



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2020 – 06:19 PM EDT

PDB ID : 6UTK
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

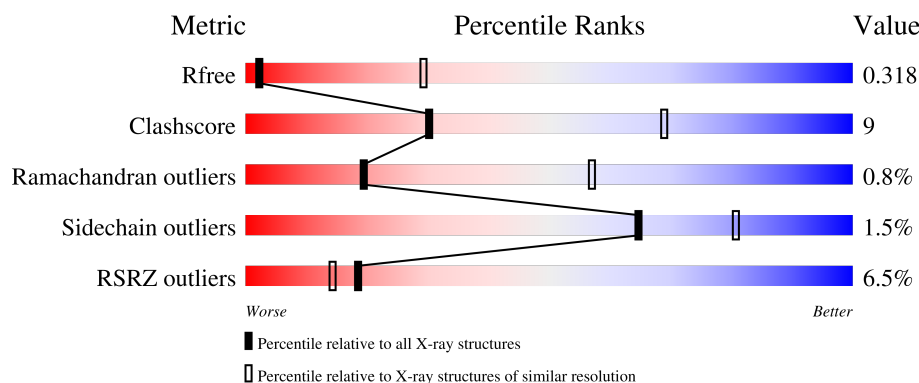
1 Overall quality at a glance

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.





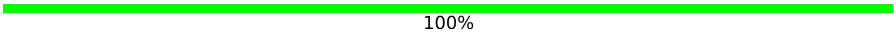
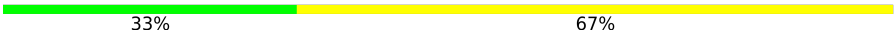

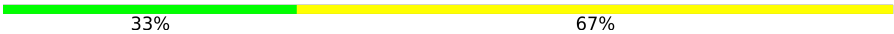
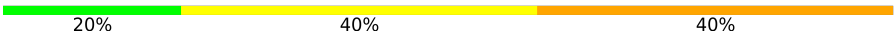

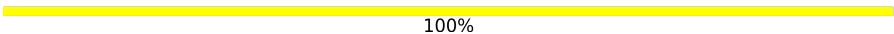
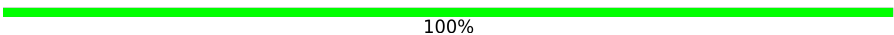


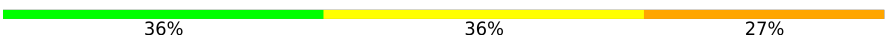



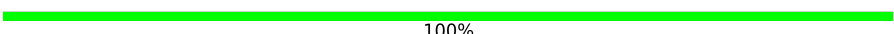
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	E	216	
3	L	213	
4	G	485	
5	T	140	

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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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	MAN	K	9	-	-	-	X
15	NAG	V	1	-	-	-	X
15	NAG	V	2	-	-	-	X
16	NAG	G	605	-	-	-	X
16	NAG	T	701	-	-	-	X
16	NAG	T	703	-	-	-	X
7	NAG	I	2	-	-	-	X
7	BMA	I	3	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	BMA	P	3	-	-	-	X
8	MAN	B	7	-	-	-	X
9	NAG	C	1	-	-	-	X
9	NAG	C	2	-	-	-	X

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			

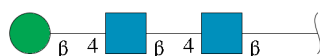
There are 9 discrepancies between the modelled and reference sequences:

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.

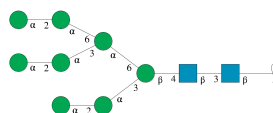
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	231	Total	C	N	O	S	0	0	0
			1747	1109	296	333	9			

- 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.



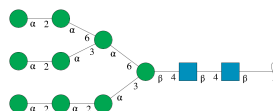
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



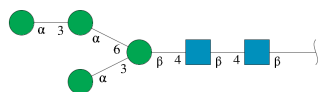
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	4	Total	C	N	O	0	0	0
			50	28	2	20			
10	M	4	Total	C	N	O	0	0	0
			50	28	2	20			

- 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.



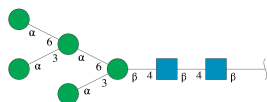
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	K	11	Total	C	N	O	0	0	0
			127	70	2	55			

- 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.



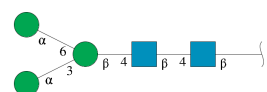
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	N	6	Total	C	N	O	0	0	0
			72	40	2	30			

- 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 (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by author).

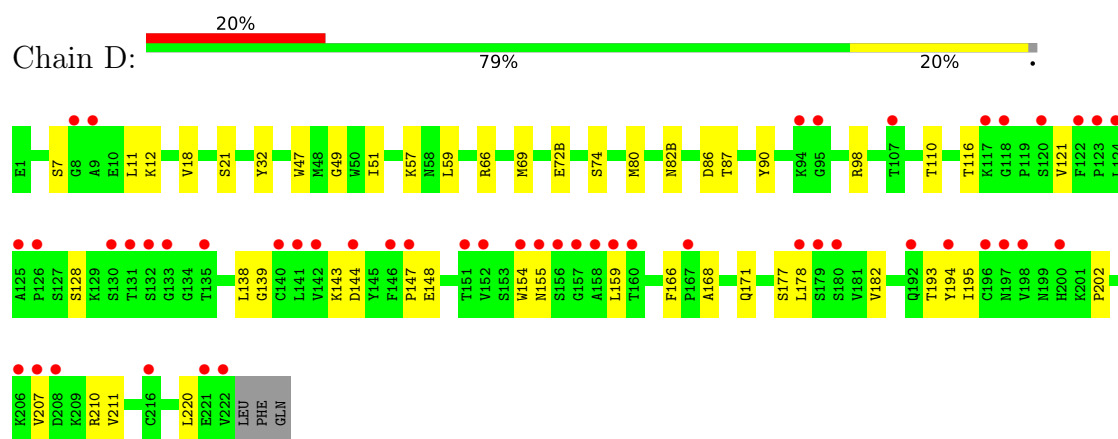


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	G	1	Total	C	N	O	0	0
			14	8	1	5		
16	T	1	Total	C	N	O	0	0
			14	8	1	5		
16	T	1	Total	C	N	O	0	0
			14	8	1	5		
16	T	1	Total	C	N	O	0	0
			14	8	1	5		

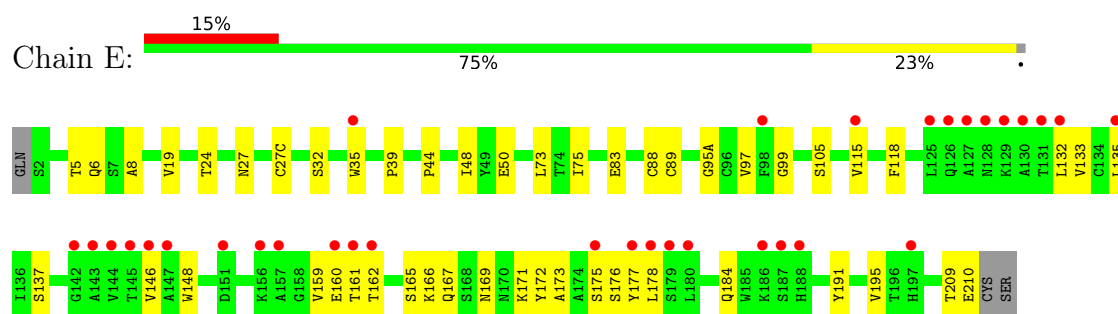
3 Residue-property plots [i](#)

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.

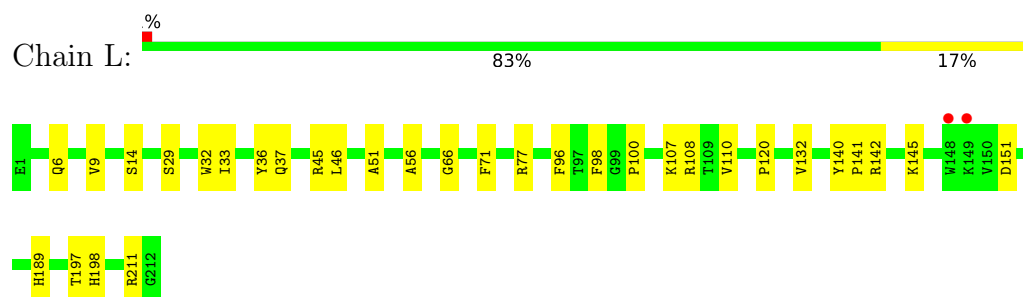
- Molecule 1: 35O22 Fab Heavy Chain



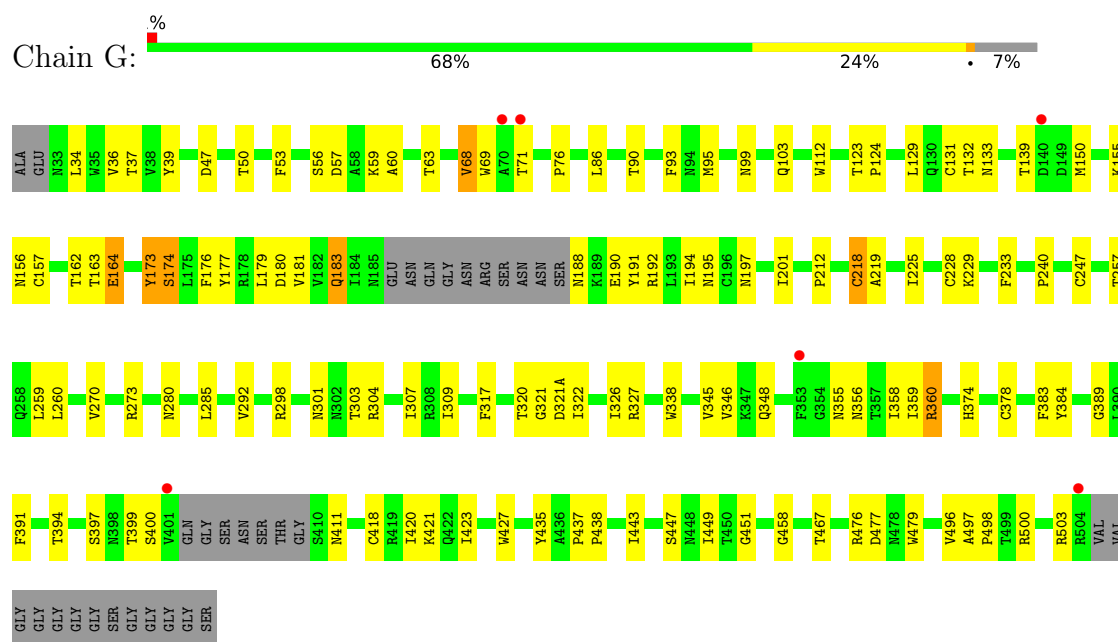
- Molecule 2: 35O22 Fab Light Chain



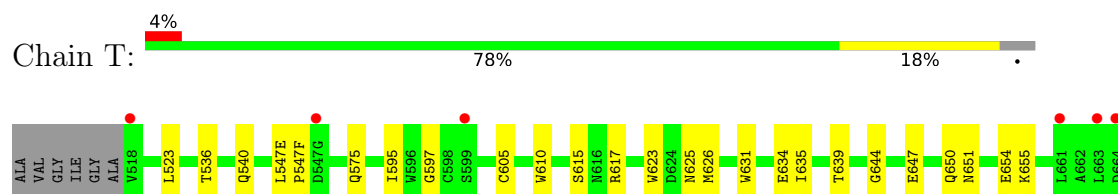
- Molecule 3: B11 Fab Light Chain



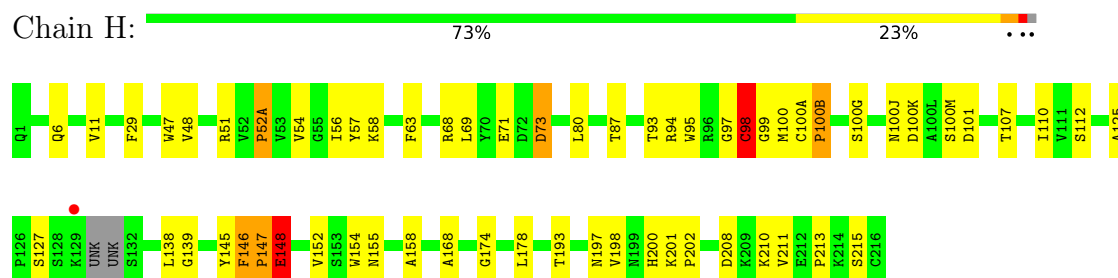
- Molecule 4: Envelope glycoprotein gp120



- 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





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



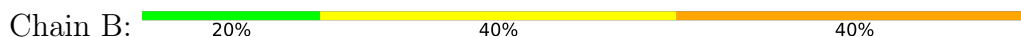
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- 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



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



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



NAG1
NAG2

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

Chain O:  100%

NAG1
NAG2

- 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:  50% 50%

NAG1
NAG2
BMA3
MAN4

- 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:  50% 50%

NAG1
NAG2
BMA3
MAN4

- 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:  36% 36% 27%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9
MAN10
MAN11

- 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%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

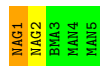
- Molecule 13: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  14% 29% 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	247.31 Å 247.31 Å 257.61 Å 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) 99.6 (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 3.77 Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.299 , 0.317 0.299 , 0.318	Depositor DCC
R_{free} test set	1491 reflections (5.01%)	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)	0.28 , 82.0	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: BMA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	D	0.25	0/1860	0.46	0/2533
2	E	0.24	0/1659	0.43	0/2269
3	L	0.25	0/1669	0.46	0/2267
4	G	0.25	0/3637	0.46	0/4939
5	T	0.23	0/1092	0.43	0/1486
6	H	0.27	0/1793	0.49	0/2442
All	All	0.25	0/11710	0.46	0/15936

There are no bond length outliers.

There are no bond angle outliers.

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	33	0
2	E	1615	0	1544	33	0
3	L	1634	0	1587	21	0
4	G	3563	0	3494	85	0
5	T	1069	0	1033	23	0
6	H	1747	0	1720	39	0
7	A	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4	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	227	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 9.

All (227) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:H:73:ASP:OD1	6:H:73:ASP:N	2.31	0.58
4:G:37:THR:HG22	5:T:605:CYS:HA	1.85	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
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
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.87	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:280:ASN:HD22	4:G:458:GLY:HA3	1.72	0.54
4:G:90:THR:HG22	4:G:240:PRO:HA	1.90	0.54
2:E:27:ASN:HA	2:E:27(C):CYS:HB2	1.90	0.54
4:G:60:ALA:HB1	4:G:71:THR:HG23	1.89	0.54
3:L:96:PHE:HB2	6:H:47:TRP:CG	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:H:168:ALA:HA	6:H:178:LEU:HB3	1.90	0.53
4:G:389:GLY:HA2	12:N:1:NAG:H83	1.90	0.53
4:G:181:VAL:HG11	4:G:192:ARG:HG2	1.90	0.53
3:L:29:SER:HB2	3:L:32:TRP:CD1	2.43	0.53
3:L:6:GLN:HG3	3:L:100:PRO:HD2	1.91	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: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
8:B:1:NAG:O4	8:B:2:NAG:N2	2.44	0.50
2:E:166:LYS:HA	2:E:172:TYR:HD1	1.77	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:G:68:VAL:HG12	4:G:69:TRP:H	1.79	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:152:VAL:HG22	6:H:198:VAL:HG22	1.97	0.47
6:H:112:SER:OG	6:H:174:GLY:O	2.26	0.47
6:H:51:ARG:HG3	6:H:57:TYR:HB3	1.97	0.47
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: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
4:G:47:ASP:N	4:G:47:ASP:OD1	2.48	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
6:H:69:LEU:HD23	6:H:80:LEU:HA	1.97	0.46
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
2:E:162:THR:HG1	2:E:175:SER:H	1.64	0.45
4:G:194:ILE:O	4:G:197:ASN:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:F:1:NAG:H4	9:F:2:NAG:H2	1.62	0.45
6:H:11:VAL:HG22	6:H:110:ILE:HB	1.99	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
6:H:93:THR:HB	6:H:100(M):SER:HB3	1.99	0.45
5:T:644:GLY:HA2	5:T:647:GLU:HG2	1.98	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
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:399:THR:OG1	4:G:400:SER:N	2.51	0.44
4:G:177:TYR:CE1	4:G:420:ILE:HB	2.53	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
4:G:181:VAL:HG13	4:G:183:GLN:H	1.81	0.43
3:L:14:SER:OG	3:L:107:LYS:HB3	2.18	0.43
1:D:69:MET:HG2	1:D:80:MET:HG3	2.00	0.43
4:G:321(A):ASP:N	4:G:321(A):ASP:OD1	2.50	0.43
4:G:285:LEU:HD21	4:G:477:ASP:HB3	2.01	0.43
6:H:58:LYS:HA	6:H:58:LYS:HD2	1.67	0.43
7:P:1:NAG:H61	7:P:2:NAG:N2	2.34	0.43
4:G:36:VAL:HG12	5:T:610:TRP:HE3	1.83	0.43
6:H:139:GLY:HA2	6:H:154:TRP:HH2	1.83	0.43
7:A:1:NAG:H61	7:A:2:NAG:N2	2.33	0.43
4:G:195:ASN:OD1	4:G:201:ILE:HB	2.18	0.43
4:G:34:LEU:HG	5:T:610:TRP:HB3	1.99	0.43
2:E:161:THR:HG23	2:E:176:SER:HB2	1.99	0.43
4:G:183:GLN:HB3	4:G:190:GLU:O	2.19	0.43
4:G:179:LEU:HD13	4:G:421:LYS:HE3	2.00	0.43
3:L:33:ILE:HB	3:L:51:ALA:HB2	2.00	0.43
2:E:184:GLN:O	2:E:191:TYR:OH	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:131:CYS:HA	4:G:157:CYS:HA	2.01	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
4:G:133:ASN:OD1	4:G:155:LYS:NZ	2.41	0.42
3:L:56:ALA:HB2	11:K:11:MAN:H4	2.01	0.42
3:L:36:TYR:HE2	3:L:98:PHE:HE1	1.68	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
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:151:ASP:OD2	3:L:189:HIS:ND1	2.44	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:179:LEU:HG	4:G:179:LEU:O	2.20	0.41
4:G:131:CYS:SG	4:G:191:TYR:HB2	2.60	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
4:G:257:THR:C	4:G:259:LEU:H	2.24	0.41
1:D:177:SER:HB2	2:E:177:TYR:HE2	1.85	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
4:G:95:MET:SD	4:G:273:ARG:HD3	2.60	0.41
4:G:86:LEU:HD22	5:T:523:LEU:O	2.21	0.41
1:D:72(B):GLU:HB2	1:D:74:SER:HB2	2.02	0.41
4:G:194:ILE:HA	4:G:194:ILE:HD13	1.89	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: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
6:H:100(J):ASN:O	11:K:5:MAN:H61	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:635:ILE:O	5:T:639:THR:N	2.54	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%)	29	66
3	L	211/213 (99%)	189 (90%)	21 (10%)	1 (0%)	29	66
4	G	447/485 (92%)	402 (90%)	40 (9%)	5 (1%)	14	51
5	T	132/140 (94%)	114 (86%)	18 (14%)	0	100	100
6	H	227/233 (97%)	205 (90%)	17 (8%)	5 (2%)	6	39
All	All	1466/1530 (96%)	1324 (90%)	130 (9%)	12 (1%)	19	57

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	186 (100%)	0	100	100
3	L	183/183 (100%)	181 (99%)	2 (1%)	73	85
4	G	405/424 (96%)	393 (97%)	12 (3%)	41	66
5	T	116/118 (98%)	116 (100%)	0	100	100
6	H	197/197 (100%)	192 (98%)	5 (2%)	47	70
All	All	1290/1317 (98%)	1271 (98%)	19 (2%)	65	81

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	77	ARG
3	L	211	ARG
4	G	57	ASP
4	G	99	ASN
4	G	164	GLU
4	G	173	TYR
4	G	180	ASP
4	G	218	CYS
4	G	229	LYS
4	G	304	ARG
4	G	327	ARG
4	G	360	ARG

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Mol	Chain	Res	Type
4	G	378	CYS
4	G	500	ARG
6	H	68	ARG
6	H	73	ASP
6	H	98	CYS
6	H	146	PHE
6	H	148	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	164	HIS
2	E	6	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	3,7	14,14,15	0.29	0	17,19,21	0.62	0
7	NAG	A	2	7	14,14,15	0.29	0	17,19,21	0.69	0
7	BMA	A	3	7	11,11,12	0.59	0	15,15,17	0.73	0
8	NAG	B	1	8,4	14,14,15	0.44	0	17,19,21	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	B	10	8	11,11,12	0.28	0	15,15,17	0.88	0
8	NAG	B	2	8	14,14,15	0.42	0	17,19,21	2.09	2 (11%)
8	BMA	B	3	8	11,11,12	1.17	1 (9%)	15,15,17	1.11	1 (6%)
8	MAN	B	4	8	11,11,12	0.65	0	15,15,17	1.72	2 (13%)
8	MAN	B	5	8	11,11,12	0.37	0	15,15,17	1.01	1 (6%)
8	MAN	B	6	8	11,11,12	0.27	0	15,15,17	0.86	0
8	MAN	B	7	8	11,11,12	0.44	0	15,15,17	1.09	2 (13%)
8	MAN	B	8	8	11,11,12	0.29	0	15,15,17	0.80	1 (6%)
8	MAN	B	9	8	11,11,12	1.04	1 (9%)	15,15,17	1.93	5 (33%)
9	NAG	C	1	9,4	14,14,15	0.43	0	17,19,21	1.26	2 (11%)
9	NAG	C	2	9	14,14,15	0.28	0	17,19,21	0.71	0
9	NAG	F	1	9,4	14,14,15	0.27	0	17,19,21	1.08	0
9	NAG	F	2	9	14,14,15	0.42	0	17,19,21	0.72	0
7	NAG	I	1	4,7	14,14,15	0.29	0	17,19,21	0.83	0
7	NAG	I	2	7	14,14,15	0.27	0	17,19,21	0.85	0
7	BMA	I	3	7	11,11,12	0.62	0	15,15,17	0.73	0
10	NAG	J	1	10,4	14,14,15	0.34	0	17,19,21	0.64	0
10	NAG	J	2	10	14,14,15	0.31	0	17,19,21	0.68	0
10	BMA	J	3	10	11,11,12	0.68	0	15,15,17	0.68	0
10	MAN	J	4	10	11,11,12	0.27	0	15,15,17	0.79	1 (6%)
11	NAG	K	1	11,4	14,14,15	0.26	0	17,19,21	0.65	0
11	MAN	K	10	11	11,11,12	0.30	0	15,15,17	1.11	1 (6%)
11	MAN	K	11	11	11,11,12	0.29	0	15,15,17	0.91	1 (6%)
11	NAG	K	2	11	14,14,15	0.32	0	17,19,21	0.83	0
11	BMA	K	3	11	11,11,12	0.55	0	15,15,17	0.87	0
11	MAN	K	4	11	11,11,12	0.25	0	15,15,17	0.98	1 (6%)
11	MAN	K	5	11	11,11,12	0.37	0	15,15,17	1.07	1 (6%)
11	MAN	K	6	11	11,11,12	0.23	0	15,15,17	0.71	0
11	MAN	K	7	11	11,11,12	0.27	0	15,15,17	0.89	0
11	MAN	K	8	11	11,11,12	0.35	0	15,15,17	1.15	2 (13%)
11	MAN	K	9	11	11,11,12	0.33	0	15,15,17	0.94	1 (6%)
10	NAG	M	1	10,4	14,14,15	0.27	0	17,19,21	0.84	0
10	NAG	M	2	10	14,14,15	0.30	0	17,19,21	0.91	1 (5%)
10	BMA	M	3	10	11,11,12	0.70	0	15,15,17	0.74	0
10	MAN	M	4	10	11,11,12	0.27	0	15,15,17	0.81	1 (6%)
12	NAG	N	1	12,4	14,14,15	0.32	0	17,19,21	1.47	3 (17%)
12	NAG	N	2	12	14,14,15	0.31	0	17,19,21	0.92	1 (5%)
12	BMA	N	3	12	11,11,12	0.86	0	15,15,17	0.90	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	N	4	12	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
12	MAN	N	5	12	11,11,12	0.31	0	15,15,17	0.86	1 (6%)
12	MAN	N	6	12	11,11,12	0.32	0	15,15,17	0.93	1 (6%)
9	NAG	O	1	9,4	14,14,15	0.30	0	17,19,21	0.65	0
9	NAG	O	2	9	14,14,15	0.28	0	17,19,21	0.74	0
7	NAG	P	1	4,7	14,14,15	0.29	0	17,19,21	0.92	0
7	NAG	P	2	7	14,14,15	0.31	0	17,19,21	0.73	0
7	BMA	P	3	7	11,11,12	0.63	0	15,15,17	0.85	0
7	NAG	Q	1	4,7	14,14,15	0.32	0	17,19,21	0.91	1 (5%)
7	NAG	Q	2	7	14,14,15	0.33	0	17,19,21	0.91	0
7	BMA	Q	3	7	11,11,12	0.61	0	15,15,17	0.82	0
13	NAG	R	1	13,4	14,14,15	0.30	0	17,19,21	0.60	0
13	NAG	R	2	13	14,14,15	0.34	0	17,19,21	1.92	3 (17%)
13	BMA	R	3	13	11,11,12	0.94	0	15,15,17	1.23	1 (6%)
13	MAN	R	4	13	11,11,12	0.69	0	15,15,17	2.00	4 (26%)
13	MAN	R	5	13	11,11,12	0.66	0	15,15,17	1.66	3 (20%)
13	MAN	R	6	13	11,11,12	0.36	0	15,15,17	0.99	1 (6%)
13	MAN	R	7	13	11,11,12	0.27	0	15,15,17	0.82	1 (6%)
14	NAG	S	1	4,14	14,14,15	0.30	0	17,19,21	1.07	2 (11%)
14	NAG	S	2	14	14,14,15	0.38	0	17,19,21	2.04	4 (23%)
14	BMA	S	3	14	11,11,12	0.62	0	15,15,17	0.78	0
14	MAN	S	4	14	11,11,12	0.24	0	15,15,17	0.81	0
14	MAN	S	5	14	11,11,12	0.25	0	15,15,17	0.83	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	0.31	0	17,19,21	1.23	2 (11%)
7	BMA	U	3	7	11,11,12	1.08	1 (9%)	15,15,17	1.27	3 (20%)
15	NAG	V	1	15,5	14,14,15	0.31	0	17,19,21	0.75	0
15	NAG	V	2	15	14,14,15	0.28	0	17,19,21	0.62	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	3,7	-	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	8,4	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	B	10	8	-	1/2/19/22	0/1/1/1
8	NAG	B	2	8	-	4/6/23/26	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	9,4	-	1/6/23/26	0/1/1/1
9	NAG	C	2	9	-	2/6/23/26	0/1/1/1
9	NAG	F	1	9,4	-	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	10,4	-	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	11,4	-	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	10,4	-	1/6/23/26	0/1/1/1
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	12,4	-	3/6/23/26	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	9,4	-	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	-	2/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	0/2/19/22	0/1/1/1
13	NAG	R	1	13,4	-	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	15,5	-	0/6/23/26	0/1/1/1
15	NAG	V	2	15	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	3	BMA	C1-C2	2.60	1.58	1.52
8	B	9	MAN	C1-C2	2.28	1.57	1.52
8	B	3	BMA	O3-C3	2.03	1.47	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	2	NAG	C2-N2-C7	6.76	132.53	122.90
14	S	2	NAG	C2-N2-C7	6.15	131.67	122.90
13	R	2	NAG	C2-N2-C7	6.00	131.45	122.90
8	B	9	MAN	C1-C2-C3	4.47	115.16	109.67
13	R	5	MAN	C1-C2-C3	4.43	115.11	109.67
12	N	1	NAG	O4-C4-C3	-4.14	100.78	110.35
13	R	4	MAN	C6-C5-C4	-3.95	103.75	113.00
13	R	4	MAN	C1-C2-C3	3.84	114.38	109.67
8	B	4	MAN	O3-C3-C2	3.74	117.15	109.99
8	B	4	MAN	O5-C1-C2	-3.67	105.11	110.77
8	B	2	NAG	C8-C7-N2	3.52	122.06	116.10
13	R	4	MAN	O5-C1-C2	-3.35	105.61	110.77
13	R	5	MAN	O5-C1-C2	-3.16	105.90	110.77
14	S	2	NAG	C8-C7-N2	3.04	121.24	116.10
13	R	4	MAN	O3-C3-C4	-2.93	103.58	110.35
13	R	2	NAG	C1-C2-N2	2.92	115.48	110.49
14	S	2	NAG	C1-C2-N2	2.85	115.36	110.49
11	K	9	MAN	O5-C1-C2	-2.82	106.42	110.77
12	N	6	MAN	O5-C1-C2	-2.80	106.45	110.77
8	B	9	MAN	O2-C2-C1	2.77	114.82	109.15
13	R	5	MAN	O5-C5-C6	2.76	111.53	107.20
13	R	3	BMA	C6-C5-C4	2.74	119.43	113.00
8	B	9	MAN	O5-C1-C2	-2.74	106.54	110.77
8	B	9	MAN	O5-C5-C6	2.74	111.49	107.20
13	R	2	NAG	C8-C7-N2	2.69	120.65	116.10
7	U	3	BMA	C1-C2-C3	-2.68	106.38	109.67
8	B	5	MAN	O5-C1-C2	-2.65	106.68	110.77
12	N	4	MAN	O5-C1-C2	-2.64	106.69	110.77
7	U	2	NAG	O4-C4-C3	-2.62	104.30	110.35
7	U	2	NAG	O5-C1-C2	-2.59	107.19	111.29
8	B	9	MAN	O2-C2-C3	2.54	115.23	110.14
8	B	3	BMA	O3-C3-C2	2.51	114.80	109.99
11	K	4	MAN	O5-C1-C2	-2.44	107.01	110.77
9	C	1	NAG	O4-C4-C5	-2.44	103.24	109.30
7	U	3	BMA	O2-C2-C3	-2.43	105.28	110.14
11	K	10	MAN	O2-C2-C1	2.41	114.08	109.15
12	N	5	MAN	O5-C1-C2	-2.38	107.09	110.77
11	K	5	MAN	C1-C2-C3	-2.32	106.82	109.67
14	S	1	NAG	O5-C1-C2	-2.30	107.65	111.29
13	R	6	MAN	O5-C1-C2	-2.29	107.23	110.77
12	N	1	NAG	C1-O5-C5	-2.27	109.12	112.19
10	M	4	MAN	O5-C1-C2	-2.24	107.31	110.77
11	K	8	MAN	O5-C1-C2	-2.23	107.33	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	7	MAN	O5-C1-C2	-2.22	107.34	110.77
14	S	1	NAG	C2-N2-C7	2.20	126.03	122.90
13	R	7	MAN	O5-C1-C2	-2.17	107.42	110.77
8	B	7	MAN	C1-C2-C3	2.16	112.33	109.67
12	N	3	BMA	O2-C2-C3	-2.14	105.85	110.14
7	Q	1	NAG	C1-O5-C5	2.12	115.07	112.19
8	B	8	MAN	O5-C1-C2	-2.10	107.52	110.77
11	K	11	MAN	C1-O5-C5	-2.10	109.34	112.19
11	K	8	MAN	O2-C2-C1	-2.10	104.86	109.15
7	U	3	BMA	O5-C1-C2	-2.10	107.53	110.77
9	C	1	NAG	O4-C4-C3	-2.09	105.51	110.35
12	N	2	NAG	O5-C1-C2	-2.09	107.99	111.29
10	J	4	MAN	O5-C1-C2	-2.08	107.55	110.77
14	S	2	NAG	O5-C1-C2	-2.08	108.00	111.29
12	N	1	NAG	O4-C4-C5	-2.08	104.14	109.30
10	M	2	NAG	O5-C1-C2	-2.05	108.05	111.29

There are no chirality outliers.

All (95) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
9	C	2	NAG	C4-C5-C6-O6
7	I	2	NAG	C4-C5-C6-O6
7	P	1	NAG	C4-C5-C6-O6
8	B	2	NAG	C8-C7-N2-C2
8	B	2	NAG	O7-C7-N2-C2
7	I	1	NAG	C8-C7-N2-C2
7	I	1	NAG	O7-C7-N2-C2
10	M	2	NAG	C8-C7-N2-C2
11	K	9	MAN	O5-C5-C6-O6
11	K	7	MAN	O5-C5-C6-O6
8	B	3	BMA	O5-C5-C6-O6
11	K	5	MAN	O5-C5-C6-O6
13	R	2	NAG	C1-C2-N2-C7
8	B	8	MAN	O5-C5-C6-O6
10	M	4	MAN	C4-C5-C6-O6
7	U	2	NAG	O5-C5-C6-O6
7	U	2	NAG	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
10	M	2	NAG	C1-C2-N2-C7
11	K	2	NAG	C8-C7-N2-C2
11	K	5	MAN	C4-C5-C6-O6
9	O	1	NAG	O5-C5-C6-O6
12	N	5	MAN	O5-C5-C6-O6
10	J	4	MAN	C4-C5-C6-O6
9	O	1	NAG	C4-C5-C6-O6
13	R	4	MAN	O5-C5-C6-O6
13	R	7	MAN	O5-C5-C6-O6
14	S	2	NAG	C1-C2-N2-C7
8	B	7	MAN	O5-C5-C6-O6
8	B	10	MAN	O5-C5-C6-O6
13	R	5	MAN	O5-C5-C6-O6
7	Q	2	NAG	O5-C5-C6-O6
11	K	3	BMA	C4-C5-C6-O6
7	U	1	NAG	O5-C5-C6-O6
13	R	2	NAG	O5-C5-C6-O6
9	F	1	NAG	O5-C5-C6-O6
13	R	6	MAN	O5-C5-C6-O6
11	K	2	NAG	O7-C7-N2-C2
7	I	3	BMA	O5-C5-C6-O6
11	K	11	MAN	O5-C5-C6-O6

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

There are no ring outliers.

24 monomers are involved in 17 short contacts:

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

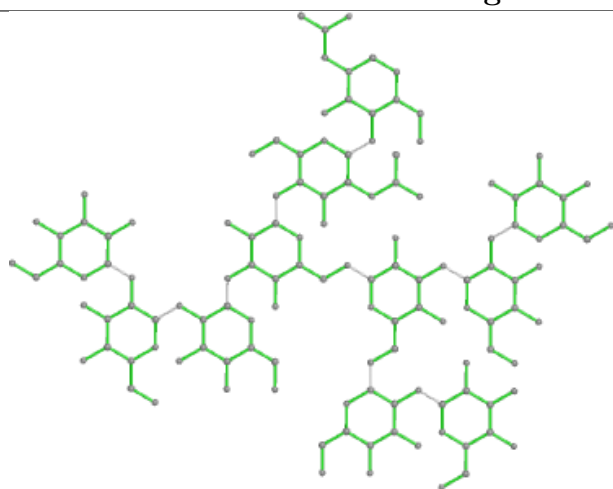
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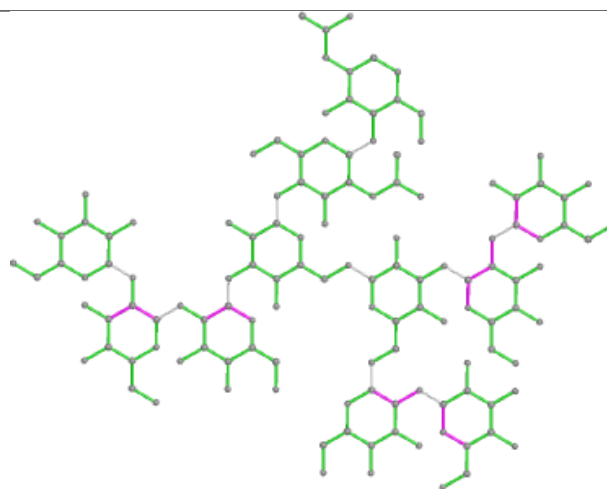
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2	NAG	1	0
13	R	4	MAN	2	0
7	A	1	NAG	1	0
11	K	10	MAN	1	0
10	J	1	NAG	1	0
11	K	11	MAN	1	0
7	P	1	NAG	1	0
11	K	7	MAN	1	0
13	R	3	BMA	1	0
9	F	2	NAG	1	0
8	B	1	NAG	1	0
12	N	1	NAG	1	0
14	S	1	NAG	1	0
13	R	2	NAG	1	0
8	B	4	MAN	1	0
8	B	3	BMA	1	0
12	N	3	BMA	1	0
13	R	5	MAN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

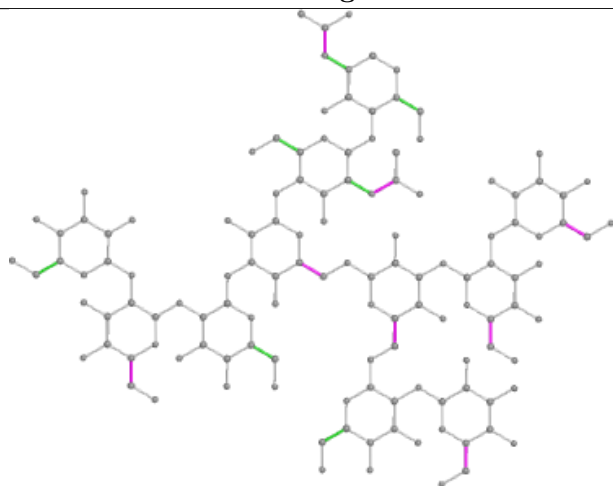
Oligosaccharide Chain K



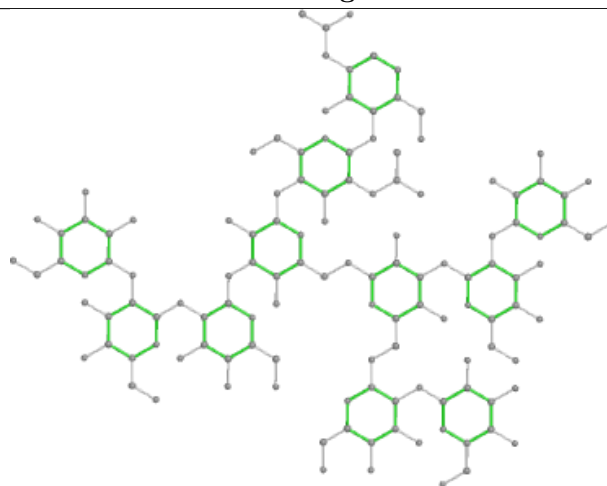
Bond lengths



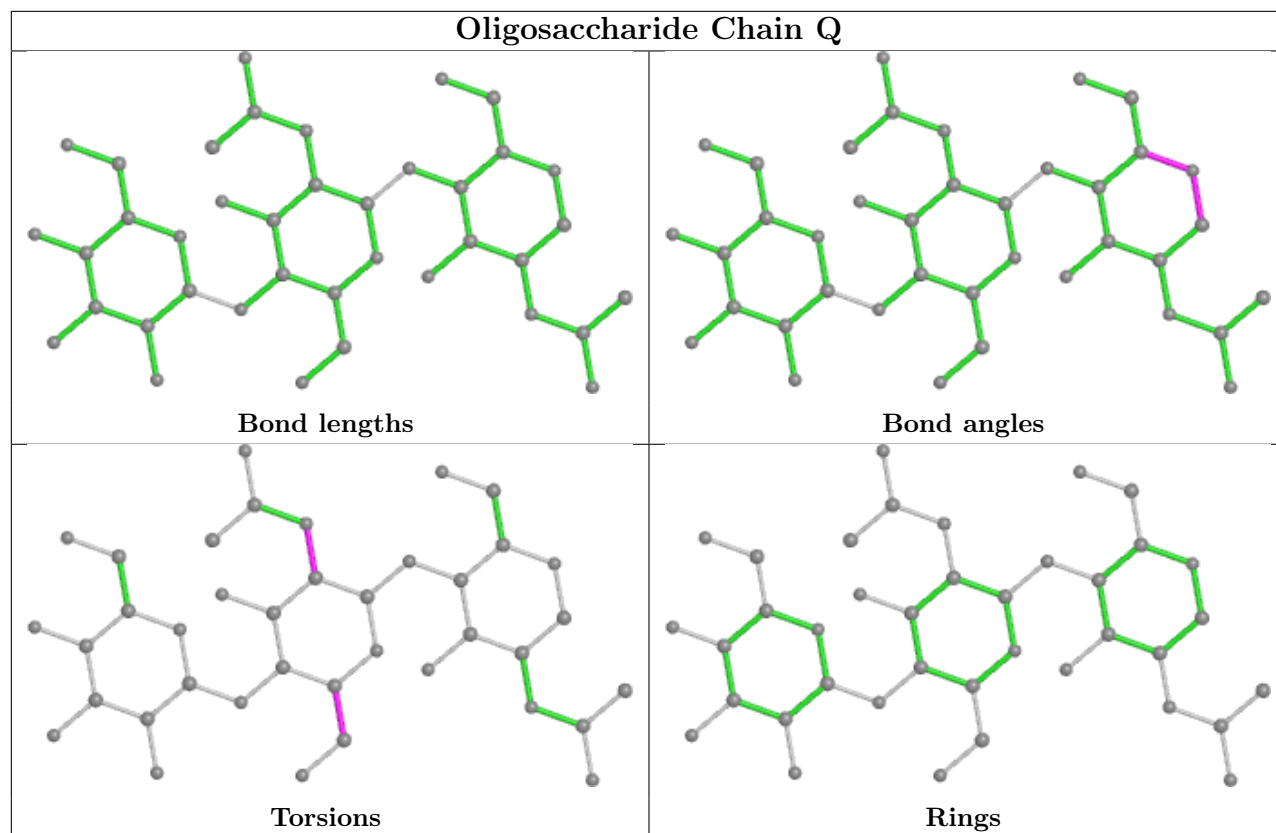
Bond angles

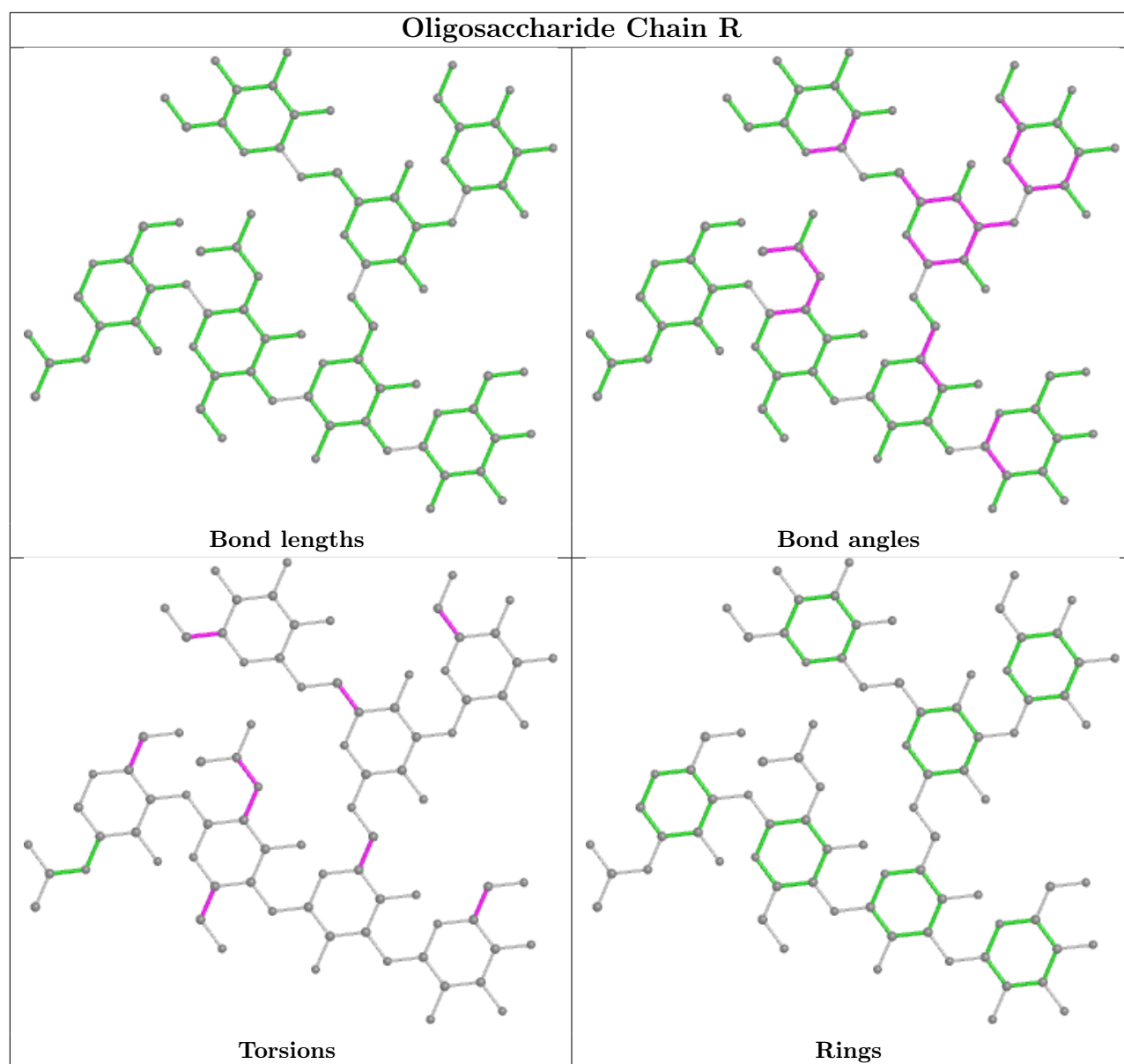


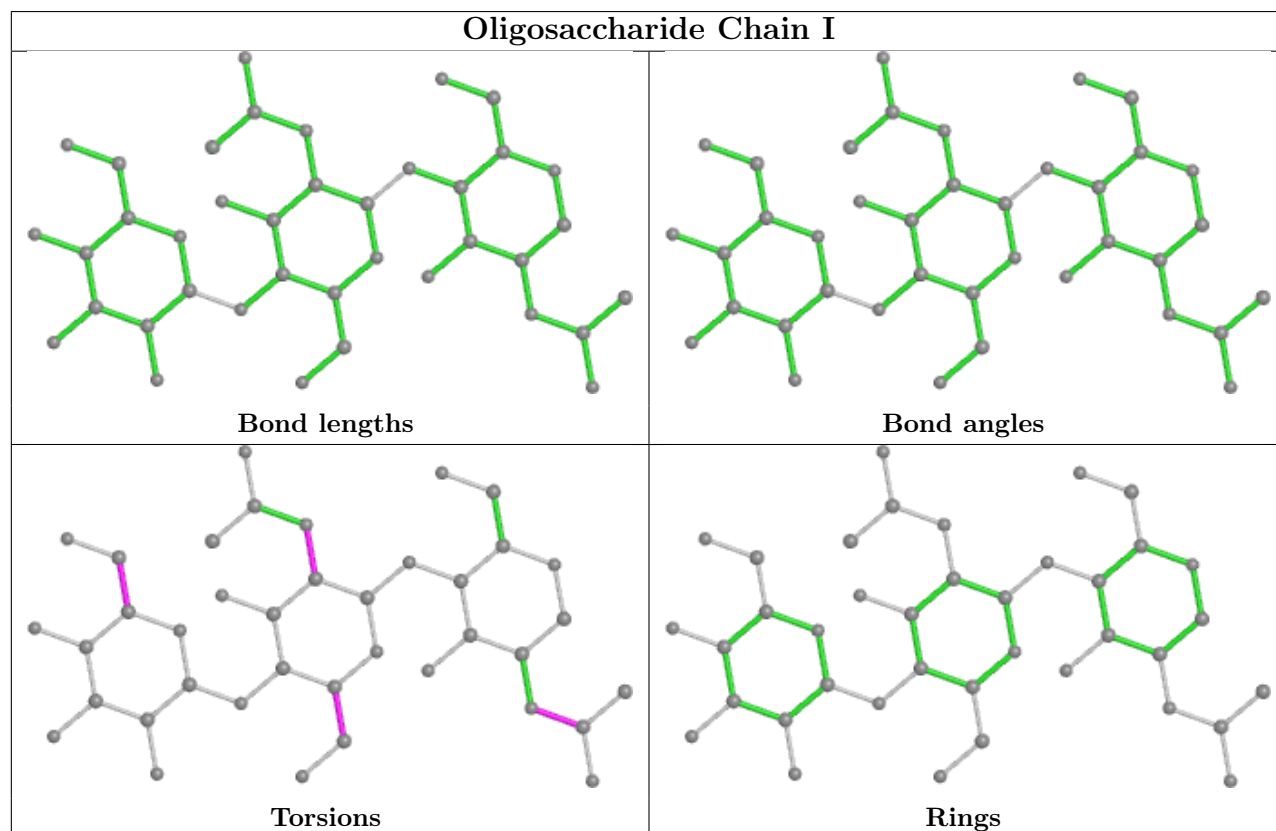
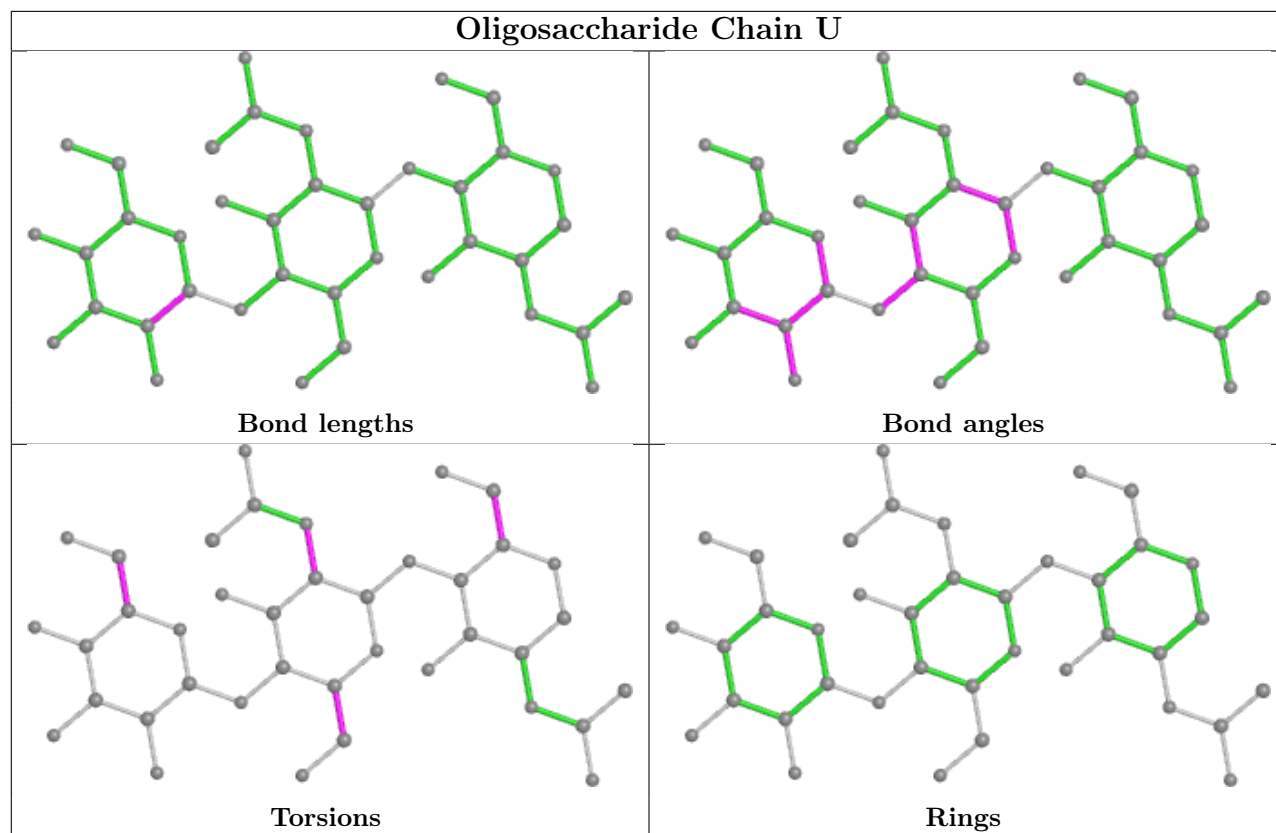
Torsions

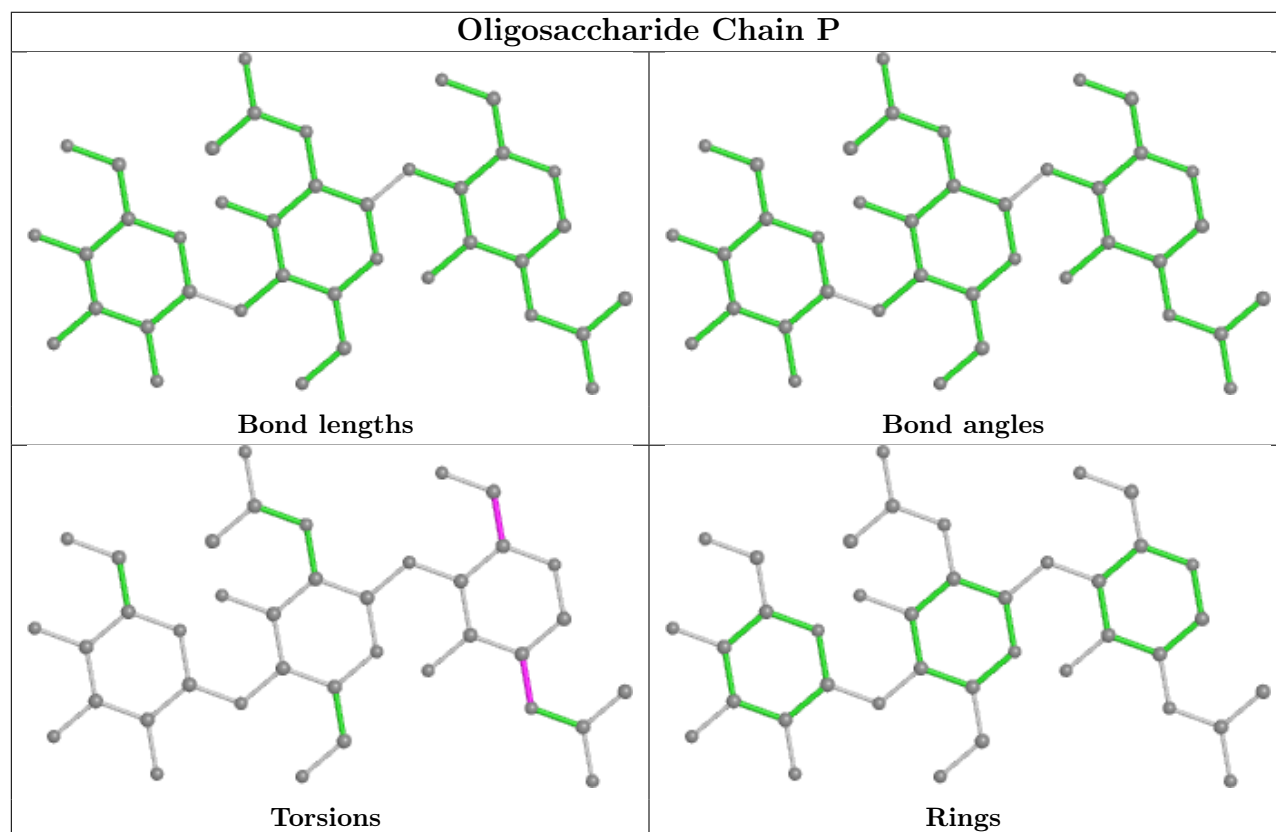
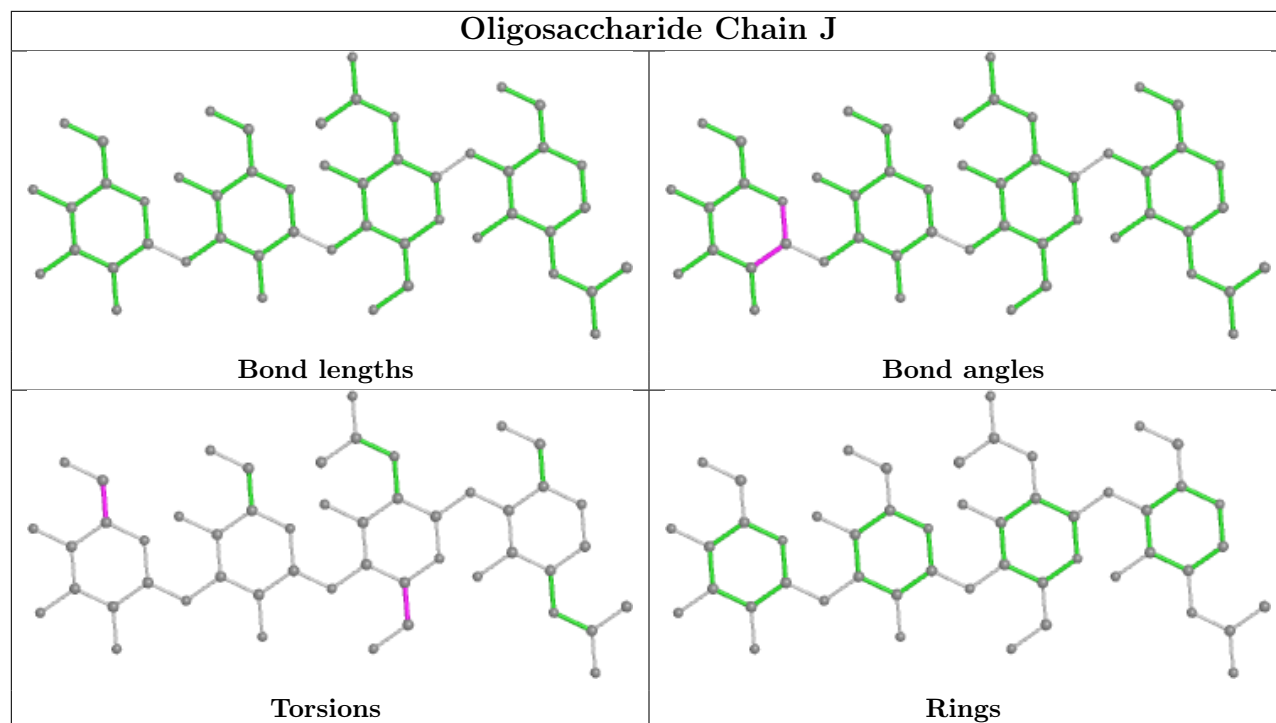


Rings

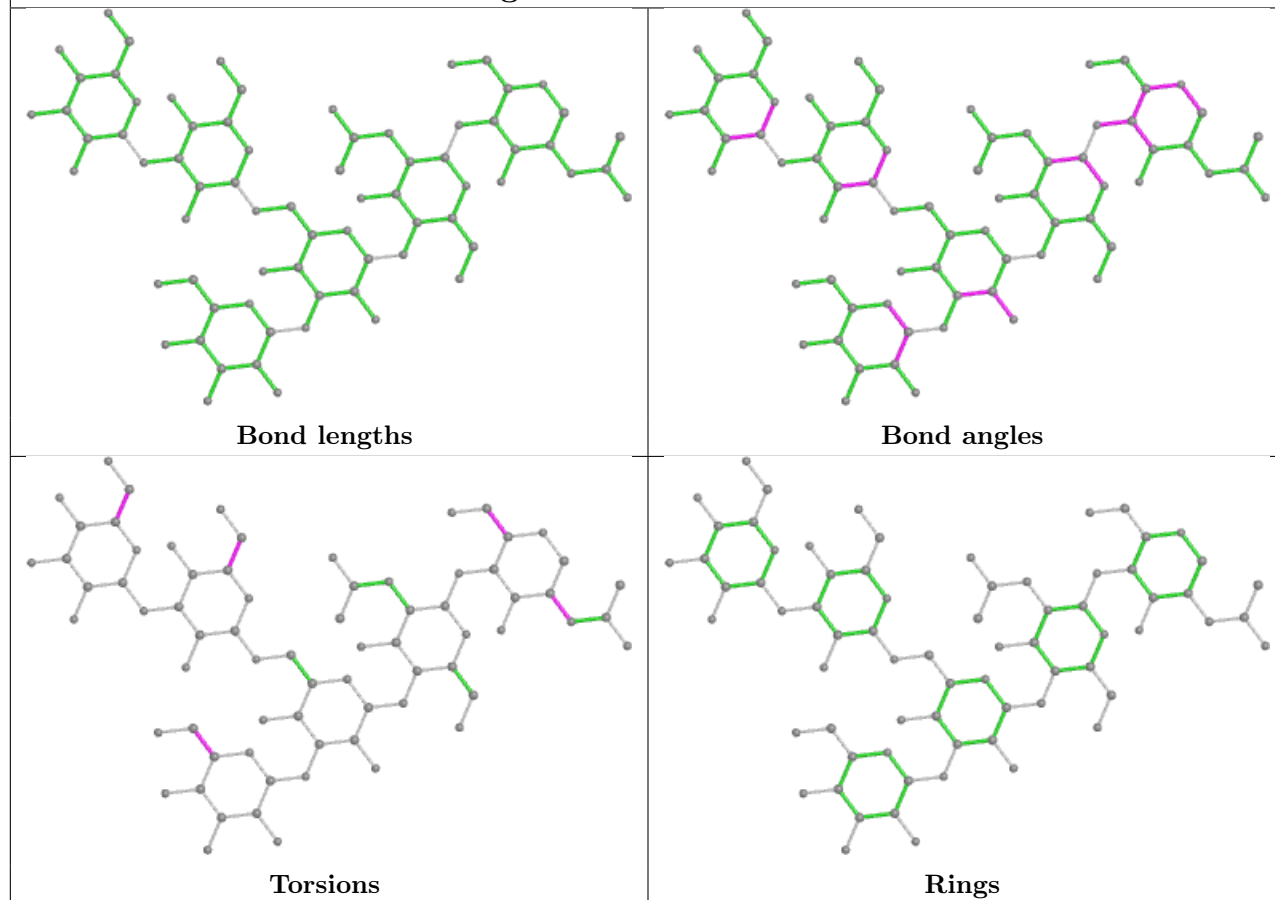




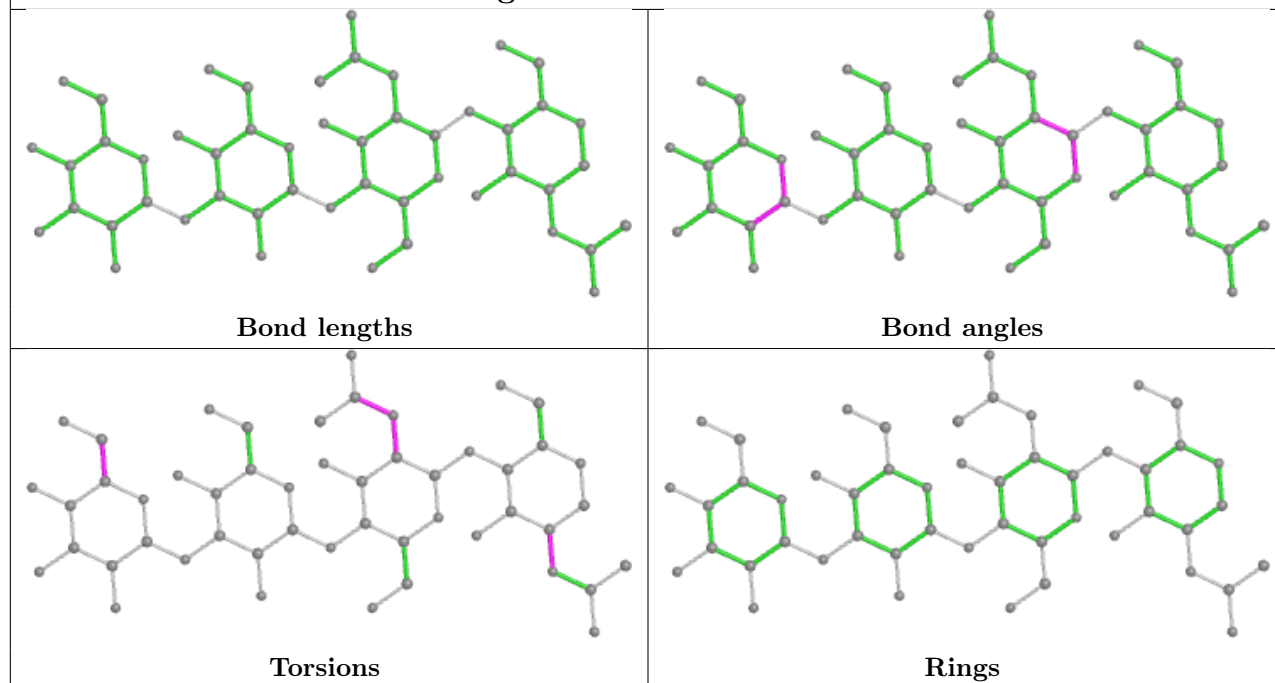


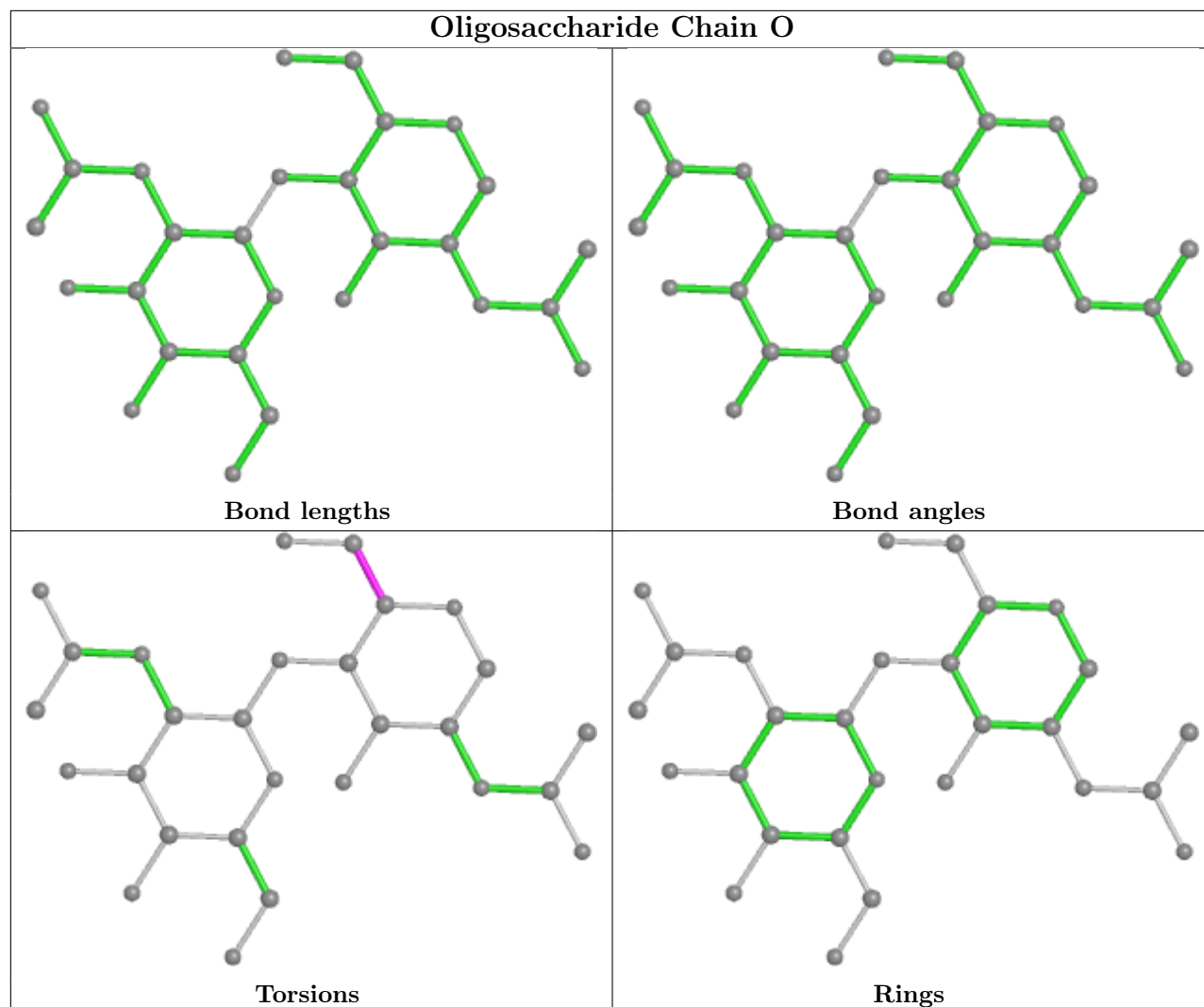


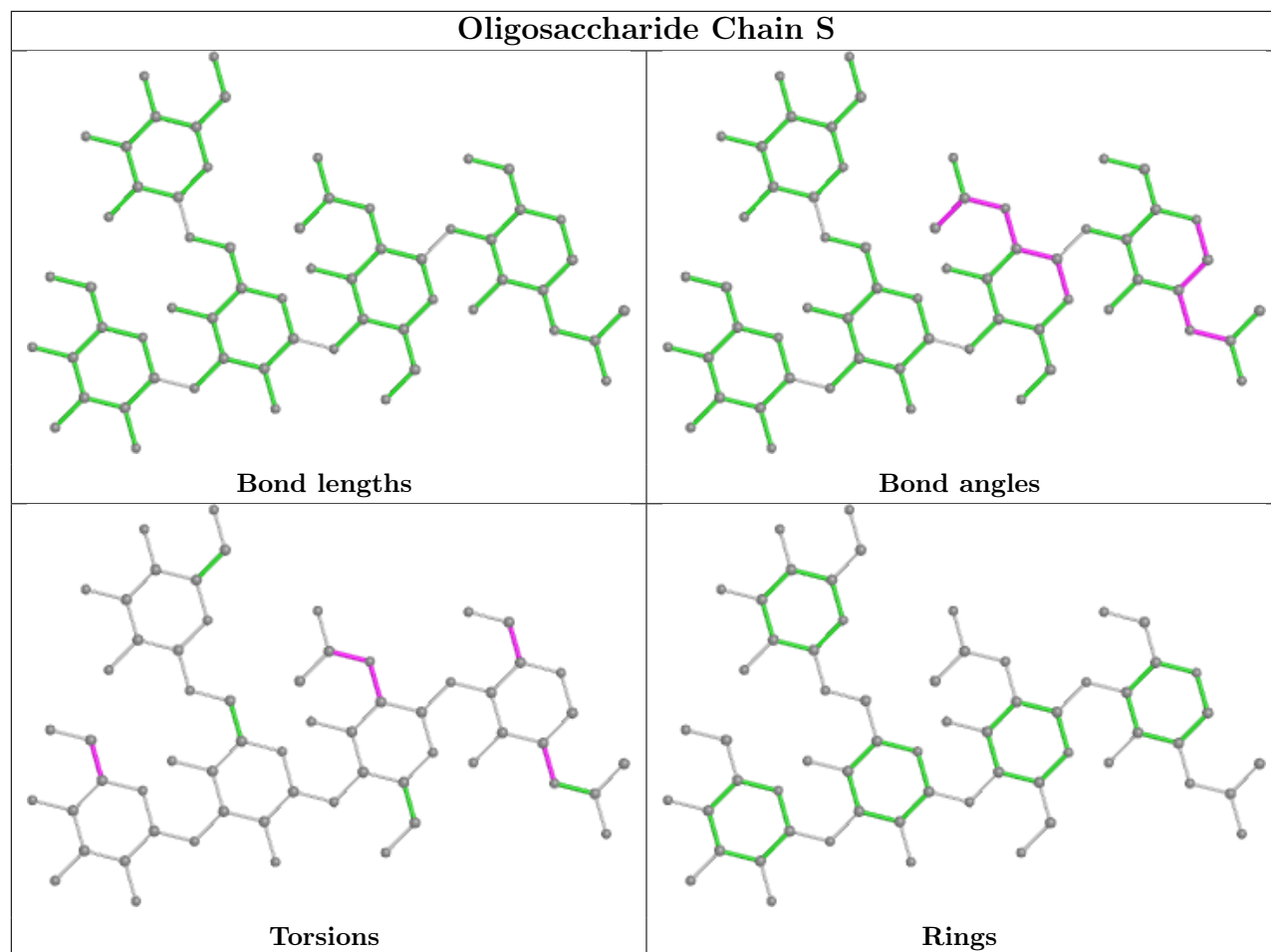
Oligosaccharide Chain N

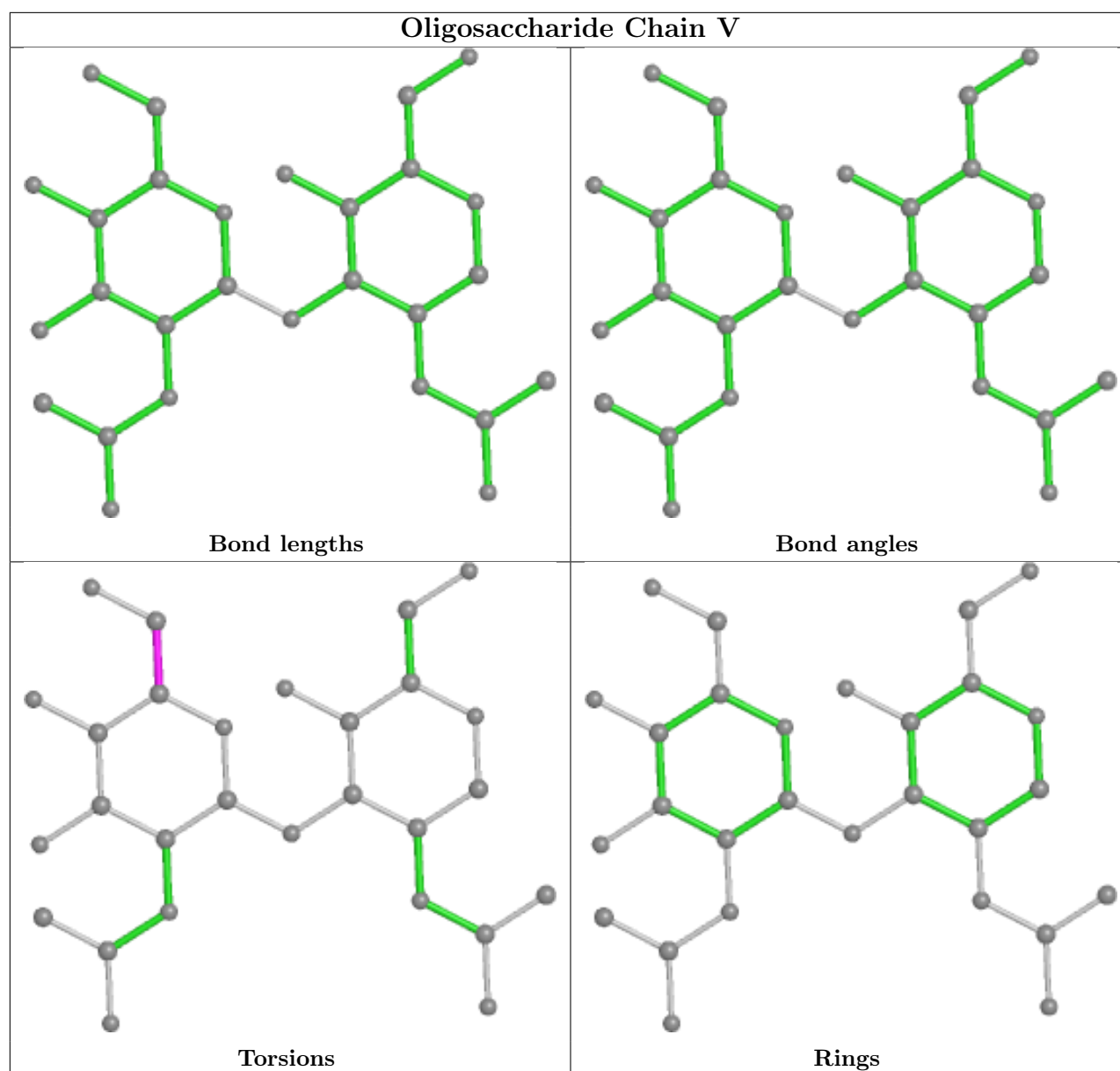


Oligosaccharide Chain M









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	601	4	14,14,15	0.31	0	17,19,21	0.64	0
16	NAG	T	701	5	14,14,15	0.30	0	17,19,21	0.86	1 (5%)
16	NAG	G	605	4	14,14,15	0.29	0	17,19,21	0.68	0
16	NAG	T	702	5	14,14,15	0.30	0	17,19,21	0.69	0
16	NAG	T	703	5	14,14,15	0.28	0	17,19,21	0.61	0
16	NAG	G	604	4	14,14,15	0.33	0	17,19,21	0.90	1 (5%)
16	NAG	G	603	4	14,14,15	0.29	0	17,19,21	0.64	0
16	NAG	G	602	4	14,14,15	0.30	0	17,19,21	0.89	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	601	4	-	4/6/23/26	0/1/1/1
16	NAG	T	701	5	-	2/6/23/26	0/1/1/1
16	NAG	G	605	4	-	0/6/23/26	0/1/1/1
16	NAG	T	702	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	604	4	-	6/6/23/26	0/1/1/1
16	NAG	G	603	4	-	0/6/23/26	0/1/1/1
16	NAG	G	602	4	-	2/6/23/26	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	2.26	115.26	112.19
16	G	604	NAG	C1-O5-C5	2.11	115.05	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

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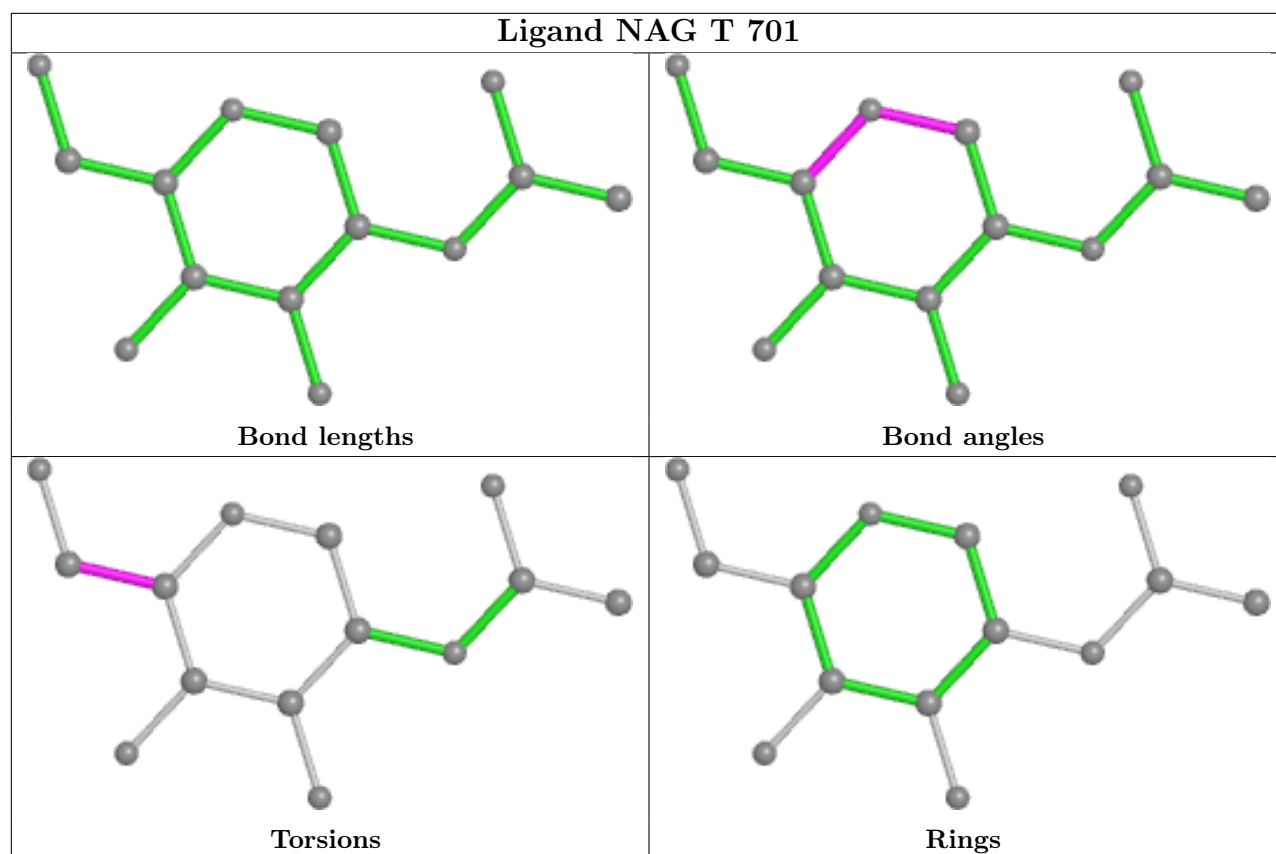
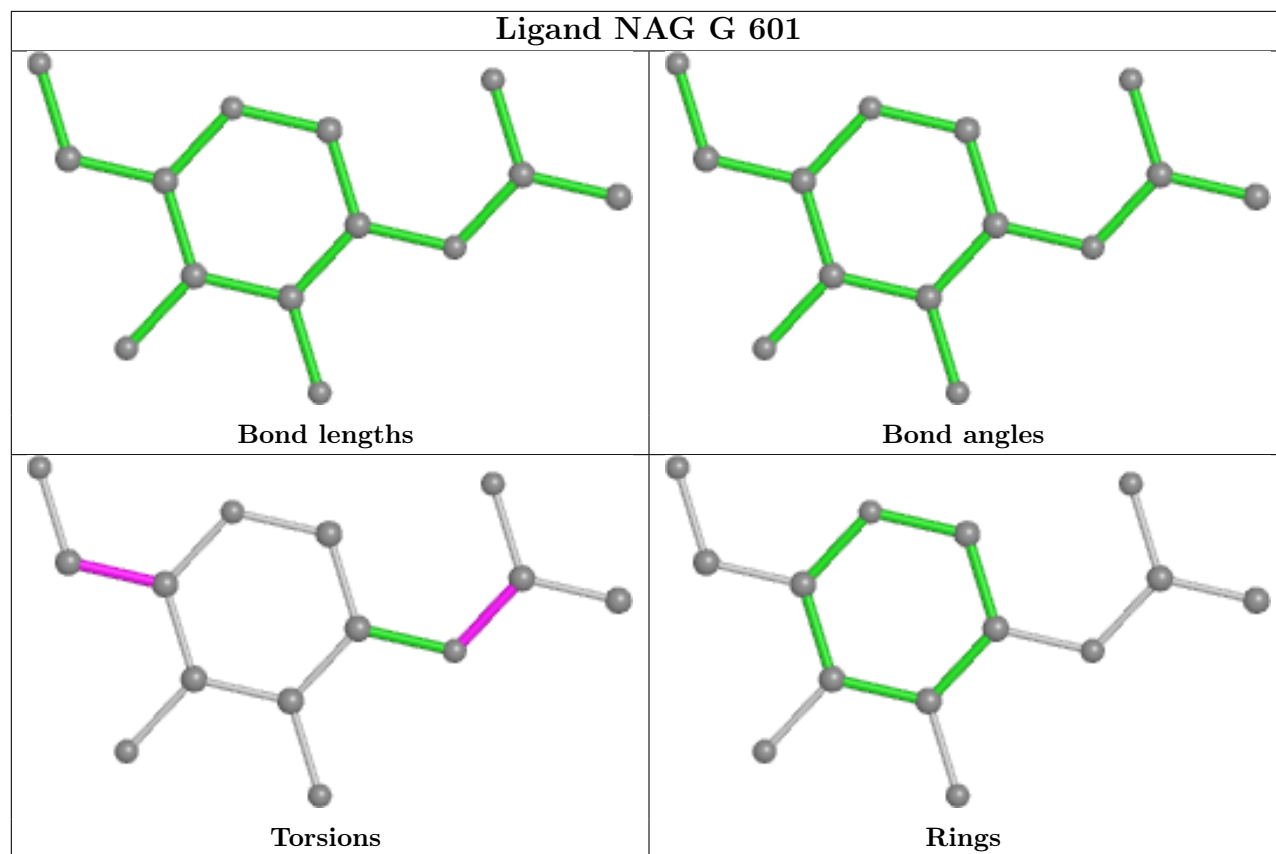
Mol	Chain	Res	Type	Atoms
16	G	601	NAG	C8-C7-N2-C2
16	G	601	NAG	O7-C7-N2-C2
16	T	703	NAG	O5-C5-C6-O6
16	G	602	NAG	O5-C5-C6-O6
16	T	701	NAG	O5-C5-C6-O6
16	G	601	NAG	O5-C5-C6-O6
16	G	604	NAG	O5-C5-C6-O6
16	T	703	NAG	C4-C5-C6-O6
16	T	701	NAG	C4-C5-C6-O6
16	T	702	NAG	C4-C5-C6-O6
16	G	604	NAG	C4-C5-C6-O6
16	G	604	NAG	C1-C2-N2-C7
16	G	604	NAG	C3-C2-N2-C7
16	G	601	NAG	C4-C5-C6-O6

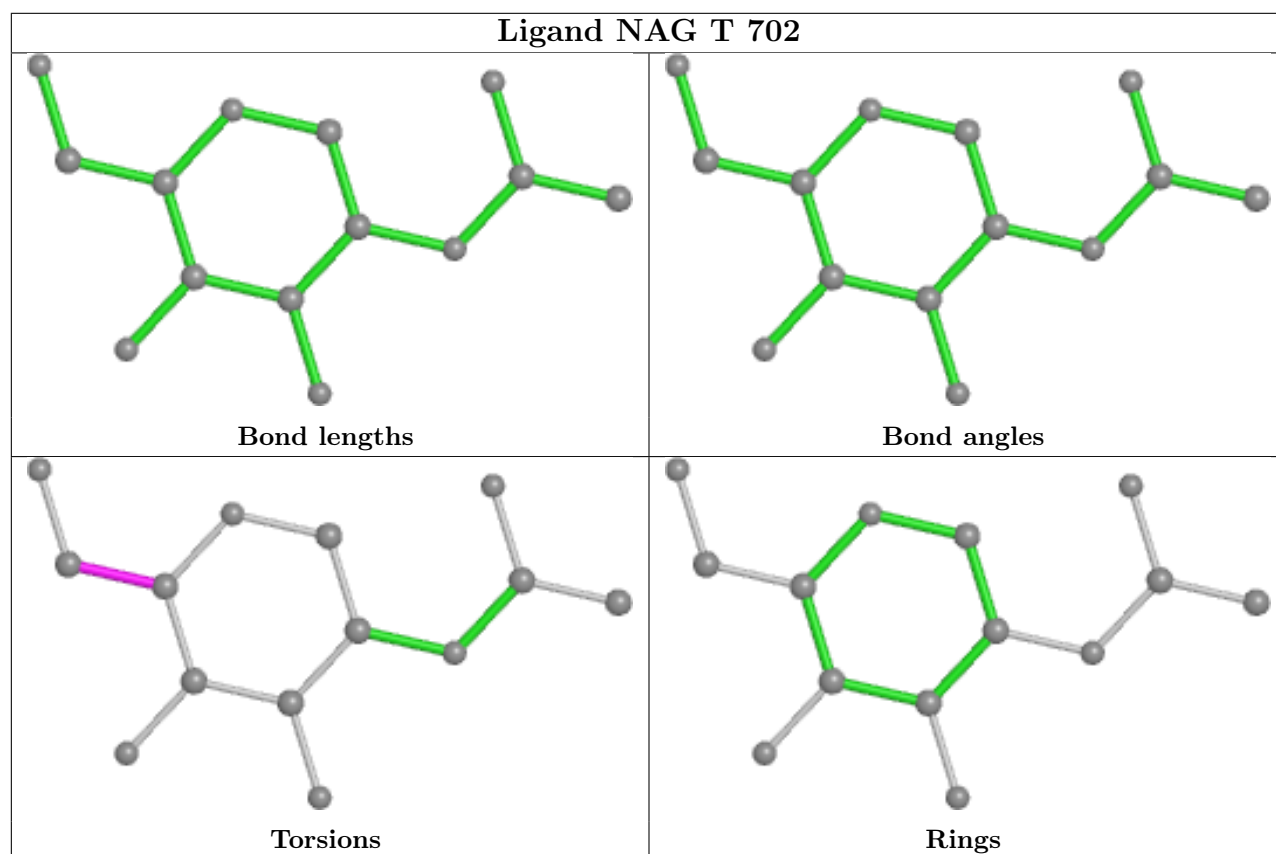
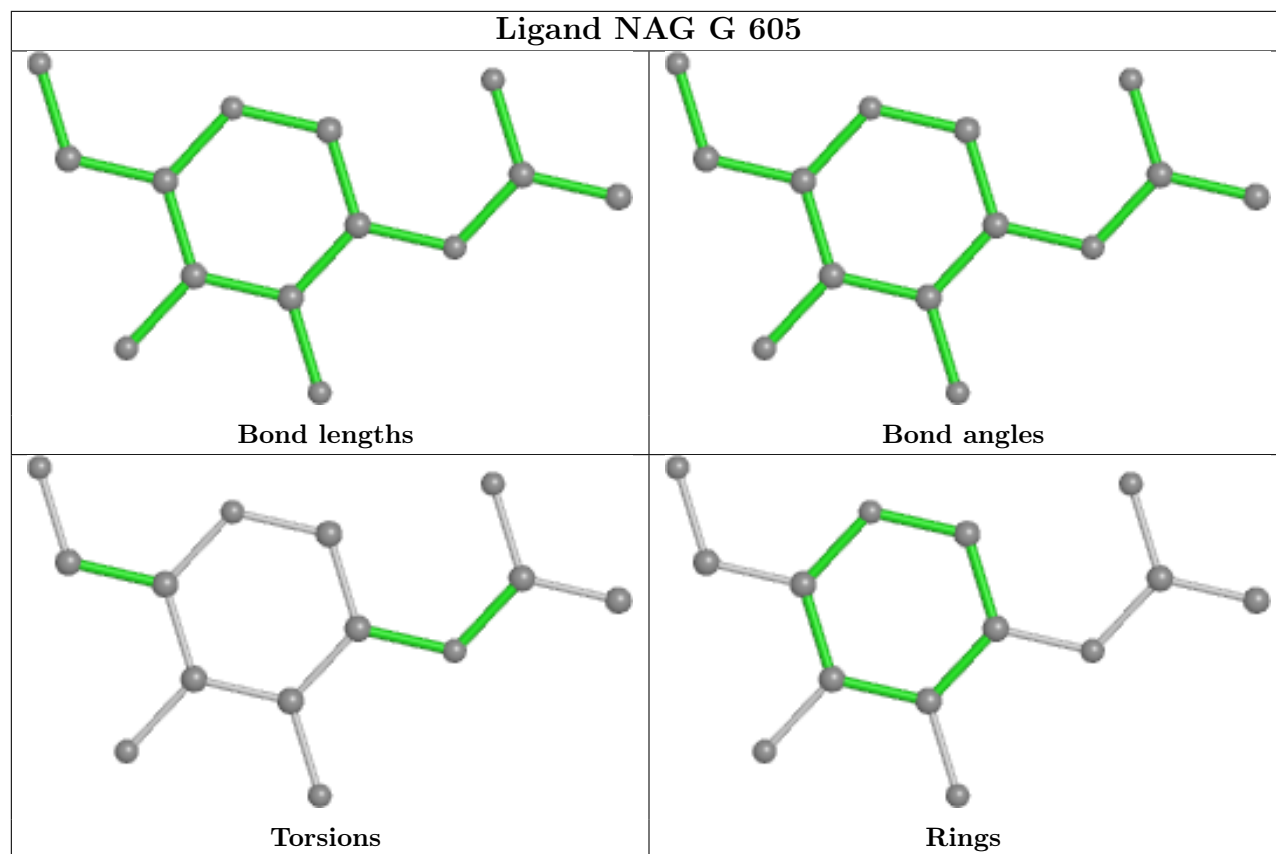
There are no ring outliers.

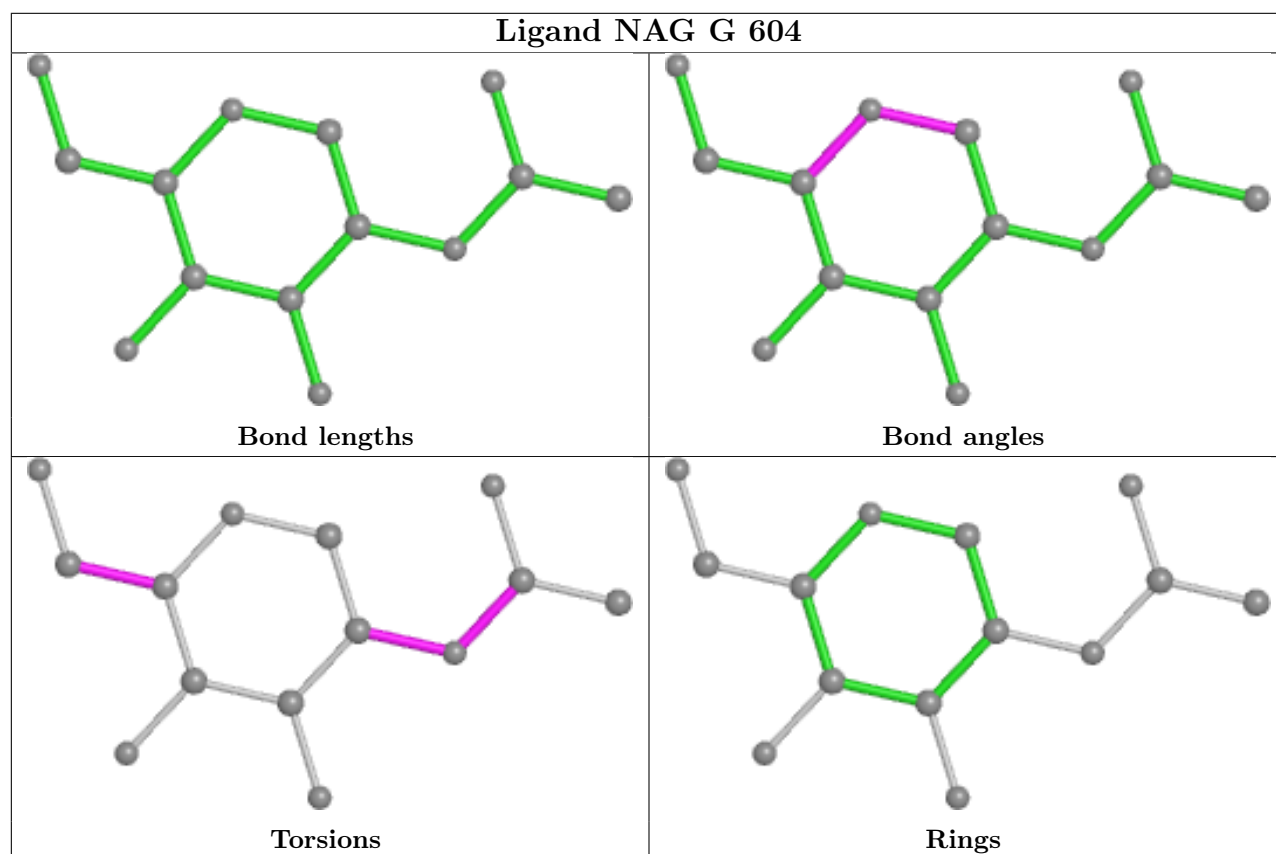
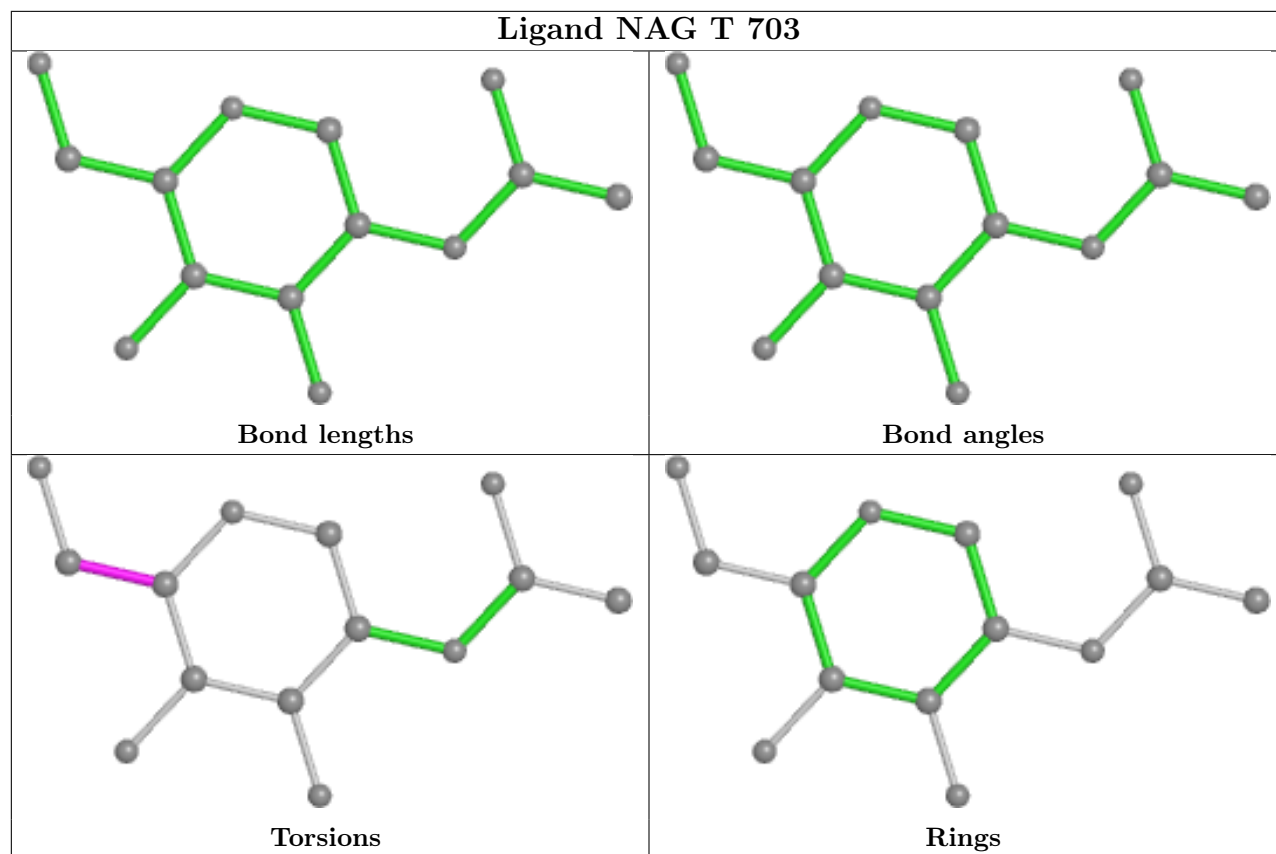
3 monomers are involved in 4 short contacts:

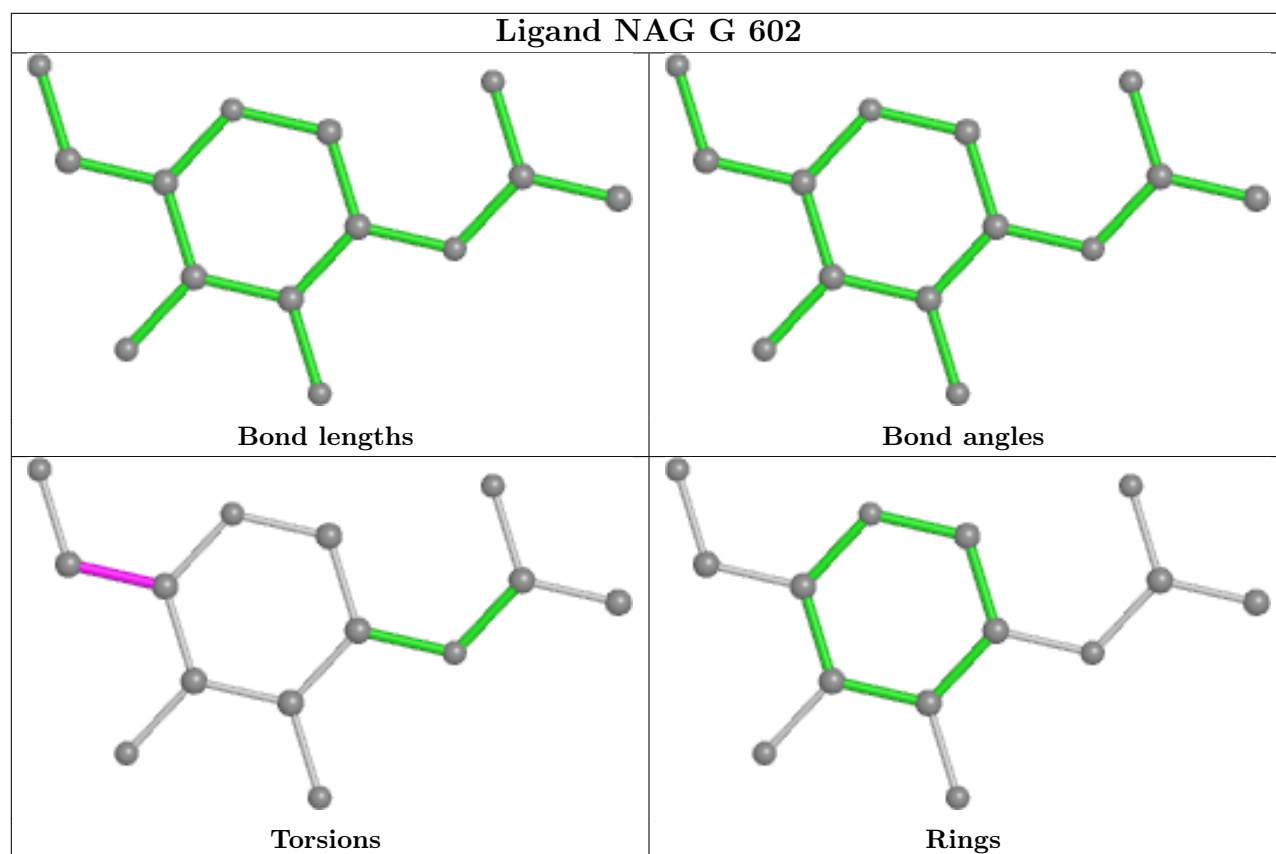
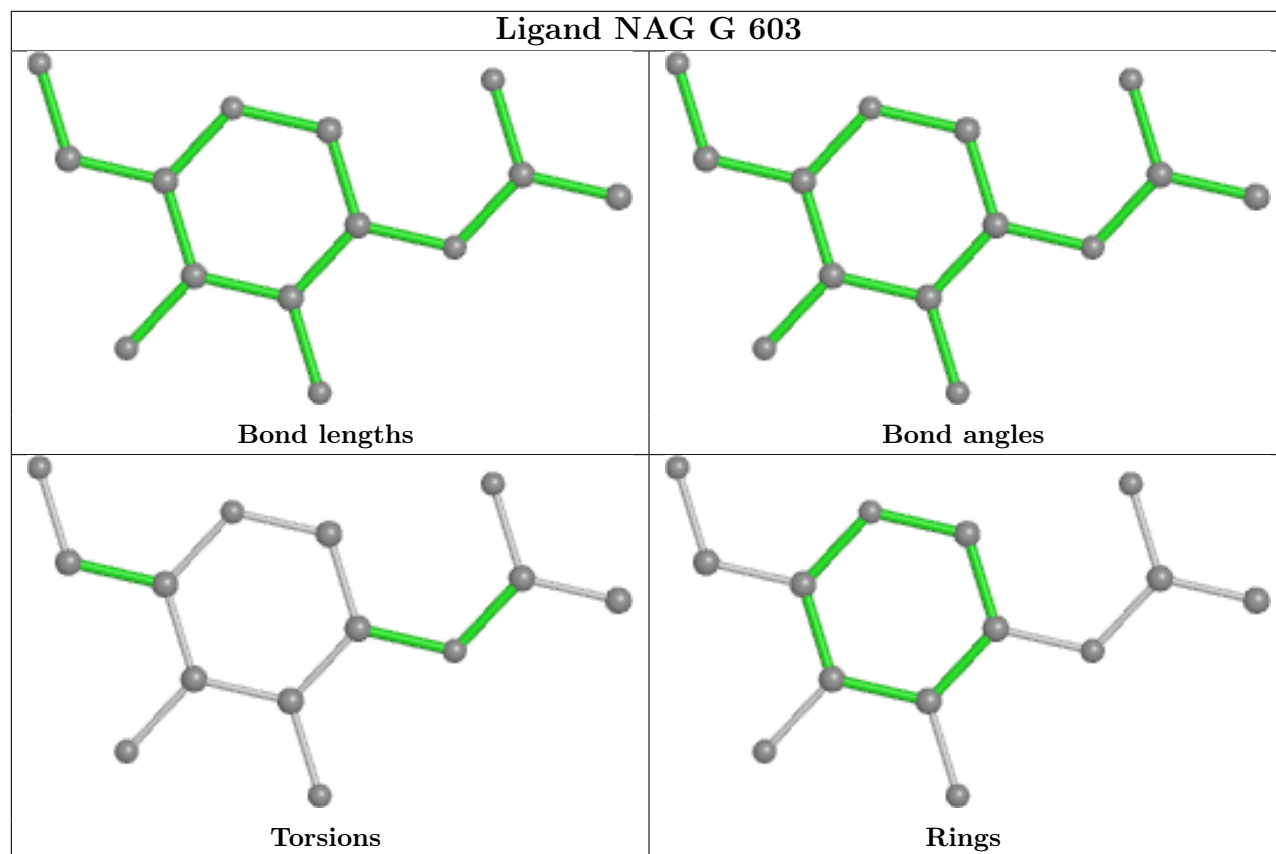
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	T	701	NAG	1	0
16	G	605	NAG	1	0
16	G	604	NAG	2	0

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%)	1.09	49 (20%) 1 1	142, 213, 331, 338	0
2	E	213/216 (98%)	0.77	33 (15%) 2 2	164, 195, 371, 388	0
3	L	213/213 (100%)	-0.06	2 (0%) 84 79	110, 133, 152, 160	0
4	G	453/485 (93%)	0.06	6 (1%) 77 70	97, 132, 174, 194	0
5	T	134/140 (95%)	0.34	6 (4%) 33 28	129, 148, 182, 189	0
6	H	231/233 (99%)	-0.03	1 (0%) 92 89	97, 123, 140, 156	0
All	All	1484/1530 (96%)	0.32	97 (6%) 18 14	97, 142, 329, 388	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	159	LEU	11.3
1	D	132	SER	10.4
1	D	208	ASP	7.6
2	E	128	ASN	7.6
1	D	131	THR	6.3
2	E	146	VAL	6.2
2	E	144	VAL	5.8
1	D	198	VAL	5.8
1	D	222	VAL	5.4
1	D	179	SER	5.4
1	D	221	GLU	5.2
1	D	207	VAL	5.2
1	D	216	CYS	5.1
2	E	161	THR	5.1
2	E	129	LYS	5.0
1	D	141	LEU	4.8
2	E	143	ALA	4.7
1	D	154	TRP	4.6
2	E	115	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
2	E	132	LEU	4.3
2	E	130	ALA	4.3
1	D	158	ALA	4.2
1	D	206	LYS	4.2
1	D	123	PRO	4.2
2	E	187	SER	4.1
1	D	140	CYS	4.1
1	D	160	THR	4.0
2	E	147	ALA	3.9
1	D	107	THR	3.9
1	D	196	CYS	3.8
1	D	200	HIS	3.8
2	E	180	LEU	3.8
1	D	192	GLN	3.6
3	L	148	TRP	3.6
2	E	131	THR	3.6
1	D	126	PRO	3.5
1	D	130	SER	3.5
1	D	94	LYS	3.5
2	E	156	LYS	3.4
2	E	157	ALA	3.4
1	D	155	ASN	3.3
1	D	122	PHE	3.2
1	D	157	GLY	3.1
2	E	162	THR	3.1
1	D	152	VAL	3.1
1	D	156	SER	3.1
2	E	188	HIS	3.1
5	T	518	VAL	3.0
1	D	180	SER	3.0
1	D	142	VAL	3.0
2	E	177	TYR	3.0
4	G	70	ALA	2.9
1	D	151	THR	2.9
1	D	197	ASN	2.9
5	T	664	ASP	2.8
2	E	186	LYS	2.8
3	L	149	LYS	2.8
2	E	175	SER	2.8
1	D	9	ALA	2.7
5	T	663	LEU	2.7
4	G	401	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
5	T	547(G)	ASP	2.7
2	E	178	LEU	2.7
2	E	35	TRP	2.6
1	D	194	TYR	2.6
4	G	504	ARG	2.6
5	T	661	LEU	2.5
1	D	120	SER	2.5
1	D	147	PRO	2.5
1	D	8	GLY	2.5
1	D	117	LYS	2.4
2	E	127	ALA	2.4
2	E	179	SER	2.4
2	E	126	GLN	2.4
6	H	129	LYS	2.3
1	D	133	GLY	2.3
1	D	167	PRO	2.3
5	T	599	SER	2.3
2	E	135	LEU	2.3
1	D	146	PHE	2.3
1	D	125	ALA	2.2
1	D	144	ASP	2.2
4	G	71	THR	2.2
1	D	95	GLY	2.2
1	D	135	THR	2.2
1	D	178	LEU	2.2
2	E	142	GLY	2.1
1	D	124	LEU	2.1
2	E	125	LEU	2.1
2	E	98	PHE	2.1
1	D	118	GLY	2.1
2	E	145	THR	2.1
2	E	197	HIS	2.1
2	E	151	ASP	2.1
4	G	140	ASP	2.0
2	E	160	GLU	2.0
4	G	353	PHE	2.0

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

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

6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	I	2	14/15	0.14	0.72	187,190,192,194	0
7	BMA	I	3	11/12	0.31	0.41	191,195,199,200	0
8	MAN	B	7	11/12	0.34	0.45	154,157,160,161	0
7	BMA	A	3	11/12	0.57	0.32	210,215,221,225	0
8	MAN	B	10	11/12	0.57	0.35	163,169,175,176	0
12	MAN	N	5	11/12	0.59	0.36	196,197,201,202	0
15	NAG	V	2	14/15	0.61	0.63	194,195,196,196	0
12	NAG	N	2	14/15	0.63	0.36	179,186,192,195	0
7	NAG	A	1	14/15	0.64	0.34	180,184,187,188	0
8	MAN	B	6	11/12	0.65	0.28	169,176,180,182	0
12	BMA	N	3	11/12	0.65	0.21	182,186,187,187	0
9	NAG	C	2	14/15	0.66	0.59	166,170,175,176	0
7	NAG	A	2	14/15	0.68	0.40	196,199,203,205	0
13	MAN	R	6	11/12	0.68	0.36	214,216,217,218	0
12	MAN	N	6	11/12	0.69	0.23	185,186,194,195	0
7	NAG	I	1	14/15	0.69	0.31	173,180,184,184	0
7	NAG	U	2	14/15	0.70	0.34	186,189,190,193	0
8	MAN	B	4	11/12	0.71	0.18	157,161,166,167	0
12	MAN	N	4	11/12	0.71	0.37	188,191,194,196	0
9	NAG	F	2	14/15	0.71	0.34	186,189,190,191	0
9	NAG	C	1	14/15	0.72	0.48	155,163,168,168	0
15	NAG	V	1	14/15	0.75	0.41	189,192,194,195	0
8	MAN	B	9	11/12	0.75	0.23	159,164,167,167	0
7	BMA	U	3	11/12	0.76	0.22	191,195,198,200	0
11	MAN	K	8	11/12	0.76	0.34	152,154,157,158	0
7	NAG	U	1	14/15	0.77	0.28	175,180,183,185	0
13	MAN	R	4	11/12	0.77	0.25	207,208,212,212	0
11	MAN	K	9	11/12	0.77	0.44	155,156,158,160	0
7	NAG	Q	1	14/15	0.77	0.34	172,173,176,177	0
12	NAG	N	1	14/15	0.78	0.29	177,182,187,187	0
7	BMA	P	3	11/12	0.78	0.42	182,185,187,188	0
7	BMA	Q	3	11/12	0.80	0.24	187,189,193,193	0
13	BMA	R	3	11/12	0.80	0.15	197,199,203,203	0
10	MAN	J	4	11/12	0.81	0.48	156,158,161,163	0
8	BMA	B	3	11/12	0.81	0.23	157,160,163,165	0
8	MAN	B	5	11/12	0.81	0.12	171,174,177,178	0

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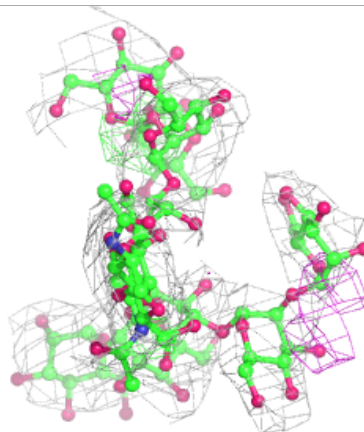
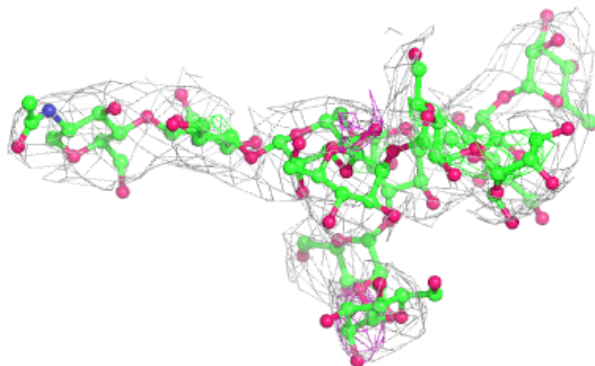
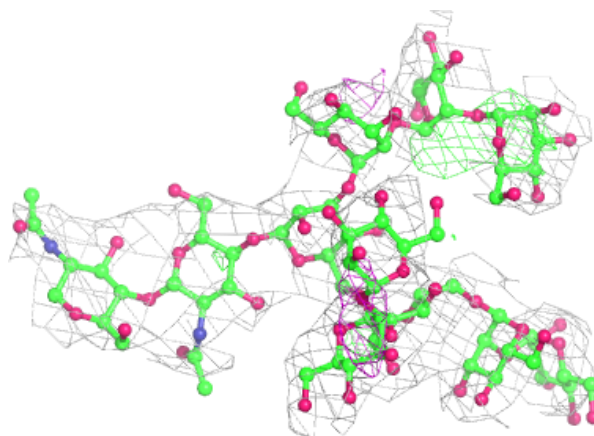
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	MAN	B	8	11/12	0.82	0.36	154,158,161,162	0
10	MAN	M	4	11/12	0.83	0.20	157,161,165,165	0
8	NAG	B	1	14/15	0.83	0.35	137,140,142,144	0
14	MAN	S	4	11/12	0.83	0.15	148,150,155,157	0
13	MAN	R	7	11/12	0.84	0.21	199,201,203,204	0
10	BMA	M	3	11/12	0.84	0.28	166,168,174,175	0
13	NAG	R	2	14/15	0.84	0.21	189,190,193,193	0
11	MAN	K	5	11/12	0.85	0.28	140,143,145,146	0
13	MAN	R	5	11/12	0.85	0.36	201,203,205,205	0
10	NAG	M	2	14/15	0.86	0.31	185,191,195,197	0
10	BMA	J	3	11/12	0.86	0.39	152,153,156,157	0
14	MAN	S	5	11/12	0.86	0.17	152,153,160,162	0
11	MAN	K	7	11/12	0.87	0.15	145,146,149,149	0
9	NAG	F	1	14/15	0.87	0.22	183,184,187,188	0
10	NAG	J	2	14/15	0.88	0.25	144,146,148,149	0
8	NAG	B	2	14/15	0.89	0.25	145,148,153,154	0
7	NAG	P	2	14/15	0.89	0.40	173,175,178,178	0
9	NAG	O	2	14/15	0.89	0.24	152,154,155,156	0
11	MAN	K	11	11/12	0.89	0.32	145,147,151,153	0
10	NAG	M	1	14/15	0.89	0.22	184,187,189,190	0
13	NAG	R	1	14/15	0.89	0.22	181,183,185,186	0
14	BMA	S	3	11/12	0.90	0.12	145,146,148,149	0
9	NAG	O	1	14/15	0.90	0.20	144,145,147,148	0
7	NAG	Q	2	14/15	0.90	0.17	173,180,184,185	0
7	NAG	P	1	14/15	0.91	0.18	157,162,164,165	0
11	MAN	K	4	11/12	0.91	0.22	142,143,146,146	0
14	NAG	S	2	14/15	0.91	0.24	139,142,145,146	0
10	NAG	J	1	14/15	0.92	0.16	137,138,141,142	0
11	NAG	K	1	14/15	0.94	0.25	139,141,146,146	0
11	BMA	K	3	11/12	0.94	0.21	142,142,144,144	0
14	NAG	S	1	14/15	0.94	0.29	140,141,143,144	0
11	MAN	K	6	11/12	0.94	0.29	139,140,142,143	0
11	MAN	K	10	11/12	0.94	0.16	147,148,151,152	0
11	NAG	K	2	14/15	0.95	0.27	140,142,145,148	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.

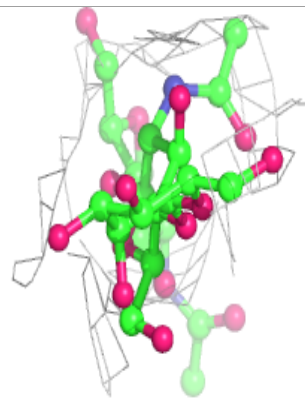
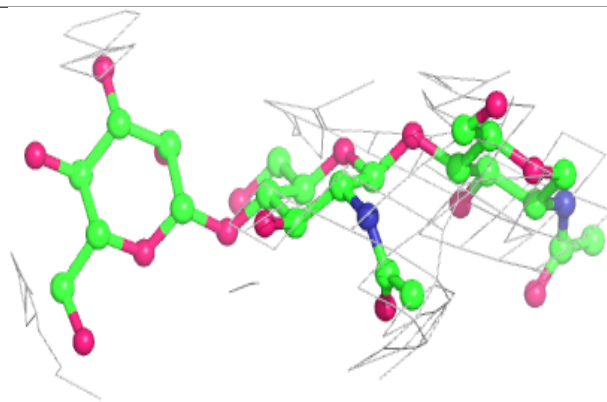
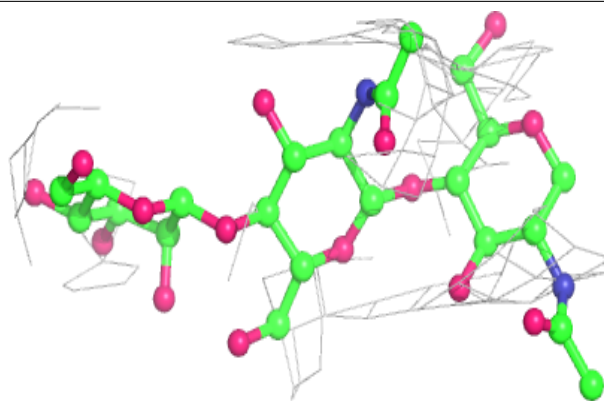
Electron density around Chain K:

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



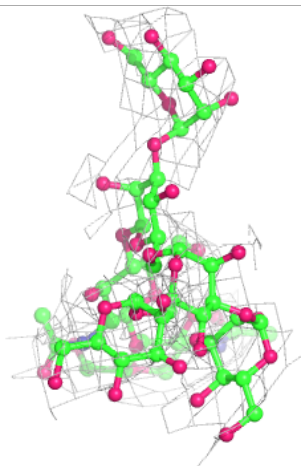
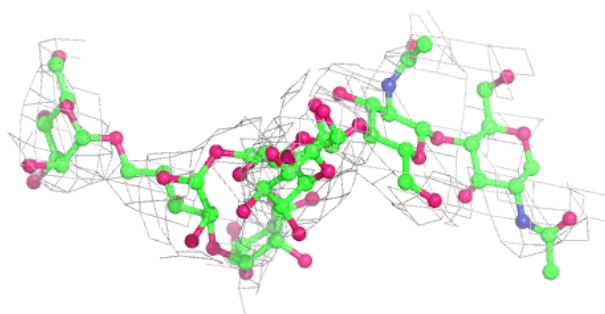
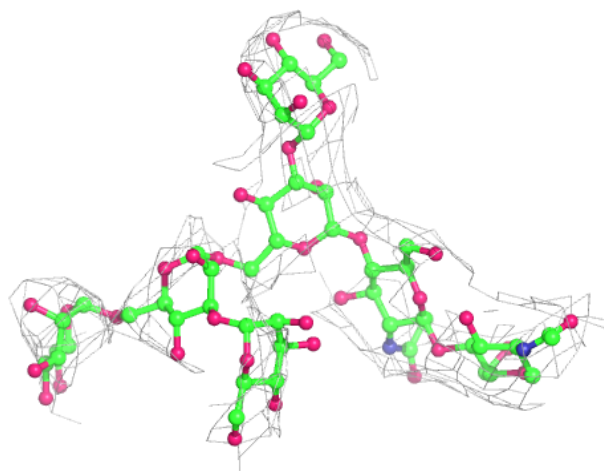
Electron density around Chain Q:

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



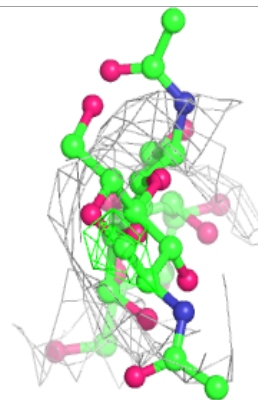
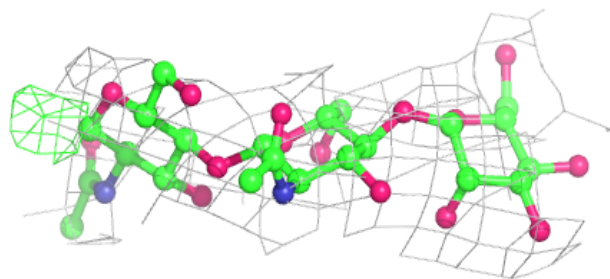
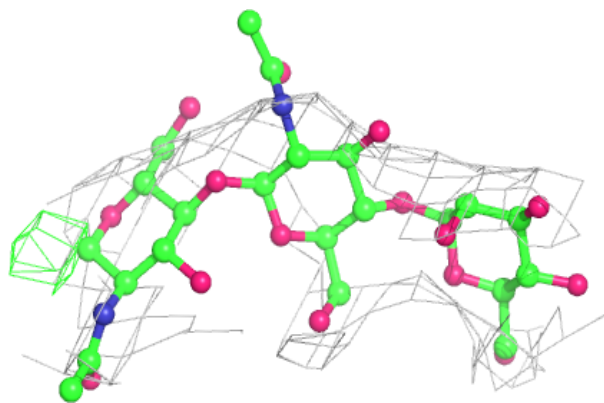
Electron density around Chain R:

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

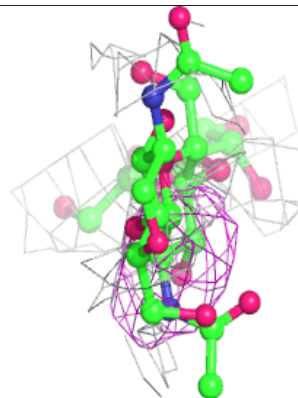
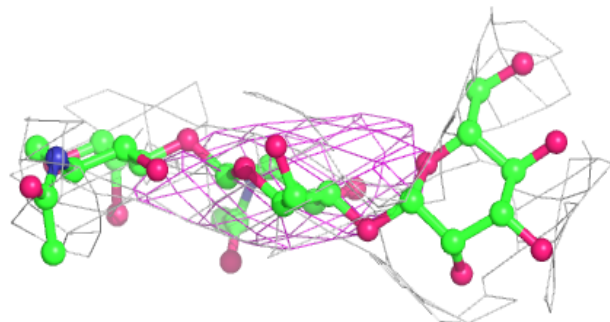
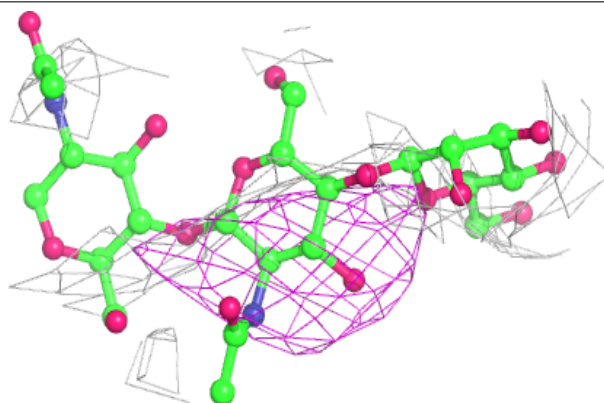


Electron density around Chain U:

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

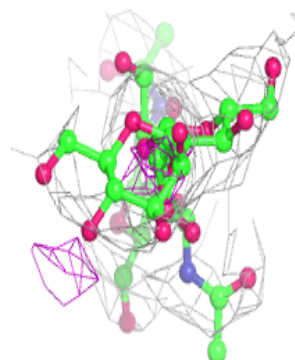
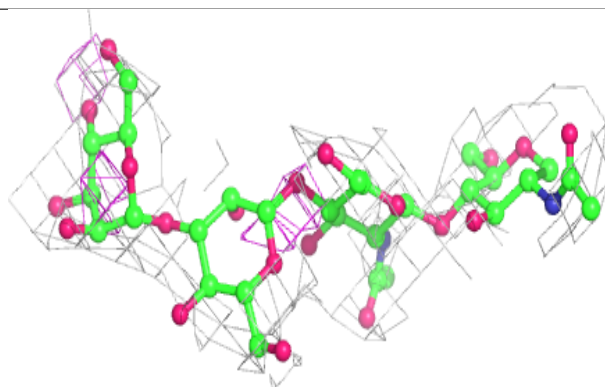
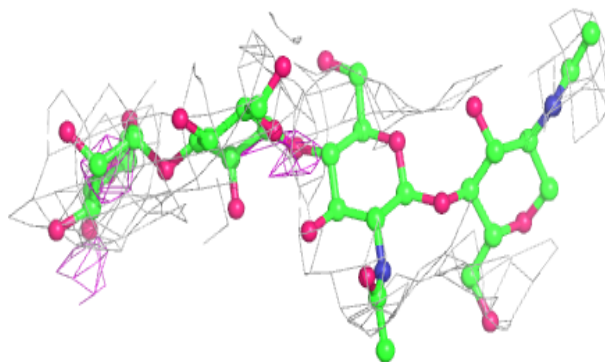
**Electron density around Chain I:**

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

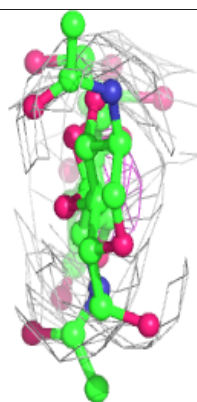
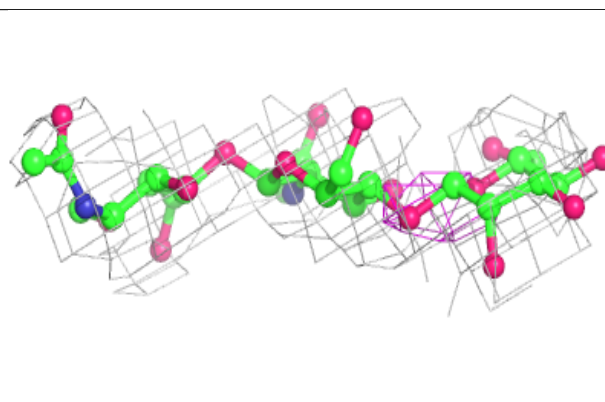
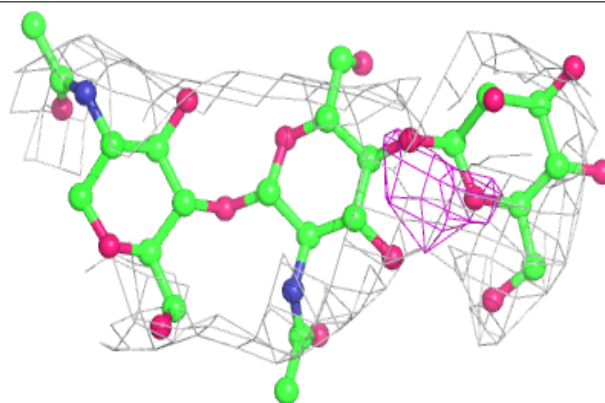


Electron density around Chain J:

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

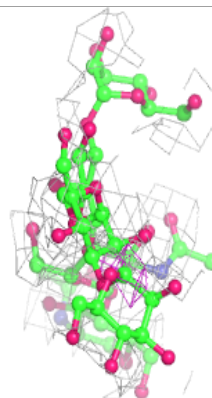
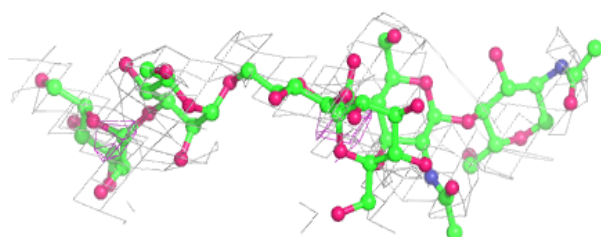
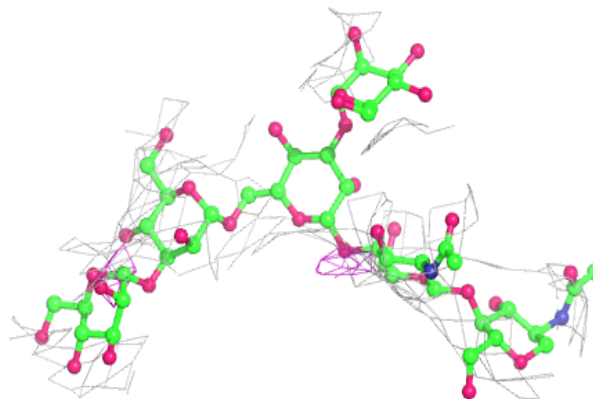
**Electron density around Chain P:**

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

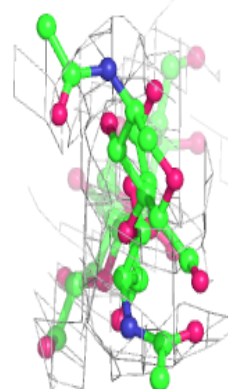
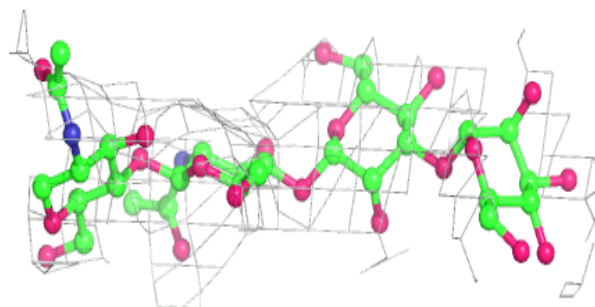
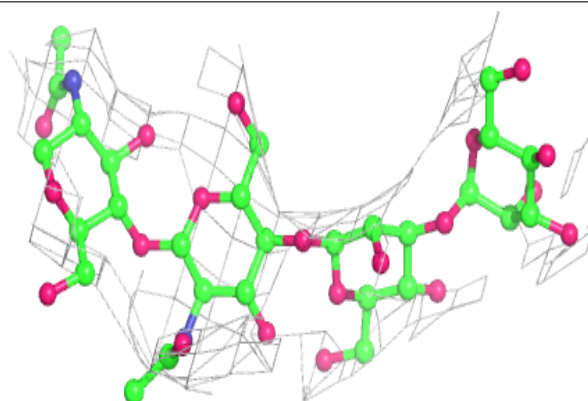


Electron density around Chain N:

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

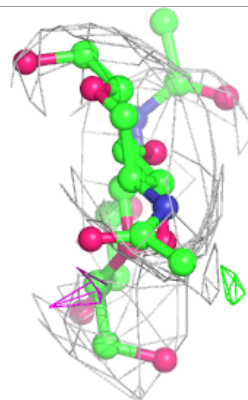
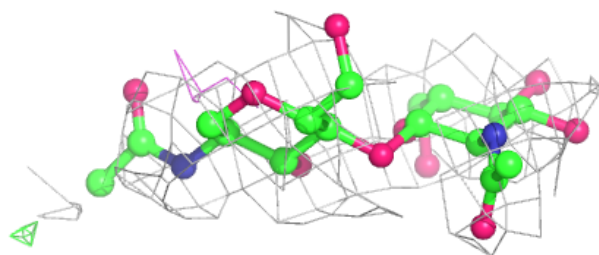
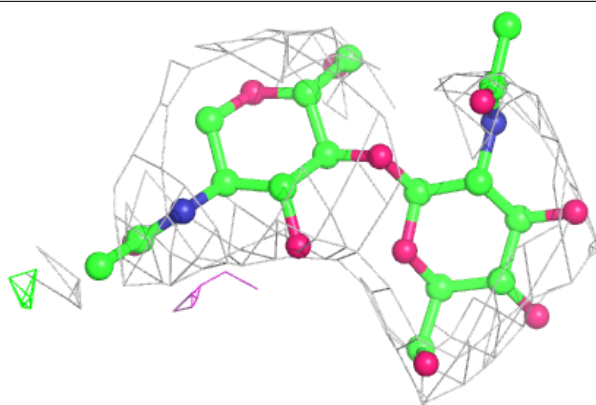
**Electron density around Chain M:**

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

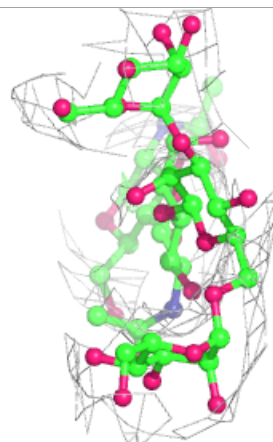
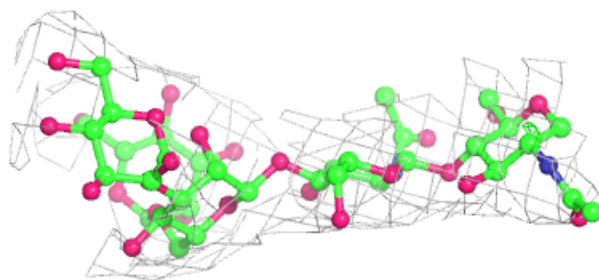
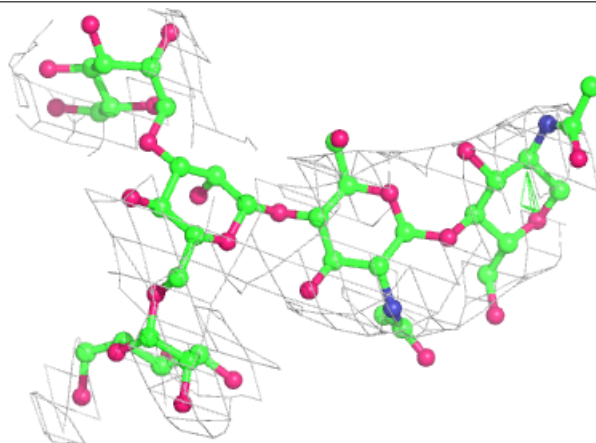


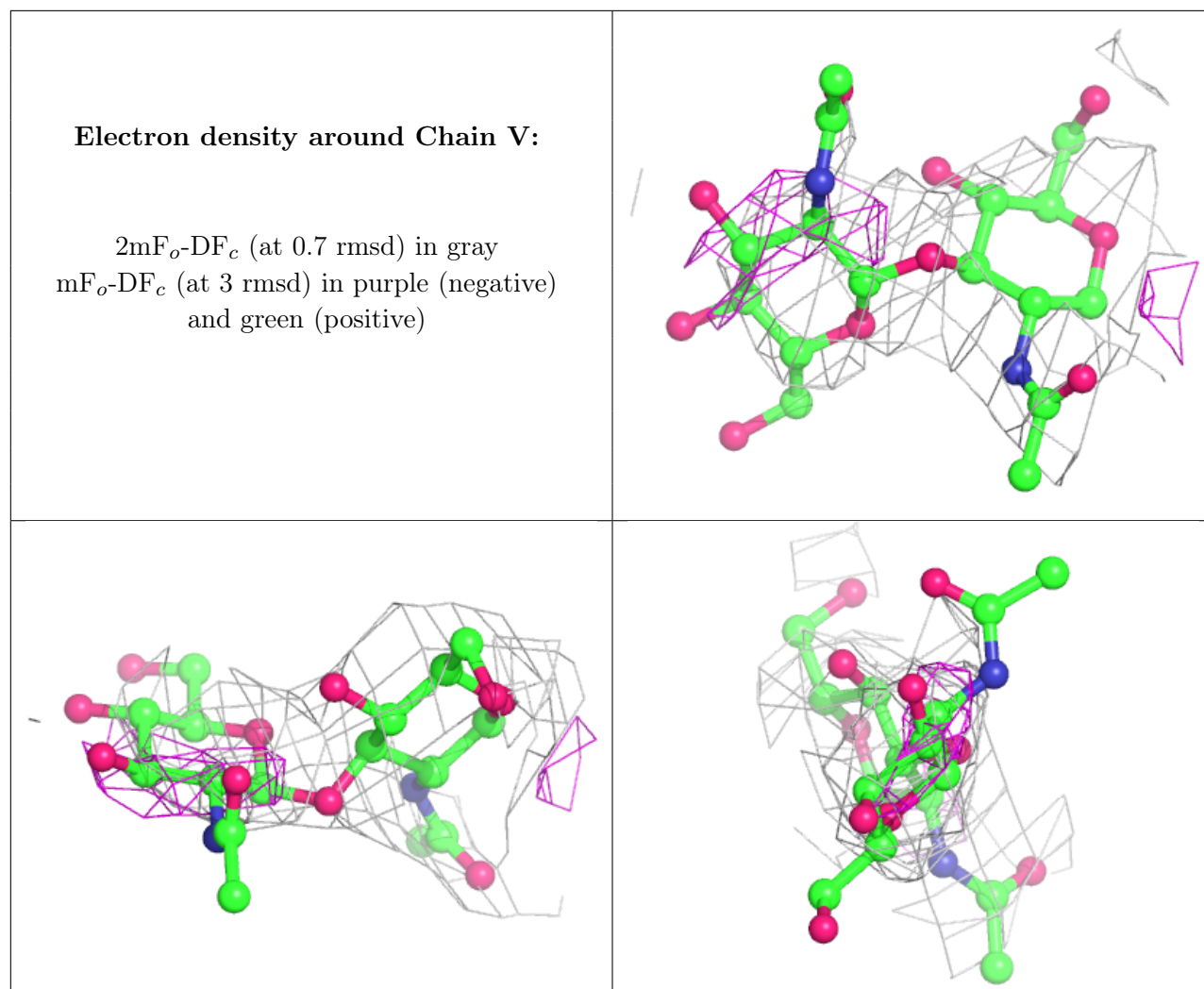
Electron density around Chain O:

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

**Electron density around Chain S:**

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



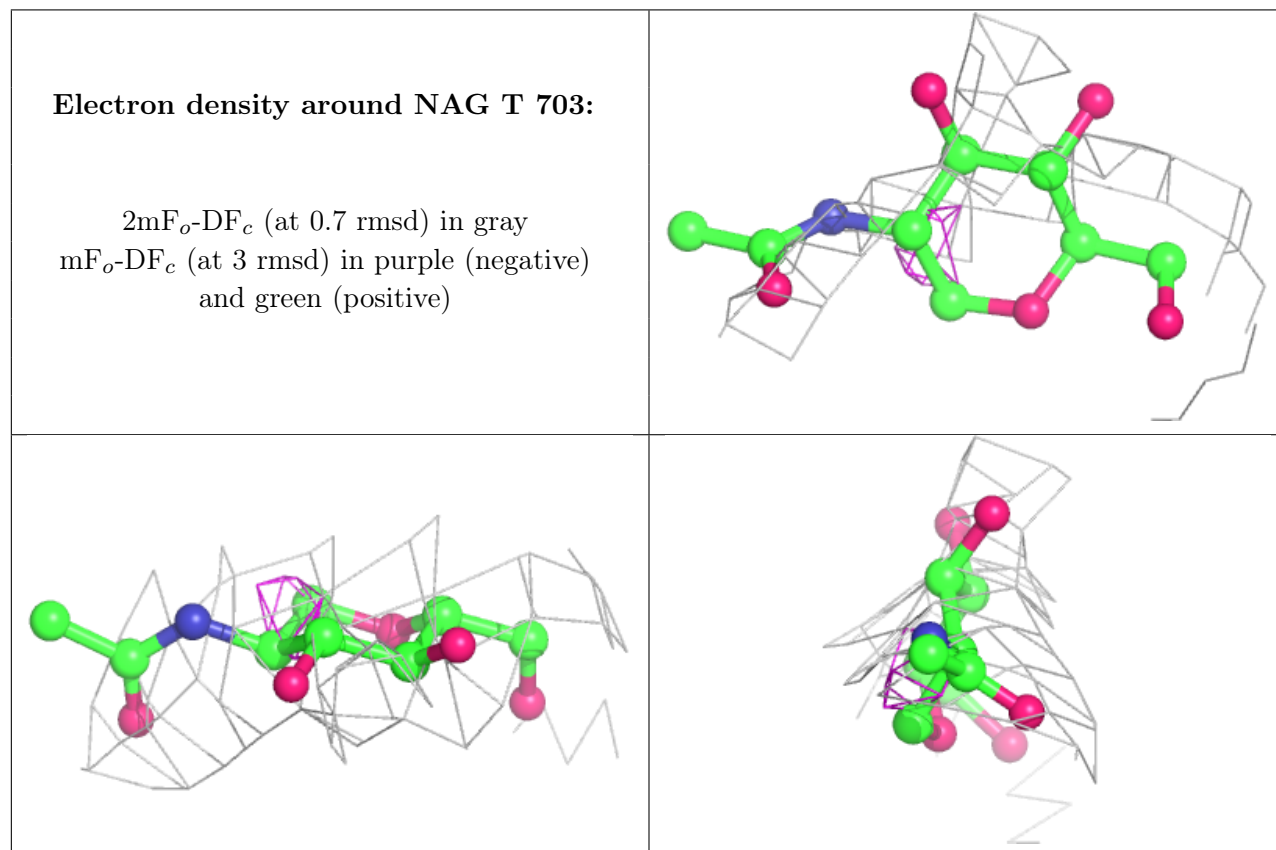


6.4 Ligands [i](#)

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.

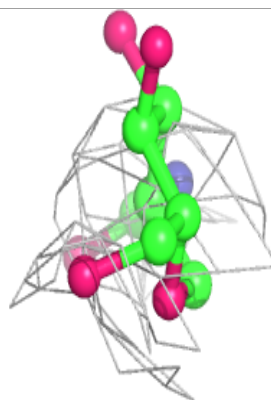
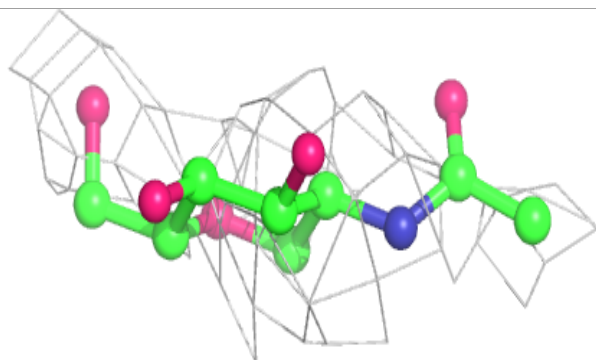
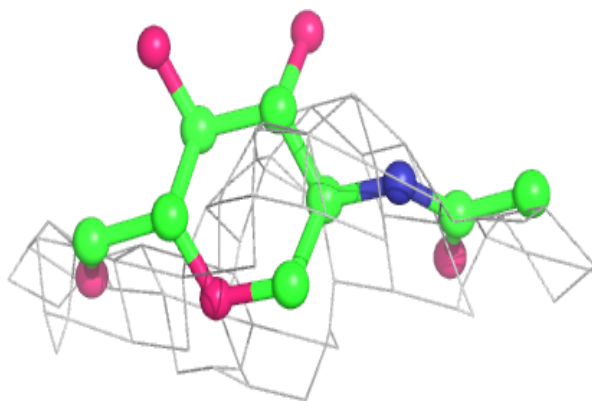
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	NAG	T	703	14/15	0.62	0.45	187,190,192,193	0
16	NAG	G	605	14/15	0.66	0.63	207,209,214,214	0
16	NAG	T	701	14/15	0.67	0.80	185,188,191,192	0
16	NAG	G	604	14/15	0.75	0.39	191,195,198,198	0
16	NAG	G	601	14/15	0.78	0.24	160,162,166,166	0
16	NAG	G	602	14/15	0.78	0.32	146,150,153,154	0
16	NAG	T	702	14/15	0.82	0.29	193,194,197,197	0
16	NAG	G	603	14/15	0.89	0.26	187,192,195,197	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.

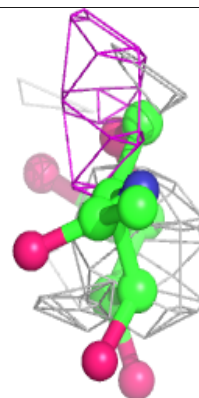
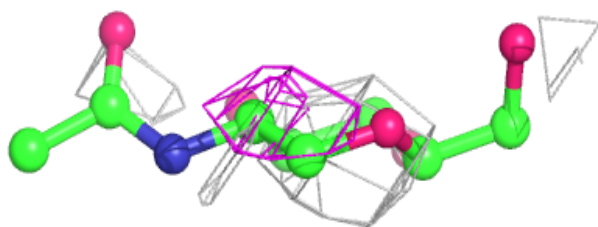
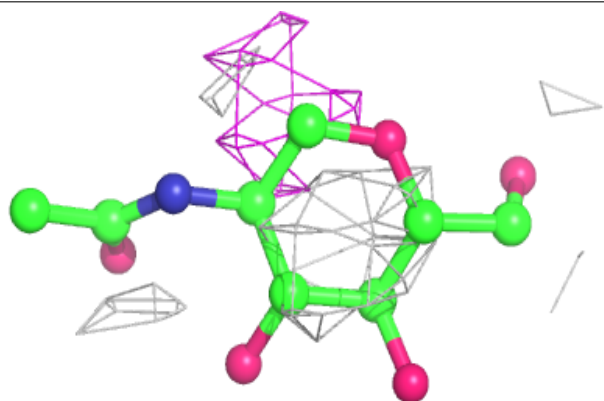


Electron density around NAG G 605:

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

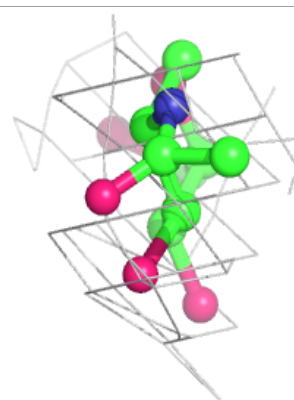
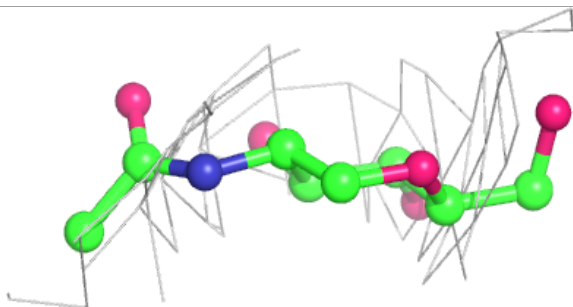
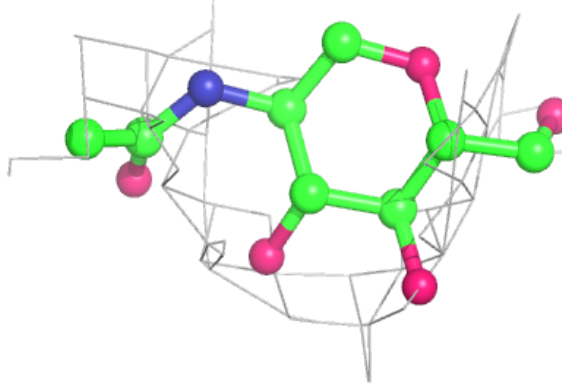
**Electron density around NAG T 701:**

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

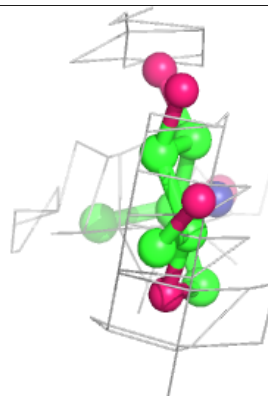
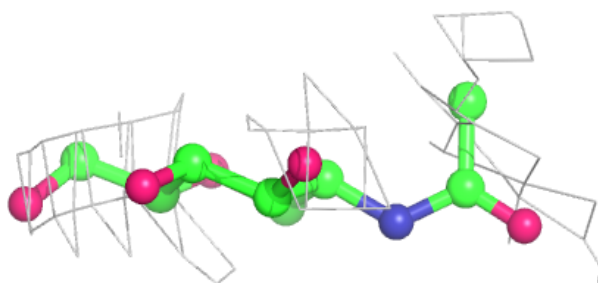
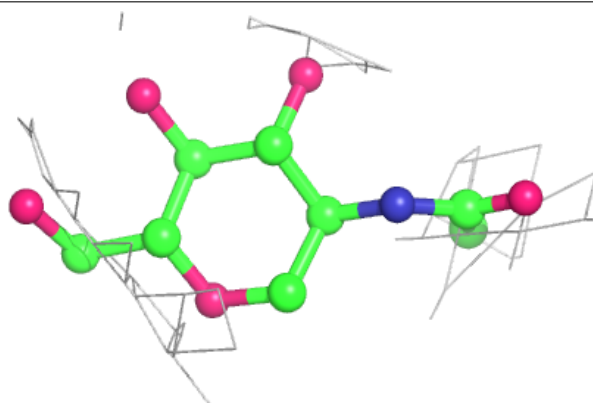


Electron density around NAG G 604:

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

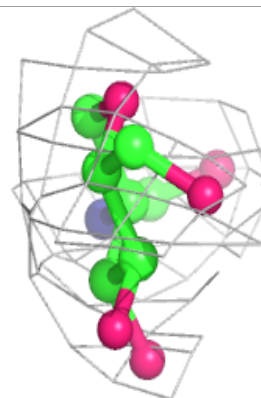
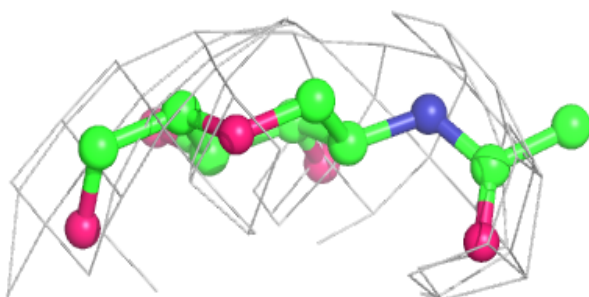
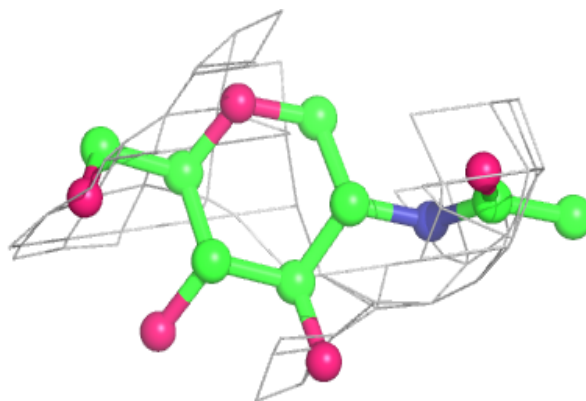
**Electron density around NAG G 601:**

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

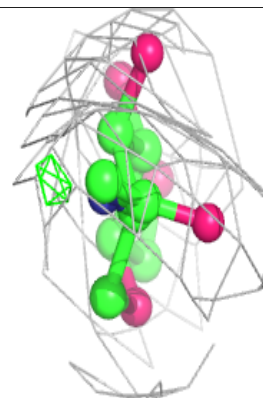
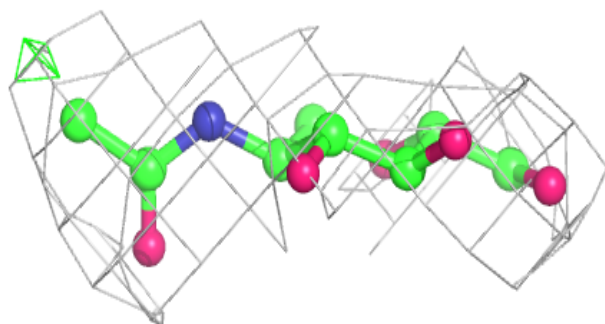
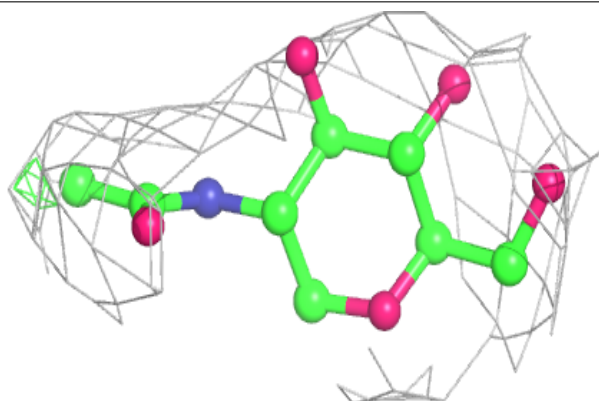


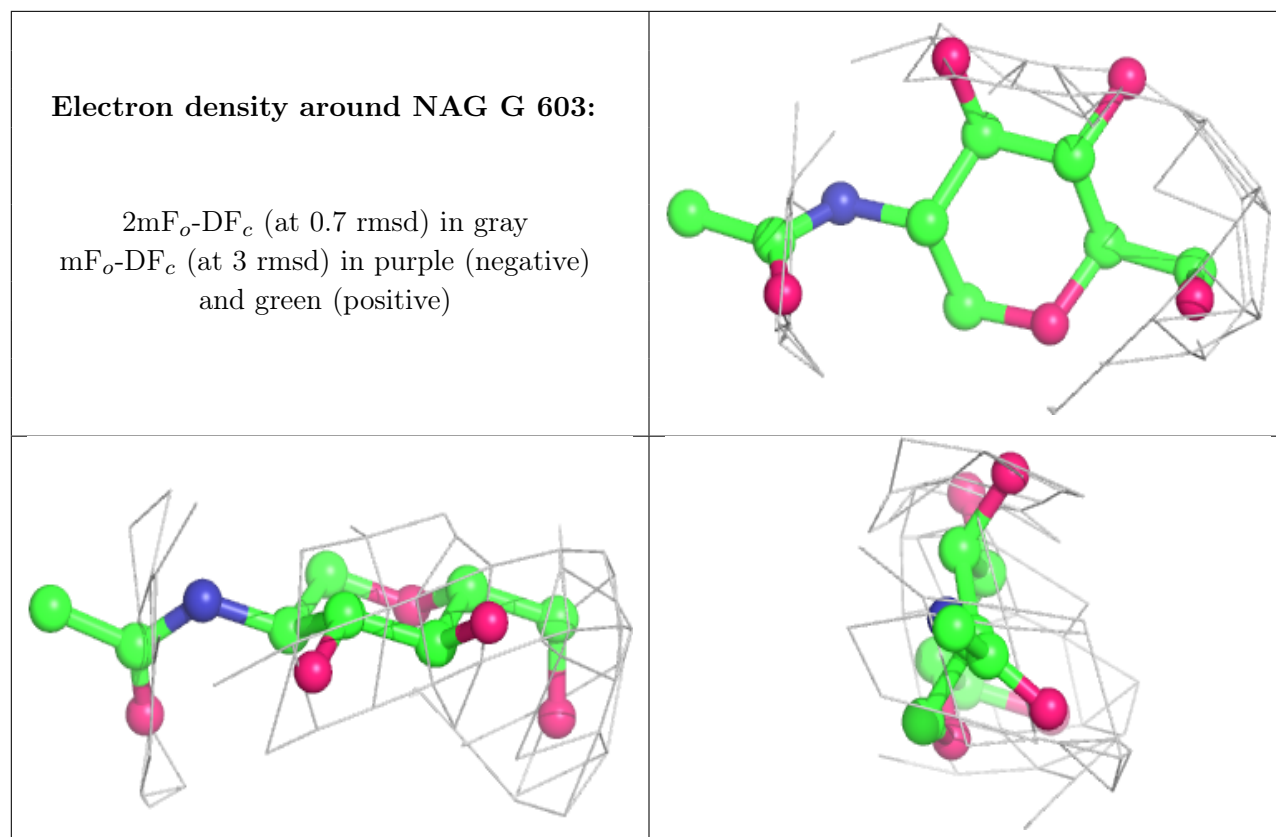
Electron density around NAG G 602:

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

**Electron density around NAG T 702:**

$2mF_o-DF_c$ (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.