



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:42 AM UTC

PDB ID : 7OL4 / pdb_00007ol4
Title : Mouse contactin-1 neurofascin-155 immunoglobulin domains adhesion complex
Authors : Chataigner, L.M.P.; Janssen, B.J.C.
Deposited on : 2021-05-19
Resolution : 4.80 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

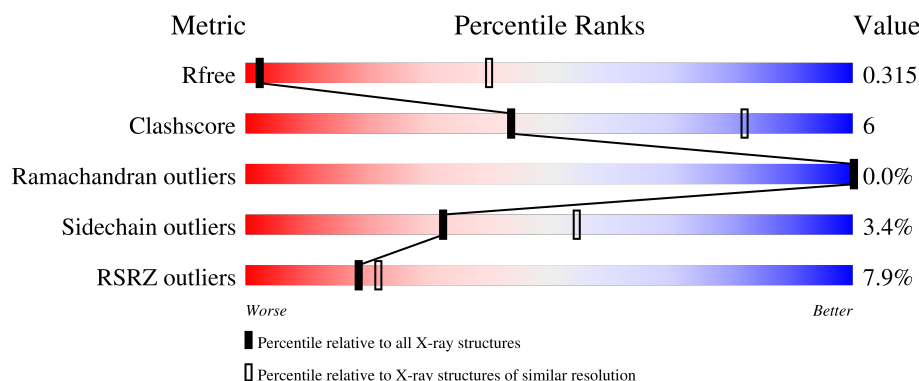
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.80 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.



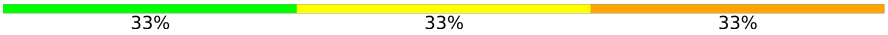
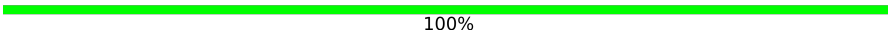
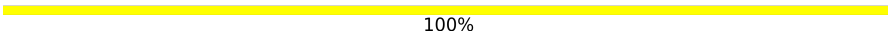
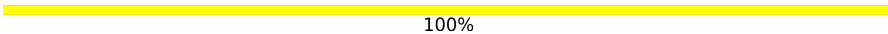
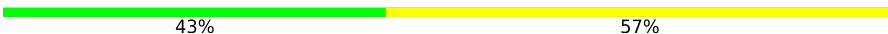
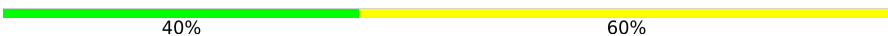
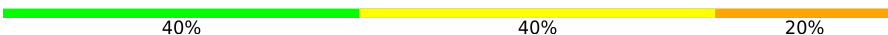
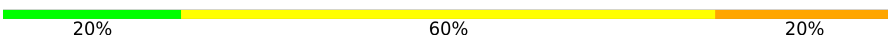
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1018 (5.66-3.94)
Clashscore	190562	1001 (5.60-3.98)
Ramachandran outliers	187476	1104 (5.70-3.90)
Sidechain outliers	187428	1085 (5.70-3.90)
RSRZ outliers	180081	1013 (5.66-3.94)

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

Mol	Chain	Length	Quality of chain
1	A	592	8% 80% 16% ..
1	B	592	8% 79% 16% ..
2	C	617	7% 78% 16% 5%
2	D	617	8% 81% 13% ..
3	E	3	100%

Continued on next page...

Continued from previous page...

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

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 19300 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 Contactin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	570	Total	C	N	O	S	0	0	0
			4515	2879	759	852	25			
1	B	568	Total	C	N	O	S	0	0	0
			4498	2870	757	846	25			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP P12960
A	20	SER	-	expression tag	UNP P12960
A	433	VAL	ILE	conflict	UNP P12960
A	605	HIS	-	expression tag	UNP P12960
A	606	HIS	-	expression tag	UNP P12960
A	607	HIS	-	expression tag	UNP P12960
A	608	HIS	-	expression tag	UNP P12960
A	609	HIS	-	expression tag	UNP P12960
A	610	HIS	-	expression tag	UNP P12960
B	19	GLY	-	expression tag	UNP P12960
B	20	SER	-	expression tag	UNP P12960
B	433	VAL	ILE	conflict	UNP P12960
B	605	HIS	-	expression tag	UNP P12960
B	606	HIS	-	expression tag	UNP P12960
B	607	HIS	-	expression tag	UNP P12960
B	608	HIS	-	expression tag	UNP P12960
B	609	HIS	-	expression tag	UNP P12960
B	610	HIS	-	expression tag	UNP P12960

- Molecule 2 is a protein called Neurofascin.

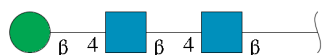
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	587	Total	C	N	O	S	0	0	0
			4648	2917	825	878	28			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	590	Total	C	N	O	S	0	0	0
			4668	2927	828	885	28			

- Molecule 3 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
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



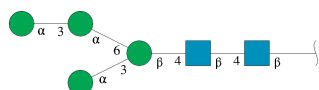
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	P	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is an oligosaccharide called 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.



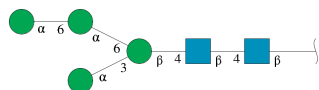
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 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
6	J	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

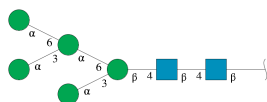
- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

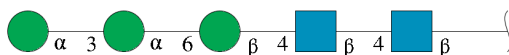
- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

copyranose.



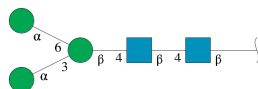
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	M	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 10 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.



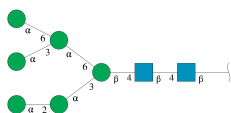
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	N	5	Total	C	N	O	0	0	0
			61	34	2	25			
10	R	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 11 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
11	O	5	Total	C	N	O	0	0	0
			61	34	2	25			
11	S	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



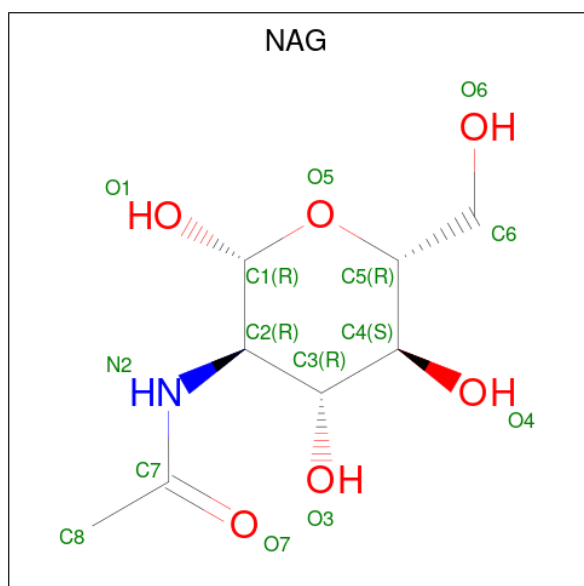
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	Q	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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
13	T	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

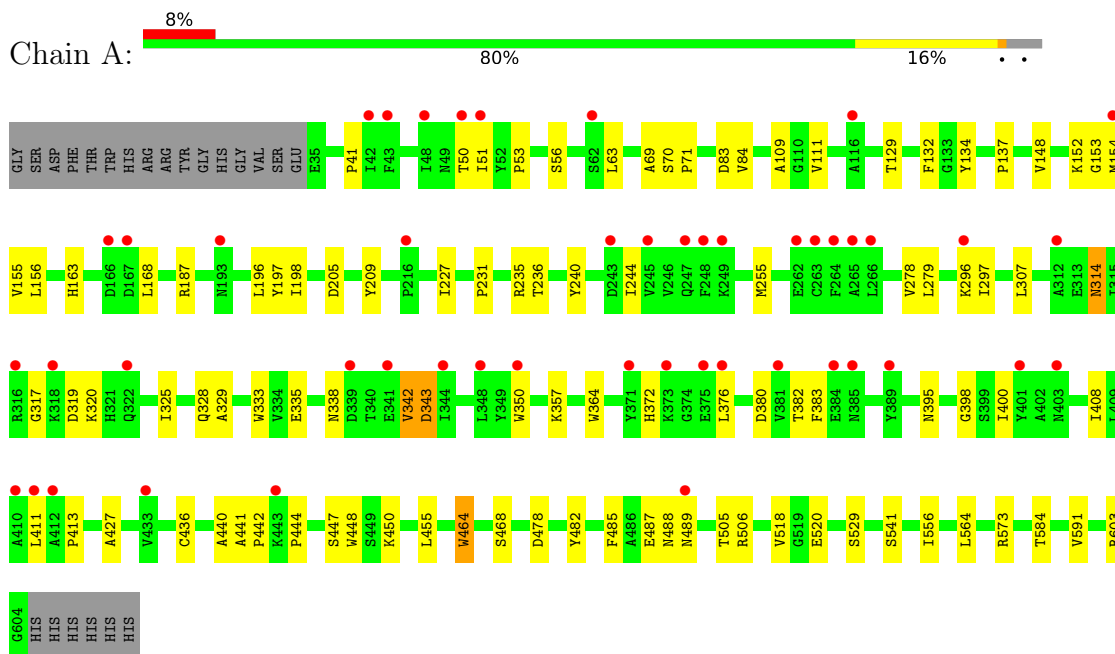


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	N	O	0	0
			14	8	1	5		
14	B	1	Total	C	N	O	0	0
			14	8	1	5		

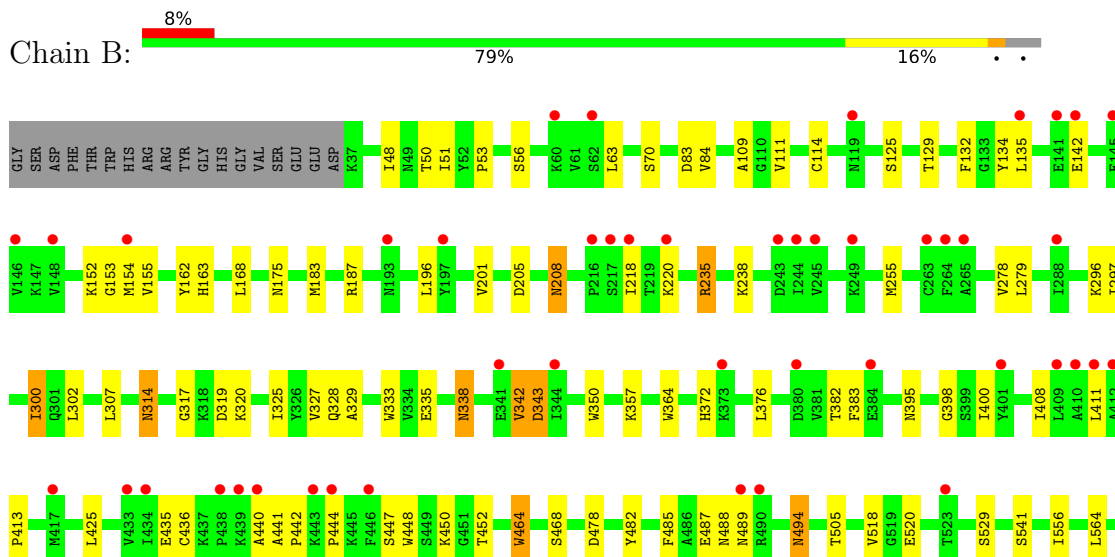
3 Residue-property plots

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

• Molecule 1: Contactin-1

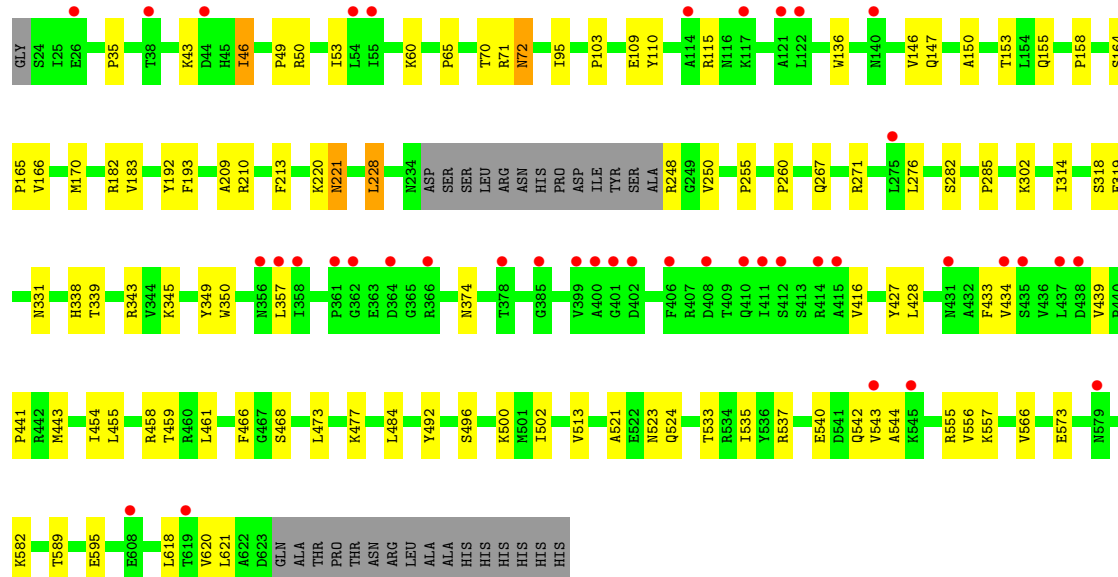
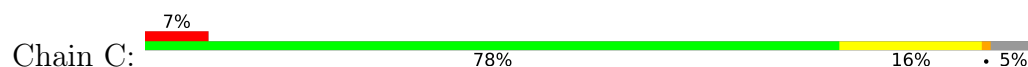


• Molecule 1: Contactin-1

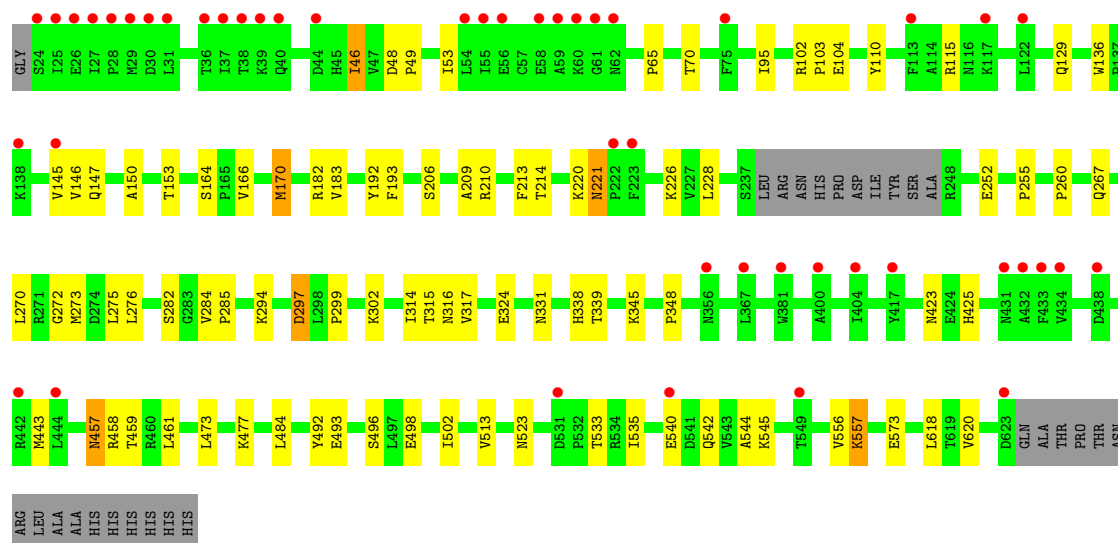
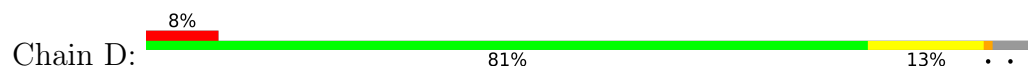




• Molecule 2: Neurofascin



• Molecule 2: Neurofascin



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





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

Chain F: 33% 33% 33%



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

Chain H: 100%



- Molecule 4: 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 G: 75% 25%



- Molecule 4: 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 P: 100%



- Molecule 5: 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 I: 25% 25% 50%

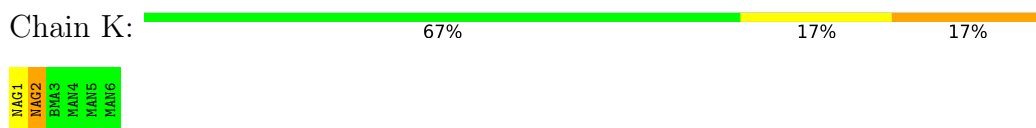


- Molecule 6: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 100%



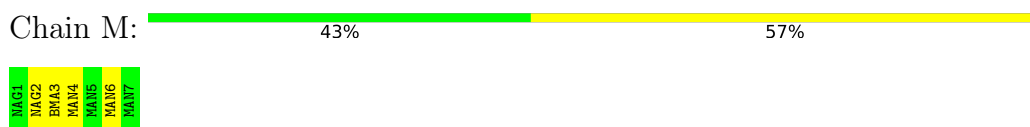
- Molecule 7: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



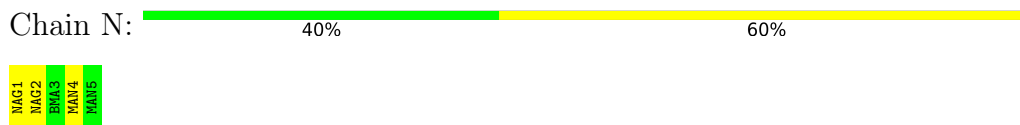
- Molecule 8: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



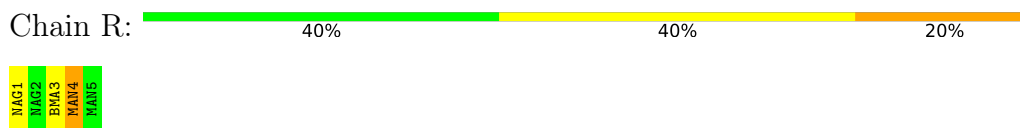
- Molecule 9: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: 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



- Molecule 10: 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



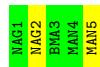
- Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





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

Chain S: 60% 40%



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

Chain Q: 38% 62%



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

Chain T: 75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	146.77Å 151.78Å 162.34Å 90.00° 111.78° 90.00°	Depositor
Resolution (Å)	75.38 – 4.80 75.38 – 4.80	Depositor EDS
% Data completeness (in resolution range)	48.0 (75.38-4.80) 48.3 (75.38-4.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 4.87Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.288 , 0.326 0.293 , 0.315	Depositor DCC
R_{free} test set	794 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	103.8	Xtriage
Anisotropy	1.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 306.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	19300	wwPDB-VP
Average B, all atoms (Å ²)	259.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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, MAN, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	0/4628	0.48	0/6291
1	B	0.19	0/4611	0.46	0/6268
2	C	0.20	0/4754	0.45	0/6450
2	D	0.20	0/4774	0.46	0/6477
All	All	0.20	0/18767	0.46	0/25486

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	A	4515	0	4412	58	1
1	B	4498	0	4402	55	0
2	C	4648	0	4577	58	0
2	D	4668	0	4591	50	0
3	E	39	0	34	0	0
3	F	39	0	34	1	0
3	H	39	0	34	0	0
4	G	50	0	43	2	0
4	P	50	0	43	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	50	0	43	3	0
6	J	72	0	61	0	0
7	K	72	0	61	4	0
8	L	61	0	52	1	0
9	M	83	0	70	0	0
10	N	61	0	52	1	0
10	R	61	0	52	1	0
11	O	61	0	52	2	0
11	S	61	0	52	0	0
12	Q	94	0	79	0	0
13	T	50	0	43	2	0
14	A	14	0	13	0	0
14	B	14	0	13	0	0
All	All	19300	0	18813	233	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (233) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:PRO:HD3	1:B:488:ASN:HD22	1.46	0.80
1:B:425:LEU:HB3	1:B:591:VAL:HG12	1.64	0.79
1:A:427:ALA:HB2	1:A:591:VAL:HB	1.64	0.78
1:A:413:PRO:HD3	1:A:488:ASN:HD22	1.47	0.78
11:O:1:NAG:H3	11:O:1:NAG:H83	1.71	0.71
7:K:2:NAG:H3	7:K:2:NAG:H83	1.77	0.67
2:C:147:GLN:HG2	2:C:228:LEU:HD12	1.75	0.67
1:B:300:ILE:HD11	1:B:327:VAL:HG22	1.80	0.64
1:A:154:MET:HG3	1:A:155:VAL:H	1.63	0.63
2:C:477:LYS:HB2	2:C:484:LEU:HD11	1.81	0.63
2:C:458:ARG:HG2	2:C:500:LYS:O	1.99	0.62
1:A:488:ASN:OD1	1:A:489:ASN:N	2.32	0.62
1:B:338:ASN:OD1	1:B:338:ASN:N	2.33	0.62
1:B:488:ASN:OD1	1:B:489:ASN:N	2.33	0.62
1:B:111:VAL:HG22	1:B:129:THR:HG22	1.82	0.62
1:B:314:ASN:HD21	1:B:317:GLY:H	1.46	0.62
1:A:314:ASN:HD21	1:A:317:GLY:H	1.46	0.61
1:A:342:VAL:HG12	1:A:343:ASP:H	1.64	0.61
1:B:342:VAL:HG12	1:B:343:ASP:H	1.66	0.60
1:A:109:ALA:HB2	1:A:132:PHE:HE2	1.67	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:ASP:O	1:B:482:TYR:OH	2.16	0.59
2:C:416:VAL:HG22	2:C:433:PHE:HB3	1.84	0.59
1:A:111:VAL:HG22	1:A:129:THR:HG22	1.85	0.58
2:C:345:LYS:HB3	2:C:374:ASN:O	2.04	0.58
2:D:182:ARG:HG2	2:D:183:VAL:HG23	1.85	0.58
2:C:182:ARG:HG2	2:C:183:VAL:HG23	1.85	0.58
1:A:478:ASP:O	1:A:482:TYR:OH	2.15	0.58
1:B:135:LEU:HD13	1:B:220:LYS:HG2	1.84	0.58
2:C:461:LEU:O	2:C:496:SER:HA	2.03	0.58
2:D:270:LEU:HA	2:D:345:LYS:O	2.04	0.57
1:B:494:ASN:OD1	1:B:494:ASN:N	2.36	0.57
2:D:285:PRO:HD2	2:D:331:ASN:HD21	1.68	0.57
1:A:464:TRP:HA	4:G:1:NAG:H5	1.86	0.56
1:B:464:TRP:HA	7:K:1:NAG:H5	1.87	0.56
1:B:135:LEU:HD12	1:B:218:ILE:HD11	1.87	0.56
2:C:166:VAL:HB	2:C:210:ARG:HB3	1.87	0.56
1:A:137:PRO:HG2	2:C:50:ARG:HD3	1.88	0.56
1:A:156:LEU:HD13	1:A:227:ILE:HD12	1.87	0.56
2:C:285:PRO:HD2	2:C:331:ASN:HD21	1.71	0.56
2:C:535:ILE:HG12	2:C:556:VAL:HG22	1.86	0.55
1:B:411:LEU:H	1:B:441:ALA:HB2	1.72	0.55
5:I:1:NAG:H4	5:I:2:NAG:N2	2.22	0.55
1:A:235:ARG:HH11	1:A:236:THR:H	1.53	0.54
1:B:109:ALA:HB2	1:B:132:PHE:HE1	1.72	0.54
8:L:2:NAG:H3	8:L:5:MAN:H2	1.89	0.54
2:D:459:THR:HB	2:D:502:ILE:HD11	1.89	0.54
1:B:413:PRO:HB3	1:B:440:ALA:HB2	1.90	0.54
2:D:477:LYS:HB2	2:D:484:LEU:HD11	1.90	0.53
2:C:533:THR:HA	2:C:557:LYS:O	2.09	0.53
2:D:275:LEU:HD23	2:D:314:ILE:HD12	1.90	0.53
1:A:413:PRO:HB3	1:A:440:ALA:HB2	1.89	0.52
2:C:248:ARG:NH1	2:C:248:ARG:HA	2.24	0.52
2:D:535:ILE:HG12	2:D:556:VAL:HG22	1.90	0.52
1:A:411:LEU:H	1:A:441:ALA:HB2	1.74	0.52
2:C:492:TYR:OH	4:P:2:NAG:H82	2.09	0.52
2:D:49:PRO:HA	2:D:103:PRO:HG2	1.92	0.52
1:A:109:ALA:HB2	1:A:132:PHE:CE2	2.44	0.52
2:C:260:PRO:HB2	2:C:338:HIS:CE1	2.46	0.51
2:C:459:THR:HB	2:C:502:ILE:HD11	1.93	0.51
2:D:166:VAL:HB	2:D:210:ARG:HB3	1.92	0.51
2:C:345:LYS:HA	2:C:374:ASN:HB3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:THR:O	2:D:110:TYR:HA	2.10	0.51
1:A:148:VAL:O	1:A:231:PRO:HA	2.12	0.50
1:B:364:TRP:CE3	1:B:376:LEU:HD22	2.46	0.50
2:C:443:MET:HG2	2:C:521:ALA:HB1	1.94	0.50
2:D:260:PRO:HB2	2:D:338:HIS:CE1	2.47	0.50
5:I:2:NAG:H3	5:I:2:NAG:H83	1.93	0.50
2:C:146:VAL:CG2	2:C:150:ALA:HB3	2.42	0.50
1:A:134:TYR:O	1:A:163:HIS:HA	2.12	0.50
2:C:248:ARG:HA	2:C:248:ARG:CZ	2.42	0.50
1:A:464:TRP:NE1	1:A:468:SER:OG	2.46	0.49
1:B:278:VAL:HG23	1:B:279:LEU:H	1.77	0.49
2:D:348:PRO:HD3	2:D:423:ASN:ND2	2.27	0.49
4:P:2:NAG:O7	4:P:2:NAG:O3	2.28	0.49
1:A:464:TRP:CE3	4:G:2:NAG:H82	2.48	0.49
10:R:3:BMA:H5	10:R:4:MAN:H5	1.94	0.49
1:A:278:VAL:HG23	1:A:279:LEU:H	1.78	0.49
7:K:1:NAG:H61	7:K:2:NAG:C7	2.42	0.48
1:B:505:THR:HA	1:B:529:SER:O	2.13	0.48
2:C:343:ARG:HD2	2:C:345:LYS:HE3	1.94	0.48
1:A:333:TRP:CE2	1:A:400:ILE:HD12	2.48	0.48
1:A:441:ALA:HB3	1:A:442:PRO:HD3	1.95	0.48
2:D:145:VAL:HG13	2:D:226:LYS:HB3	1.96	0.48
1:B:109:ALA:HB2	1:B:132:PHE:CE1	2.48	0.48
1:B:208:ASN:N	1:B:208:ASN:HD22	2.12	0.48
1:B:464:TRP:HE3	7:K:2:NAG:O7	1.96	0.48
2:C:544:ALA:O	2:C:620:VAL:HA	2.13	0.48
2:D:221:ASN:OD1	2:D:221:ASN:N	2.47	0.48
1:A:395:ASN:OD1	1:A:398:GLY:N	2.45	0.48
1:A:505:THR:HA	1:A:529:SER:O	2.14	0.48
2:C:146:VAL:O	2:C:228:LEU:HG	2.14	0.47
2:D:147:GLN:HG2	2:D:228:LEU:HD12	1.95	0.47
3:F:1:NAG:H62	3:F:2:NAG:C7	2.44	0.47
1:A:154:MET:HG3	1:A:155:VAL:N	2.28	0.47
1:B:278:VAL:HG21	1:B:307:LEU:HB2	1.97	0.47
2:D:146:VAL:CG2	2:D:150:ALA:HB3	2.44	0.47
2:D:166:VAL:O	2:D:209:ALA:HA	2.14	0.47
2:C:443:MET:HE2	2:C:523:ASN:HB2	1.96	0.47
1:B:333:TRP:CE2	1:B:400:ILE:HD12	2.49	0.47
2:C:43:LYS:NZ	2:C:427:TYR:O	2.48	0.47
1:A:447:SER:OG	1:A:485:PHE:HB2	2.13	0.47
1:B:328:GLN:HA	1:B:357:LYS:HG2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:ALA:HB3	1:B:442:PRO:HD3	1.96	0.47
2:C:70:THR:O	2:C:110:TYR:HA	2.15	0.47
1:B:255:MET:N	1:B:328:GLN:O	2.48	0.47
1:B:464:TRP:NE1	1:B:468:SER:OG	2.48	0.47
13:T:1:NAG:O7	13:T:1:NAG:H3	2.15	0.47
1:B:447:SER:OG	1:B:485:PHE:HB2	2.14	0.46
2:C:46:ILE:HD12	2:C:213:PHE:CE1	2.50	0.46
2:C:136:TRP:CH2	2:C:220:LYS:HD2	2.50	0.46
2:D:275:LEU:HB2	2:D:317:VAL:HG11	1.95	0.46
1:A:319:ASP:OD1	1:A:320:LYS:N	2.48	0.46
2:C:454:ILE:HD12	2:C:455:LEU:N	2.31	0.46
2:D:136:TRP:CH2	2:D:220:LYS:HD2	2.50	0.46
1:B:436:CYS:HB2	1:B:448:TRP:CZ2	2.51	0.46
2:D:443:MET:HE2	2:D:523:ASN:HB2	1.98	0.46
1:A:278:VAL:HG21	1:A:307:LEU:HB2	1.96	0.46
2:C:302:LYS:HD3	2:C:314:ILE:HG23	1.98	0.46
1:A:50:THR:C	1:A:51:ILE:HG13	2.41	0.46
1:A:83:ASP:OD1	1:A:84:VAL:N	2.49	0.46
1:B:485:PHE:CD1	1:B:494:ASN:HB3	2.51	0.46
2:C:271:ARG:HD3	2:C:349:TYR:CE2	2.49	0.46
1:A:53:PRO:HB2	1:A:56:SER:HB2	1.98	0.46
1:B:153:GLY:HA2	1:B:201:VAL:HG23	1.98	0.46
2:C:439:VAL:H	2:C:468:SER:HB2	1.81	0.46
2:D:345:LYS:HB3	2:D:425:HIS:NE2	2.30	0.45
11:O:1:NAG:H3	11:O:1:NAG:C8	2.43	0.45
1:B:83:ASP:OD1	1:B:84:VAL:N	2.48	0.45
1:A:328:GLN:HA	1:A:357:LYS:HG2	1.96	0.45
1:A:163:HIS:CD2	1:A:168:LEU:HD11	2.51	0.45
1:A:255:MET:N	1:A:328:GLN:O	2.48	0.45
1:B:50:THR:C	1:B:51:ILE:HG13	2.41	0.45
2:C:49:PRO:HA	2:C:103:PRO:HG2	1.98	0.45
2:D:252:GLU:HA	2:D:284:VAL:HG11	1.98	0.45
2:D:544:ALA:O	2:D:620:VAL:HA	2.16	0.45
2:C:166:VAL:O	2:C:209:ALA:HA	2.16	0.45
2:C:473:LEU:HA	2:C:513:VAL:O	2.17	0.45
2:D:473:LEU:HA	2:D:513:VAL:O	2.17	0.45
1:B:235:ARG:CZ	1:B:235:ARG:HA	2.47	0.45
2:C:318:SER:HB3	10:N:1:NAG:H81	1.99	0.45
1:B:395:ASN:OD1	1:B:398:GLY:N	2.46	0.45
1:A:152:LYS:HE2	1:A:240:TYR:CZ	2.53	0.44
1:B:329:ALA:HB3	1:B:357:LYS:H	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:183:VAL:HG22	2:C:193:PHE:HA	1.99	0.44
2:C:350:TRP:NE1	2:C:428:LEU:HD13	2.31	0.44
1:A:244:ILE:HG13	1:A:319:ASP:HB3	1.98	0.44
1:A:187:ARG:NH2	1:A:205:ASP:OD1	2.49	0.44
1:B:319:ASP:OD1	1:B:320:LYS:N	2.50	0.44
2:D:299:PRO:HB2	2:D:302:LYS:HG2	1.99	0.44
2:C:543:VAL:HG12	2:C:621:LEU:HD11	1.99	0.44
2:D:492:TYR:CD2	13:T:1:NAG:H61	2.52	0.44
2:D:542:GLN:HG3	2:D:618:LEU:HD13	2.00	0.44
1:A:70:SER:OG	1:A:71:PRO:HD3	2.18	0.44
1:A:329:ALA:HB3	1:A:357:LYS:H	1.82	0.44
2:D:294:LYS:HB2	2:D:324:GLU:HB2	1.99	0.44
1:A:364:TRP:CE3	1:A:376:LEU:HD22	2.53	0.44
2:D:183:VAL:HG22	2:D:193:PHE:HA	1.99	0.44
2:C:248:ARG:NH1	2:C:250:VAL:HG12	2.33	0.44
2:C:542:GLN:HG3	2:C:618:LEU:HD13	1.99	0.44
2:D:46:ILE:HA	2:D:129:GLN:O	2.18	0.44
1:A:63:LEU:HD23	1:A:63:LEU:HA	1.83	0.43
1:B:53:PRO:HB2	1:B:56:SER:HB2	2.00	0.43
2:C:357:LEU:HB2	2:C:434:VAL:HG22	2.00	0.43
1:A:153:GLY:HA3	1:A:198:ILE:O	2.19	0.43
2:C:221:ASN:OD1	2:C:221:ASN:N	2.49	0.43
2:D:533:THR:HA	2:D:557:LYS:O	2.19	0.43
1:B:556:ILE:O	1:B:573:ARG:NH2	2.51	0.43
2:C:345:LYS:HD2	2:C:374:ASN:CG	2.44	0.43
1:B:134:TYR:O	1:B:163:HIS:HA	2.19	0.43
2:D:270:LEU:O	2:D:273:MET:HB2	2.19	0.43
1:B:187:ARG:NH2	1:B:205:ASP:OD1	2.50	0.43
2:C:35:PRO:HA	2:C:60:LYS:O	2.19	0.43
1:A:444:PRO:HB3	1:A:488:ASN:HA	2.00	0.43
1:B:63:LEU:HD23	1:B:63:LEU:HA	1.83	0.43
2:D:48:ASP:OD2	2:D:214:THR:HA	2.19	0.43
2:D:65:PRO:HA	2:D:115:ARG:O	2.18	0.43
1:A:155:VAL:HG22	1:A:197:TYR:HA	2.01	0.42
1:A:444:PRO:HB2	1:A:487:GLU:O	2.19	0.42
1:A:436:CYS:HB2	1:A:448:TRP:CZ2	2.53	0.42
2:C:72:ASN:HD22	2:C:109:GLU:HB2	1.84	0.42
1:A:518:VAL:HG13	1:A:603:ARG:O	2.19	0.42
1:A:556:ILE:O	1:A:573:ARG:NH2	2.53	0.42
2:D:53:ILE:HG22	2:D:95:ILE:HB	2.02	0.42
1:B:114:CYS:HB3	1:B:125:SER:OG	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:255:PRO:HA	2:D:282:SER:O	2.19	0.42
1:A:205:ASP:O	1:A:209:TYR:OH	2.31	0.42
2:C:71:ARG:HA	2:C:109:GLU:O	2.20	0.42
2:C:153:THR:HG23	2:C:192:TYR:CE1	2.54	0.42
2:D:272:GLY:HA2	2:D:316:ASN:HB2	2.00	0.42
2:D:348:PRO:HD3	2:D:423:ASN:HD21	1.84	0.42
5:I:1:NAG:O4	5:I:2:NAG:H2	2.20	0.42
1:A:450:LYS:HB2	1:A:455:LEU:HD11	2.01	0.42
2:D:458:ARG:NH1	2:D:498:GLU:OE2	2.52	0.42
1:A:155:VAL:HA	1:A:196:LEU:O	2.19	0.42
1:B:163:HIS:CD2	1:B:168:LEU:HD11	2.54	0.42
2:C:65:PRO:HA	2:C:115:ARG:O	2.20	0.42
1:A:296:LYS:O	1:A:297:ILE:HD13	2.19	0.42
2:D:153:THR:HG23	2:D:192:TYR:CE1	2.53	0.42
1:B:444:PRO:HB3	1:B:488:ASN:HA	2.02	0.42
1:B:518:VAL:HG13	1:B:603:ARG:O	2.20	0.42
2:D:457:ASN:HD22	2:D:457:ASN:HA	1.45	0.42
1:A:541:SER:OG	1:A:584:THR:HB	2.20	0.41
2:C:53:ILE:HG22	2:C:95:ILE:HB	2.01	0.41
4:P:3:BMA:H61	4:P:4:MAN:H2	1.79	0.41
1:A:325:ILE:HD13	1:A:325:ILE:HA	1.85	0.41
2:C:165:PRO:HB2	2:C:209:ALA:HB1	2.02	0.41
1:A:278:VAL:HG23	1:A:279:LEU:N	2.35	0.41
2:D:46:ILE:HD12	2:D:213:PHE:HE2	1.85	0.41
1:B:296:LYS:O	1:B:297:ILE:HD13	2.20	0.41
2:D:535:ILE:HG23	2:D:556:VAL:HG22	2.03	0.41
2:D:294:LYS:HD2	2:D:324:GLU:HG3	2.03	0.41
2:D:458:ARG:HD2	2:D:498:GLU:OE2	2.20	0.41
1:B:541:SER:OG	1:B:584:THR:HB	2.20	0.41
1:A:154:MET:CG	1:A:155:VAL:H	2.31	0.41
1:B:325:ILE:HD13	1:B:325:ILE:HA	1.86	0.41
2:C:136:TRP:CH2	2:C:158:PRO:HA	2.56	0.41
1:B:278:VAL:HG23	1:B:279:LEU:N	2.36	0.41
2:C:255:PRO:HA	2:C:282:SER:O	2.20	0.41
2:D:170:MET:O	2:D:206:SER:OG	2.36	0.41
2:C:537:ARG:HB2	2:C:555:ARG:HB2	2.03	0.41
2:D:314:ILE:HG22	2:D:315:THR:N	2.36	0.41
2:D:461:LEU:O	2:D:496:SER:HA	2.21	0.41
1:B:155:VAL:HA	1:B:196:LEU:O	2.20	0.40
1:A:41:PRO:HA	1:A:69:ALA:HB2	2.02	0.40
2:C:441:PRO:HA	2:C:466:PHE:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:102:ARG:NH2	2:D:104:GLU:OE2	2.54	0.40
2:D:297:ASP:OD1	2:D:297:ASP:N	2.54	0.40
1:B:134:TYR:CE1	1:B:162:TYR:HB2	2.57	0.40
2:C:319:GLU:OE1	2:C:319:GLU:N	2.52	0.40
2:C:582:LYS:HB3	2:C:589:THR:OG1	2.22	0.40
1:B:450:LYS:O	1:B:452:THR:N	2.52	0.40
2:C:523:ASN:OD1	2:C:524:GLN:N	2.55	0.40
1:B:444:PRO:HB2	1:B:487:GLU:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LYS:NZ	1:A:380:ASP:OD2[2_656]	2.17	0.03

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	A	568/592 (96%)	521 (92%)	47 (8%)	0	100	100
1	B	566/592 (96%)	520 (92%)	45 (8%)	1 (0%)	43	78
2	C	583/617 (94%)	546 (94%)	37 (6%)	0	100	100
2	D	586/617 (95%)	556 (95%)	30 (5%)	0	100	100
All	All	2303/2418 (95%)	2143 (93%)	159 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	175	ASN

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	A	494/513 (96%)	480 (97%)	14 (3%)	38	59
1	B	492/513 (96%)	466 (95%)	26 (5%)	20	42
2	C	520/545 (95%)	506 (97%)	14 (3%)	39	60
2	D	523/545 (96%)	509 (97%)	14 (3%)	39	60
All	All	2029/2116 (96%)	1961 (97%)	68 (3%)	32	54

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	314	ASN
1	A	335	GLU
1	A	338	ASN
1	A	342	VAL
1	A	343	ASP
1	A	350	TRP
1	A	372	HIS
1	A	382	THR
1	A	383	PHE
1	A	408	ILE
1	A	464	TRP
1	A	506	ARG
1	A	520	GLU
1	A	564	LEU
1	B	48	ILE
1	B	70	SER
1	B	142	GLU
1	B	152	LYS
1	B	154	MET
1	B	183	MET
1	B	208	ASN
1	B	235	ARG
1	B	238	LYS
1	B	300	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	302	LEU
1	B	314	ASN
1	B	335	GLU
1	B	338	ASN
1	B	342	VAL
1	B	343	ASP
1	B	350	TRP
1	B	372	HIS
1	B	382	THR
1	B	383	PHE
1	B	408	ILE
1	B	435	GLU
1	B	464	TRP
1	B	494	ASN
1	B	520	GLU
1	B	564	LEU
2	C	46	ILE
2	C	72	ASN
2	C	155	GLN
2	C	164	SER
2	C	170	MET
2	C	221	ASN
2	C	228	LEU
2	C	267	GLN
2	C	276	LEU
2	C	339	THR
2	C	540	GLU
2	C	566	VAL
2	C	573	GLU
2	C	595	GLU
2	D	46	ILE
2	D	164	SER
2	D	170	MET
2	D	221	ASN
2	D	267	GLN
2	D	276	LEU
2	D	297	ASP
2	D	339	THR
2	D	457	ASN
2	D	493	GLU
2	D	540	GLU
2	D	545	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	557	LYS
2	D	573	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	A	257	GLN
1	A	321	HIS
1	A	372	HIS
1	A	385	ASN
1	B	257	GLN
1	B	321	HIS
1	B	385	ASN
2	C	62	ASN
2	C	72	ASN
2	C	129	GLN
2	C	309	ASN
2	C	490	HIS
2	D	33	GLN
2	D	62	ASN
2	D	129	GLN
2	D	230	ASN
2	D	309	ASN
2	D	490	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

77 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	$\# Z > 2$
3	NAG	E	1	3,1	14,14,15	0.31	0	17,19,21	0.55	0
3	NAG	E	2	3	14,14,15	0.53	0	17,19,21	0.53	0
3	BMA	E	3	3	11,11,12	0.68	0	15,15,17	0.68	0
3	NAG	F	1	3,1	14,14,15	0.24	0	17,19,21	0.52	0
3	NAG	F	2	3	14,14,15	0.42	0	17,19,21	1.01	1 (5%)
3	BMA	F	3	3	11,11,12	0.74	0	15,15,17	0.74	0
4	NAG	G	1	4,1	14,14,15	0.27	0	17,19,21	0.47	0
4	NAG	G	2	4	14,14,15	0.42	0	17,19,21	0.96	1 (5%)
4	BMA	G	3	4	11,11,12	1.04	1 (9%)	15,15,17	1.30	1 (6%)
4	MAN	G	4	4	11,11,12	0.87	1 (9%)	15,15,17	0.92	0
3	NAG	H	1	3,1	14,14,15	0.30	0	17,19,21	0.69	0
3	NAG	H	2	3	14,14,15	0.60	0	17,19,21	0.56	0
3	BMA	H	3	3	11,11,12	0.57	0	15,15,17	0.69	0
5	NAG	I	1	5,1	14,14,15	0.63	1 (7%)	17,19,21	0.84	0
5	NAG	I	2	5	14,14,15	1.70	2 (14%)	17,19,21	1.47	2 (11%)
5	BMA	I	3	5	11,11,12	0.96	0	15,15,17	0.82	0
5	MAN	I	4	5	11,11,12	0.71	0	15,15,17	0.77	1 (6%)
6	NAG	J	1	6,1	14,14,15	1.26	1 (7%)	17,19,21	1.23	1 (5%)
6	NAG	J	2	6	14,14,15	0.82	0	17,19,21	1.58	2 (11%)
6	BMA	J	3	6	11,11,12	1.64	4 (36%)	15,15,17	0.94	0
6	MAN	J	4	6	11,11,12	1.29	1 (9%)	15,15,17	1.21	0
6	MAN	J	5	6	11,11,12	0.79	1 (9%)	15,15,17	0.87	0
6	MAN	J	6	6	11,11,12	0.88	0	15,15,17	0.79	1 (6%)
7	NAG	K	1	7,1	14,14,15	0.23	0	17,19,21	0.39	0
7	NAG	K	2	7	14,14,15	0.55	0	17,19,21	1.19	1 (5%)
7	BMA	K	3	7	11,11,12	0.62	0	15,15,17	0.84	0
7	MAN	K	4	7	11,11,12	0.75	0	15,15,17	0.73	0
7	MAN	K	5	7	11,11,12	0.69	0	15,15,17	0.75	0
7	MAN	K	6	7	11,11,12	0.67	0	15,15,17	0.72	0
8	NAG	L	1	8,1	14,14,15	0.30	0	17,19,21	0.61	0
8	NAG	L	2	8	14,14,15	0.30	0	17,19,21	0.67	1 (5%)
8	BMA	L	3	8	11,11,12	0.66	0	15,15,17	0.62	0
8	MAN	L	4	8	11,11,12	0.62	0	15,15,17	0.86	0
8	MAN	L	5	8	11,11,12	0.87	1 (9%)	15,15,17	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	M	1	9,2	14,14,15	0.21	0	17,19,21	0.33	0
9	NAG	M	2	9	14,14,15	0.59	0	17,19,21	0.77	1 (5%)
9	BMA	M	3	9	11,11,12	1.20	2 (18%)	15,15,17	0.69	0
9	MAN	M	4	9	11,11,12	0.56	0	15,15,17	0.76	1 (6%)
9	MAN	M	5	9	11,11,12	0.68	0	15,15,17	0.69	0
9	MAN	M	6	9	11,11,12	0.75	0	15,15,17	0.79	1 (6%)
9	MAN	M	7	9	11,11,12	0.68	0	15,15,17	0.64	0
10	NAG	N	1	10,2	14,14,15	0.24	0	17,19,21	0.44	0
10	NAG	N	2	10	14,14,15	0.45	0	17,19,21	0.82	1 (5%)
10	BMA	N	3	10	11,11,12	0.73	0	15,15,17	0.65	0
10	MAN	N	4	10	11,11,12	0.70	0	15,15,17	0.77	1 (6%)
10	MAN	N	5	10	11,11,12	0.65	0	15,15,17	0.75	0
11	NAG	O	1	2,11	14,14,15	1.01	1 (7%)	17,19,21	1.28	1 (5%)
11	NAG	O	2	11	14,14,15	0.47	0	17,19,21	0.80	1 (5%)
11	BMA	O	3	11	11,11,12	1.02	0	15,15,17	1.05	1 (6%)
11	MAN	O	4	11	11,11,12	0.91	1 (9%)	15,15,17	1.04	2 (13%)
11	MAN	O	5	11	11,11,12	0.94	0	15,15,17	0.92	0
4	NAG	P	1	4,2	14,14,15	0.88	1 (7%)	17,19,21	0.53	0
4	NAG	P	2	4	14,14,15	0.49	0	17,19,21	0.67	0
4	BMA	P	3	4	11,11,12	0.49	0	15,15,17	0.54	0
4	MAN	P	4	4	11,11,12	0.68	0	15,15,17	0.69	0
12	NAG	Q	1	2,12	14,14,15	0.31	0	17,19,21	0.42	0
12	NAG	Q	2	12	14,14,15	0.79	1 (7%)	17,19,21	0.86	1 (5%)
12	BMA	Q	3	12	11,11,12	2.06	3 (27%)	15,15,17	1.45	2 (13%)
12	MAN	Q	4	12	11,11,12	1.01	0	15,15,17	1.19	1 (6%)
12	MAN	Q	5	12	11,11,12	0.72	0	15,15,17	0.91	0
12	MAN	Q	6	12	11,11,12	1.13	1 (9%)	15,15,17	1.39	3 (20%)
12	MAN	Q	7	12	11,11,12	0.78	0	15,15,17	0.75	1 (6%)
12	MAN	Q	8	12	11,11,12	0.73	0	15,15,17	0.86	0
10	NAG	R	1	10,2	14,14,15	0.19	0	17,19,21	0.78	1 (5%)
10	NAG	R	2	10	14,14,15	0.52	0	17,19,21	0.51	0
10	BMA	R	3	10	11,11,12	0.54	0	15,15,17	0.71	0
10	MAN	R	4	10	11,11,12	0.86	0	15,15,17	0.97	1 (6%)
10	MAN	R	5	10	11,11,12	0.64	0	15,15,17	0.81	0
11	NAG	S	1	2,11	14,14,15	0.31	0	17,19,21	0.50	0
11	NAG	S	2	11	14,14,15	0.59	0	17,19,21	0.66	1 (5%)
11	BMA	S	3	11	11,11,12	0.69	0	15,15,17	0.57	0
11	MAN	S	4	11	11,11,12	0.66	0	15,15,17	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MAN	S	5	11	11,11,12	0.60	0	15,15,17	0.75	1 (6%)
13	NAG	T	1	13,2	14,14,15	1.11	1 (7%)	17,19,21	1.28	3 (17%)
13	NAG	T	2	13	14,14,15	0.81	0	17,19,21	0.98	2 (11%)
13	BMA	T	3	13	11,11,12	0.91	0	15,15,17	0.93	1 (6%)
13	MAN	T	4	13	11,11,12	0.91	1 (9%)	15,15,17	0.88	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
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
3	BMA	H	3	3	-	1/2/19/22	0/1/1/1
5	NAG	I	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	I	2	5	-	6/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	MAN	I	4	5	-	0/2/19/22	0/1/1/1
6	NAG	J	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
6	MAN	J	5	6	-	0/2/19/22	0/1/1/1
6	MAN	J	6	6	-	0/2/19/22	0/1/1/1
7	NAG	K	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	4/6/23/26	0/1/1/1
7	BMA	K	3	7	-	0/2/19/22	0/1/1/1
7	MAN	K	4	7	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	K	5	7	-	0/2/19/22	0/1/1/1
7	MAN	K	6	7	-	0/2/19/22	0/1/1/1
8	NAG	L	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	L	2	8	-	1/6/23/26	0/1/1/1
8	BMA	L	3	8	-	2/2/19/22	0/1/1/1
8	MAN	L	4	8	-	2/2/19/22	0/1/1/1
8	MAN	L	5	8	-	1/2/19/22	0/1/1/1
9	NAG	M	1	9,2	-	1/6/23/26	0/1/1/1
9	NAG	M	2	9	-	0/6/23/26	0/1/1/1
9	BMA	M	3	9	-	0/2/19/22	0/1/1/1
9	MAN	M	4	9	-	0/2/19/22	0/1/1/1
9	MAN	M	5	9	-	0/2/19/22	0/1/1/1
9	MAN	M	6	9	-	0/2/19/22	0/1/1/1
9	MAN	M	7	9	-	0/2/19/22	0/1/1/1
10	NAG	N	1	10,2	-	1/6/23/26	0/1/1/1
10	NAG	N	2	10	-	0/6/23/26	0/1/1/1
10	BMA	N	3	10	-	2/2/19/22	0/1/1/1
10	MAN	N	4	10	-	0/2/19/22	0/1/1/1
10	MAN	N	5	10	-	1/2/19/22	0/1/1/1
11	NAG	O	1	2,11	-	3/6/23/26	0/1/1/1
11	NAG	O	2	11	-	2/6/23/26	0/1/1/1
11	BMA	O	3	11	-	0/2/19/22	0/1/1/1
11	MAN	O	4	11	-	1/2/19/22	0/1/1/1
11	MAN	O	5	11	-	0/2/19/22	0/1/1/1
4	NAG	P	1	4,2	-	1/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	BMA	P	3	4	-	0/2/19/22	0/1/1/1
4	MAN	P	4	4	-	1/2/19/22	0/1/1/1
12	NAG	Q	1	2,12	-	0/6/23/26	0/1/1/1
12	NAG	Q	2	12	-	1/6/23/26	0/1/1/1
12	BMA	Q	3	12	-	0/2/19/22	0/1/1/1
12	MAN	Q	4	12	-	1/2/19/22	0/1/1/1
12	MAN	Q	5	12	-	0/2/19/22	0/1/1/1
12	MAN	Q	6	12	-	2/2/19/22	0/1/1/1
12	MAN	Q	7	12	-	0/2/19/22	0/1/1/1
12	MAN	Q	8	12	-	0/2/19/22	0/1/1/1
10	NAG	R	1	10,2	-	0/6/23/26	0/1/1/1
10	NAG	R	2	10	-	0/6/23/26	0/1/1/1
10	BMA	R	3	10	-	1/2/19/22	0/1/1/1
10	MAN	R	4	10	-	0/2/19/22	0/1/1/1
10	MAN	R	5	10	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	S	1	2,11	-	0/6/23/26	0/1/1/1
11	NAG	S	2	11	-	0/6/23/26	0/1/1/1
11	BMA	S	3	11	-	0/2/19/22	0/1/1/1
11	MAN	S	4	11	-	0/2/19/22	0/1/1/1
11	MAN	S	5	11	-	0/2/19/22	0/1/1/1
13	NAG	T	1	13,2	-	2/6/23/26	0/1/1/1
13	NAG	T	2	13	-	2/6/23/26	0/1/1/1
13	BMA	T	3	13	-	1/2/19/22	0/1/1/1
13	MAN	T	4	13	-	1/2/19/22	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	2	NAG	C1-C2	5.16	1.59	1.52
12	Q	3	BMA	O5-C1	-4.18	1.36	1.43
6	J	1	NAG	O5-C1	-3.95	1.37	1.43
12	Q	3	BMA	C2-C3	3.59	1.58	1.52
5	I	2	NAG	O5-C1	3.57	1.49	1.43
12	Q	3	BMA	O3-C3	3.40	1.51	1.43
6	J	4	MAN	O5-C1	-3.37	1.38	1.43
11	O	1	NAG	C1-C2	3.10	1.56	1.52
13	T	1	NAG	C1-C2	3.07	1.56	1.52
4	P	1	NAG	O5-C1	-3.03	1.38	1.43
12	Q	6	MAN	O5-C1	-2.99	1.38	1.43
6	J	3	BMA	O5-C5	-2.76	1.38	1.43
6	J	3	BMA	O5-C1	-2.63	1.39	1.43
12	Q	2	NAG	C1-C2	2.54	1.55	1.52
8	L	5	MAN	C1-C2	2.52	1.58	1.52
13	T	4	MAN	C1-C2	2.47	1.58	1.52
4	G	4	MAN	C1-C2	2.24	1.57	1.52
6	J	5	MAN	C1-C2	2.22	1.57	1.52
11	O	4	MAN	C1-C2	2.22	1.57	1.52
9	M	3	BMA	O5-C1	-2.21	1.40	1.43
6	J	3	BMA	C1-C2	2.19	1.57	1.52
9	M	3	BMA	C2-C3	2.15	1.55	1.52
5	I	1	NAG	C1-C2	2.07	1.55	1.52
4	G	3	BMA	C6-C5	2.07	1.58	1.51
6	J	3	BMA	C2-C3	2.06	1.55	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	2	NAG	C1-O5-C5	5.13	119.06	112.19
5	I	2	NAG	C2-N2-C7	4.72	129.22	122.90
11	O	1	NAG	C2-N2-C7	4.30	128.66	122.90
4	G	3	BMA	O5-C5-C6	4.27	115.97	107.66
7	K	2	NAG	C2-N2-C7	4.02	128.29	122.90
12	Q	3	BMA	C1-O5-C5	3.66	117.09	112.19
3	F	2	NAG	C1-O5-C5	3.14	116.40	112.19
5	I	2	NAG	C1-C2-N2	3.00	115.16	110.43
12	Q	4	MAN	O2-C2-C3	-2.86	104.24	110.15
13	T	3	BMA	O5-C5-C6	2.80	113.12	107.66
6	J	2	NAG	O4-C4-C5	-2.65	102.80	109.32
12	Q	2	NAG	O4-C4-C5	-2.61	102.89	109.32
6	J	1	NAG	O3-C3-C2	-2.48	104.26	109.40
10	R	1	NAG	O4-C4-C3	-2.34	104.86	110.38
13	T	2	NAG	C1-C2-N2	2.33	114.11	110.43
13	T	1	NAG	C3-C4-C5	2.33	114.45	110.23
10	N	2	NAG	C1-O5-C5	2.32	115.30	112.19
12	Q	6	MAN	C1-C2-C3	2.30	113.00	109.64
13	T	1	NAG	O4-C4-C5	-2.28	103.70	109.32
13	T	2	NAG	O5-C1-C2	-2.27	107.78	111.29
12	Q	6	MAN	O6-C6-C5	-2.27	103.62	111.33
4	G	2	NAG	C1-C2-N2	2.26	114.00	110.43
12	Q	3	BMA	O6-C6-C5	-2.24	103.72	111.33
8	L	2	NAG	C1-O5-C5	2.22	115.16	112.19
11	O	2	NAG	C1-O5-C5	2.22	115.16	112.19
9	M	6	MAN	O2-C2-C3	-2.15	105.69	110.15
13	T	1	NAG	C2-N2-C7	2.14	125.77	122.90
9	M	4	MAN	O2-C2-C3	-2.12	105.76	110.15
12	Q	6	MAN	O3-C3-C4	-2.11	105.41	110.38
11	O	3	BMA	C6-C5-C4	2.11	118.19	113.02
11	S	2	NAG	C1-O5-C5	2.06	114.95	112.19
10	N	4	MAN	O2-C2-C3	-2.06	105.89	110.15
11	O	4	MAN	C1-O5-C5	2.05	114.94	112.19
10	R	4	MAN	O2-C2-C3	-2.05	105.91	110.15
12	Q	7	MAN	O2-C2-C3	-2.05	105.91	110.15
11	S	5	MAN	O2-C2-C3	-2.04	105.94	110.15
9	M	2	NAG	C1-O5-C5	2.03	114.90	112.19
6	J	6	MAN	O2-C2-C3	-2.02	105.97	110.15
11	O	4	MAN	O2-C2-C3	-2.01	105.98	110.15
5	I	4	MAN	O2-C2-C3	-2.01	105.98	110.15

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C1-C2-N2-C7
13	T	2	NAG	O5-C5-C6-O6
13	T	2	NAG	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
6	J	3	BMA	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
6	J	3	BMA	C4-C5-C6-O6
8	L	4	MAN	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
6	J	2	NAG	C8-C7-N2-C2
6	J	2	NAG	O7-C7-N2-C2
7	K	1	NAG	C8-C7-N2-C2
7	K	1	NAG	O7-C7-N2-C2
7	K	2	NAG	C8-C7-N2-C2
7	K	2	NAG	O7-C7-N2-C2
11	O	1	NAG	C8-C7-N2-C2
11	O	1	NAG	O7-C7-N2-C2
12	Q	4	MAN	O5-C5-C6-O6
10	N	3	BMA	C4-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
12	Q	6	MAN	O5-C5-C6-O6
10	N	3	BMA	O5-C5-C6-O6
8	L	3	BMA	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
10	N	5	MAN	O5-C5-C6-O6
8	L	4	MAN	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
4	P	4	MAN	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
13	T	1	NAG	O5-C5-C6-O6
12	Q	6	MAN	C4-C5-C6-O6
10	R	3	BMA	O5-C5-C6-O6
13	T	4	MAN	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
8	L	5	MAN	O5-C5-C6-O6
11	O	4	MAN	O5-C5-C6-O6
13	T	1	NAG	C3-C2-N2-C7
8	L	2	NAG	O5-C5-C6-O6
12	Q	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	G	3	BMA	C4-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
3	H	1	NAG	C1-C2-N2-C7
11	O	2	NAG	C1-C2-N2-C7
3	E	2	NAG	O5-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
13	T	3	BMA	C4-C5-C6-O6
3	H	1	NAG	C3-C2-N2-C7
4	P	2	NAG	C3-C2-N2-C7
5	I	2	NAG	C3-C2-N2-C7
7	K	2	NAG	C3-C2-N2-C7
11	O	1	NAG	C3-C2-N2-C7
7	K	4	MAN	C4-C5-C6-O6
7	K	4	MAN	O5-C5-C6-O6
8	L	3	BMA	C4-C5-C6-O6
4	P	2	NAG	C1-C2-N2-C7
5	I	2	NAG	C1-C2-N2-C7
7	K	2	NAG	C1-C2-N2-C7
10	N	1	NAG	C1-C2-N2-C7
11	O	2	NAG	C3-C2-N2-C7
9	M	1	NAG	O5-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6

There are no ring outliers.

18 monomers are involved in 20 short contacts:

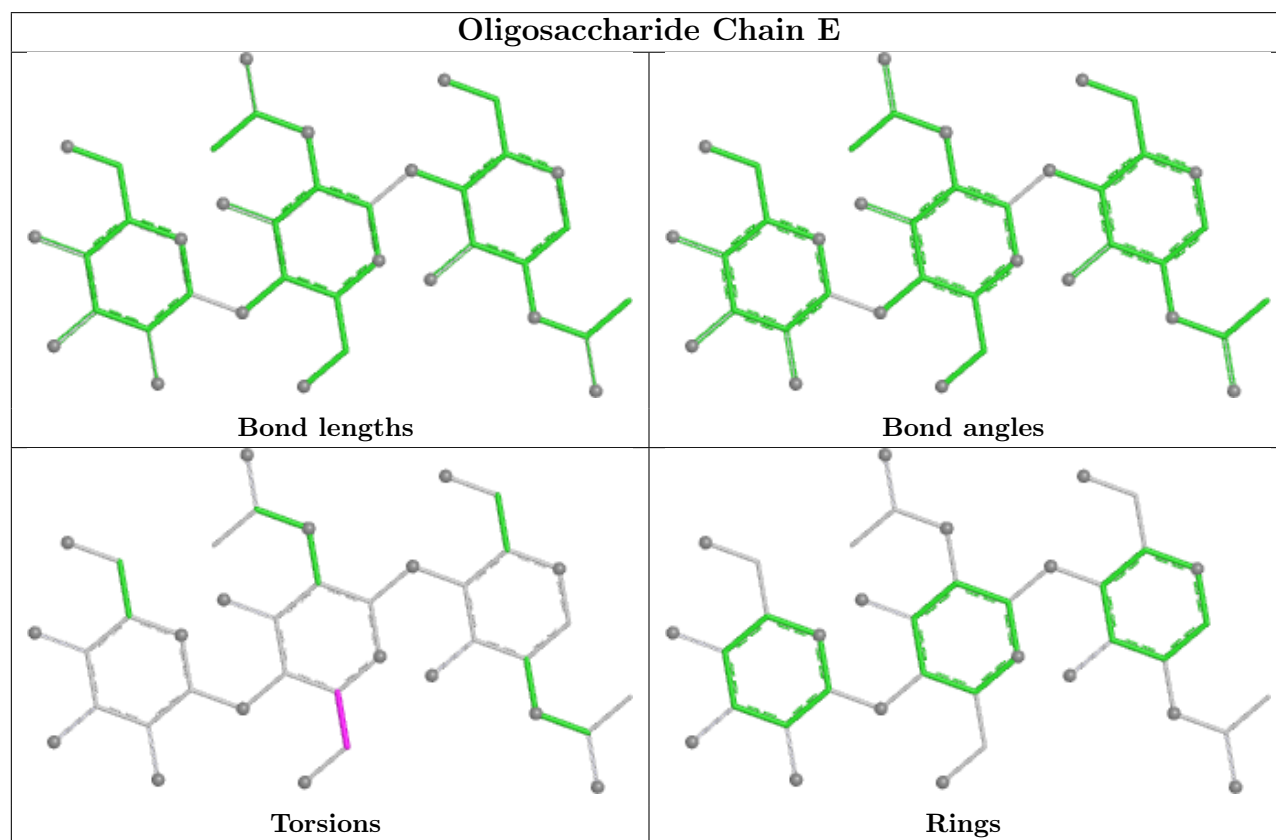
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	O	1	NAG	2	0
8	L	2	NAG	1	0
4	G	1	NAG	1	0
8	L	5	MAN	1	0
13	T	1	NAG	2	0
5	I	1	NAG	2	0
4	P	2	NAG	2	0
7	K	1	NAG	2	0
4	P	3	BMA	1	0
10	R	3	BMA	1	0
4	P	4	MAN	1	0
7	K	2	NAG	3	0
10	R	4	MAN	1	0
4	G	2	NAG	1	0
3	F	2	NAG	1	0

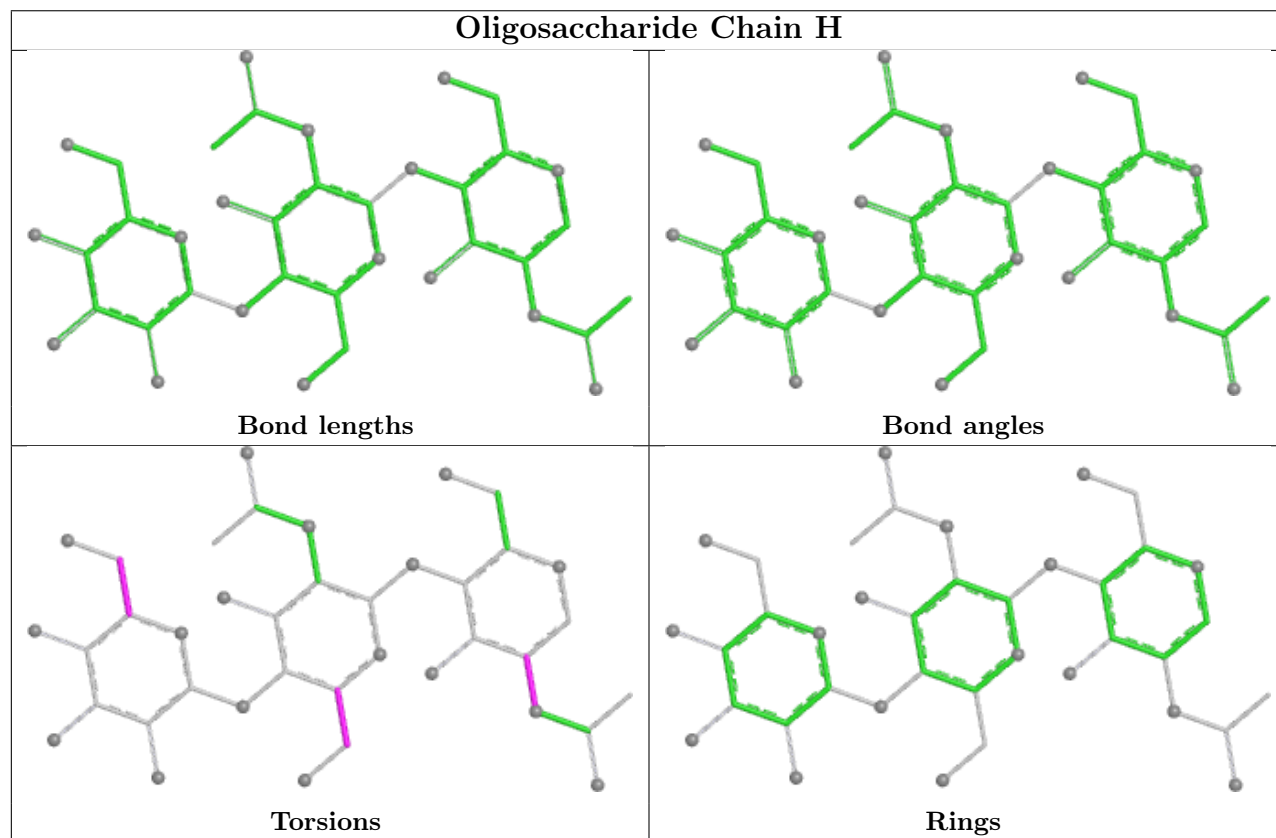
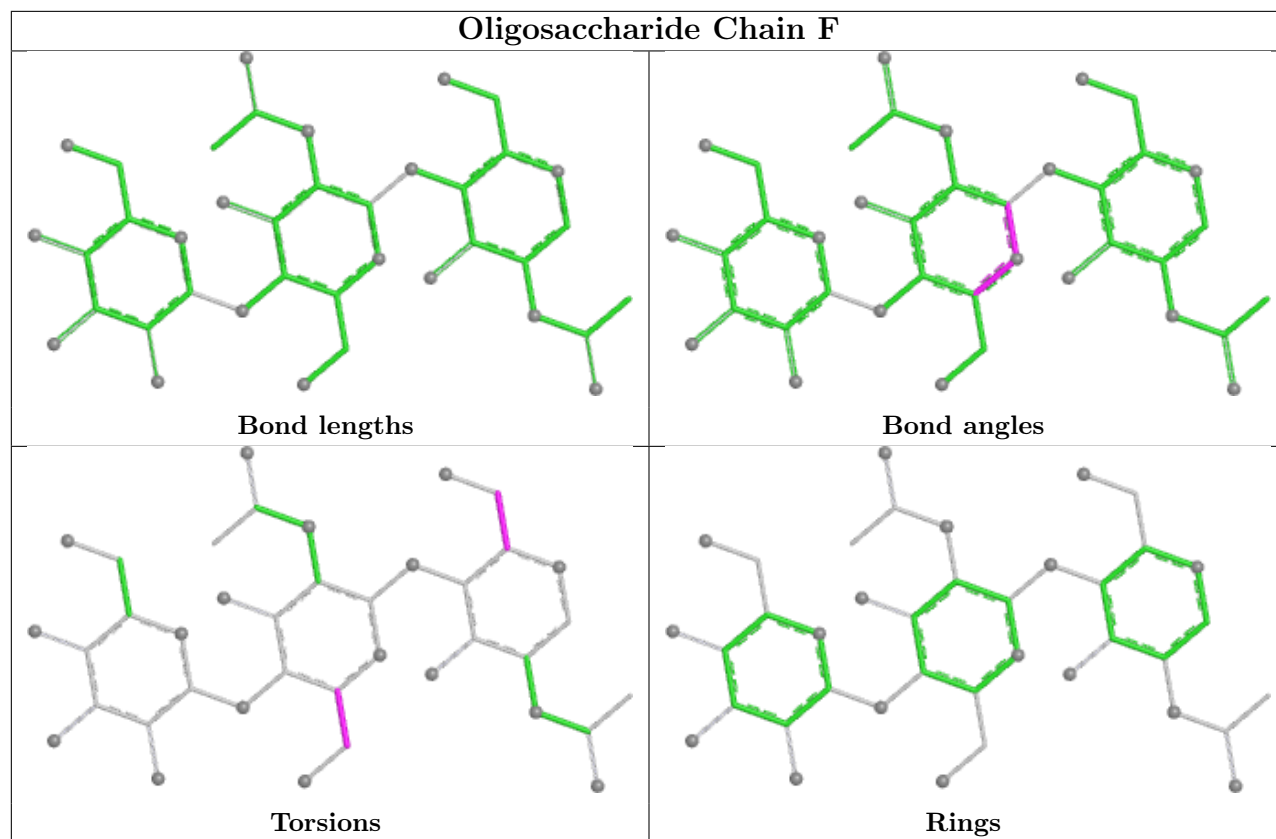
Continued on next page...

Continued from previous page...

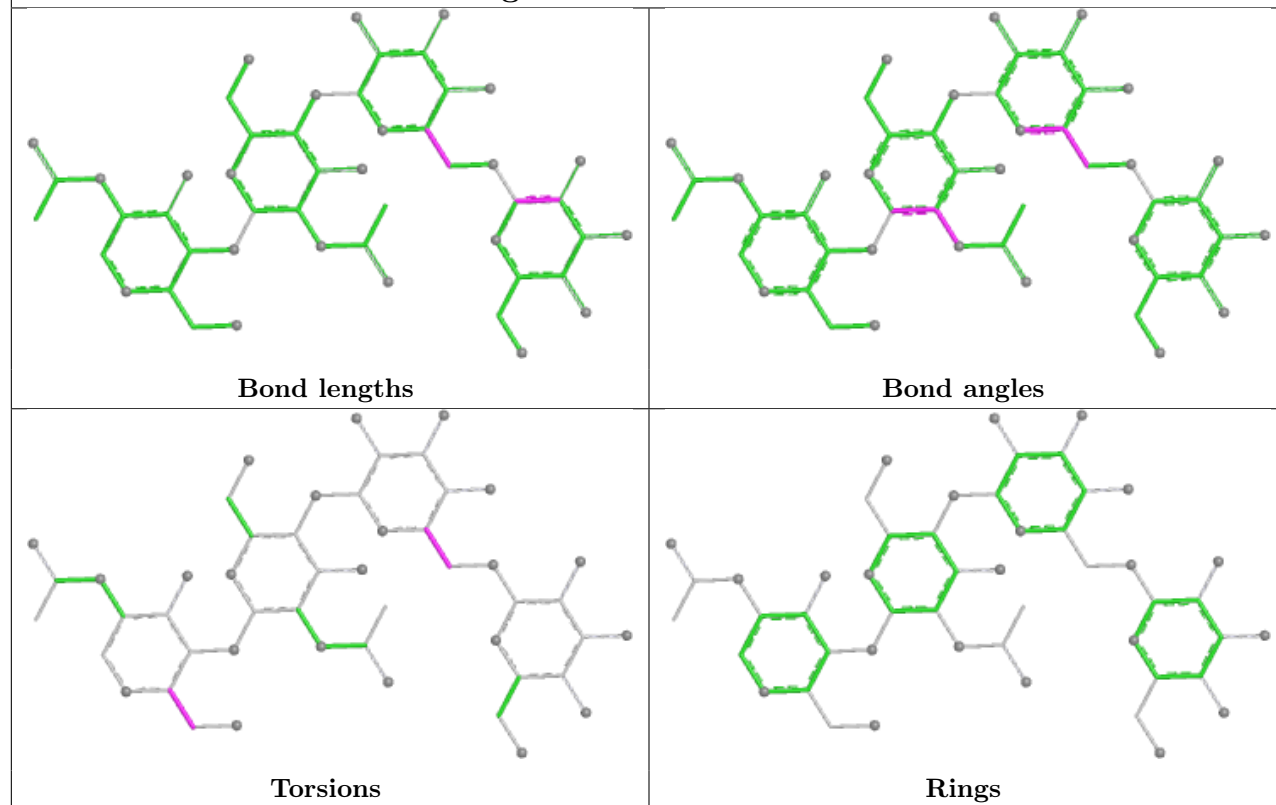
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	2	NAG	3	0
10	N	1	NAG	1	0
3	F	1	NAG	1	0

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

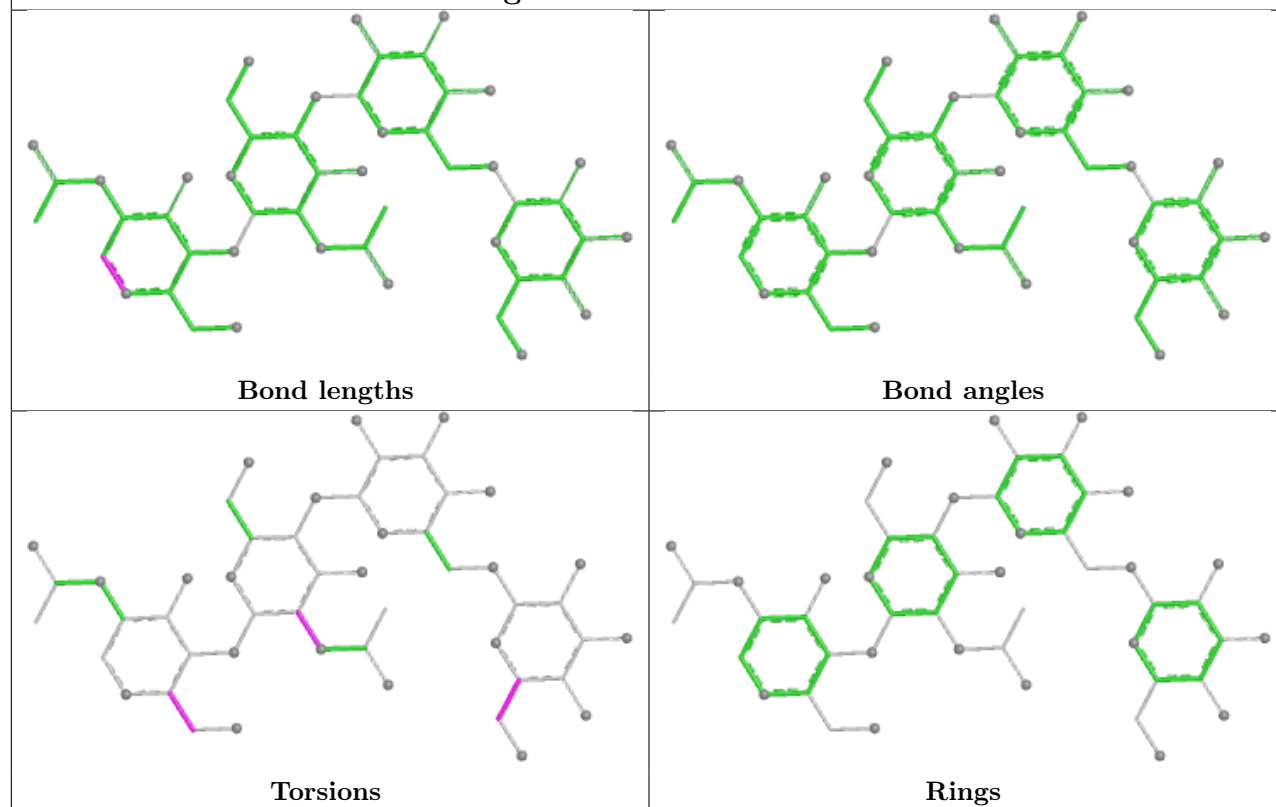


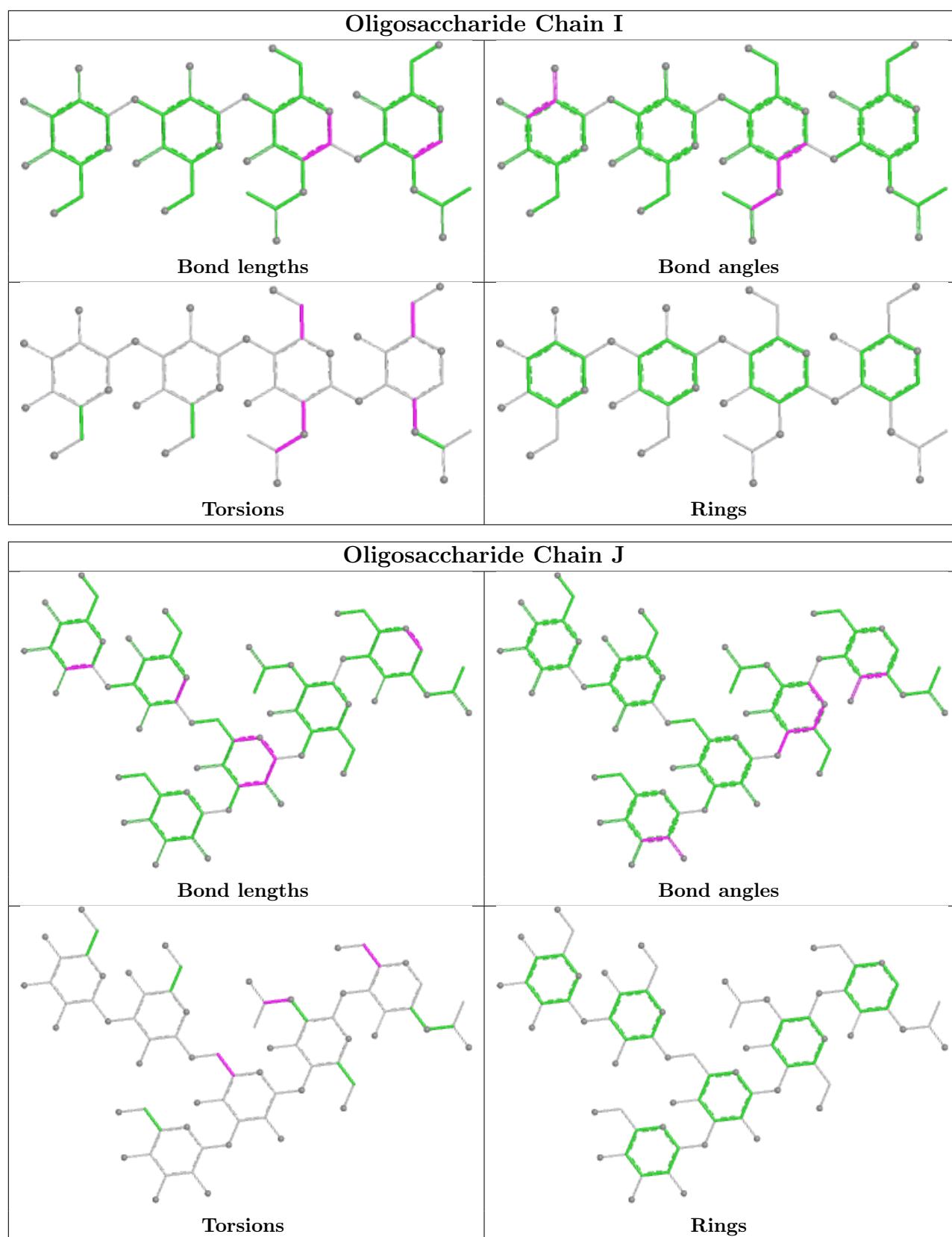


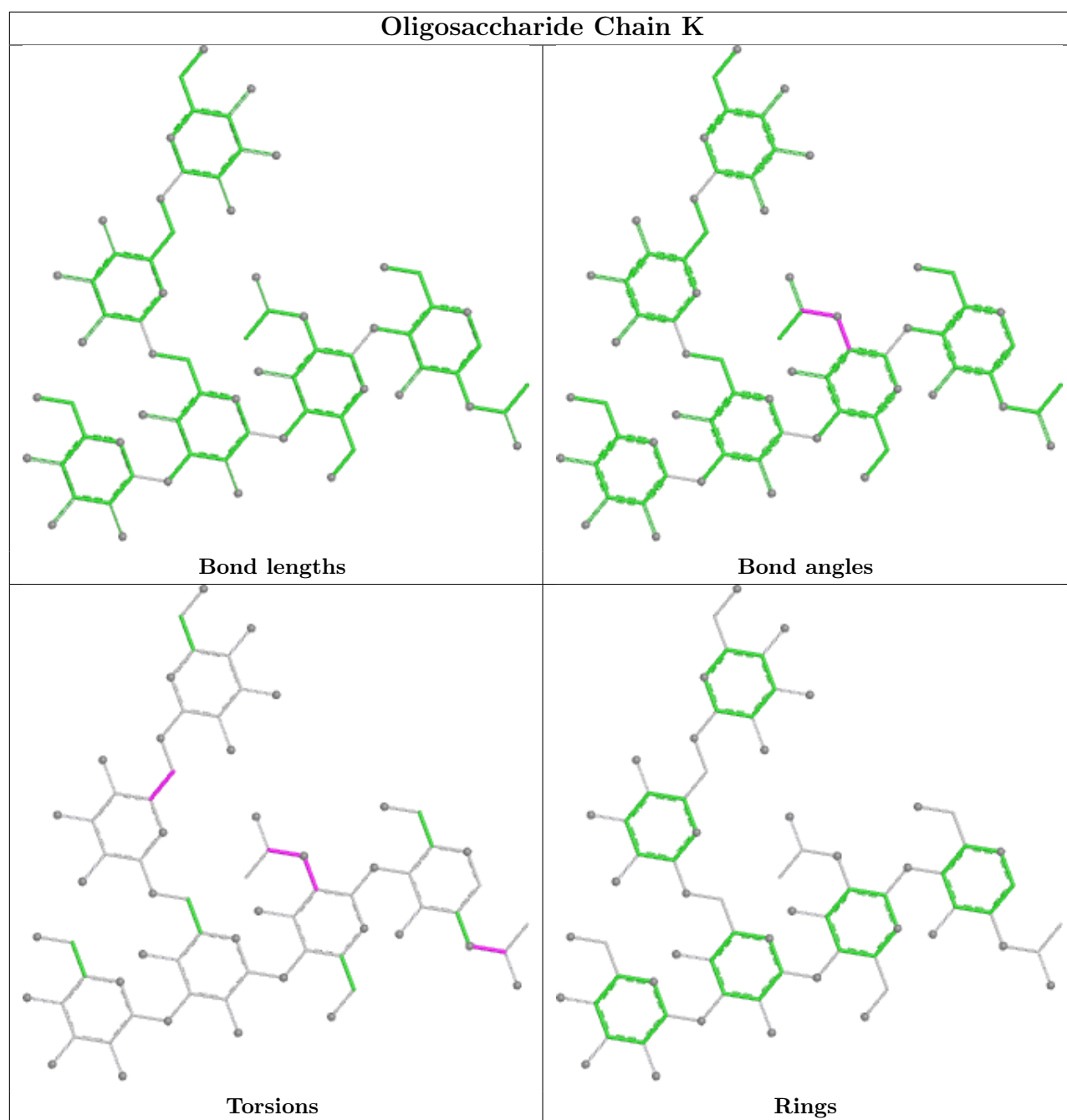
Oligosaccharide Chain G

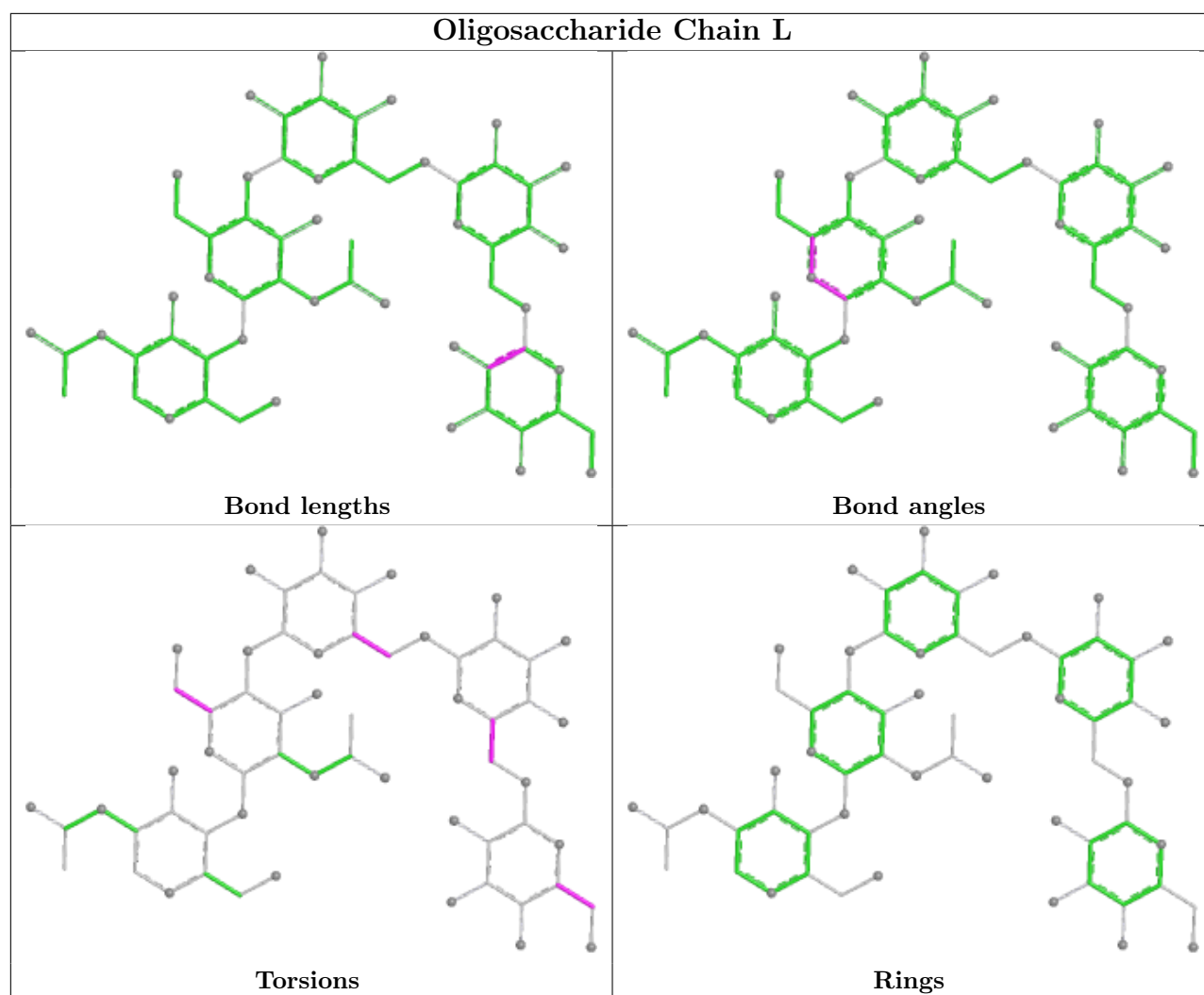


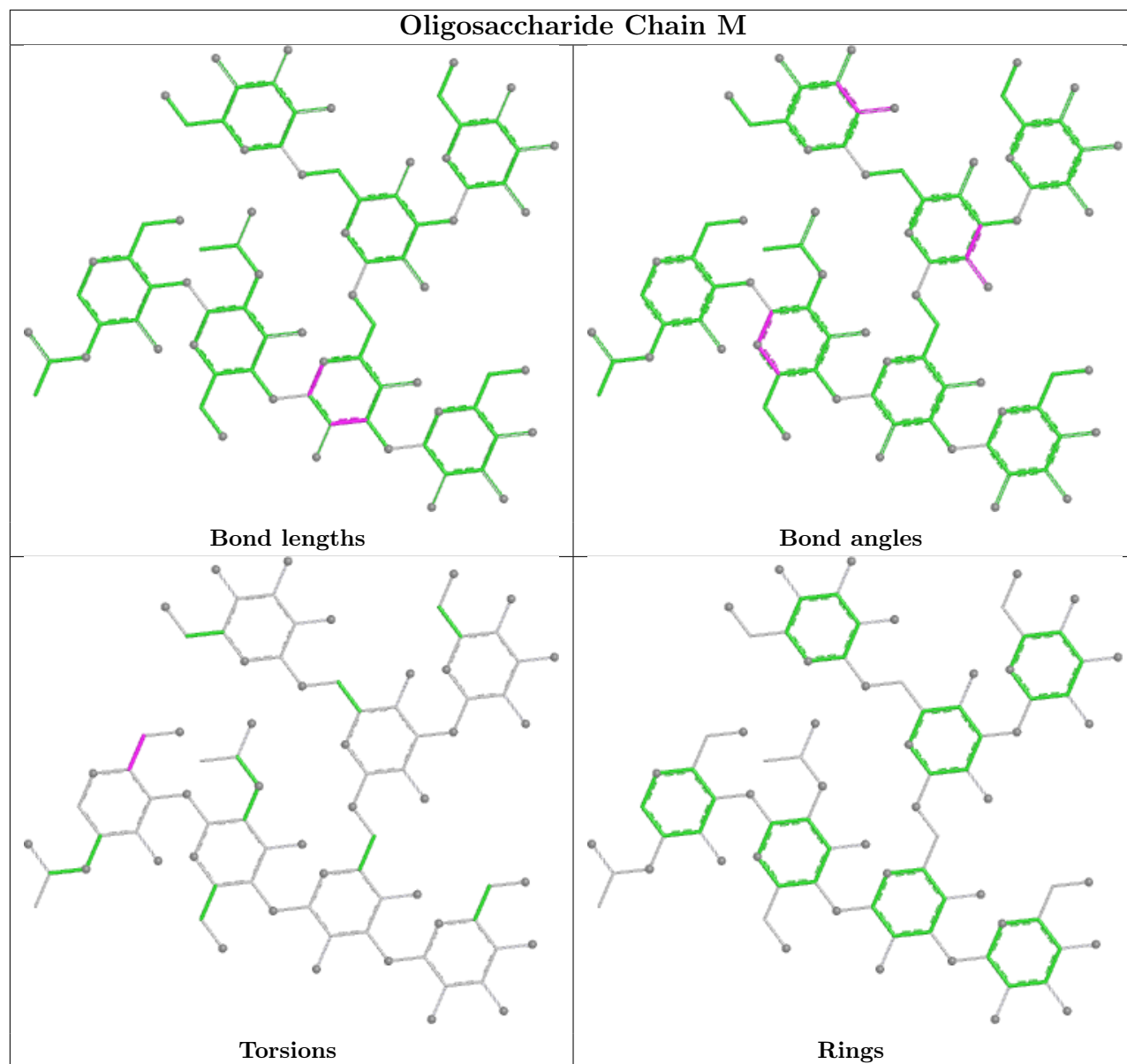
Oligosaccharide Chain P

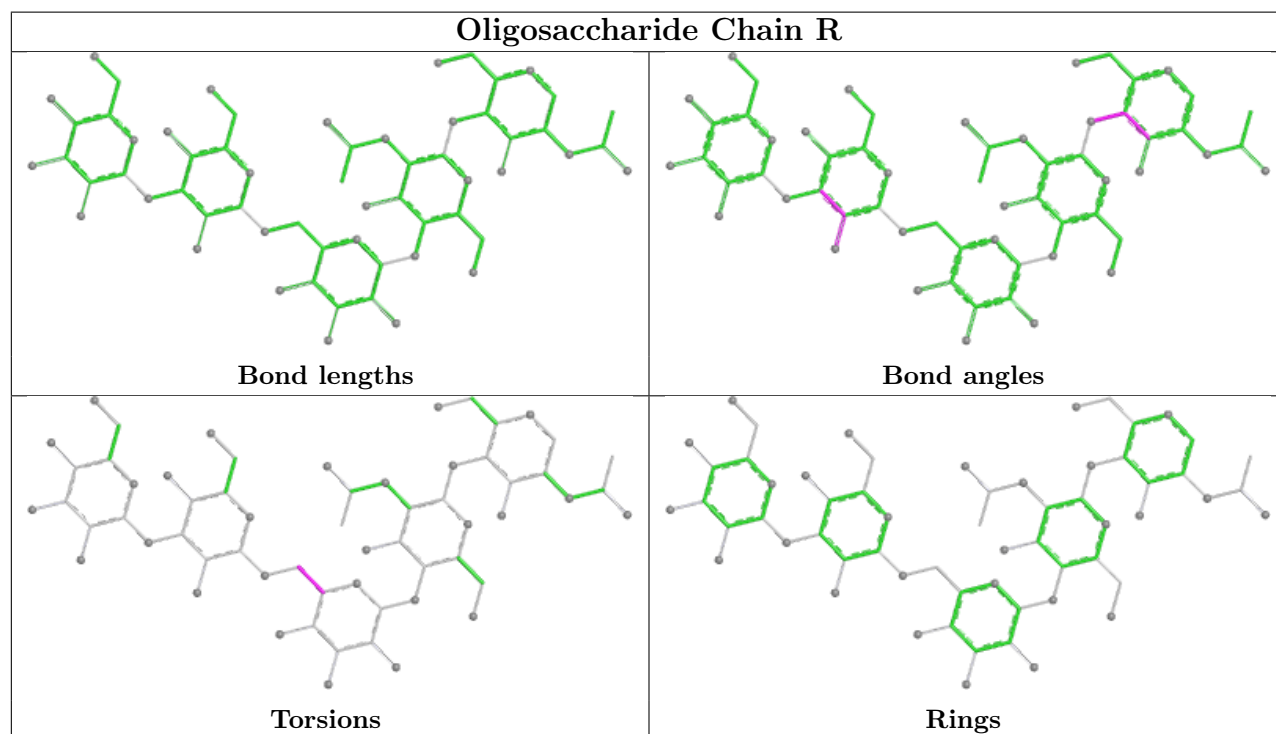
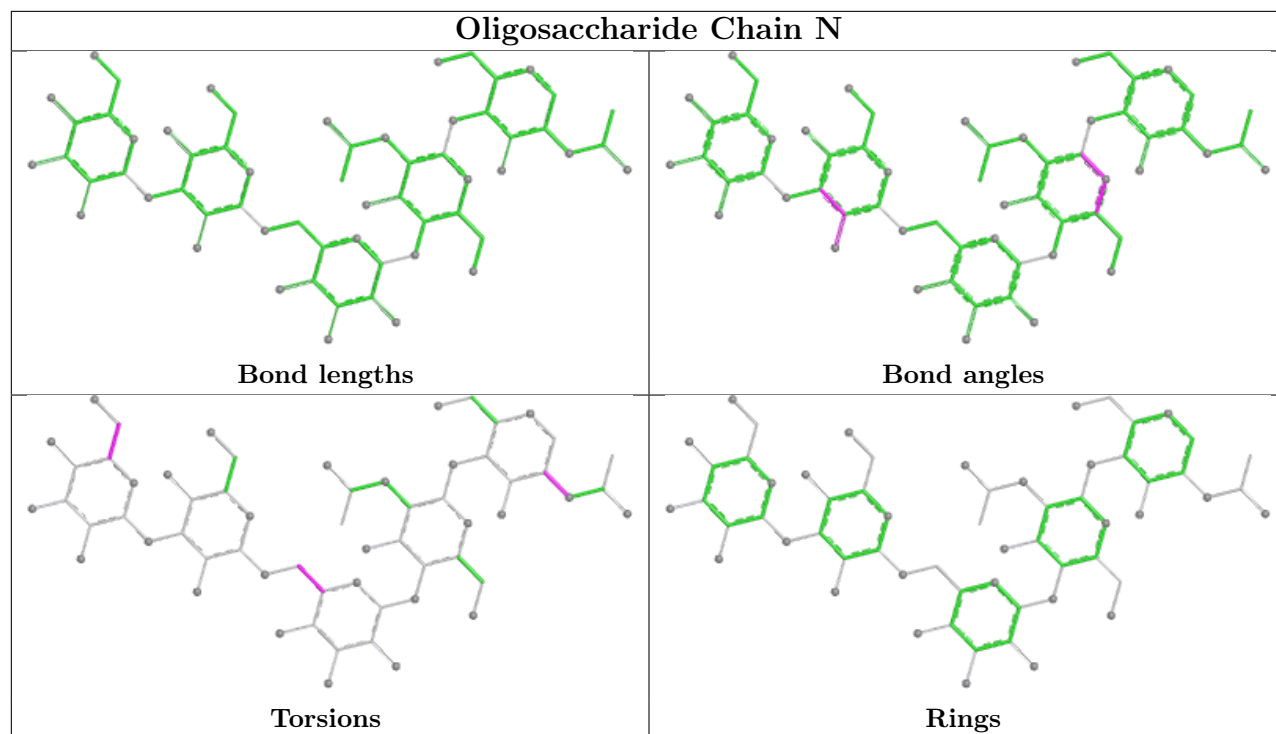


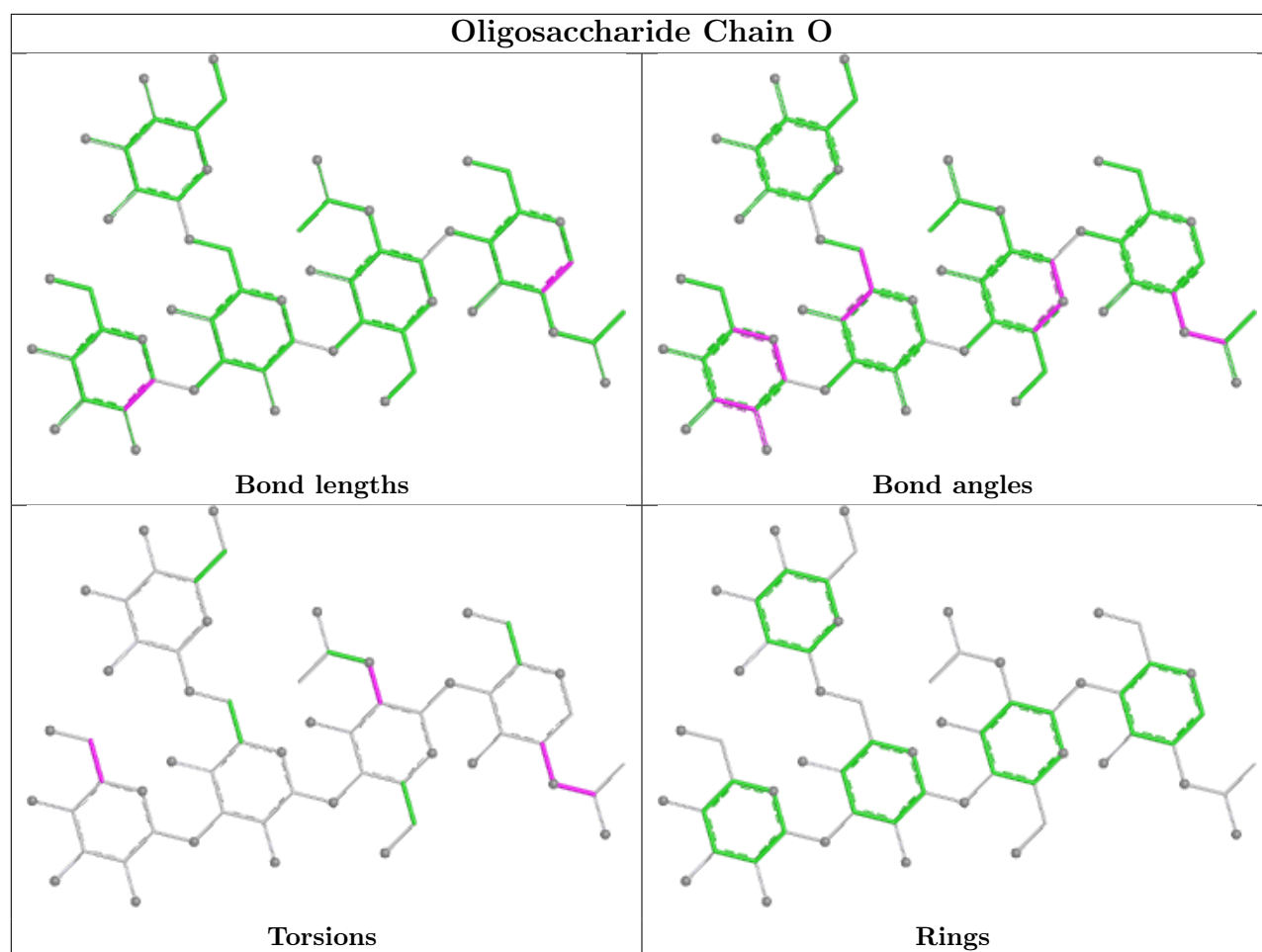


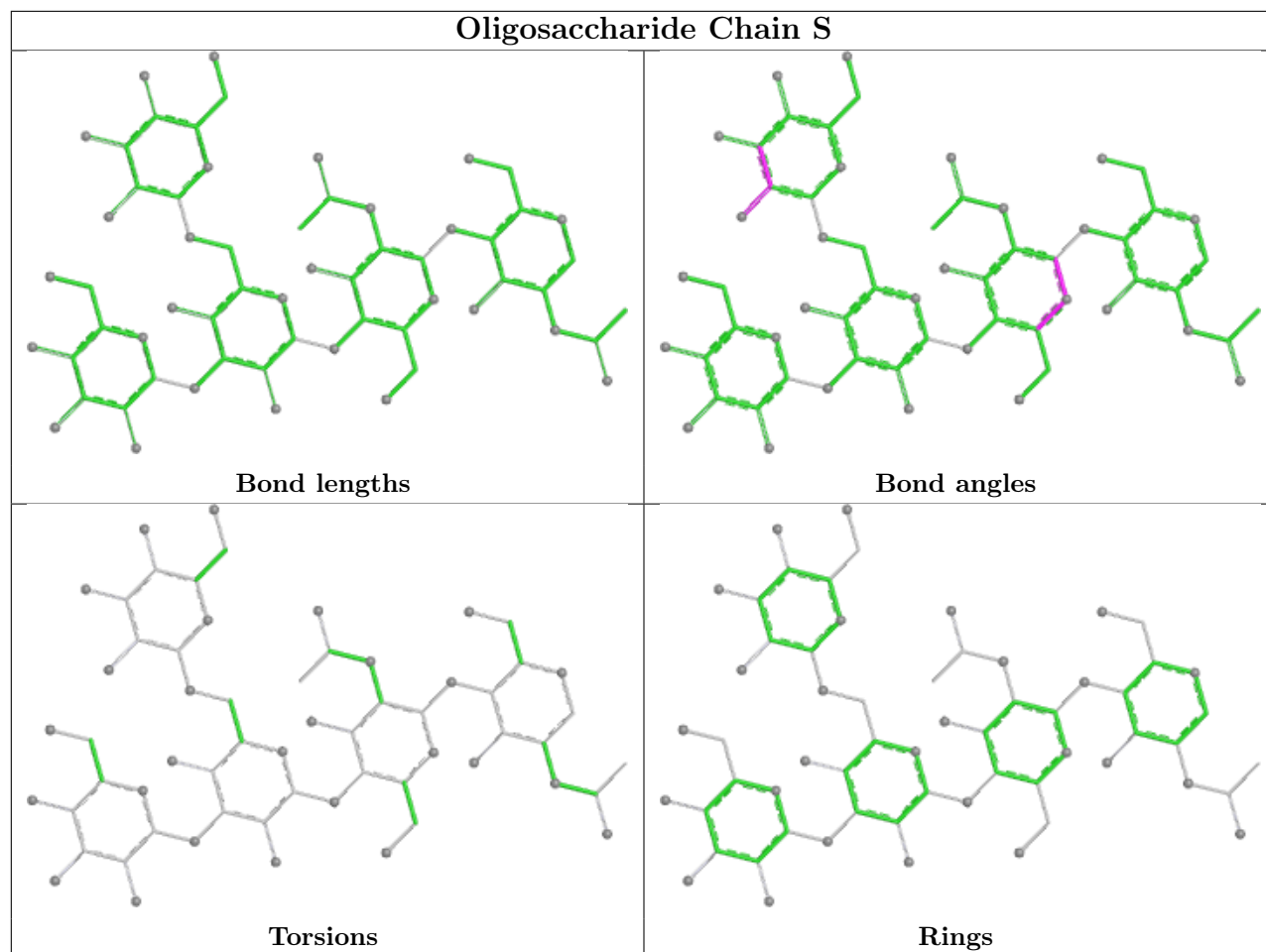


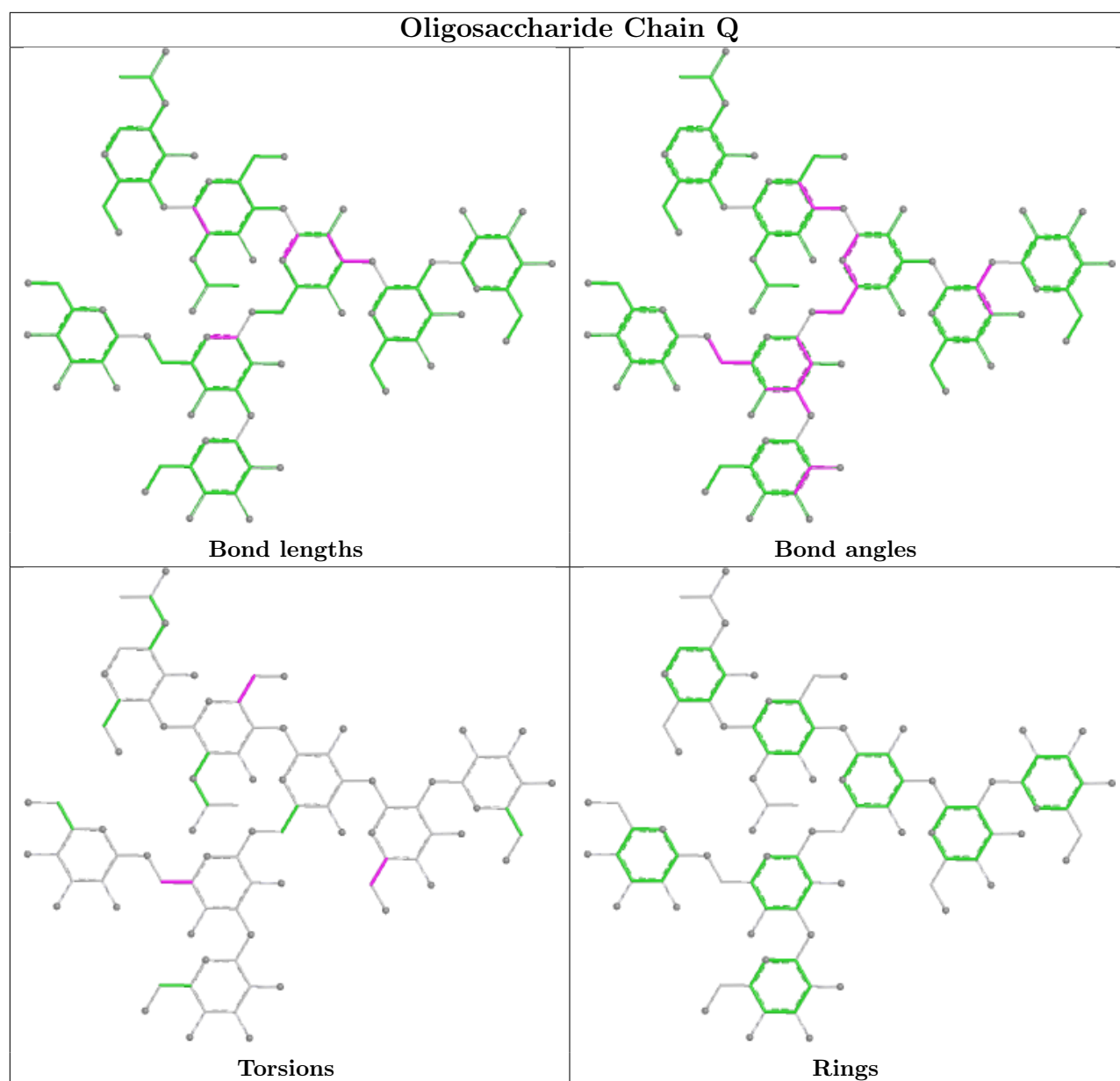


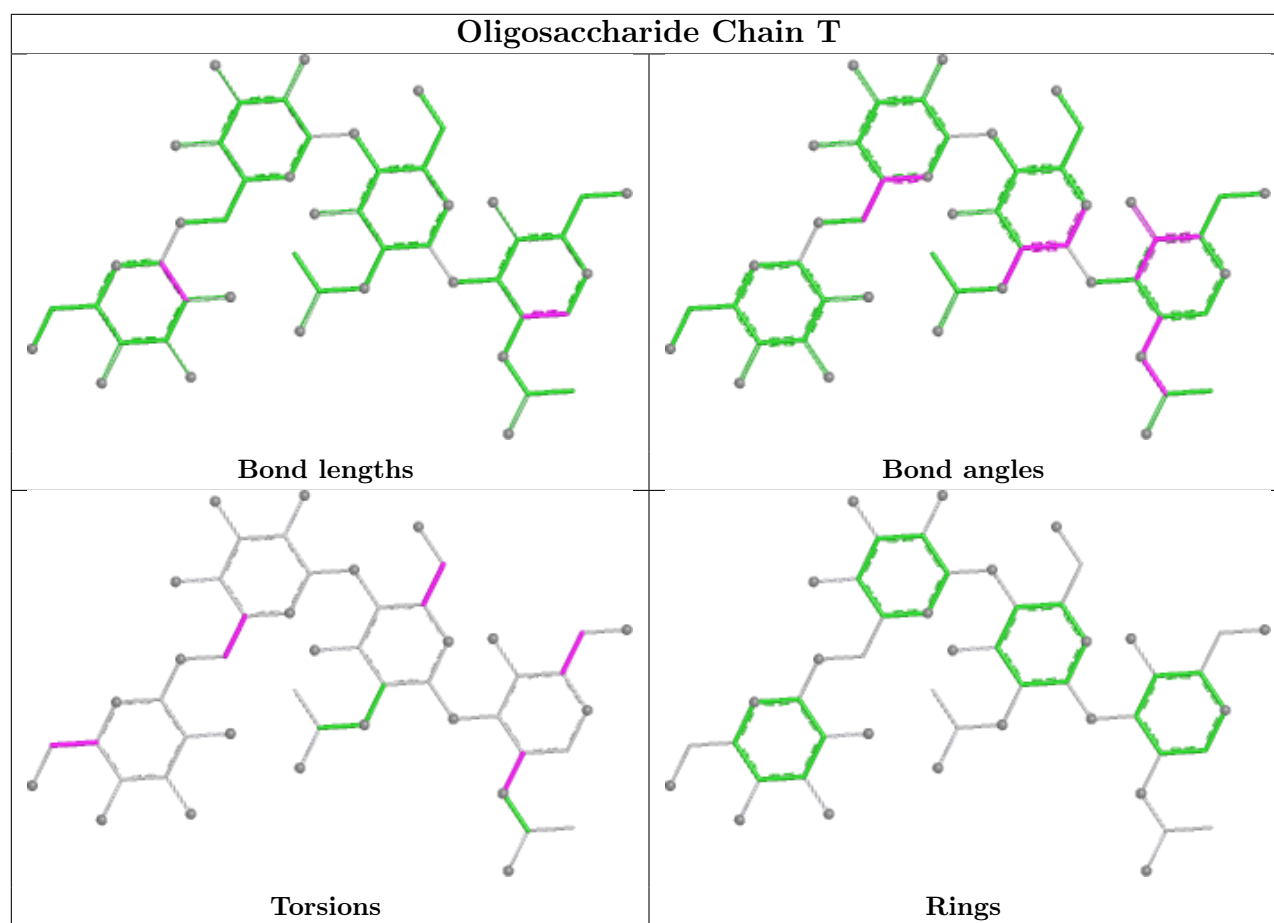












5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	NAG	B	701	1	14,14,15	0.20	0	17,19,21	0.53	0
14	NAG	A	701	1	14,14,15	0.23	0	17,19,21	0.85	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	B	701	1	-	0/6/23/26	0/1/1/1
14	NAG	A	701	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	701	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

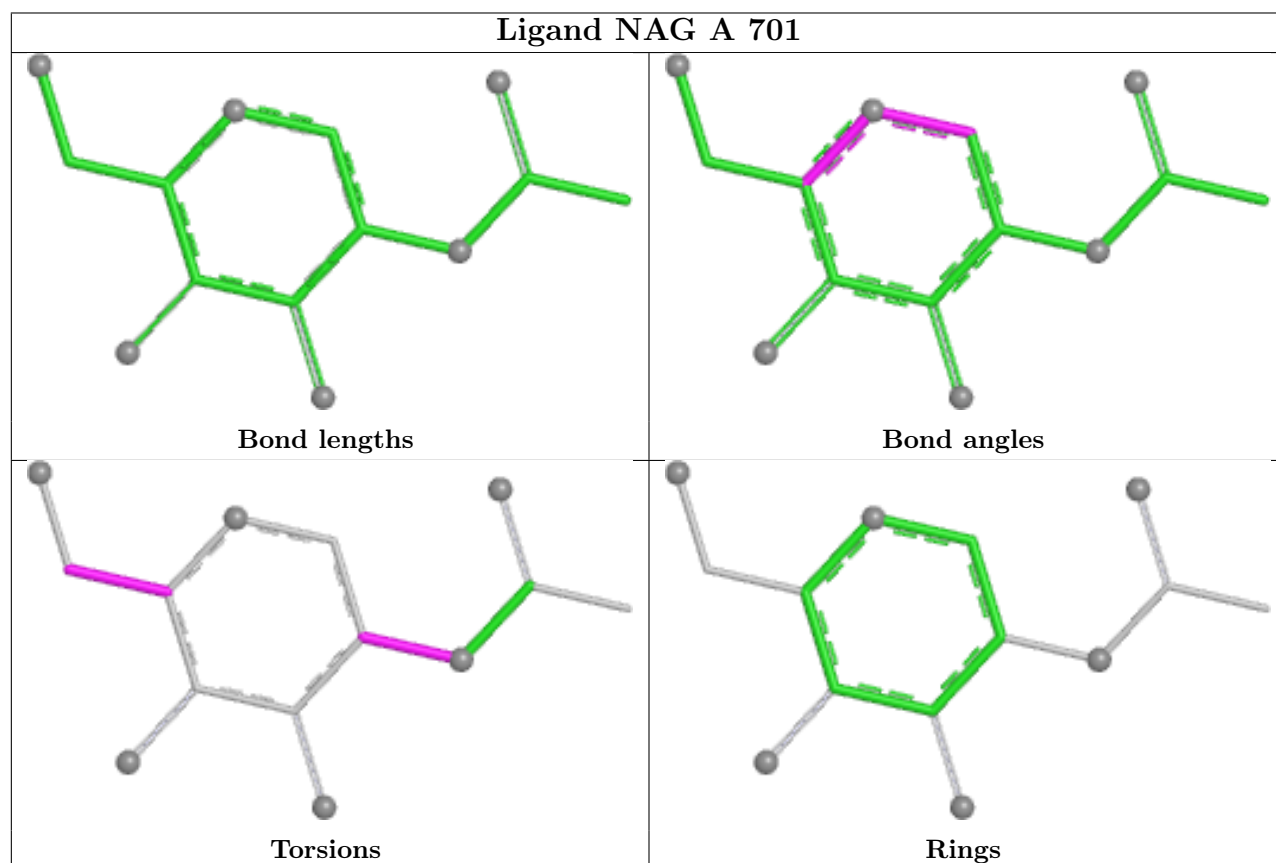
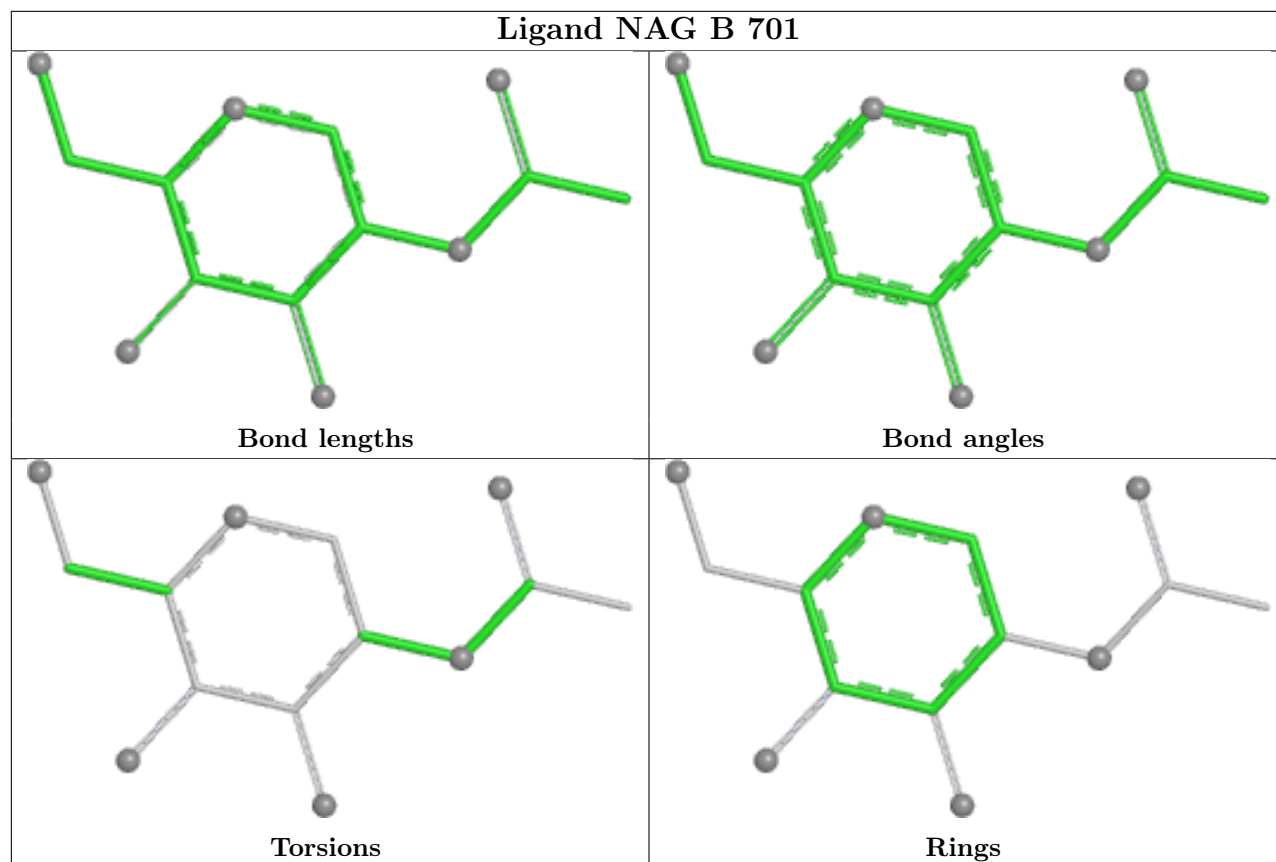
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	701	NAG	C4-C5-C6-O6
14	A	701	NAG	O5-C5-C6-O6
14	A	701	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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	A	570/592 (96%)	0.40	48 (8%)	17	21	146, 197, 466, 505	0
1	B	568/592 (95%)	0.25	47 (8%)	17	21	129, 204, 445, 539	0
2	C	587/617 (95%)	0.31	41 (6%)	22	25	132, 306, 471, 519	0
2	D	590/617 (95%)	0.30	47 (7%)	18	22	136, 250, 328, 487	0
All	All	2315/2418 (95%)	0.31	183 (7%)	18	22	129, 226, 458, 539	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	435	SER	15.6
2	C	434	VAL	11.2
1	B	443	LYS	11.2
2	C	358	ILE	9.4
2	D	26	GLU	8.5
1	B	410	ALA	8.2
1	A	243	ASP	7.7
1	B	243	ASP	7.5
2	D	36	THR	6.6
2	C	122	LEU	6.5
2	D	60	LYS	6.2
2	D	138	LYS	6.2
2	C	55	ILE	6.2
2	D	29	MET	6.1
1	B	411	LEU	6.0
1	A	443	LYS	5.9
2	C	357	LEU	5.8
2	C	26	GLU	5.8
2	D	25	ILE	5.6
1	A	249	LYS	5.6
2	D	56	GLU	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	316	ARG	5.1
1	A	167	ASP	5.1
1	B	439	LYS	5.0
1	B	409	LEU	4.9
1	B	412	ALA	4.8
2	C	411	ILE	4.7
2	D	540	GLU	4.7
2	C	362	GLY	4.7
2	C	543	VAL	4.6
1	B	433	VAL	4.6
2	D	417	TYR	4.6
2	D	31	LEU	4.5
1	B	216	PRO	4.4
1	B	154	MET	4.4
1	A	265	ALA	4.3
2	C	117	LYS	4.3
2	C	54	LEU	4.3
1	B	440	ALA	4.2
2	C	410	GLN	4.2
1	A	376	LEU	4.1
2	D	44	ASP	4.1
1	A	42	ILE	4.1
1	B	489	ASN	4.0
1	A	154	MET	4.0
2	C	400	ALA	4.0
2	D	438	ASP	4.0
1	B	197	TYR	4.0
2	C	361	PRO	4.0
1	A	403	ASN	4.0
1	B	344	ILE	4.0
2	C	414	ARG	3.9
2	D	30	ASP	3.9
1	B	142	GLU	3.9
2	C	608	GLU	3.8
2	D	431	ASN	3.8
2	D	432	ALA	3.8
1	A	264	PHE	3.8
1	B	217	SER	3.8
1	B	264	PHE	3.8
1	A	263	CYS	3.8
1	A	341	GLU	3.7
2	D	434	VAL	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	341	GLU	3.6
2	C	121	ALA	3.6
1	B	490	ARG	3.6
2	D	59	ALA	3.5
1	A	410	ALA	3.5
2	C	401	GLY	3.4
1	A	401	TYR	3.4
1	B	446	PHE	3.3
2	C	408	ASP	3.3
2	C	438	ASP	3.3
2	D	549	THR	3.3
1	A	43	PHE	3.3
1	A	384	GLU	3.3
2	C	437	LEU	3.3
2	C	356	ASN	3.2
2	D	27	ILE	3.2
1	A	266	LEU	3.2
1	B	245	VAL	3.2
1	A	348	LEU	3.1
2	D	75	PHE	3.1
2	D	40	GLN	3.1
1	B	119	ASN	3.1
1	A	262	GLU	3.1
2	C	114	ALA	3.1
2	D	38	THR	3.1
2	C	399	VAL	3.0
1	A	385	ASN	3.0
1	B	193	ASN	3.0
2	D	531	ASP	3.0
1	A	116	ALA	3.0
2	C	412	SER	2.9
1	B	373	LYS	2.9
1	B	135	LEU	2.9
1	B	604	GLY	2.9
1	A	344	ILE	2.9
1	A	350	TRP	2.8
2	D	623	ASP	2.8
1	B	145	GLU	2.7
2	D	37	ILE	2.7
2	C	44	ASP	2.7
2	D	24	SER	2.7
1	A	248	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	220	LYS	2.7
2	C	406	PHE	2.7
1	B	263	CYS	2.6
2	D	223	PHE	2.6
2	C	579	ASN	2.6
2	D	62	ASN	2.6
1	A	62	SER	2.6
1	A	318	LYS	2.6
2	C	431	ASN	2.6
1	A	389	TYR	2.6
2	D	28	PRO	2.6
2	D	222	PRO	2.6
2	C	385	GLY	2.6
1	B	380	ASP	2.5
2	D	55	ILE	2.5
2	D	39	LYS	2.5
1	A	247	GLN	2.5
1	B	444	PRO	2.5
2	D	113	PHE	2.5
1	A	381	VAL	2.5
2	D	400	ALA	2.5
1	A	312	ALA	2.5
2	C	545	LYS	2.5
1	A	339	ASP	2.5
1	B	401	TYR	2.5
2	C	140	ASN	2.5
2	C	415	ALA	2.5
2	D	122	LEU	2.4
1	B	288	ILE	2.4
1	B	434	ILE	2.4
1	B	141	GLU	2.4
2	D	442	ARG	2.4
1	A	433	VAL	2.4
1	B	62	SER	2.4
1	A	193	ASN	2.4
2	D	58	GLU	2.3
1	A	50	THR	2.3
1	A	245	VAL	2.3
1	A	373	LYS	2.3
1	A	48	ILE	2.3
2	C	364	ASP	2.3
1	A	322	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	61	GLY	2.2
1	B	218	ILE	2.2
1	B	60	LYS	2.2
2	D	117	LYS	2.2
1	A	371	TYR	2.2
2	D	444	LEU	2.2
2	C	366	ARG	2.2
1	A	51	ILE	2.2
1	A	411	LEU	2.2
1	B	384	GLU	2.2
1	A	412	ALA	2.2
1	B	265	ALA	2.2
1	B	438	PRO	2.2
2	D	367	LEU	2.2
1	A	166	ASP	2.2
1	B	417	MET	2.2
1	A	216	PRO	2.2
2	C	378	THR	2.2
2	D	404	ILE	2.2
2	D	54	LEU	2.1
1	B	146	VAL	2.1
2	C	402	ASP	2.1
2	D	145	VAL	2.1
2	C	275	LEU	2.1
2	D	433	PHE	2.1
1	B	148	VAL	2.1
1	A	489	ASN	2.1
1	B	244	ILE	2.1
2	C	619	THR	2.1
2	D	356	ASN	2.1
2	D	381	TRP	2.1
1	B	523	THR	2.0
1	A	375	GLU	2.0
1	A	296	LYS	2.0
2	C	38	THR	2.0
1	B	249	LYS	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
12	MAN	Q	4	11/12	0.00	0.12	309,315,325,329	0
5	MAN	I	4	11/12	0.10	0.13	274,296,310,322	0
10	MAN	N	4	11/12	0.18	0.14	443,476,500,506	0
11	MAN	S	5	11/12	0.31	0.12	339,353,369,372	0
9	MAN	M	5	11/12	0.34	0.12	326,335,344,348	0
4	MAN	P	4	11/12	0.41	0.17	317,326,337,339	0
6	MAN	J	5	11/12	0.45	0.13	248,252,256,258	0
11	MAN	S	4	11/12	0.47	0.15	417,433,450,455	0
4	MAN	G	4	11/12	0.51	0.12	238,245,252,257	0
7	MAN	K	4	11/12	0.53	0.12	272,281,293,296	0
7	BMA	K	3	11/12	0.53	0.09	287,293,305,307	0
5	BMA	I	3	11/12	0.56	0.12	235,247,268,272	0
6	BMA	J	3	11/12	0.56	0.07	257,267,284,285	0
3	BMA	F	3	11/12	0.57	0.10	265,277,297,298	0
11	MAN	O	4	11/12	0.57	0.15	375,385,392,393	0
11	NAG	S	2	14/15	0.57	0.13	323,347,367,370	0
6	NAG	J	2	14/15	0.58	0.19	219,233,249,251	0
10	BMA	N	3	11/12	0.58	0.14	485,499,518,522	0
13	BMA	T	3	11/12	0.58	0.10	283,290,302,305	0
13	MAN	T	4	11/12	0.59	0.14	298,309,319,321	0
6	MAN	J	6	11/12	0.61	0.09	275,291,311,318	0
9	NAG	M	2	14/15	0.61	0.15	289,298,304,308	0
10	BMA	R	3	11/12	0.62	0.10	382,397,420,428	0
11	MAN	O	5	11/12	0.62	0.14	319,323,332,336	0
9	MAN	M	4	11/12	0.63	0.09	309,318,326,331	0
12	MAN	Q	7	11/12	0.63	0.15	312,322,329,334	0
3	NAG	H	2	14/15	0.64	0.12	247,261,270,274	0
7	MAN	K	5	11/12	0.64	0.12	303,308,315,315	0
10	MAN	R	5	11/12	0.64	0.15	430,448,486,490	0
4	BMA	P	3	11/12	0.65	0.09	337,349,359,366	0
11	BMA	S	3	11/12	0.65	0.09	373,385,407,411	0
11	NAG	S	1	14/15	0.66	0.12	310,321,331,336	0
10	NAG	R	2	14/15	0.68	0.16	334,359,375,380	0
9	MAN	M	7	11/12	0.70	0.09	297,302,307,311	0
4	NAG	P	2	14/15	0.71	0.19	336,347,359,366	0
10	MAN	N	5	11/12	0.71	0.10	391,417,427,435	0
10	MAN	R	4	11/12	0.71	0.12	377,409,438,440	0

Continued on next page...

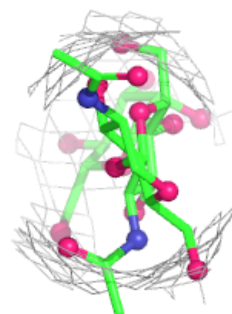
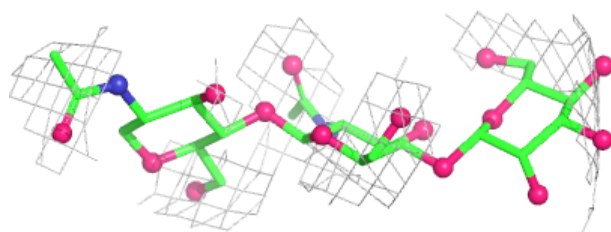
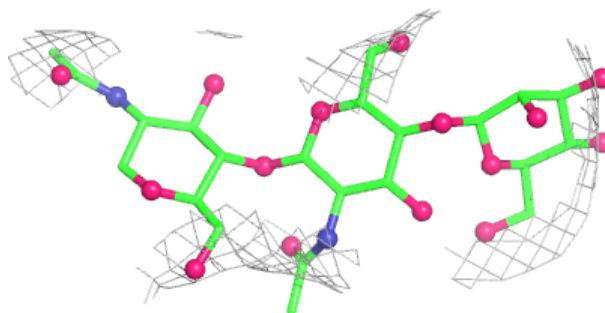
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	BMA	O	3	11/12	0.72	0.07	338,353,362,368	0
6	MAN	J	4	11/12	0.72	0.13	268,277,288,293	0
9	BMA	M	3	11/12	0.72	0.09	299,302,316,318	0
12	BMA	Q	3	11/12	0.75	0.07	291,300,304,310	0
3	BMA	H	3	11/12	0.76	0.11	270,280,290,294	0
9	NAG	M	1	14/15	0.78	0.12	278,286,298,303	0
4	BMA	G	3	11/12	0.78	0.09	240,242,247,248	0
10	NAG	R	1	14/15	0.79	0.15	297,311,329,334	0
12	MAN	Q	5	11/12	0.79	0.09	316,326,333,338	0
6	NAG	J	1	14/15	0.79	0.24	195,206,216,222	0
11	NAG	O	2	14/15	0.79	0.09	343,351,365,368	0
5	NAG	I	2	14/15	0.79	0.12	188,202,220,227	0
7	MAN	K	6	11/12	0.80	0.20	294,307,323,330	0
9	MAN	M	6	11/12	0.81	0.10	305,311,324,327	0
4	NAG	G	2	14/15	0.83	0.08	233,236,238,241	0
10	NAG	N	1	14/15	0.83	0.10	331,374,408,414	0
12	MAN	Q	6	11/12	0.83	0.07	290,299,310,314	0
10	NAG	N	2	14/15	0.84	0.10	425,448,481,481	0
11	NAG	O	1	14/15	0.84	0.07	357,374,395,402	0
8	NAG	L	1	14/15	0.84	0.14	221,228,238,241	0
3	NAG	F	2	14/15	0.86	0.06	228,239,250,255	0
3	NAG	F	1	14/15	0.86	0.14	184,206,224,226	0
8	BMA	L	3	11/12	0.87	0.06	257,267,277,280	0
13	NAG	T	2	14/15	0.87	0.18	264,269,276,279	0
8	MAN	L	5	11/12	0.87	0.09	233,241,244,249	0
3	BMA	E	3	11/12	0.87	0.08	277,295,322,329	0
8	NAG	L	2	14/15	0.88	0.10	229,236,248,252	0
4	NAG	P	1	14/15	0.88	0.15	343,362,376,385	0
7	NAG	K	2	14/15	0.89	0.16	273,280,287,291	0
12	NAG	Q	1	14/15	0.90	0.09	256,260,265,266	0
12	MAN	Q	8	11/12	0.91	0.11	285,291,298,303	0
3	NAG	E	2	14/15	0.91	0.08	220,246,274,275	0
5	NAG	I	1	14/15	0.92	0.10	163,170,184,185	0
4	NAG	G	1	14/15	0.92	0.10	229,233,239,239	0
3	NAG	H	1	14/15	0.93	0.14	226,240,253,255	0
3	NAG	E	1	14/15	0.94	0.09	200,207,226,227	0
13	NAG	T	1	14/15	0.94	0.16	252,254,260,261	0
7	NAG	K	1	14/15	0.94	0.19	262,266,272,276	0
12	NAG	Q	2	14/15	0.94	0.09	270,274,284,285	0
8	MAN	L	4	11/12	0.94	0.08	249,261,274,278	0

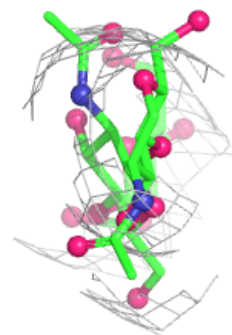
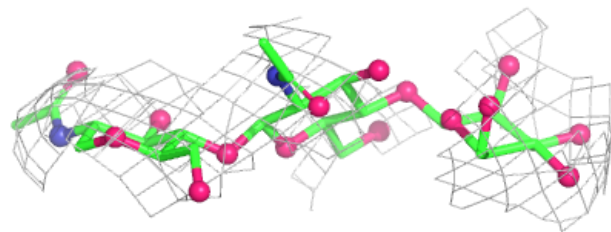
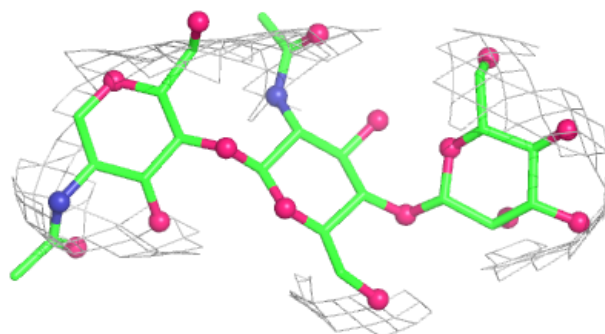
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

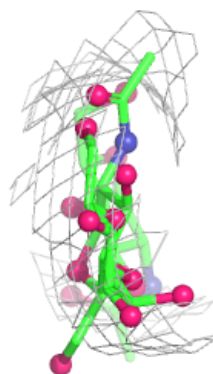
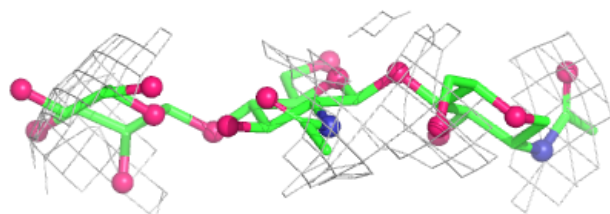
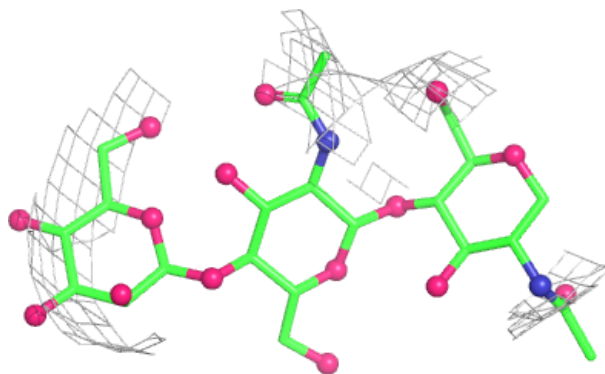
**Electron density around Chain F:**

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

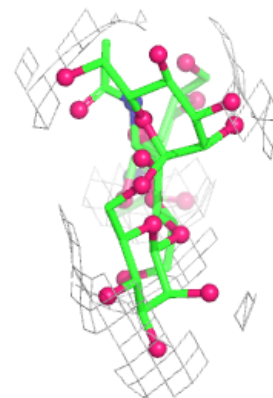
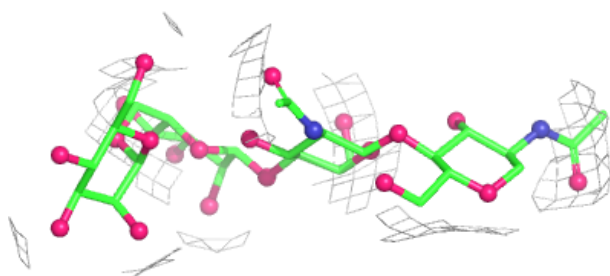
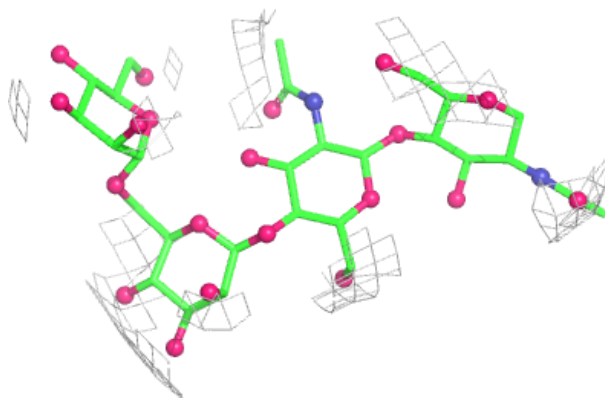


Electron density around Chain H:

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

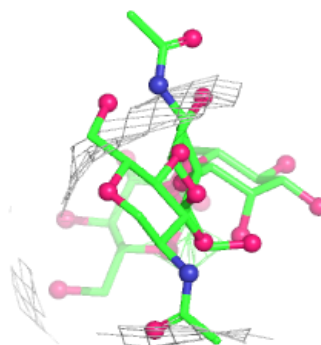
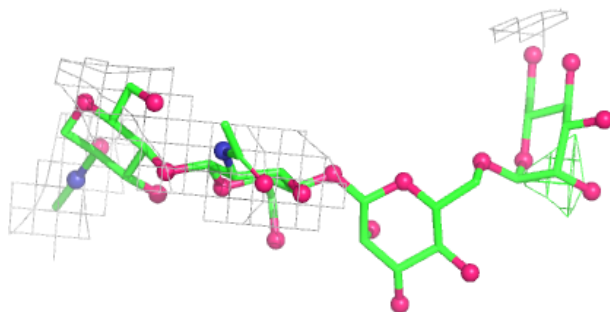
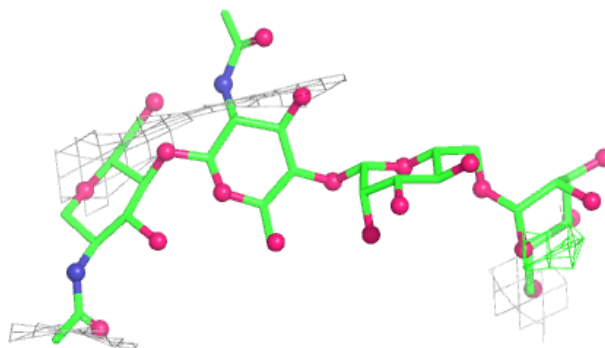
**Electron density around Chain G:**

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

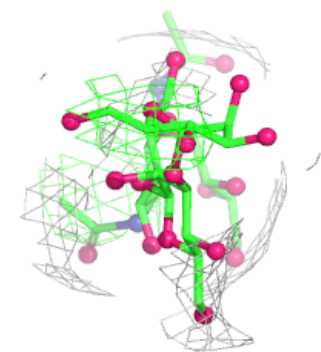
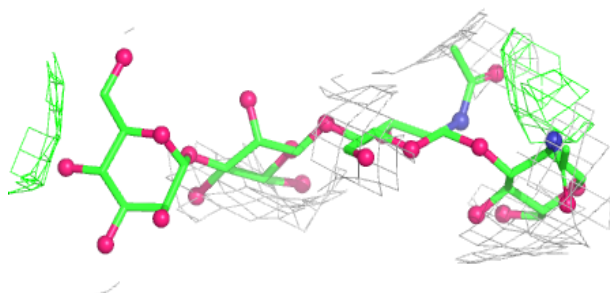
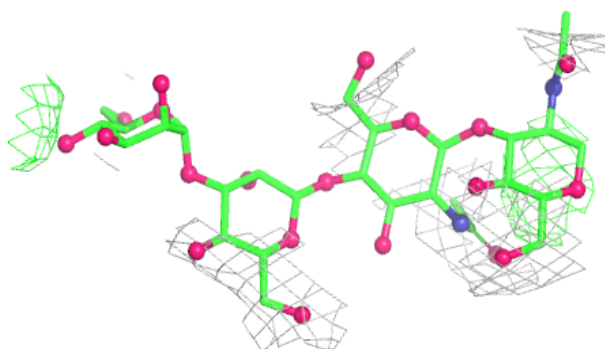


Electron density around Chain P:

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

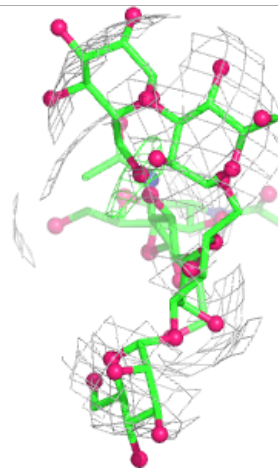
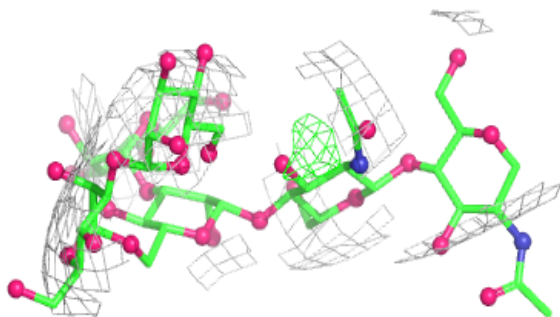
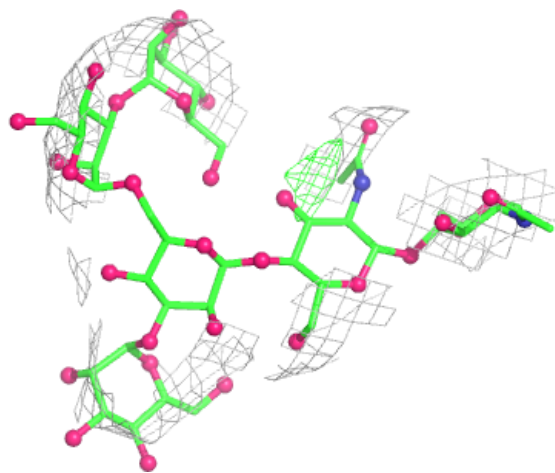
**Electron density around Chain I:**

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



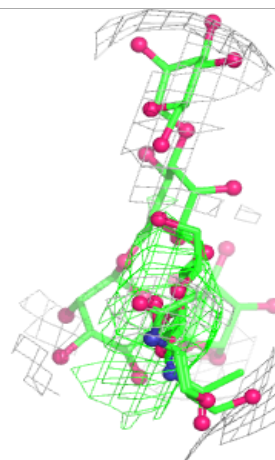
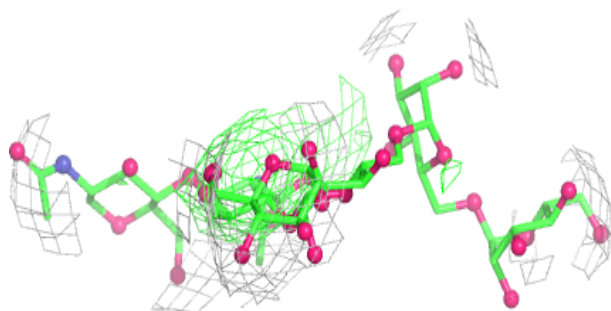
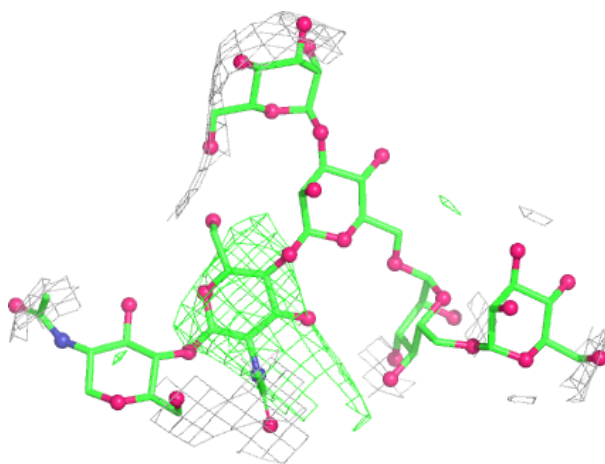
Electron density around Chain J:

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



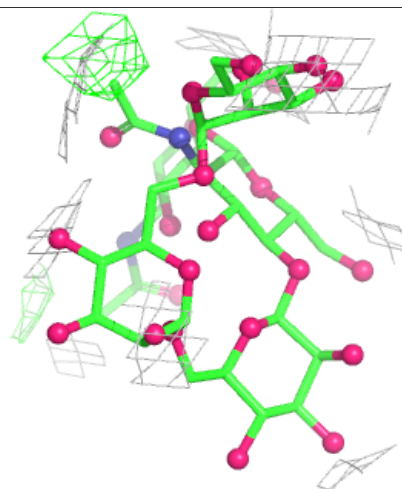
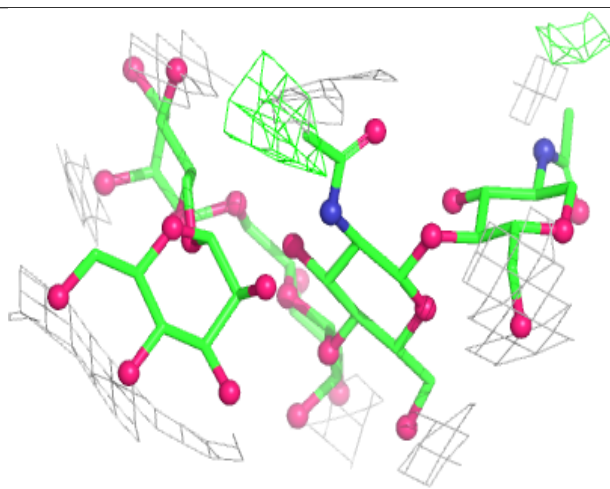
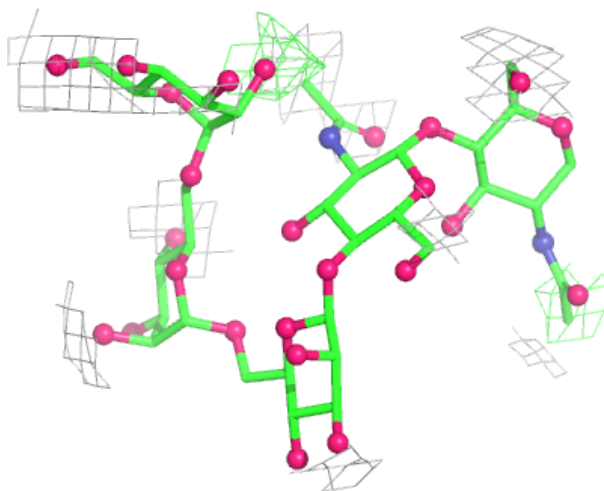
Electron density around Chain K:

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



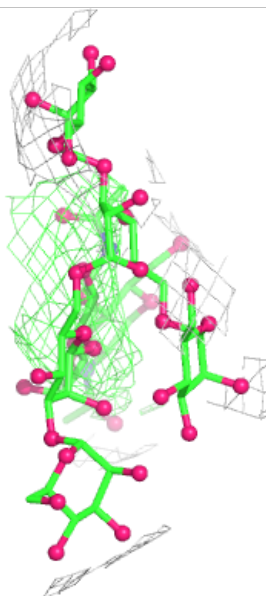
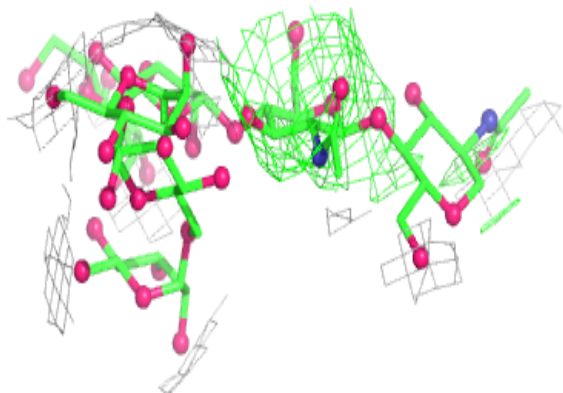
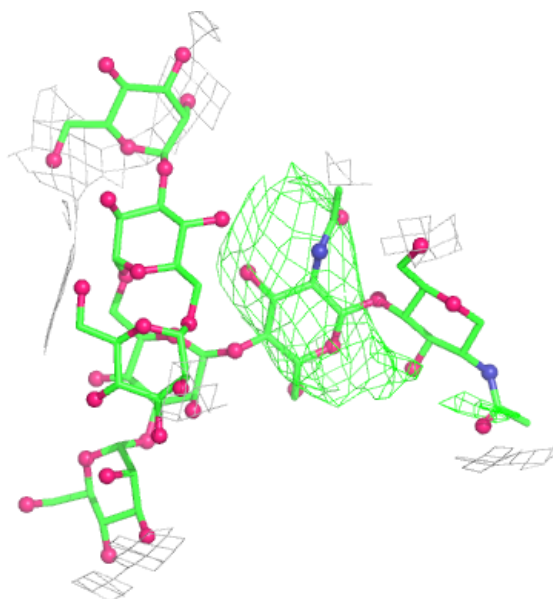
Electron density around Chain L:

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



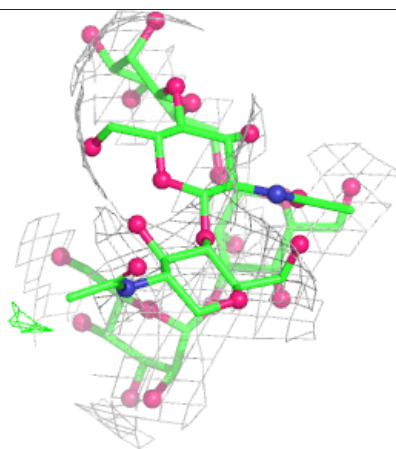
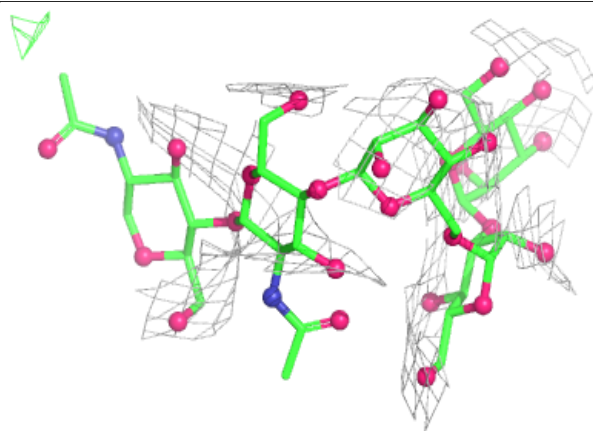
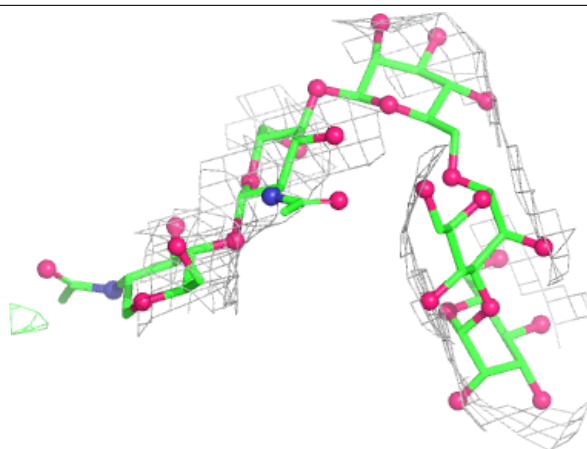
Electron density around Chain M:

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



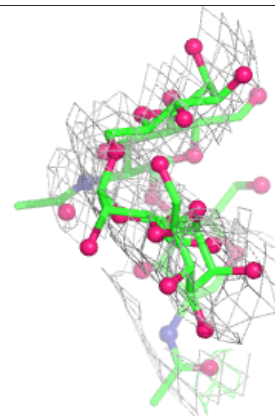
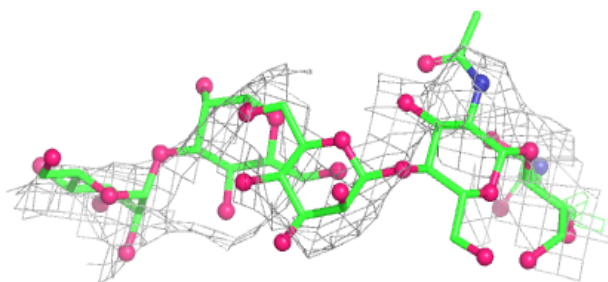
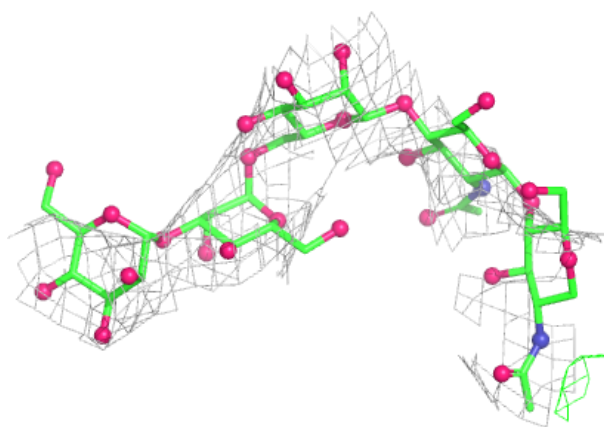
Electron density around Chain N:

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



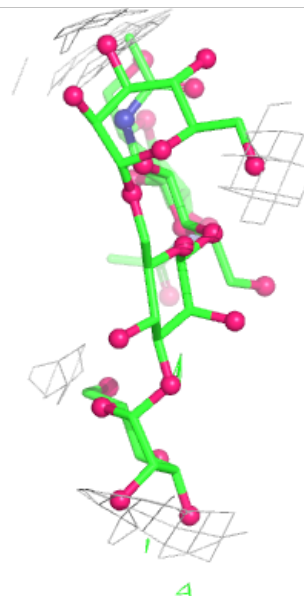
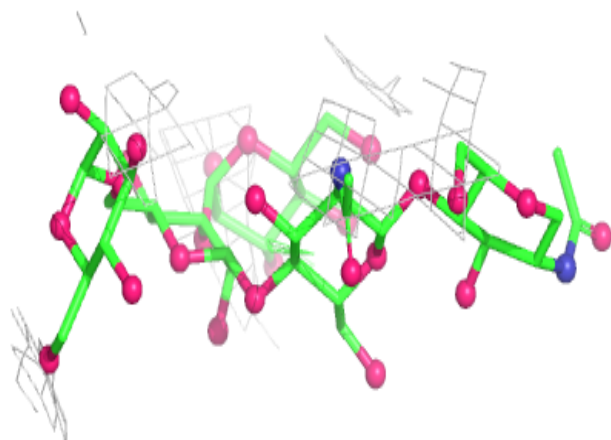
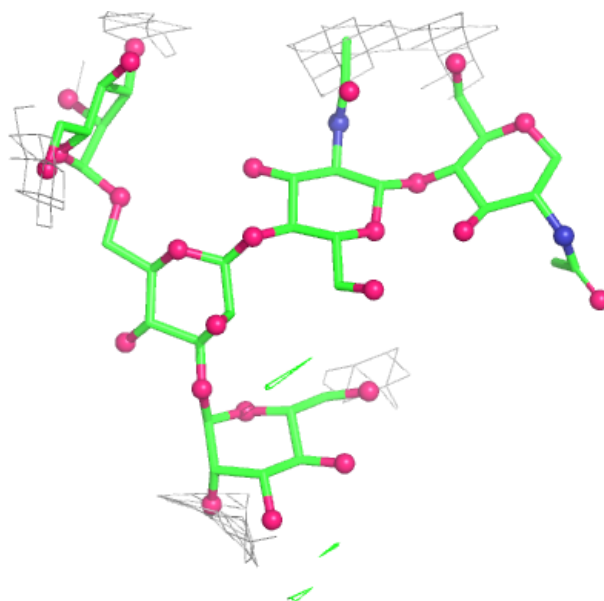
Electron density around Chain R:

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



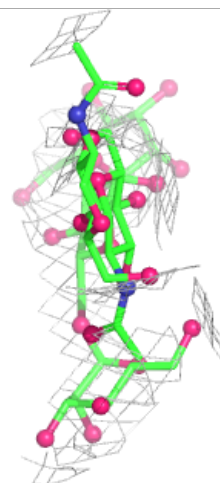
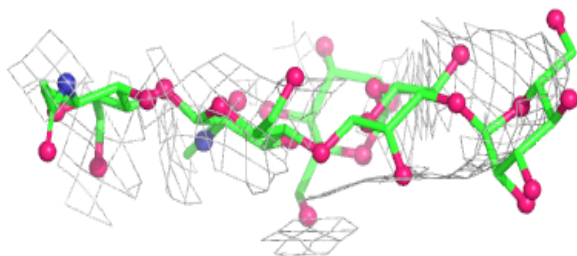
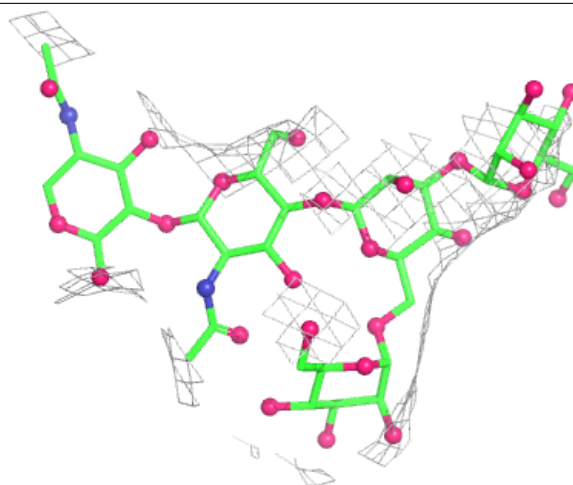
Electron density around Chain O:

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



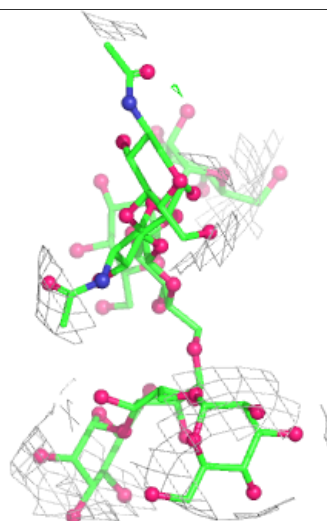
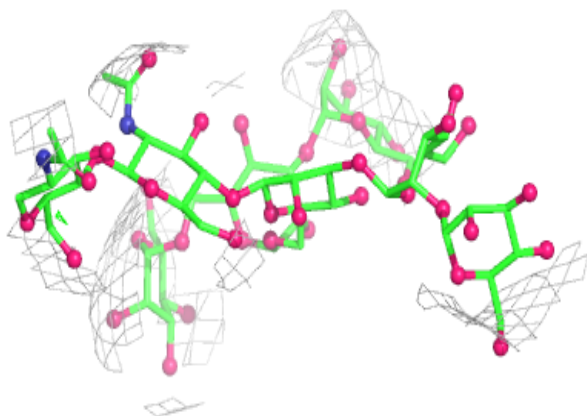
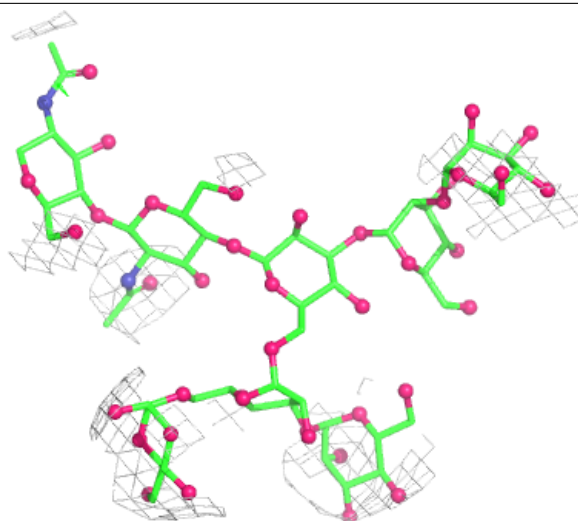
Electron density around Chain S:

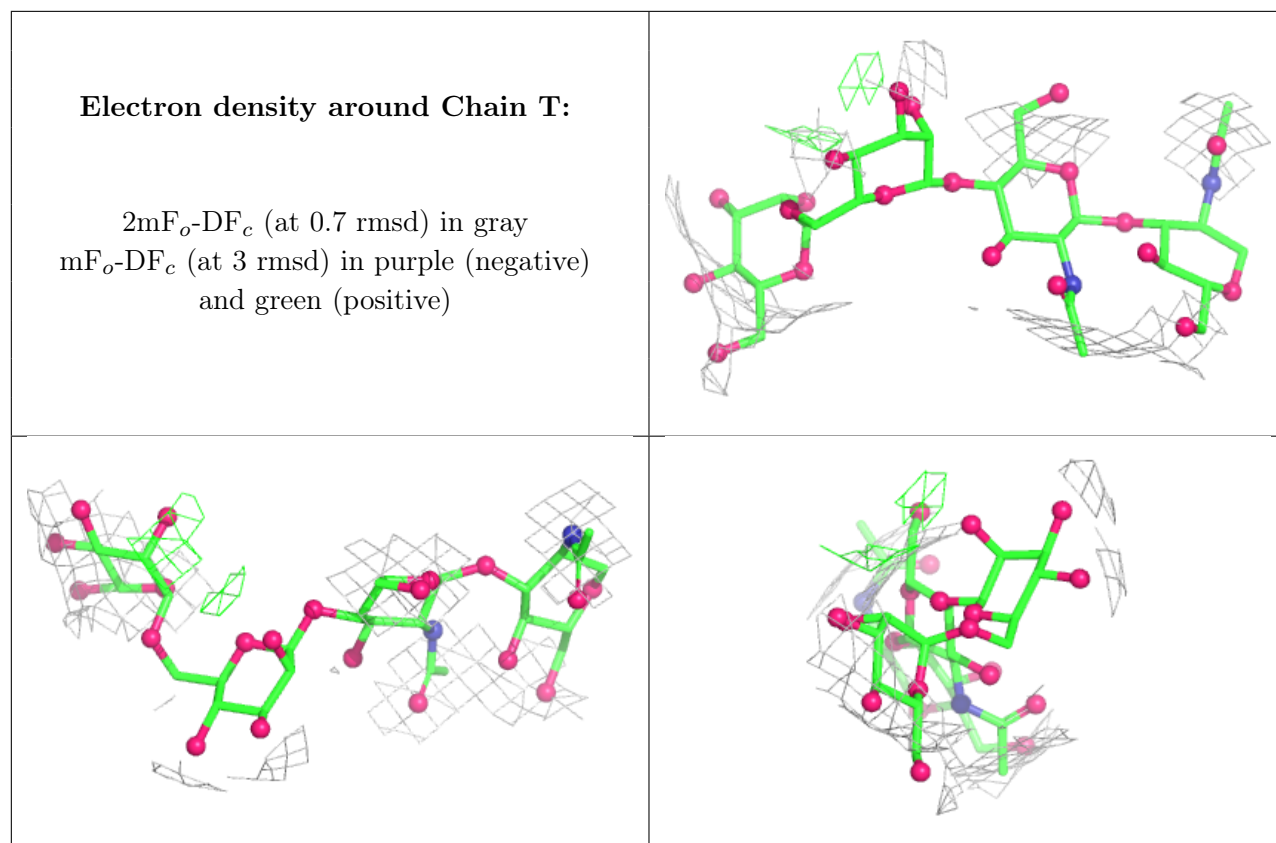
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.4 Ligands [i](#)

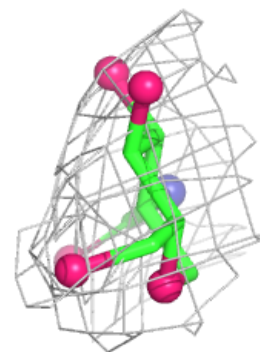
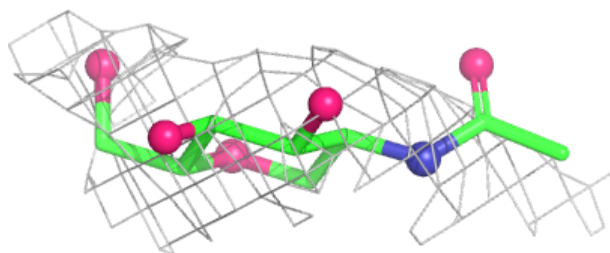
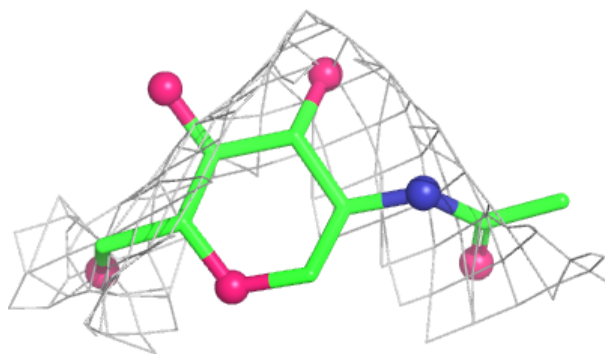
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	NAG	B	701	14/15	0.63	0.11	234,239,246,246	0
14	NAG	A	701	14/15	0.79	0.07	192,196,202,203	0

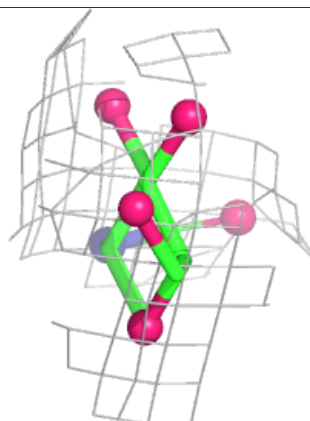
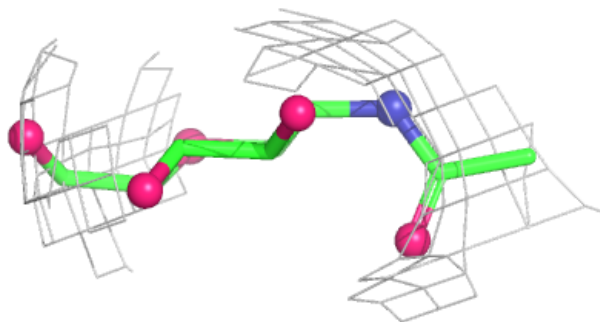
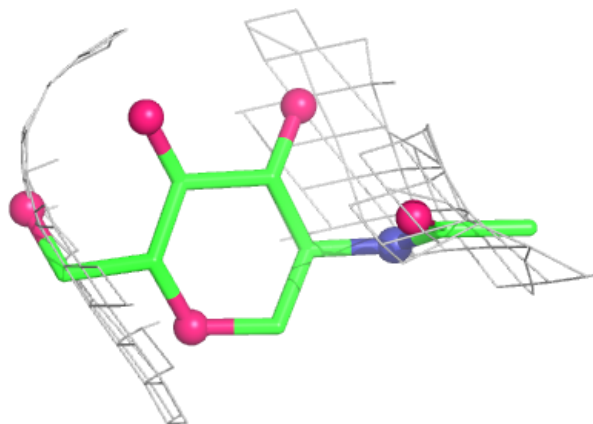
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG B 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 A 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 ⓘ

There are no such residues in this entry.