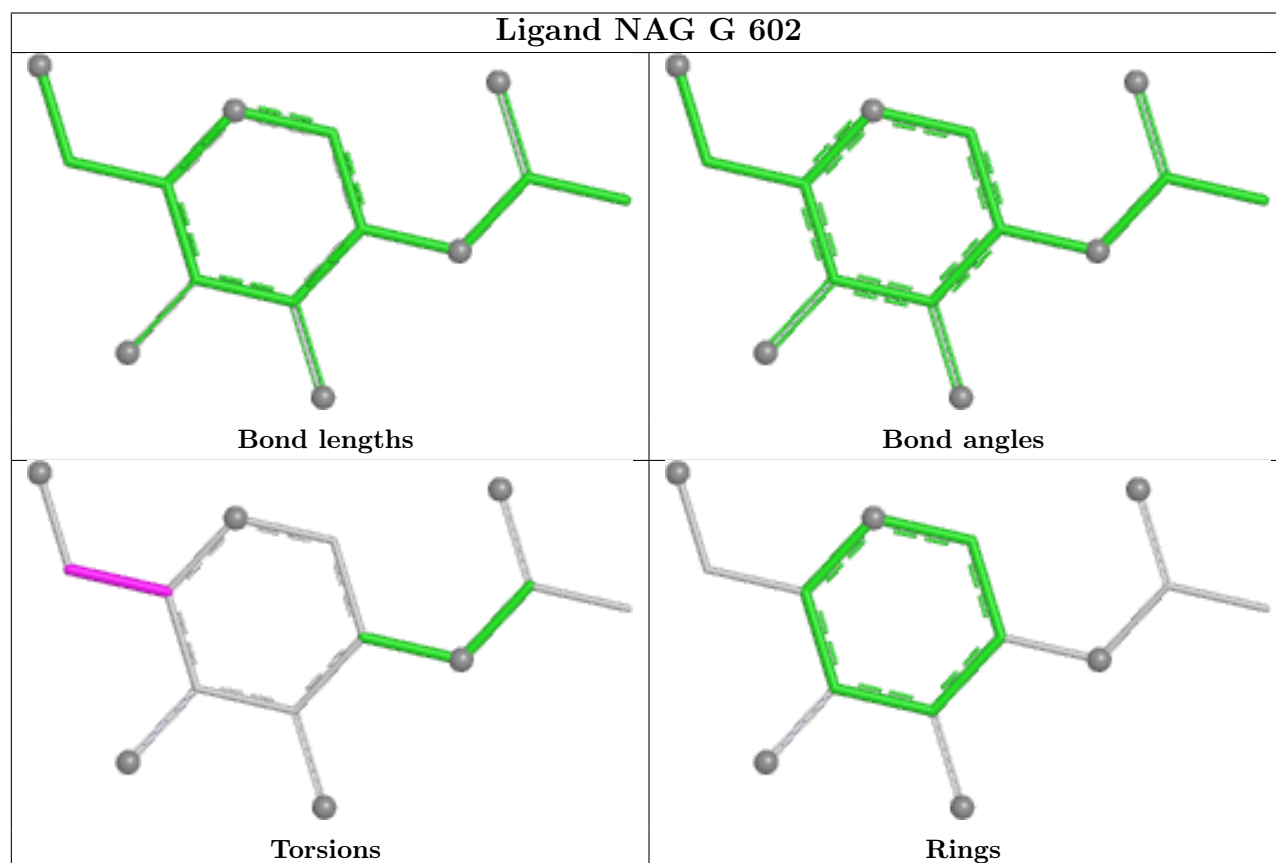
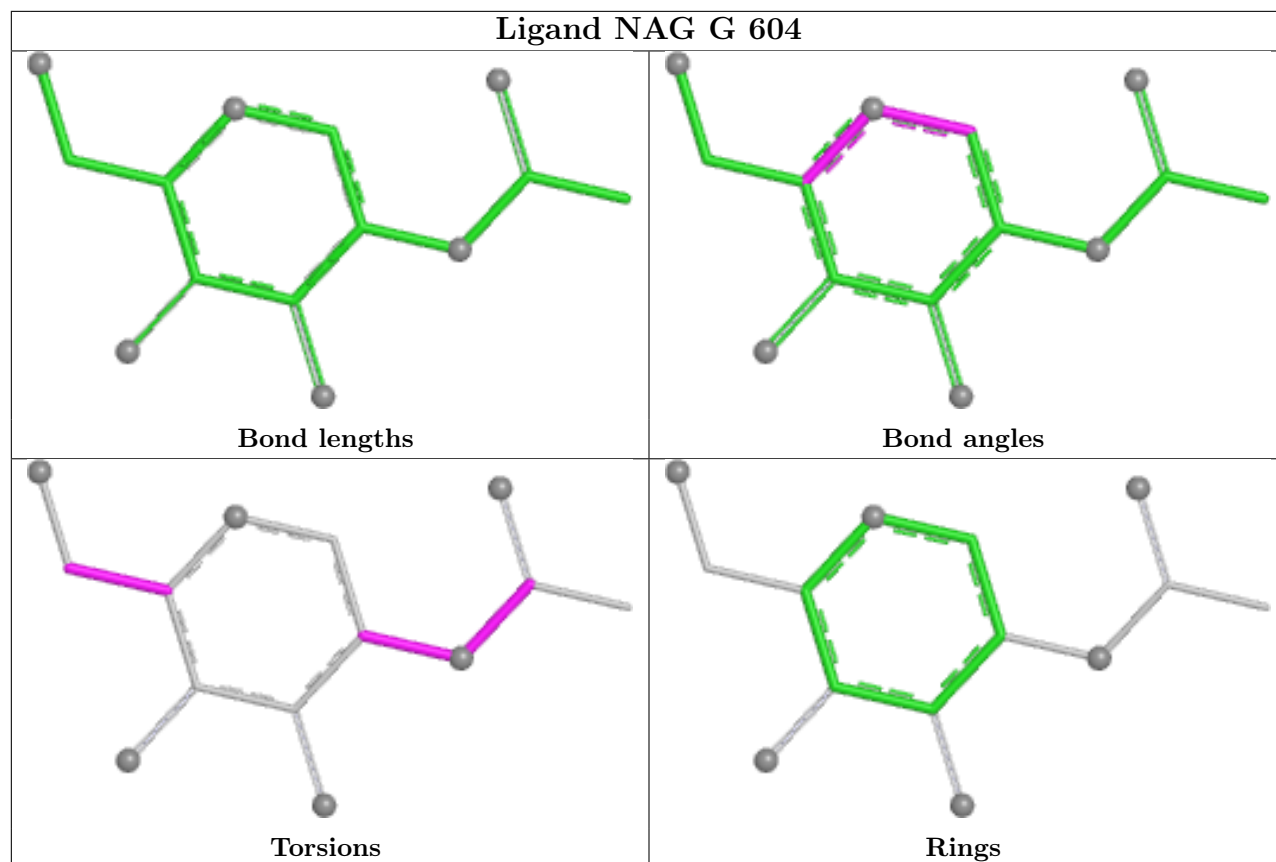
Mol	Chain	Res	Type	Atoms
16	G	602	NAG	O5-C5-C6-O6
16	T	703	NAG	O5-C5-C6-O6
16	G	601	NAG	C8-C7-N2-C2
16	G	601	NAG	O7-C7-N2-C2
16	T	701	NAG	O5-C5-C6-O6
16	T	703	NAG	C4-C5-C6-O6
16	G	601	NAG	O5-C5-C6-O6
16	G	604	NAG	O5-C5-C6-O6
16	T	701	NAG	C4-C5-C6-O6
16	G	604	NAG	C4-C5-C6-O6
16	T	702	NAG	C4-C5-C6-O6
16	G	604	NAG	C3-C2-N2-C7
16	G	601	NAG	C4-C5-C6-O6

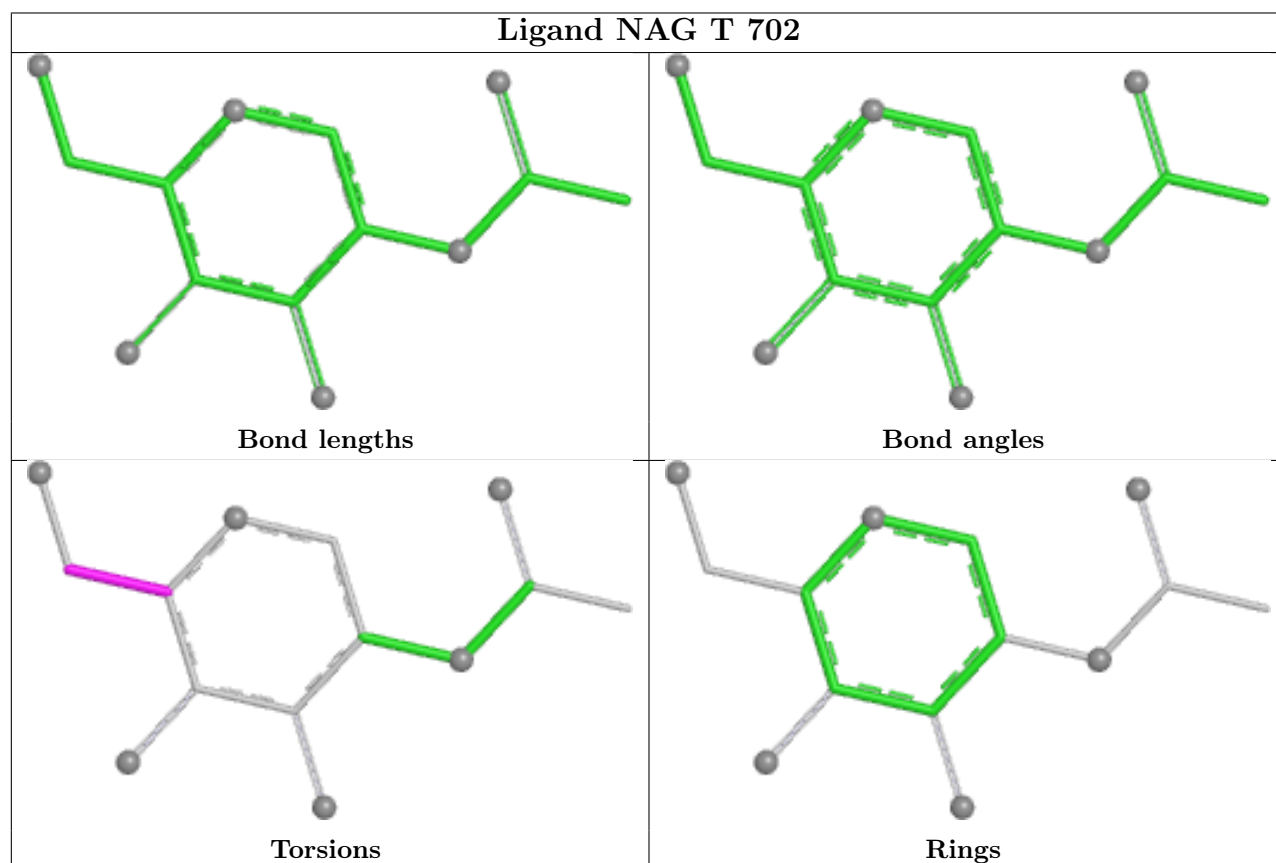
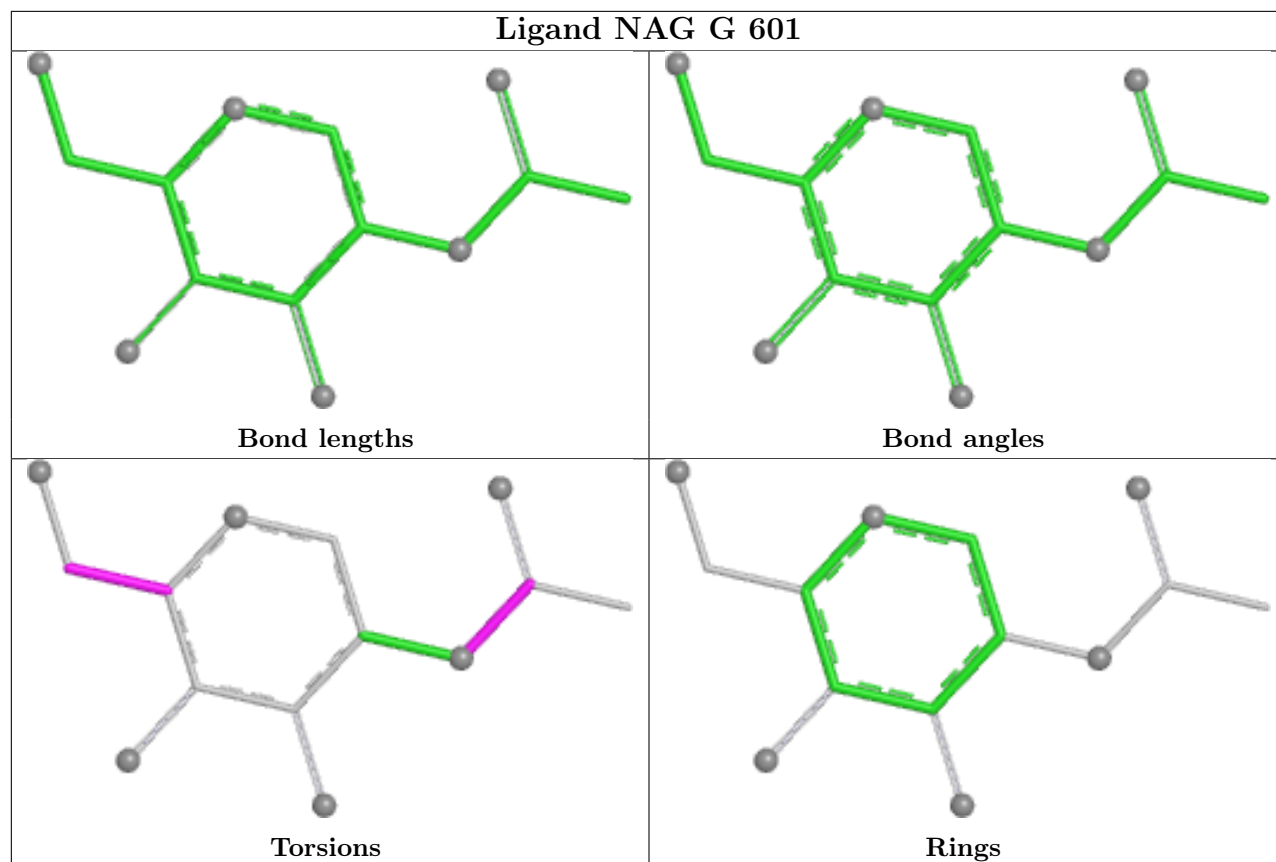
There are no ring outliers.

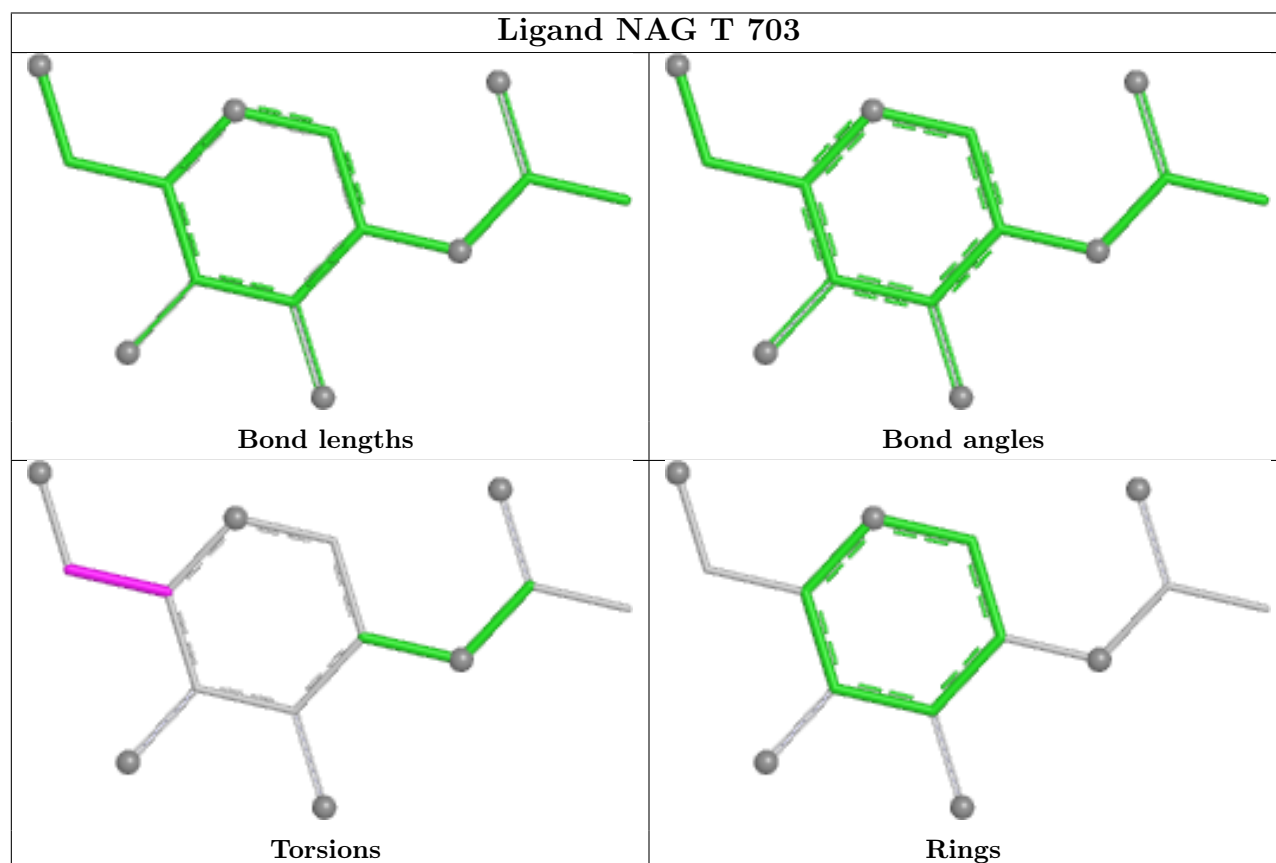
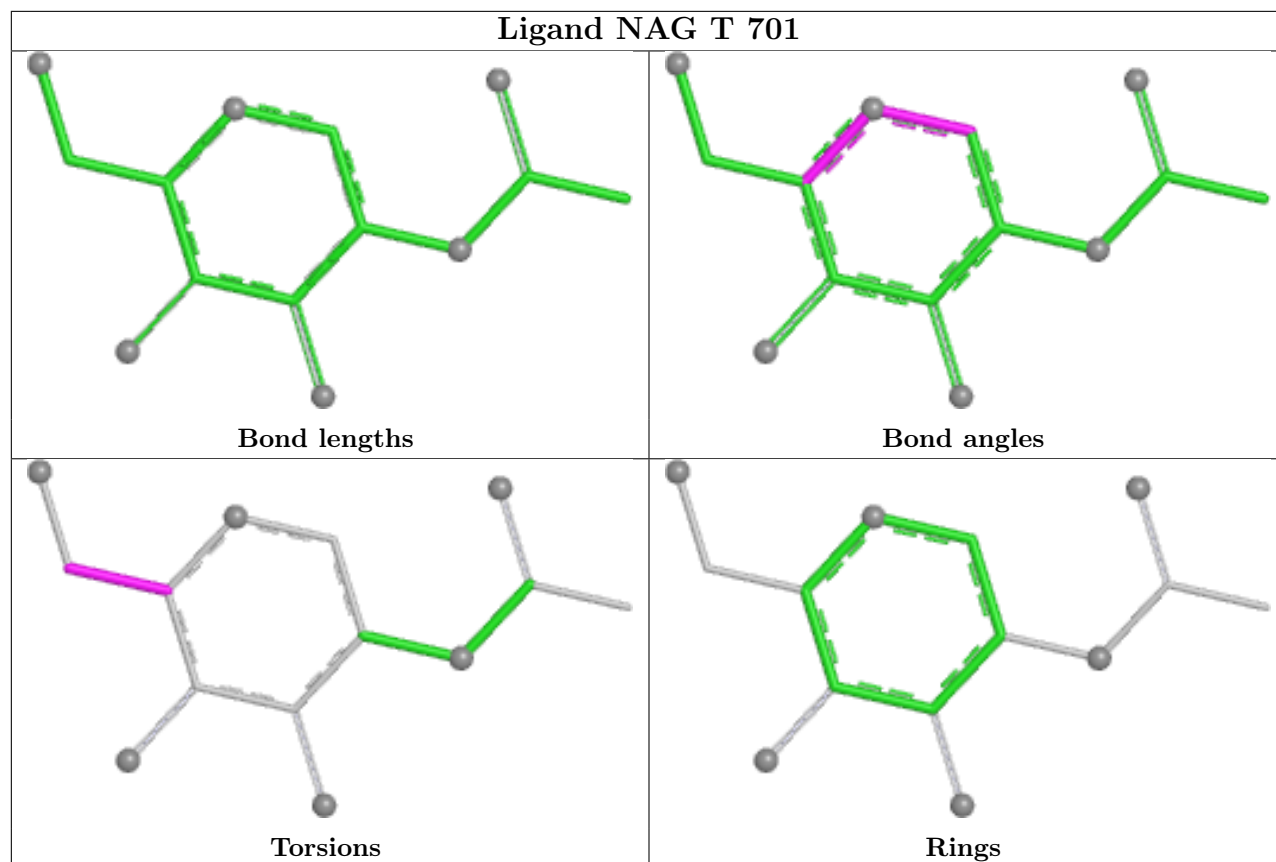
3 monomers are involved in 4 short contacts:

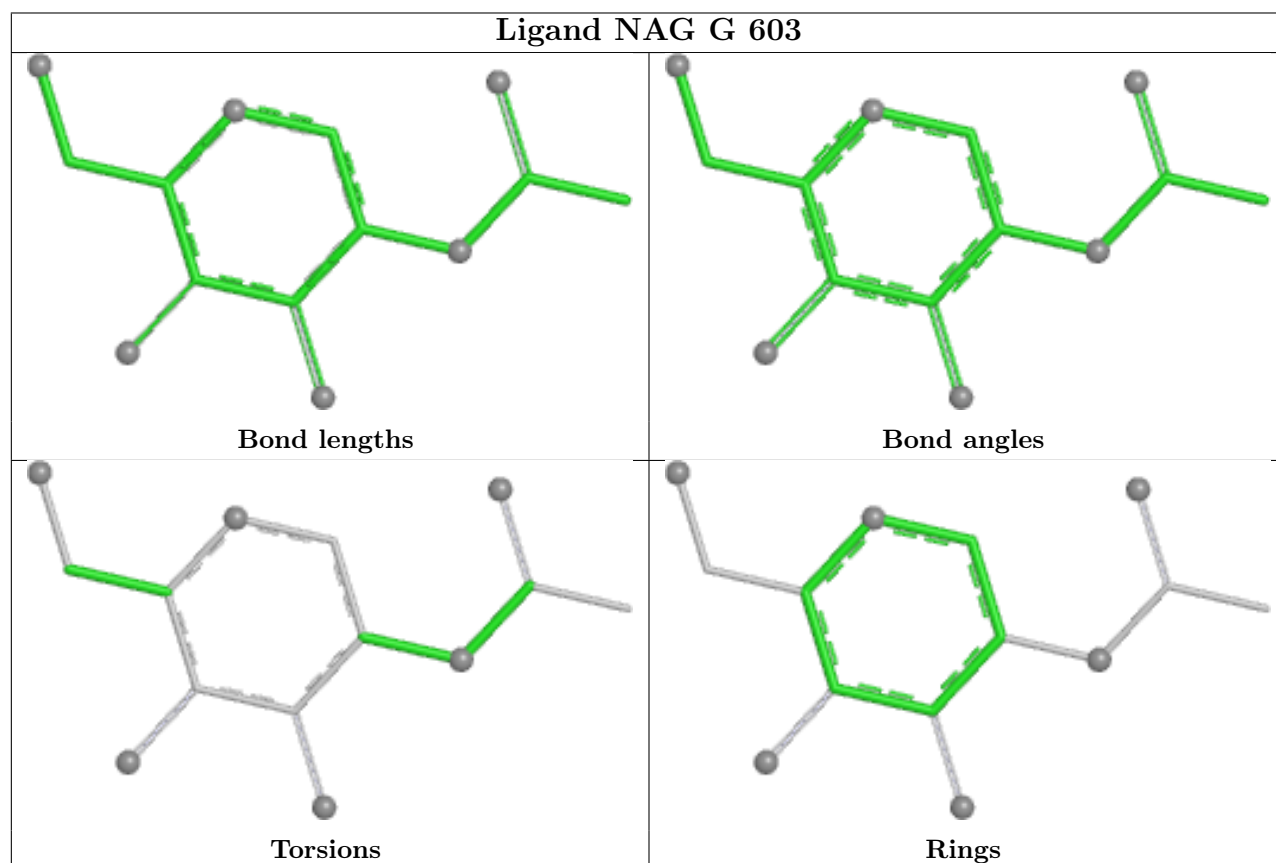
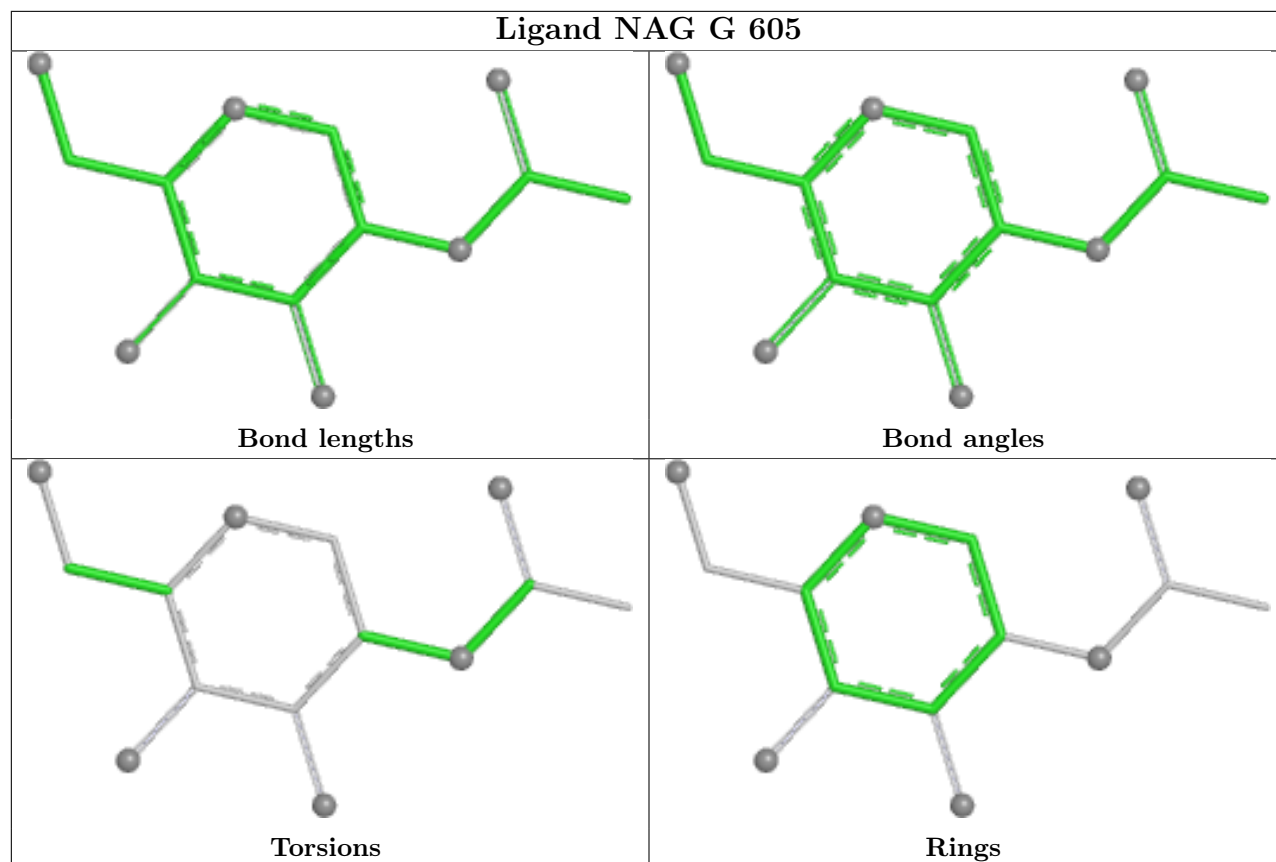
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	604	NAG	2	0
16	T	701	NAG	1	0
16	G	605	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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	D	240/243 (98%)	0.33	4 (1%) 69 47	142, 213, 331, 338	0
2	E	213/216 (98%)	0.36	7 (3%) 49 34	164, 195, 371, 388	0
3	L	213/213 (100%)	0.29	5 (2%) 61 42	110, 133, 152, 160	0
4	G	453/485 (93%)	0.36	10 (2%) 62 44	97, 132, 174, 194	0
5	T	134/140 (95%)	0.65	7 (5%) 33 25	129, 148, 182, 189	0
6	H	231/233 (99%)	0.06	1 (0%) 88 74	97, 123, 140, 156	0
All	All	1484/1530 (96%)	0.33	34 (2%) 61 42	97, 142, 329, 388	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	144	VAL	4.8
4	G	180	ASP	3.8
5	T	601	LYS	3.7
4	G	152	GLY	3.4
5	T	547(G)	ASP	3.2
2	E	18	SER	3.1
4	G	47	ASP	2.8
6	H	113	ALA	2.6
5	T	518	VAL	2.6
3	L	212	GLY	2.6
4	G	289	ASN	2.5
2	E	163	THR	2.5
1	D	152	VAL	2.5
3	L	146	VAL	2.4
5	T	659	ASP	2.4
1	D	138	LEU	2.3
4	G	70	ALA	2.3
2	E	113	PRO	2.3
4	G	338	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
4	G	134	VAL	2.3
2	E	161	THR	2.2
3	L	190	LYS	2.2
1	D	207	VAL	2.2
1	D	151	THR	2.2
3	L	148	TRP	2.1
5	T	519	PHE	2.1
4	G	415	THR	2.1
2	E	197	HIS	2.1
4	G	195	ASN	2.1
3	L	147	GLN	2.1
4	G	328	GLN	2.1
5	T	632	ASP	2.0
2	E	35	TRP	2.0
5	T	660	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	A	1	14/15	-	-	180,184,187,188	0
7	NAG	A	2	14/15	-	-	196,199,203,205	0
7	BMA	A	3	11/12	-	-	210,215,221,225	0
7	NAG	I	1	14/15	-0.02	0.16	173,180,184,184	0
10	NAG	J	2	14/15	0.01	0.13	144,146,148,149	0
7	BMA	I	3	11/12	-	-	191,195,199,200	0
11	NAG	K	2	14/15	0.06	0.17	140,142,145,148	0
7	BMA	Q	3	11/12	0.14	0.11	187,189,193,193	0
7	BMA	P	3	11/12	-	-	182,185,187,188	0
15	NAG	V	2	14/15	0.22	0.14	194,195,196,196	0
7	NAG	I	2	14/15	0.23	0.12	187,190,192,194	0
7	BMA	U	3	11/12	0.25	0.10	191,195,198,200	0
13	BMA	R	3	11/12	0.34	0.12	197,199,203,203	0

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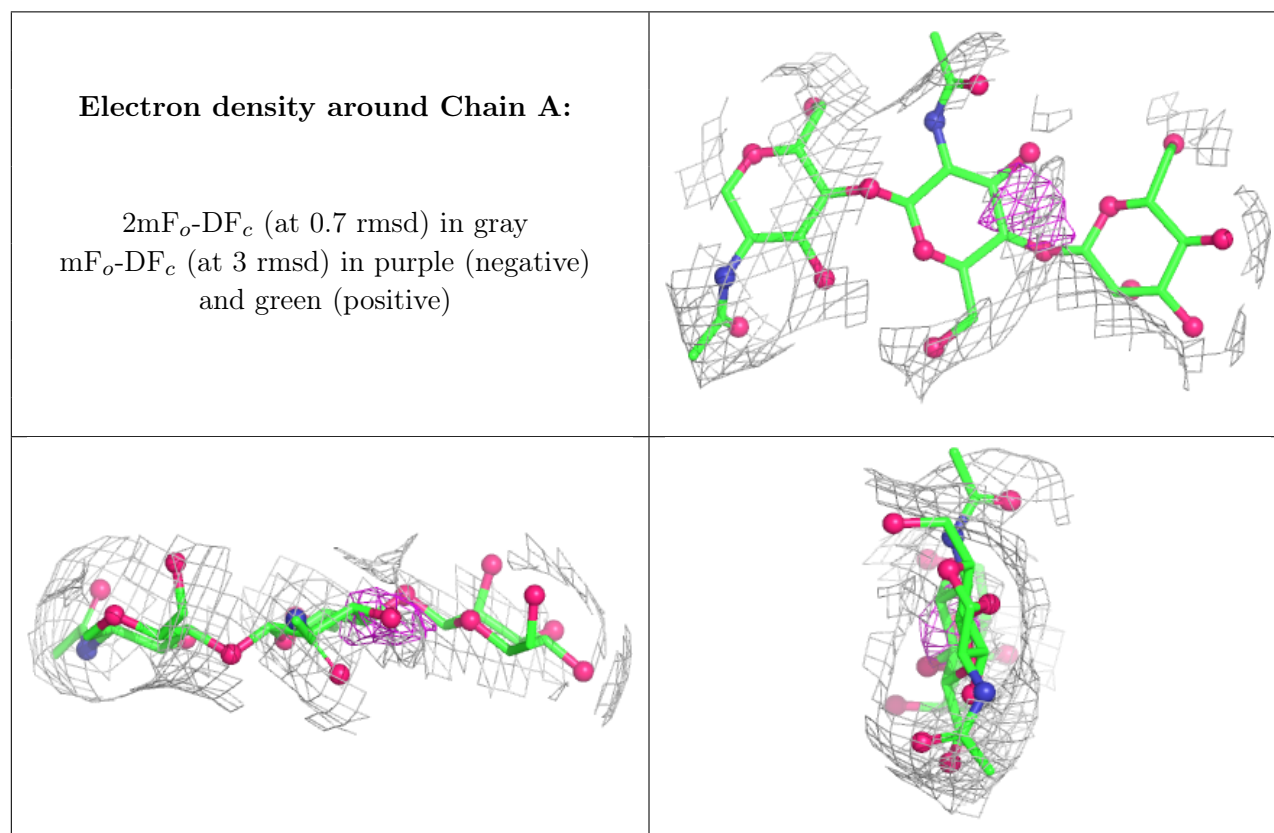
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	NAG	V	1	14/15	0.41	0.15	189,192,194,195	0
11	BMA	K	3	11/12	0.42	0.12	142,142,144,144	0
8	NAG	B	1	14/15	-	-	137,140,142,144	0
8	NAG	B	2	14/15	-	-	145,148,153,154	0
8	BMA	B	3	11/12	-	-	157,160,163,165	0
8	MAN	B	4	11/12	-	-	157,161,166,167	0
8	MAN	B	5	11/12	-	-	171,174,177,178	0
8	MAN	B	6	11/12	-	-	169,176,180,182	0
8	MAN	B	7	11/12	-	-	154,157,160,161	0
8	MAN	B	8	11/12	-	-	154,158,161,162	0
8	MAN	B	9	11/12	-	-	159,164,167,167	0
8	MAN	B	10	11/12	-	-	163,169,175,176	0
9	NAG	C	1	14/15	-	-	155,163,168,168	0
9	NAG	C	2	14/15	-	-	166,170,175,176	0
9	NAG	F	1	14/15	-	-	183,184,187,188	0
9	NAG	F	2	14/15	-	-	186,189,190,191	0
12	MAN	N	4	11/12	0.45	0.10	188,191,194,196	0
14	MAN	S	5	11/12	0.49	0.12	152,153,160,162	0
14	MAN	S	4	11/12	0.56	0.10	148,150,155,157	0
9	NAG	O	2	14/15	0.59	0.10	152,154,155,156	0
10	BMA	J	3	11/12	-	-	152,153,156,157	0
10	MAN	J	4	11/12	-	-	156,158,161,163	0
12	BMA	N	3	11/12	0.61	0.08	182,186,187,187	0
7	NAG	P	2	14/15	0.64	0.11	173,175,178,178	0
11	NAG	K	1	14/15	0.66	0.12	139,141,146,146	0
7	NAG	U	2	14/15	0.68	0.14	186,189,190,193	0
10	NAG	J	1	14/15	0.69	0.13	137,138,141,142	0
7	NAG	U	1	14/15	0.72	0.18	175,180,183,185	0
13	NAG	R	2	14/15	0.74	0.11	189,190,193,193	0
11	MAN	K	4	11/12	-	-	142,143,146,146	0
11	MAN	K	5	11/12	-	-	140,143,145,146	0
11	MAN	K	6	11/12	-	-	139,140,142,143	0
11	MAN	K	7	11/12	-	-	145,146,149,149	0
11	MAN	K	8	11/12	-	-	152,154,157,158	0
11	MAN	K	9	11/12	-	-	155,156,158,160	0
11	MAN	K	10	11/12	-	-	147,148,151,152	0
11	MAN	K	11	11/12	-	-	145,147,151,153	0
13	NAG	R	1	14/15	0.76	0.16	181,183,185,186	0
7	NAG	P	1	14/15	0.76	0.13	157,162,164,165	0
7	NAG	Q	2	14/15	0.76	0.10	173,180,184,185	0
14	BMA	S	3	11/12	0.76	0.08	145,146,148,149	0
12	MAN	N	5	11/12	-	-	196,197,201,202	0

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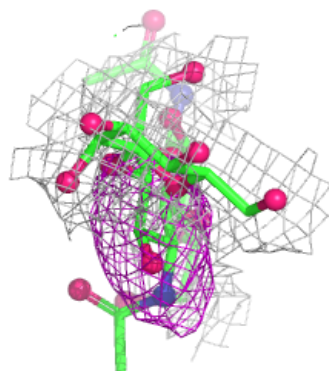
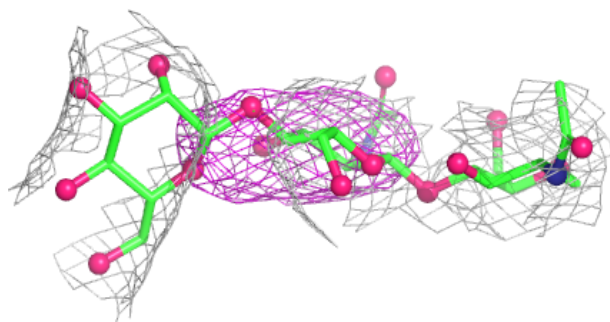
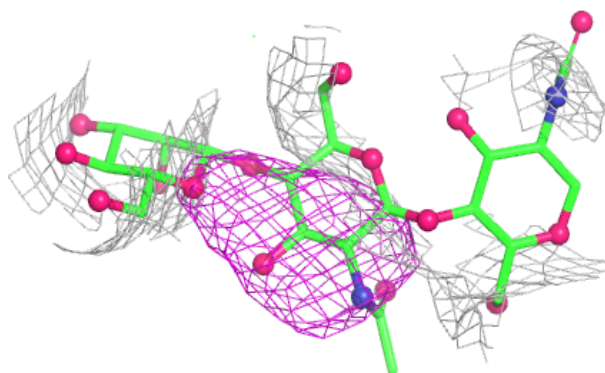
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	MAN	N	6	11/12	-	-	185,186,194,195	0
7	NAG	Q	1	14/15	0.80	0.10	172,173,176,177	0
12	NAG	N	2	14/15	0.80	0.08	179,186,192,195	0
12	NAG	N	1	14/15	0.82	0.09	177,182,187,187	0
13	MAN	R	4	11/12	-	-	207,208,212,212	0
13	MAN	R	5	11/12	-	-	201,203,205,205	0
13	MAN	R	6	11/12	-	-	214,216,217,218	0
13	MAN	R	7	11/12	-	-	199,201,203,204	0
14	NAG	S	2	14/15	0.83	0.11	139,142,145,146	0
9	NAG	O	1	14/15	0.84	0.09	144,145,147,148	0
10	BMA	M	3	11/12	0.86	0.12	166,168,174,175	0
10	MAN	M	4	11/12	0.87	0.13	157,161,165,165	0
10	NAG	M	2	14/15	0.90	0.15	185,191,195,197	0
10	NAG	M	1	14/15	0.94	0.11	184,187,189,190	0
14	NAG	S	1	14/15	0.94	0.11	140,141,143,144	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.

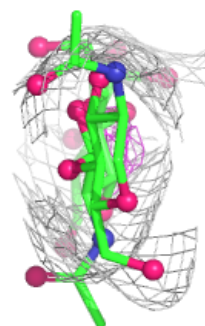
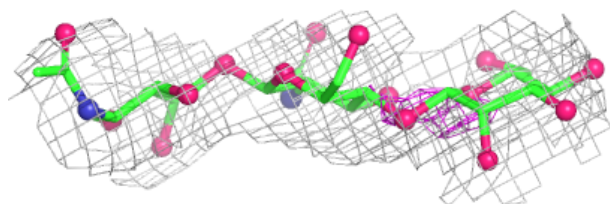
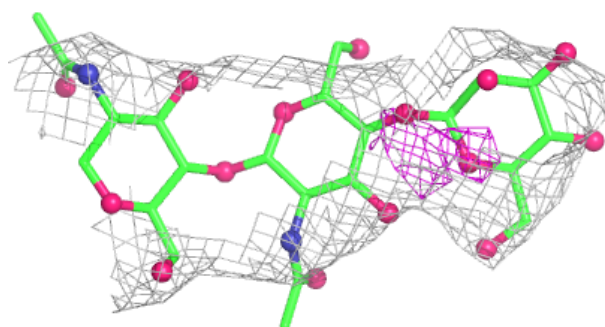


Electron density around Chain I:

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

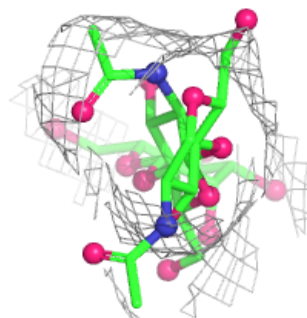
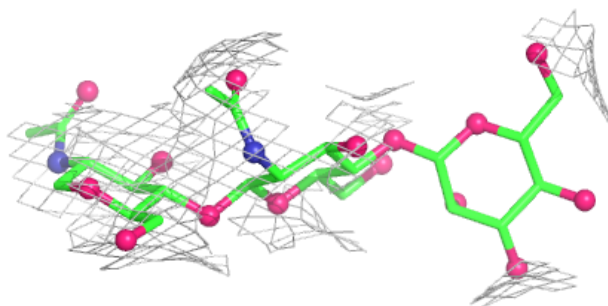
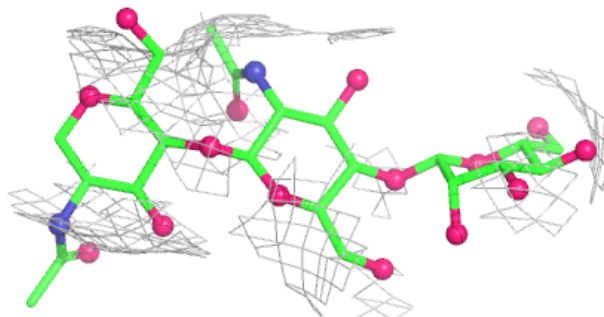
**Electron density around Chain P:**

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

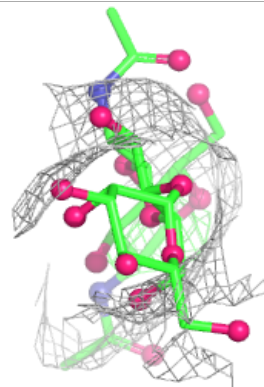
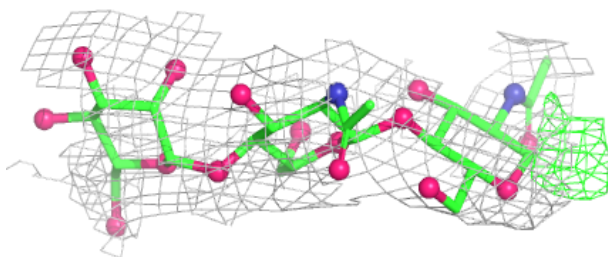
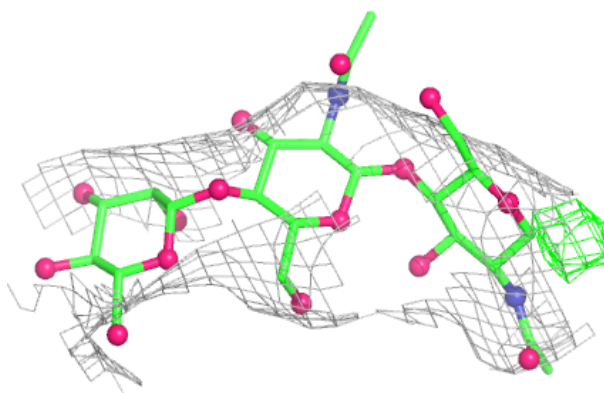


Electron density around Chain Q:

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

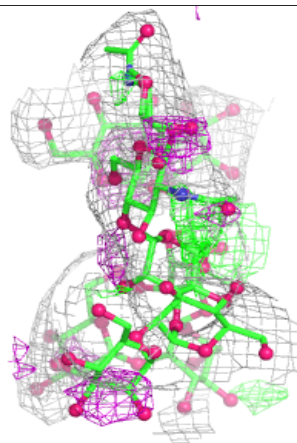
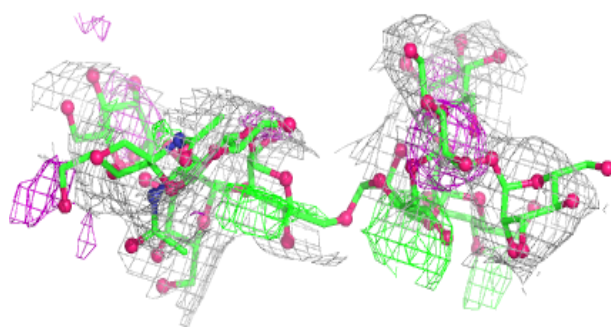
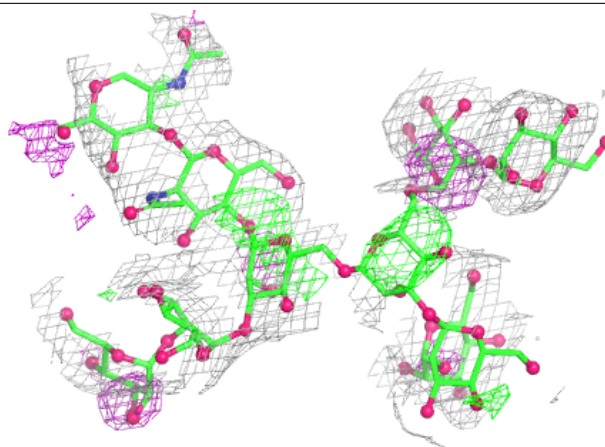
**Electron density around Chain U:**

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



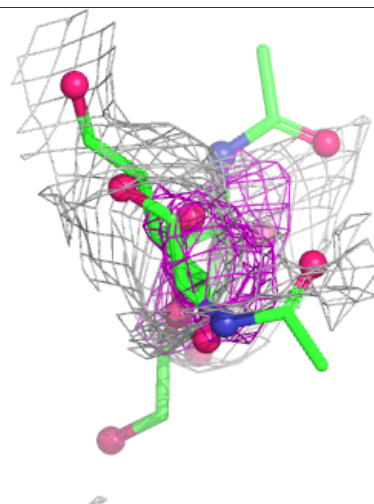
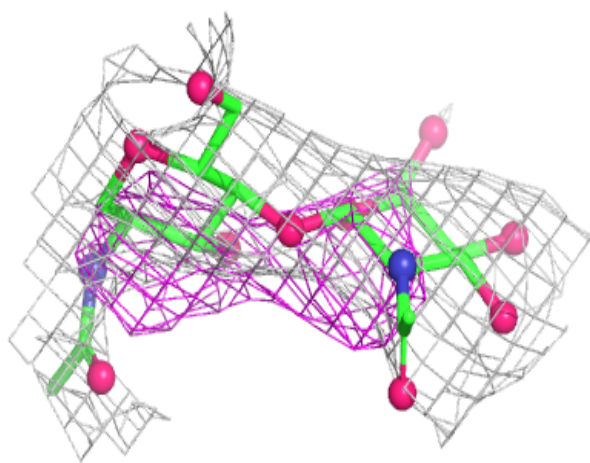
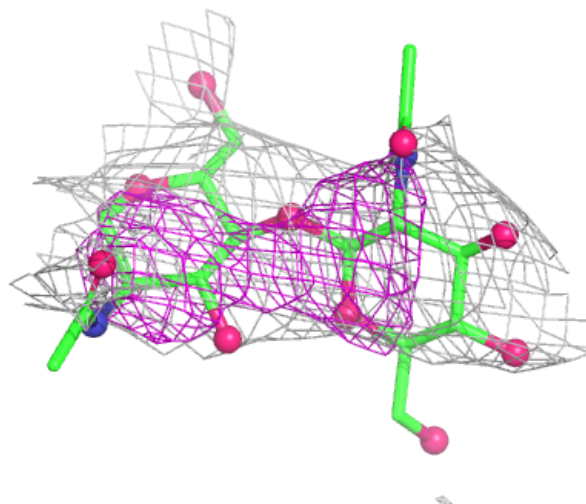
Electron density around Chain B:

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



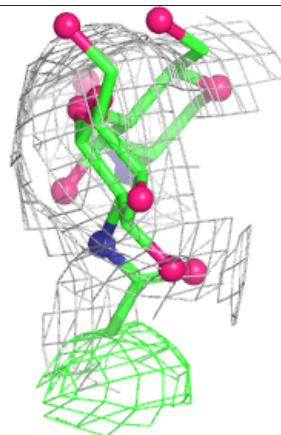
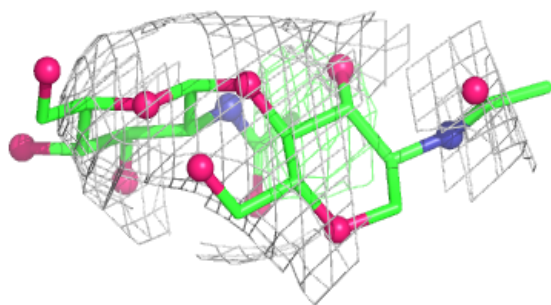
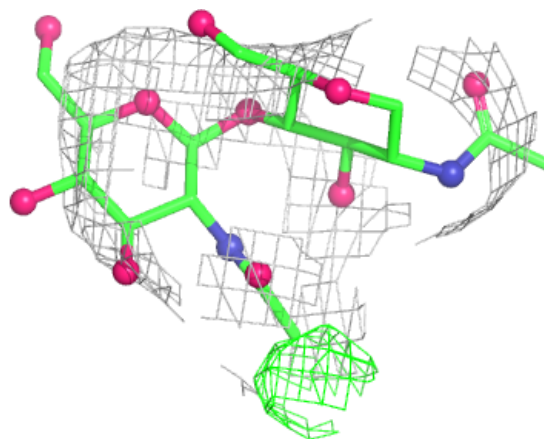
Electron density around Chain C:

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



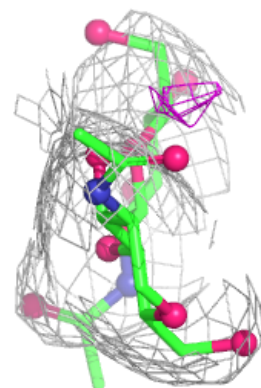
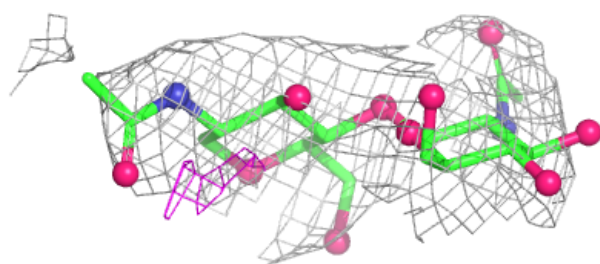
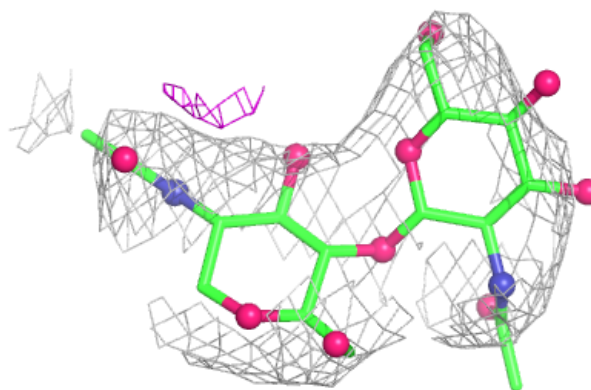
Electron density around Chain F:

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

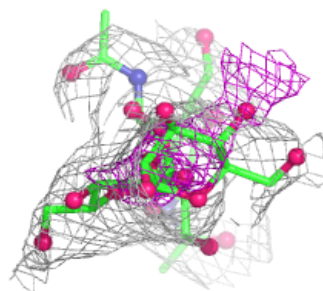
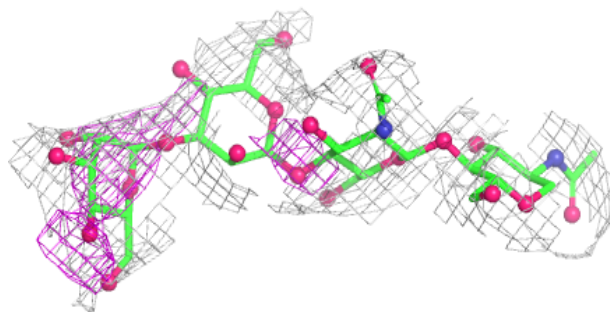
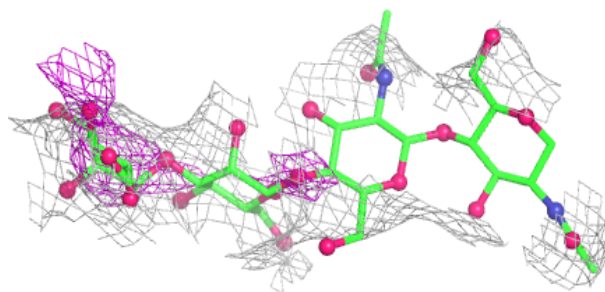


Electron density around Chain O:

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

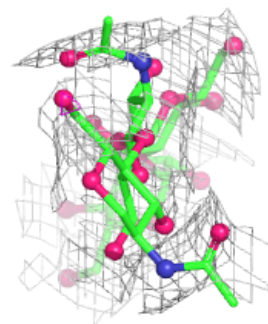
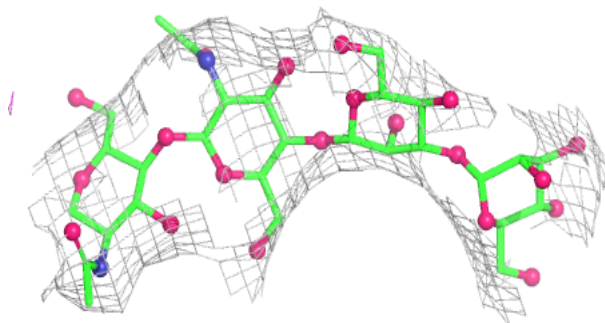
**Electron density around Chain J:**

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

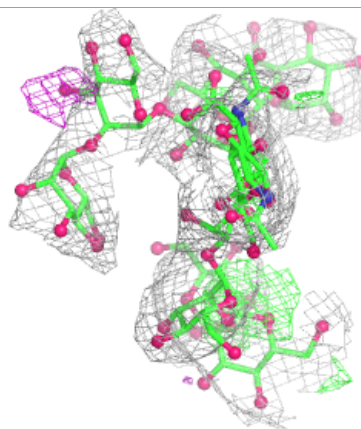
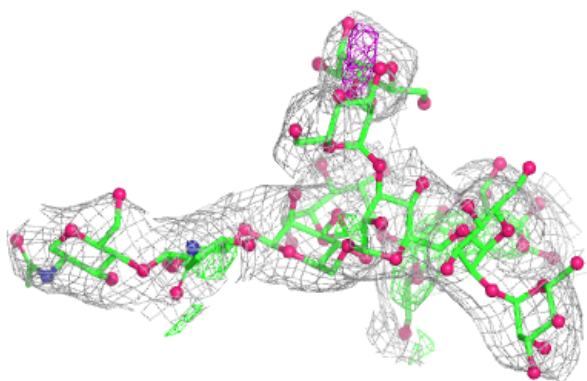
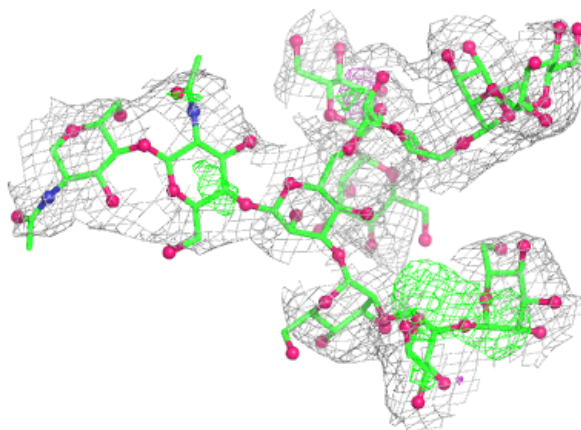


Electron density around Chain M:

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

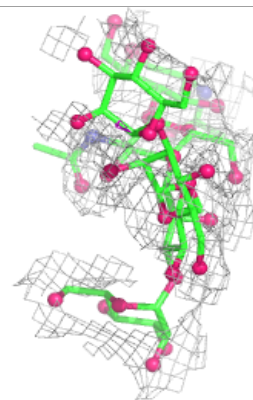
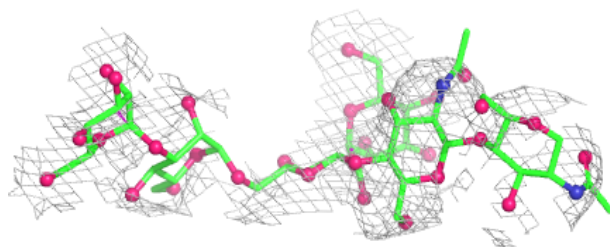
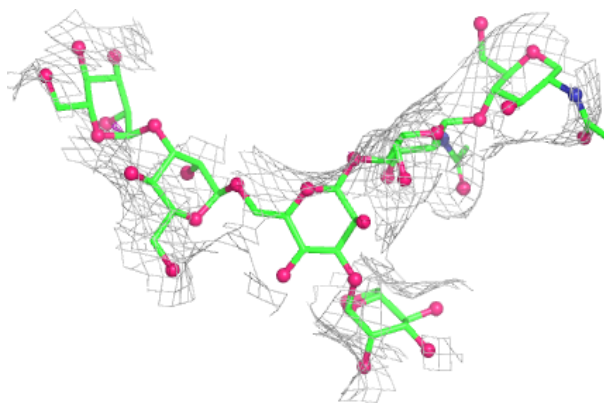
**Electron density around Chain K:**

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



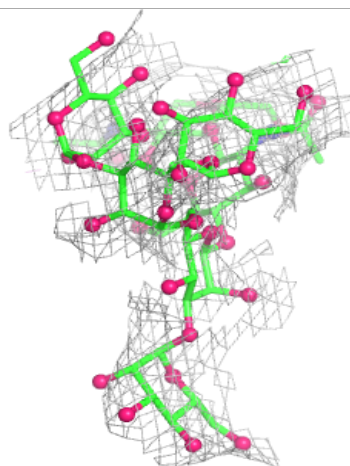
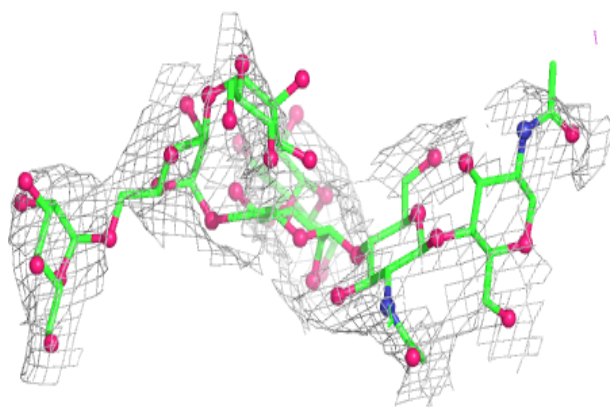
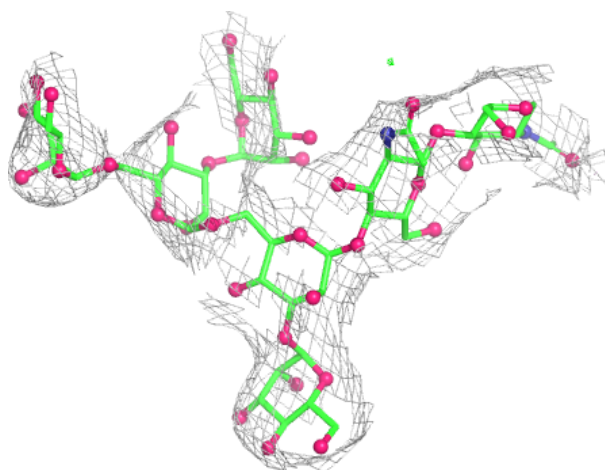
Electron density around Chain N:

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



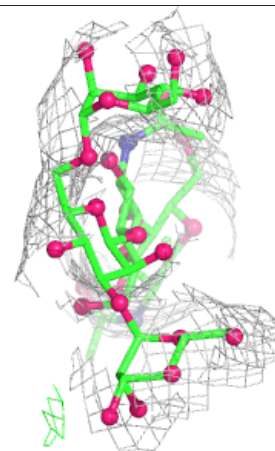
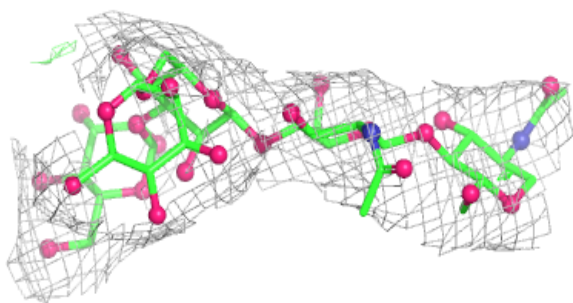
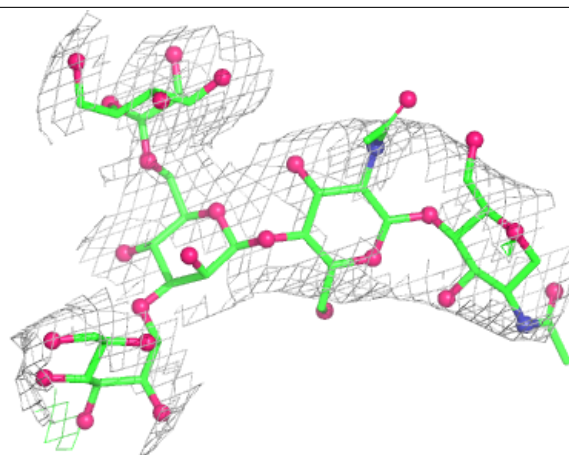
Electron density around Chain R:

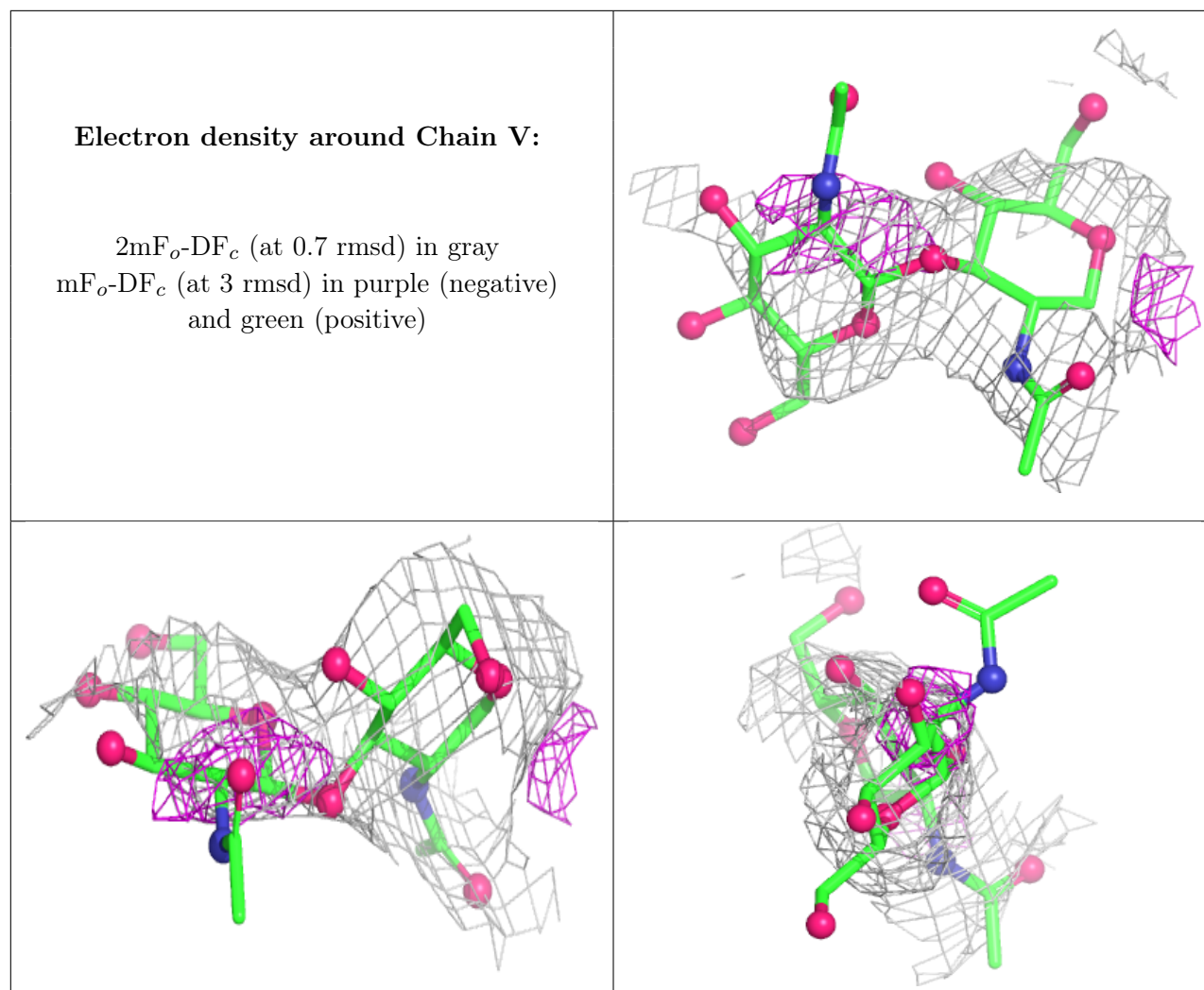
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain S:

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



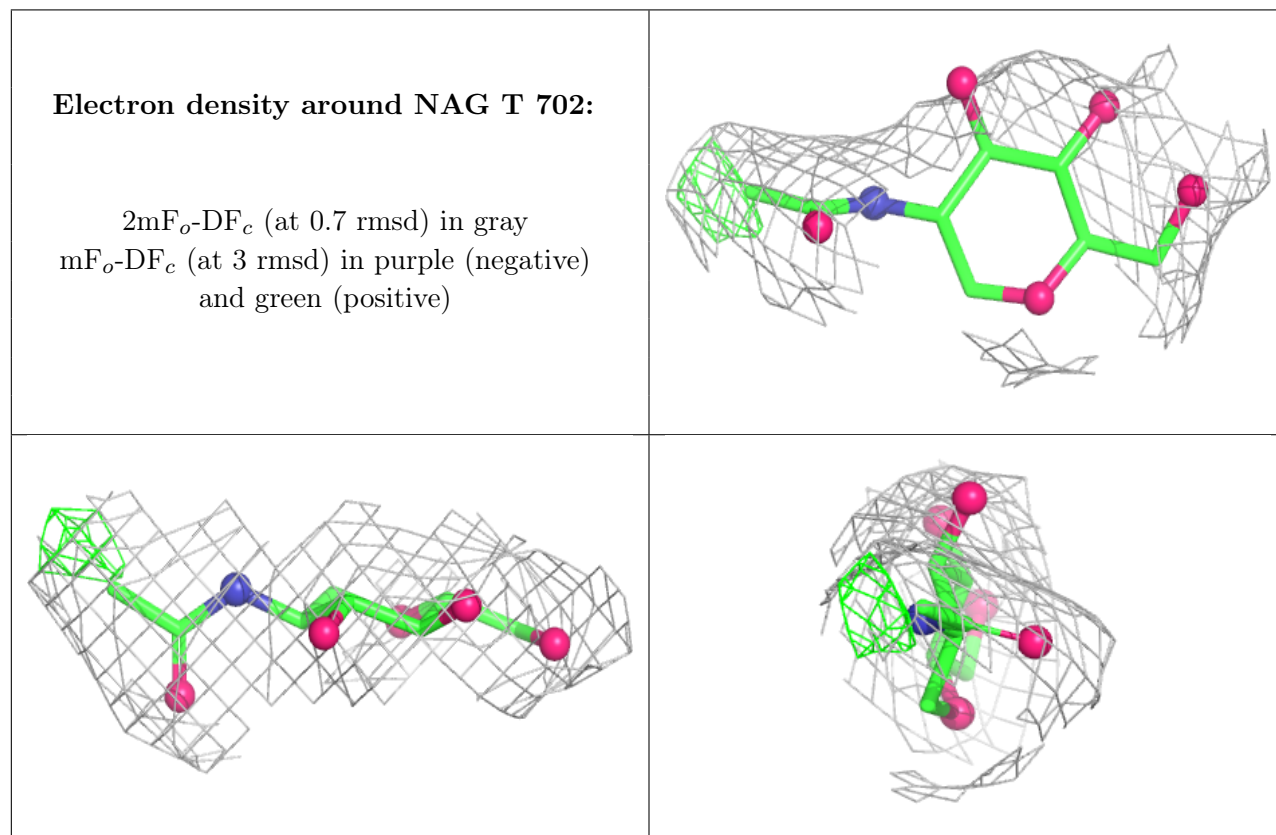


6.4 Ligands [i](#)

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.

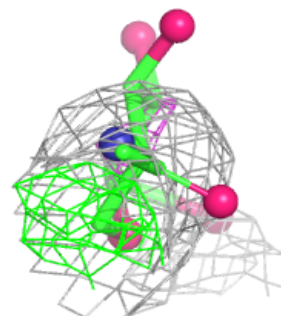
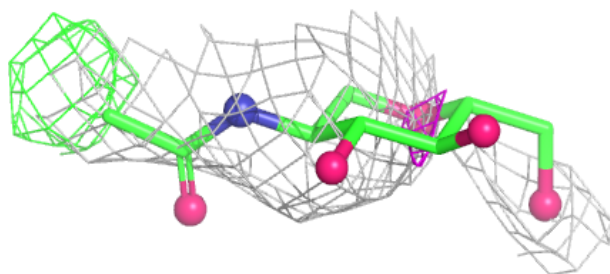
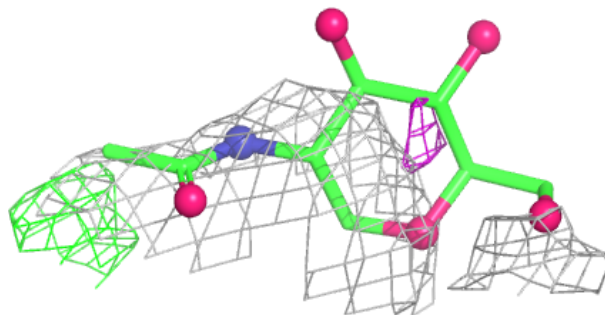
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	NAG	T	702	14/15	0.07	0.12	193,194,197,197	0
16	NAG	G	605	14/15	0.13	0.14	207,209,214,214	0
16	NAG	T	703	14/15	0.24	0.14	187,190,192,193	0
16	NAG	G	601	14/15	0.56	0.10	160,162,166,166	0
16	NAG	G	603	14/15	0.62	0.10	187,192,195,197	0
16	NAG	G	604	14/15	0.72	0.12	191,195,198,198	0
16	NAG	G	602	14/15	0.73	0.12	146,150,153,154	0
16	NAG	T	701	14/15	0.78	0.14	185,188,191,192	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

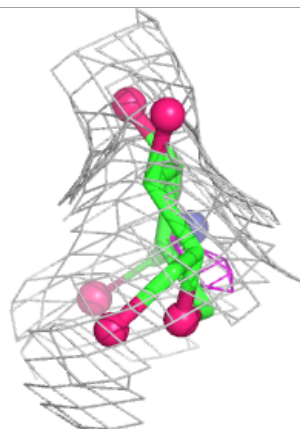
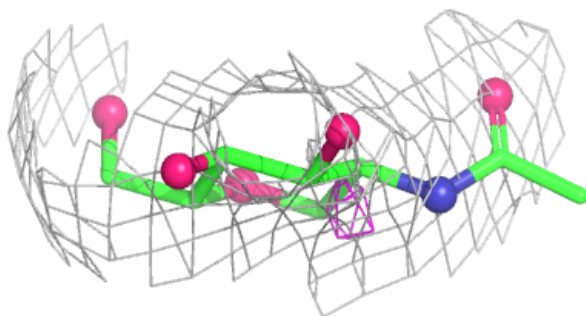
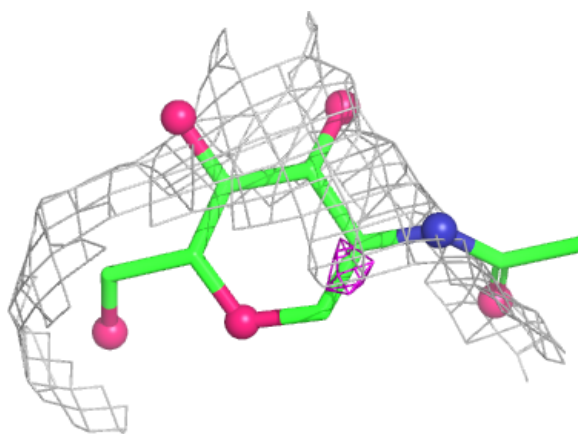


Electron density around NAG G 605:

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

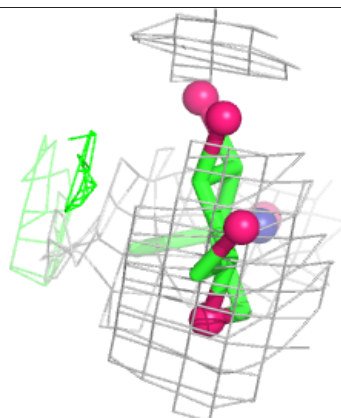
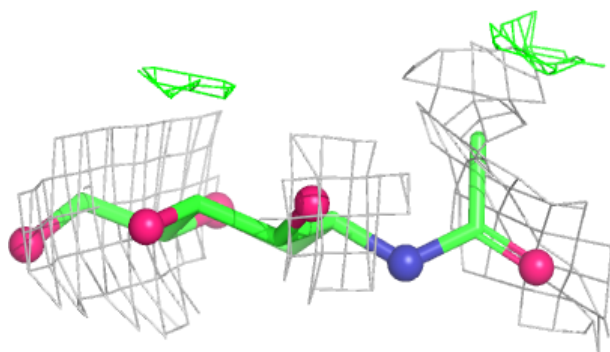
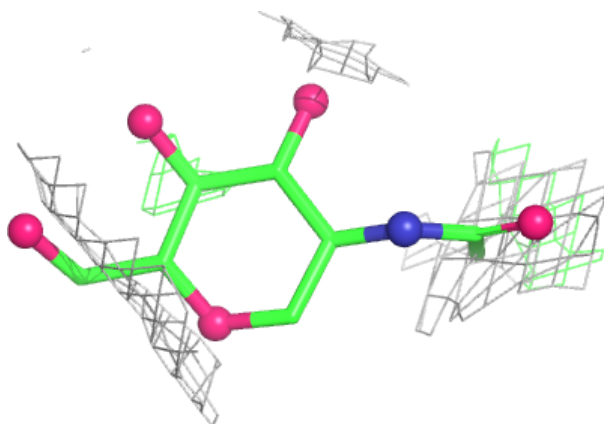
**Electron density around NAG T 703:**

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

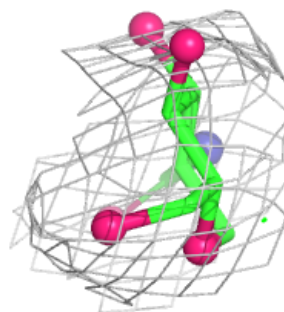
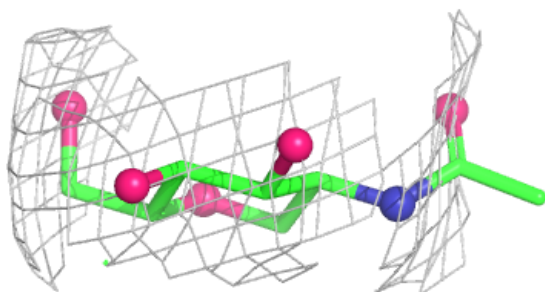
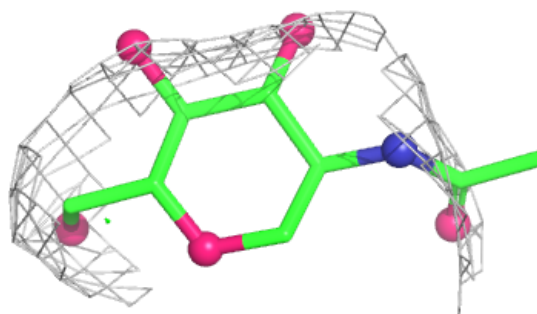


Electron density around NAG G 601:

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

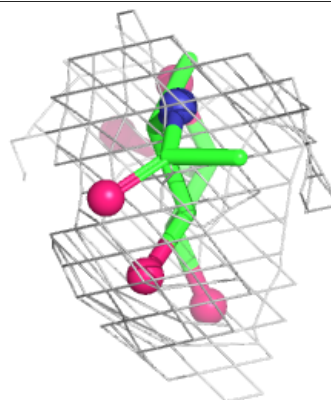
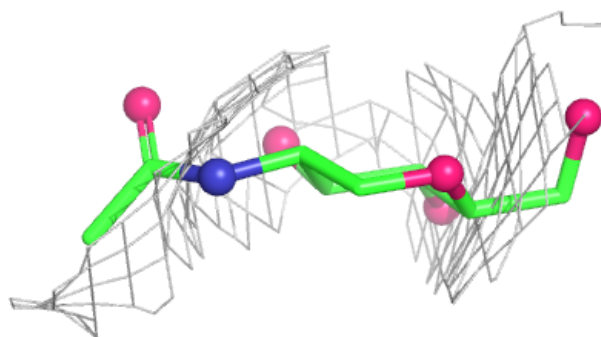
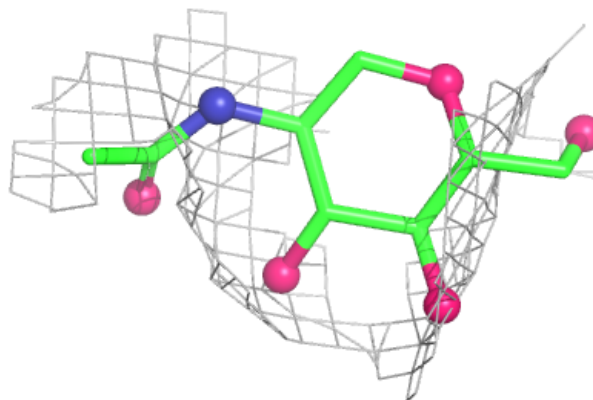
**Electron density around NAG G 603:**

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

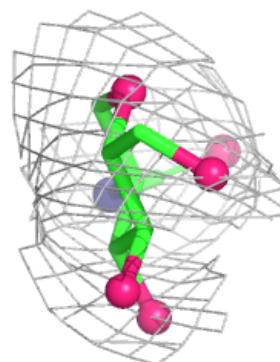
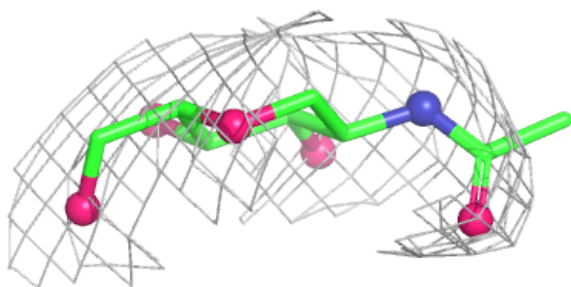
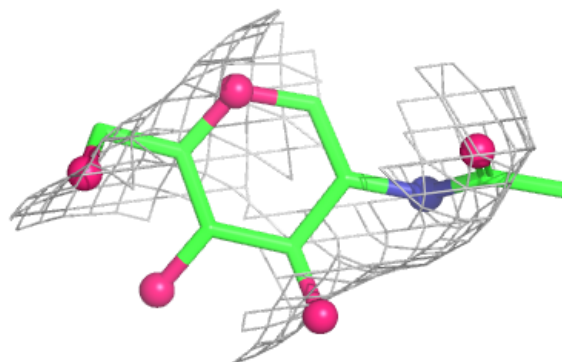


Electron density around NAG G 604:

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

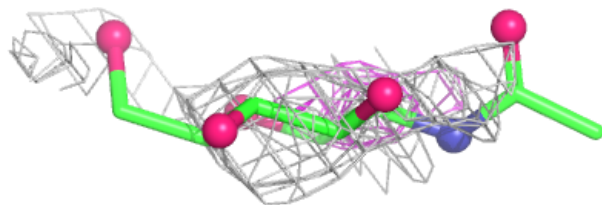
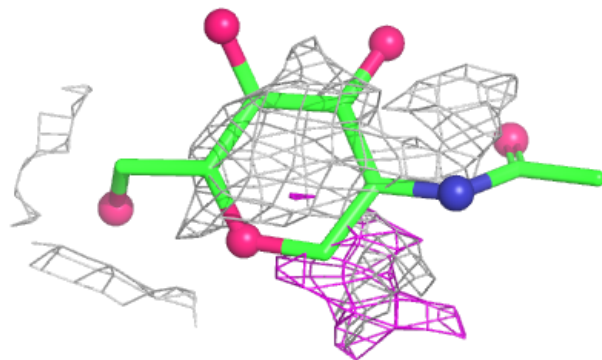
**Electron density around NAG G 602:**

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



Electron density around NAG T 701:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.