



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 25, 2026 – 05:28 AM UTC

PDB ID : 6JBS / pdb_00006jbs
Title : Bifunctional xylosidase/glucosidase LXYL
Authors : Gong, W.M.; Yang, L.Y.
Deposited on : 2019-01-26
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

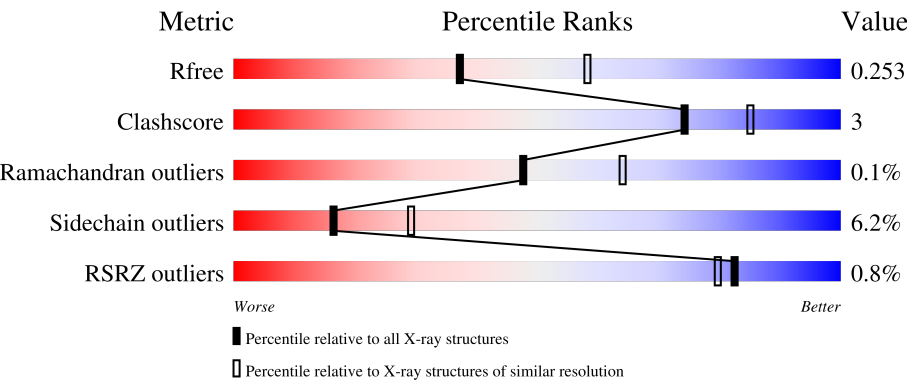
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	809	85%8%• 6%
1	B	809	% 84%8%• 6%
1	C	809	% 84%8%• 6%
1	D	809	% 86%7%• 6%
2	E	3	33%67%

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Mol	Chain	Length	Quality of chain
2	N	3	100%
3	F	7	14% 86%
4	G	6	33% 67%
5	H	3	100%
5	K	3	33% 67%
6	I	7	100%
6	L	7	29% 71%
6	O	7	14% 86%
7	J	2	50% 50%
8	M	5	100%
9	P	7	29% 71%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 25512 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 Beta-D-xylosidase/beta-D-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	762	Total	C	N	O	S	0	1	0
			5752	3640	963	1132	17			
1	B	761	Total	C	N	O	S	0	0	0
			5744	3635	962	1130	17			
1	C	761	Total	C	N	O	S	0	0	0
			5744	3635	962	1130	17			
1	D	761	Total	C	N	O	S	0	0	0
			5744	3635	962	1130	17			

There are 24 discrepancies between the modelled and reference sequences:

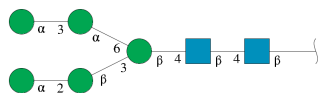
Chain	Residue	Modelled	Actual	Comment	Reference
A	804	HIS	-	expression tag	UNP G8GLP2
A	805	HIS	-	expression tag	UNP G8GLP2
A	806	HIS	-	expression tag	UNP G8GLP2
A	807	HIS	-	expression tag	UNP G8GLP2
A	808	HIS	-	expression tag	UNP G8GLP2
A	809	HIS	-	expression tag	UNP G8GLP2
B	804	HIS	-	expression tag	UNP G8GLP2
B	805	HIS	-	expression tag	UNP G8GLP2
B	806	HIS	-	expression tag	UNP G8GLP2
B	807	HIS	-	expression tag	UNP G8GLP2
B	808	HIS	-	expression tag	UNP G8GLP2
B	809	HIS	-	expression tag	UNP G8GLP2
C	804	HIS	-	expression tag	UNP G8GLP2
C	805	HIS	-	expression tag	UNP G8GLP2
C	806	HIS	-	expression tag	UNP G8GLP2
C	807	HIS	-	expression tag	UNP G8GLP2
C	808	HIS	-	expression tag	UNP G8GLP2
C	809	HIS	-	expression tag	UNP G8GLP2
D	804	HIS	-	expression tag	UNP G8GLP2
D	805	HIS	-	expression tag	UNP G8GLP2
D	806	HIS	-	expression tag	UNP G8GLP2

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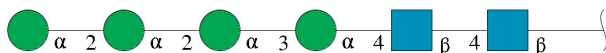
Chain	Residue	Modelled	Actual	Comment	Reference
D	807	HIS	-	expression tag	UNP G8GLP2
D	808	HIS	-	expression tag	UNP G8GLP2
D	809	HIS	-	expression tag	UNP G8GLP2

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- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[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.

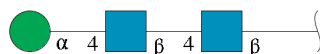


- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



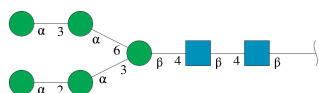
WORLD WIDE
PDB
PROTEIN DATA BANK

- Molecule 5 is an oligosaccharide called alpha-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
5	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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.



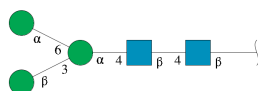
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	7	Total	C	N	O	0	0	0
			83	46	2	35			
6	L	7	Total	C	N	O	0	0	0
			83	46	2	35			
6	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



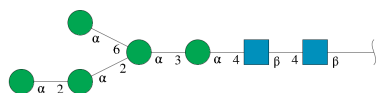
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



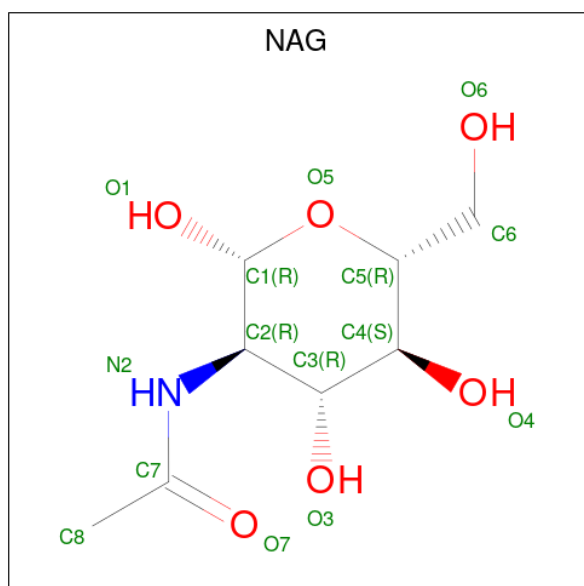
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	M	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-alpha-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
9	P	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



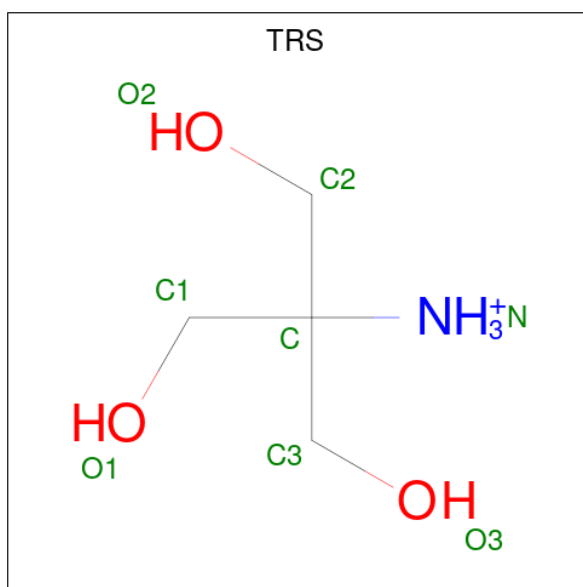
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			13	8	1	4		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	B	1	Total	C	N	O	0	0
			14	8	1	5		
10	B	1	Total	C	N	O	0	0
			13	8	1	4		
10	B	1	Total	C	N	O	0	0
			14	8	1	5		
10	B	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			13	8	1	4		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	C	1	Total	C	N	O	0	0
			14	8	1	5		
10	D	1	Total	C	N	O	0	0
			14	8	1	5		
10	D	1	Total	C	N	O	0	0
			13	8	1	4		
10	D	1	Total	C	N	O	0	0
			14	8	1	5		
10	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			8	4	1	3		
11	B	1	Total	C	N	O	0	0
			8	4	1	3		
11	C	1	Total	C	N	O	0	0
			8	4	1	3		
11	D	1	Total	C	N	O	0	0
			8	4	1	3		

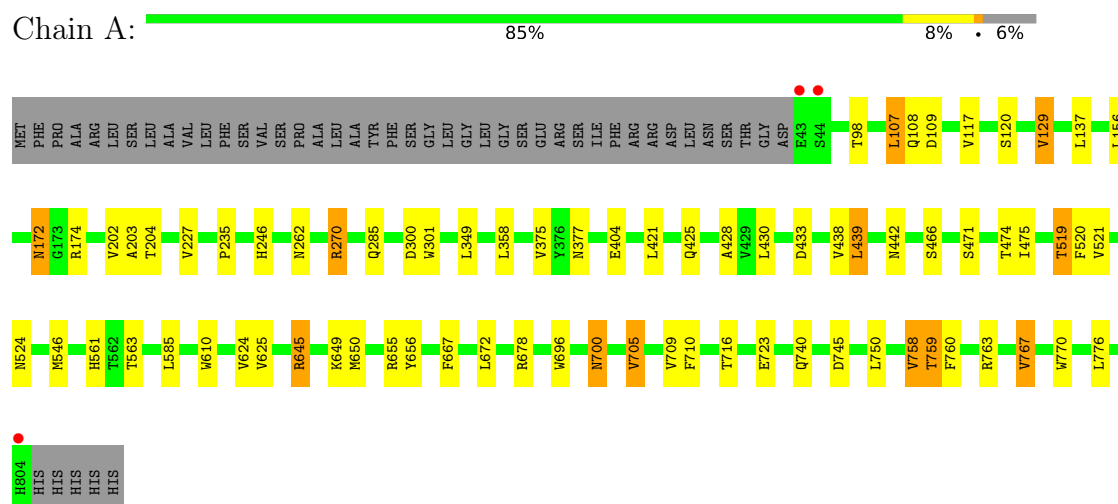
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	402	Total	O	0	0
			402	402		
12	B	311	Total	O	0	0
			311	311		
12	C	398	Total	O	0	0
			398	398		
12	D	433	Total	O	0	0
			433	433		

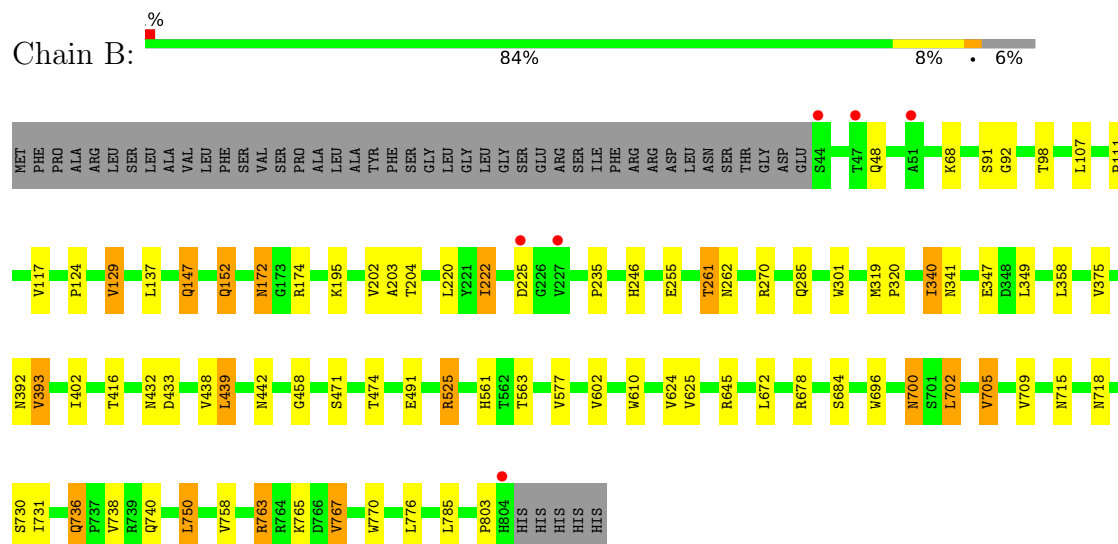
3 Residue-property plots [i](#)

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.

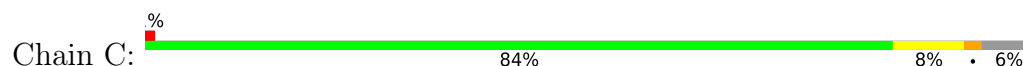
- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

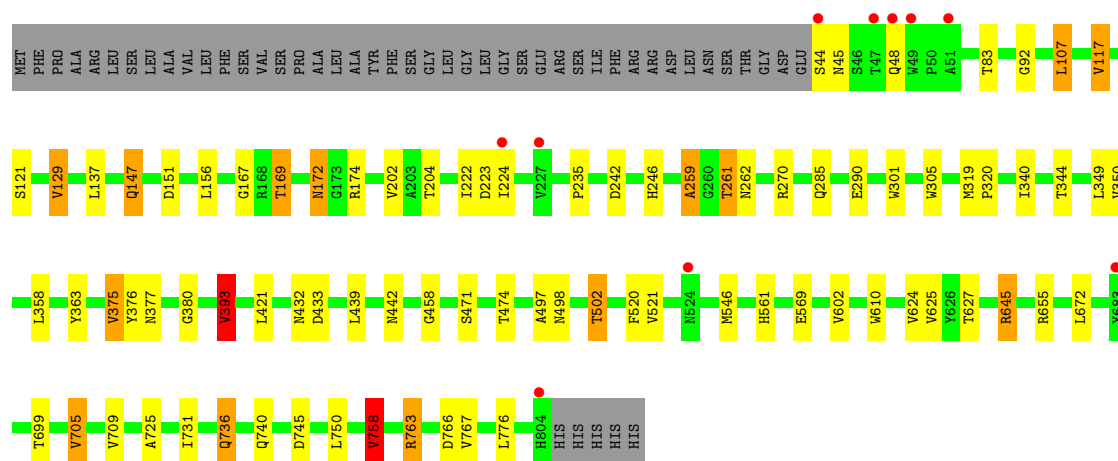


- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

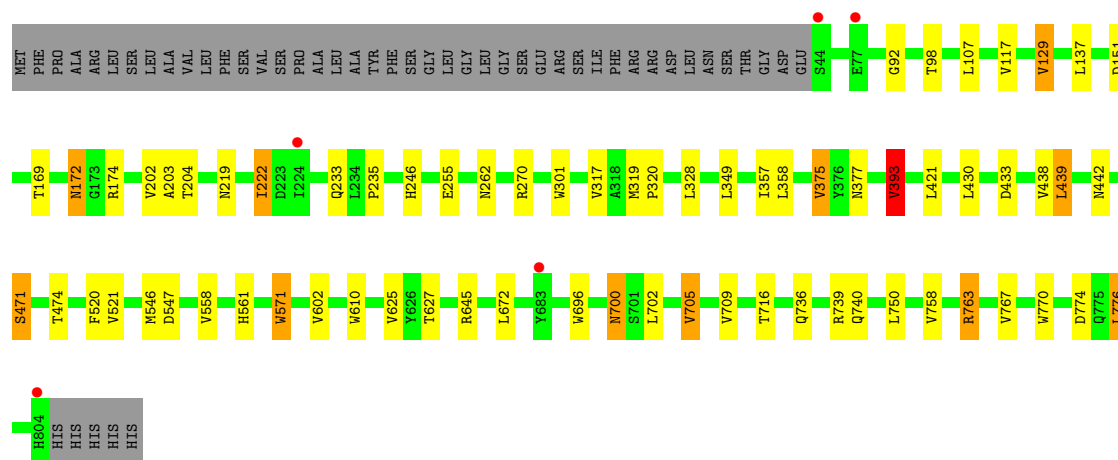
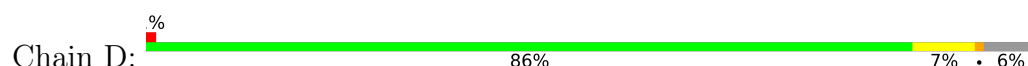


- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase





- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase



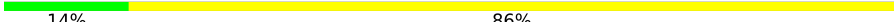
- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 3: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-3)-[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 F:  14% 86%

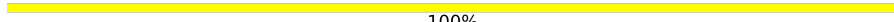


- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  33% 67%

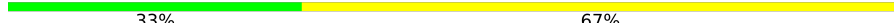


- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

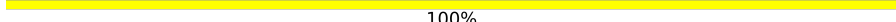


- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  33% 67%

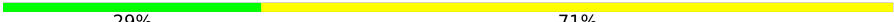


- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

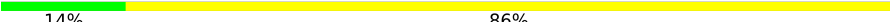


- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  29% 71%



- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 O:  14% 86%

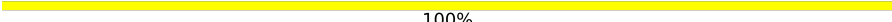


- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

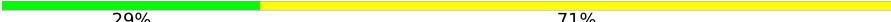


- Molecule 8: beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%



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

Chain P:  29% 71%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	131.91Å 131.91Å 385.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.40) 99.7 (50.00-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.184 , 0.251 0.190 , 0.253	Depositor DCC
R_{free} test set	6872 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25512	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.67	0/5896	0.88	4/8067 (0.0%)
1	B	0.66	0/5885	0.87	7/8052 (0.1%)
1	C	0.67	0/5885	0.88	9/8052 (0.1%)
1	D	0.66	0/5885	0.86	4/8052 (0.0%)
All	All	0.66	0/23551	0.87	24/32223 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	259	ALA	N-CA-C	6.69	121.27	113.18
1	C	129	VAL	N-CA-CB	6.68	119.62	110.54
1	B	261	THR	CB-CA-C	-6.40	100.24	109.84
1	C	169	THR	CB-CA-C	-6.36	101.96	109.47
1	A	767	VAL	N-CA-CB	-6.02	104.34	112.16

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	259	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	C	699	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5752	0	5533	38	0
1	B	5744	0	5526	37	0
1	C	5744	0	5526	38	0
1	D	5744	0	5526	35	0
2	E	39	0	34	0	0
2	N	39	0	34	0	0
3	F	83	0	70	0	0
4	G	72	0	61	0	0
5	H	39	0	34	0	0
5	K	39	0	34	0	0
6	I	83	0	70	0	0
6	L	83	0	70	0	0
6	O	83	0	70	0	0
7	J	28	0	25	0	0
8	M	61	0	52	0	0
9	P	83	0	69	0	0
10	A	55	0	50	0	0
10	B	55	0	50	1	0
10	C	55	0	50	0	0
10	D	55	0	50	0	0
11	A	8	0	12	2	0
11	B	8	0	12	0	0
11	C	8	0	12	0	0
11	D	8	0	12	0	0
12	A	402	0	0	2	0
12	B	311	0	0	5	0
12	C	398	0	0	3	0
12	D	433	0	0	0	0
All	All	25512	0	22982	146	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 3.

The worst 5 of 146 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:525:ARG:NH2	12:B:1001:HOH:O	1.99	0.95
1:C:319:MET:SD	12:C:1344:HOH:O	2.26	0.92
1:C:497:ALA:HB1	1:C:502:THR:HG21	1.59	0.85
1:B:696:TRP:HA	1:B:700:ASN:HD21	1.43	0.83
1:C:319:MET:HE3	1:C:320:PRO:HA	1.59	0.83

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	A	761/809 (94%)	733 (96%)	28 (4%)	0	100	100
1	B	759/809 (94%)	727 (96%)	30 (4%)	2 (0%)	36	50
1	C	759/809 (94%)	729 (96%)	28 (4%)	2 (0%)	36	50
1	D	759/809 (94%)	730 (96%)	29 (4%)	0	100	100
All	All	3038/3236 (94%)	2919 (96%)	115 (4%)	4 (0%)	48	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	803	PRO
1	C	224	ILE
1	B	225	ASP
1	C	167	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	613/654 (94%)	578 (94%)	35 (6%)	18	33
1	B	612/654 (94%)	569 (93%)	43 (7%)	14	24
1	C	612/654 (94%)	573 (94%)	39 (6%)	16	28
1	D	612/654 (94%)	577 (94%)	35 (6%)	18	33
All	All	2449/2616 (94%)	2297 (94%)	152 (6%)	16	29

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	767	VAL
1	D	705	VAL
1	D	117	VAL
1	D	393	VAL
1	D	767	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	736	GLN
1	D	700	ASN
1	C	262	ASN
1	D	676	HIS
1	D	246	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

60 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$
2	NAG	E	1	2,1	14,14,15	1.00	1 (7%)	17,19,21	1.38	1 (5%)
2	NAG	E	2	2	14,14,15	0.58	0	17,19,21	1.22	2 (11%)
2	BMA	E	3	2	11,11,12	0.63	0	15,15,17	0.72	0
3	NAG	F	1	3,1	14,14,15	1.20	1 (7%)	17,19,21	1.12	1 (5%)
3	NAG	F	2	3	14,14,15	0.54	0	17,19,21	0.92	0
3	BMA	F	3	3	11,11,12	0.60	0	15,15,17	1.58	1 (6%)
3	BMA	F	4	3	11,11,12	0.64	0	15,15,17	1.26	2 (13%)
3	MAN	F	5	3	11,11,12	0.71	0	15,15,17	1.65	1 (6%)
3	MAN	F	6	3	11,11,12	0.93	0	15,15,17	3.08	5 (33%)
3	MAN	F	7	3	11,11,12	0.25	0	15,15,17	0.83	1 (6%)
4	NAG	G	1	4,1	14,14,15	0.44	0	17,19,21	0.74	0
4	NAG	G	2	4	14,14,15	0.38	0	17,19,21	0.86	0
4	MAN	G	3	4	11,11,12	0.69	0	15,15,17	1.67	3 (20%)
4	MAN	G	4	4	11,11,12	0.68	0	15,15,17	1.78	1 (6%)
4	MAN	G	5	4	11,11,12	0.66	0	15,15,17	2.02	1 (6%)
4	MAN	G	6	4	11,11,12	0.49	0	15,15,17	1.14	1 (6%)
5	NAG	H	1	5,1	14,14,15	0.96	1 (7%)	17,19,21	1.20	2 (11%)
5	NAG	H	2	5	14,14,15	0.39	0	17,19,21	0.81	1 (5%)
5	MAN	H	3	5	11,11,12	0.68	0	15,15,17	1.17	2 (13%)
6	NAG	I	1	6,1	14,14,15	1.06	1 (7%)	17,19,21	1.52	3 (17%)
6	NAG	I	2	6	14,14,15	0.47	0	17,19,21	0.87	1 (5%)
6	BMA	I	3	6	11,11,12	0.27	0	15,15,17	0.93	1 (6%)
6	MAN	I	4	6	11,11,12	0.48	0	15,15,17	1.03	1 (6%)
6	MAN	I	5	6	11,11,12	0.52	0	15,15,17	1.37	2 (13%)
6	MAN	I	6	6	11,11,12	0.76	0	15,15,17	2.42	4 (26%)
6	MAN	I	7	6	11,11,12	0.39	0	15,15,17	0.86	1 (6%)
7	NAG	J	1	7,1	14,14,15	0.30	0	17,19,21	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	J	2	7	14,14,15	0.61	0	17,19,21	1.07	1 (5%)
5	NAG	K	1	5,1	14,14,15	1.14	1 (7%)	17,19,21	1.02	1 (5%)
5	NAG	K	2	5	14,14,15	0.52	0	17,19,21	1.06	0
5	MAN	K	3	5	11,11,12	0.54	0	15,15,17	0.95	1 (6%)
6	NAG	L	1	6,1	14,14,15	1.10	1 (7%)	17,19,21	0.97	1 (5%)
6	NAG	L	2	6	14,14,15	0.50	0	17,19,21	1.03	0
6	BMA	L	3	6	11,11,12	0.45	0	15,15,17	0.92	0
6	MAN	L	4	6	11,11,12	0.65	0	15,15,17	2.04	3 (20%)
6	MAN	L	5	6	11,11,12	0.69	0	15,15,17	0.89	1 (6%)
6	MAN	L	6	6	11,11,12	0.78	0	15,15,17	3.08	4 (26%)
6	MAN	L	7	6	11,11,12	0.48	0	15,15,17	0.89	1 (6%)
8	NAG	M	1	8,1	14,14,15	0.45	0	17,19,21	1.01	1 (5%)
8	NAG	M	2	8	14,14,15	0.43	0	17,19,21	1.05	1 (5%)
8	MAN	M	3	8	11,11,12	0.53	0	15,15,17	1.65	4 (26%)
8	BMA	M	4	8	11,11,12	0.62	0	15,15,17	1.52	3 (20%)
8	MAN	M	5	8	11,11,12	0.87	0	15,15,17	1.31	2 (13%)
2	NAG	N	1	2,1	14,14,15	0.92	1 (7%)	17,19,21	1.02	1 (5%)
2	NAG	N	2	2	14,14,15	0.55	0	17,19,21	1.22	2 (11%)
2	BMA	N	3	2	11,11,12	0.65	0	15,15,17	1.06	2 (13%)
6	NAG	O	1	6,1	14,14,15	1.09	1 (7%)	17,19,21	0.79	0
6	NAG	O	2	6	14,14,15	0.29	0	17,19,21	0.73	0
6	BMA	O	3	6	11,11,12	0.38	0	15,15,17	1.13	2 (13%)
6	MAN	O	4	6	11,11,12	0.54	0	15,15,17	1.39	1 (6%)
6	MAN	O	5	6	11,11,12	0.59	0	15,15,17	2.08	1 (6%)
6	MAN	O	6	6	11,11,12	0.70	0	15,15,17	3.05	2 (13%)
6	MAN	O	7	6	11,11,12	0.32	0	15,15,17	1.03	1 (6%)
9	NAG	P	1	9,1	14,14,15	0.39	0	17,19,21	0.91	0
9	NAG	P	2	9	14,14,15	0.45	0	17,19,21	0.93	0
9	MAN	P	3	9	11,11,12	0.67	0	15,15,17	2.14	3 (20%)
9	MAN	P	4	9	11,11,12	0.60	0	15,15,17	2.24	1 (6%)
9	MAN	P	5	9	11,11,12	0.45	0	15,15,17	1.64	2 (13%)
9	MAN	P	6	9	11,11,12	0.30	0	15,15,17	1.28	1 (6%)
9	MAN	P	7	9	11,11,12	0.87	0	15,15,17	2.23	5 (33%)

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
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	BMA	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	1/2/19/22	0/1/1/1
3	MAN	F	6	3	-	1/2/19/22	0/1/1/1
3	MAN	F	7	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	MAN	G	3	4	-	1/2/19/22	0/1/1/1
4	MAN	G	4	4	-	2/2/19/22	0/1/1/1
4	MAN	G	5	4	-	2/2/19/22	0/1/1/1
4	MAN	G	6	4	-	2/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	MAN	H	3	5	-	1/2/19/22	0/1/1/1
6	NAG	I	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	1/6/23/26	0/1/1/1
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1
6	MAN	I	4	6	-	0/2/19/22	0/1/1/1
6	MAN	I	5	6	-	0/2/19/22	0/1/1/1
6	MAN	I	6	6	-	2/2/19/22	0/1/1/1
6	MAN	I	7	6	-	0/2/19/22	0/1/1/1
7	NAG	J	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
5	NAG	K	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	2/6/23/26	0/1/1/1
5	MAN	K	3	5	-	2/2/19/22	1/1/1/1
6	NAG	L	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	0/2/19/22	0/1/1/1
6	MAN	L	4	6	-	1/2/19/22	0/1/1/1
6	MAN	L	5	6	-	0/2/19/22	0/1/1/1
6	MAN	L	6	6	-	1/2/19/22	0/1/1/1
6	MAN	L	7	6	-	0/2/19/22	0/1/1/1
8	NAG	M	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	M	2	8	-	1/6/23/26	0/1/1/1

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

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	O4-C4	-4.21	1.32	1.43
6	L	1	NAG	O4-C4	-3.98	1.33	1.43
5	K	1	NAG	O4-C4	-3.95	1.33	1.43
6	O	1	NAG	O4-C4	-3.62	1.34	1.43
6	I	1	NAG	O4-C4	-3.58	1.34	1.43

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	6	MAN	C1-O5-C5	10.19	125.85	112.19
6	O	6	MAN	C1-O5-C5	9.94	125.51	112.19
3	F	6	MAN	C1-O5-C5	9.58	125.02	112.19
9	P	4	MAN	C1-O5-C5	7.96	122.86	112.19
6	I	6	MAN	C1-O5-C5	7.17	121.80	112.19

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

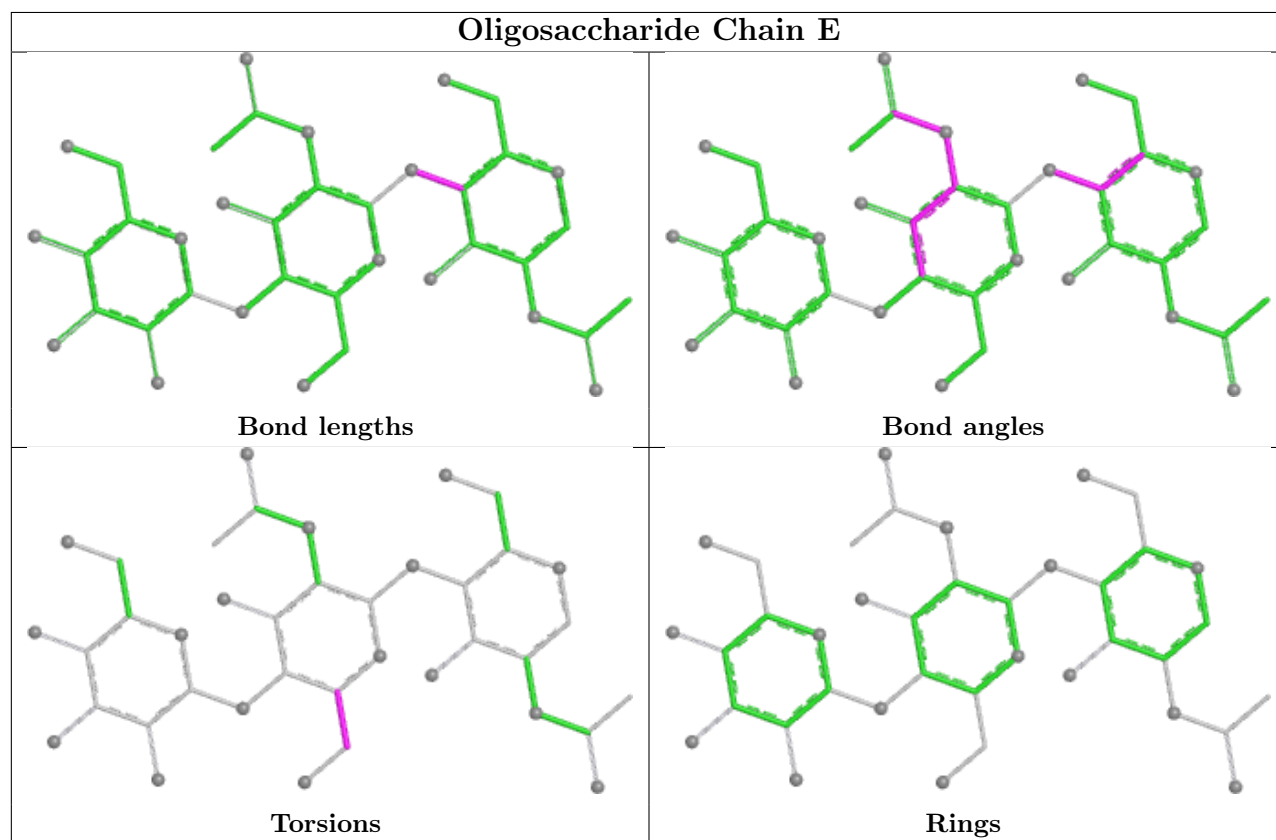
Mol	Chain	Res	Type	Atoms
5	K	3	MAN	O5-C5-C6-O6
6	O	6	MAN	O5-C5-C6-O6
4	G	6	MAN	C4-C5-C6-O6
4	G	5	MAN	C4-C5-C6-O6
4	G	6	MAN	O5-C5-C6-O6

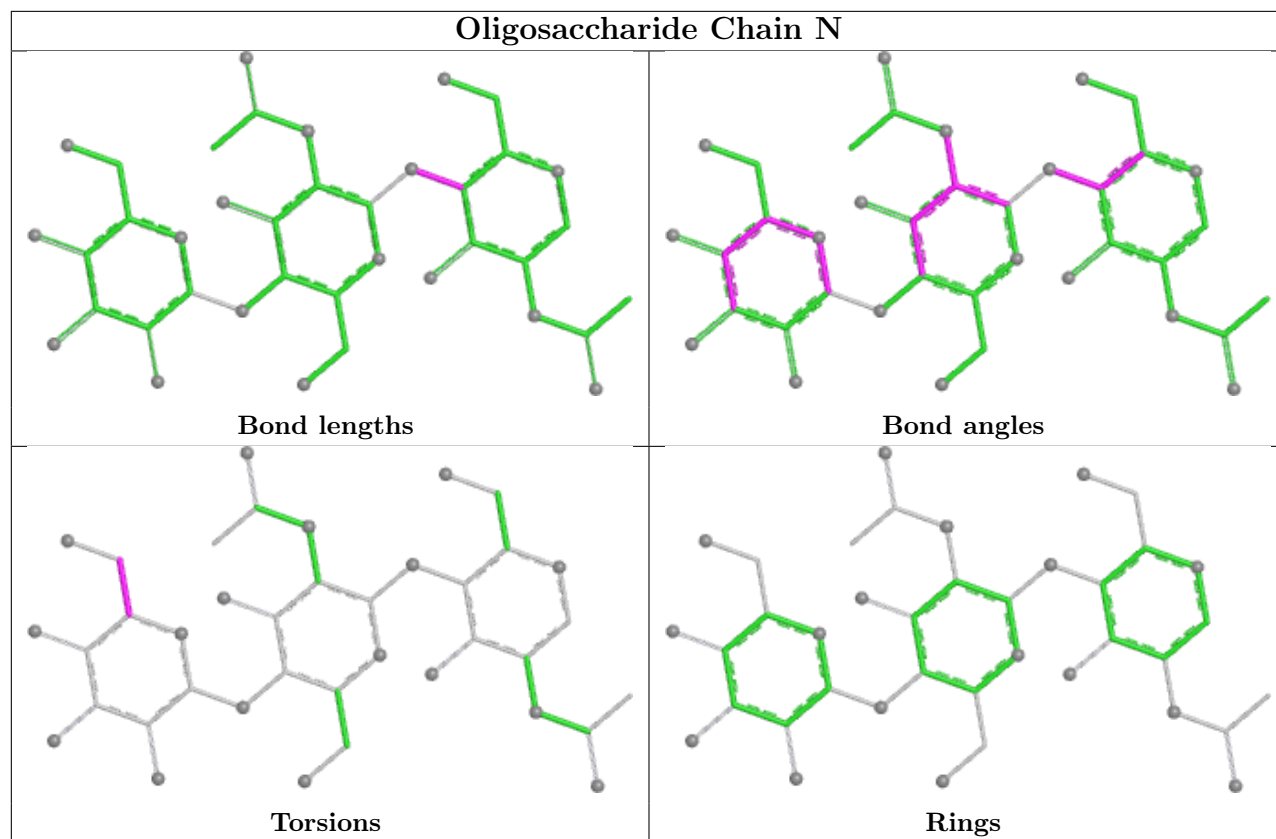
All (2) ring outliers are listed below:

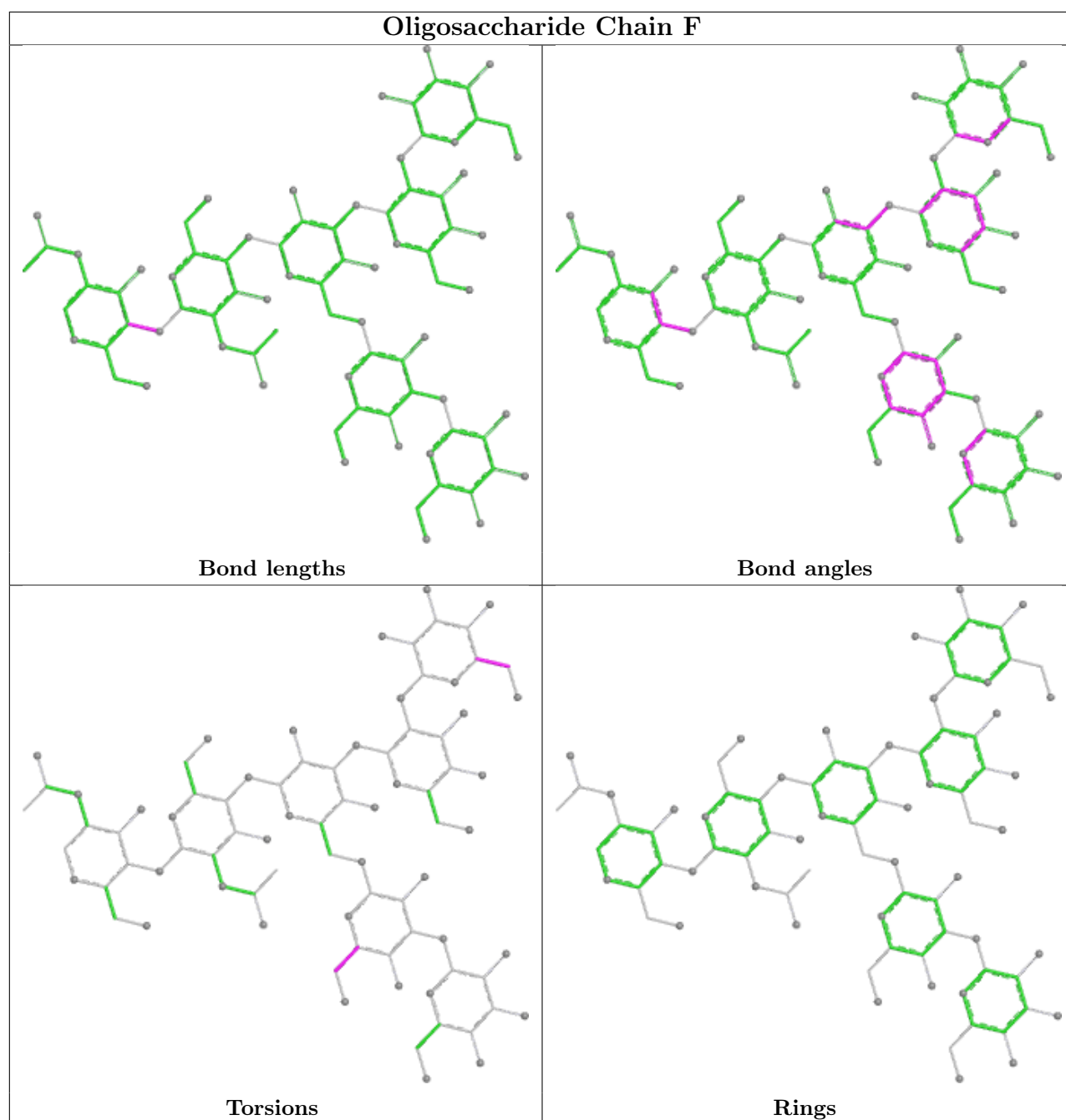
Mol	Chain	Res	Type	Atoms
9	P	3	MAN	C1-C2-C3-C4-C5-O5
5	K	3	MAN	C1-C2-C3-C4-C5-O5

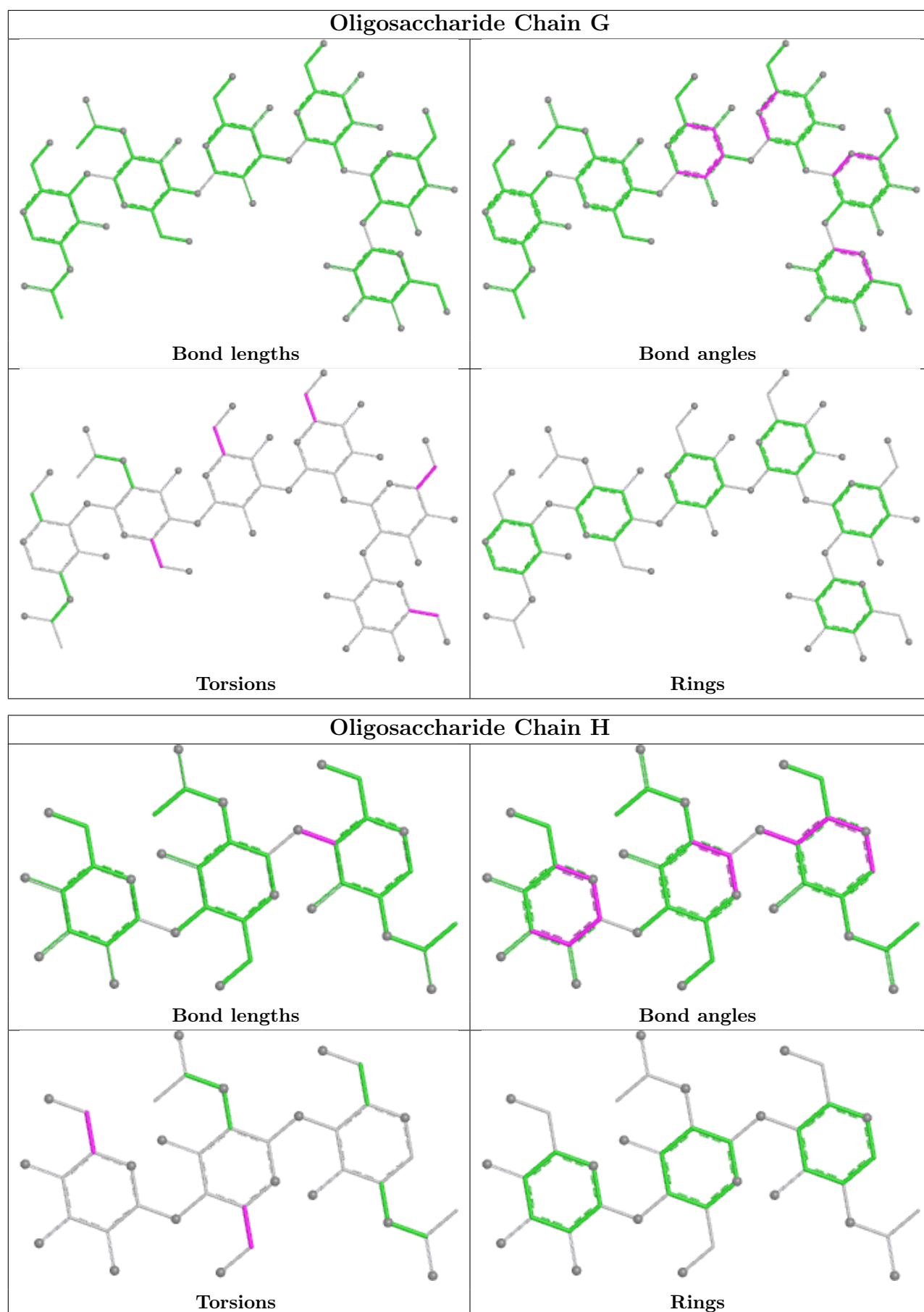
No monomer is involved in short contacts.

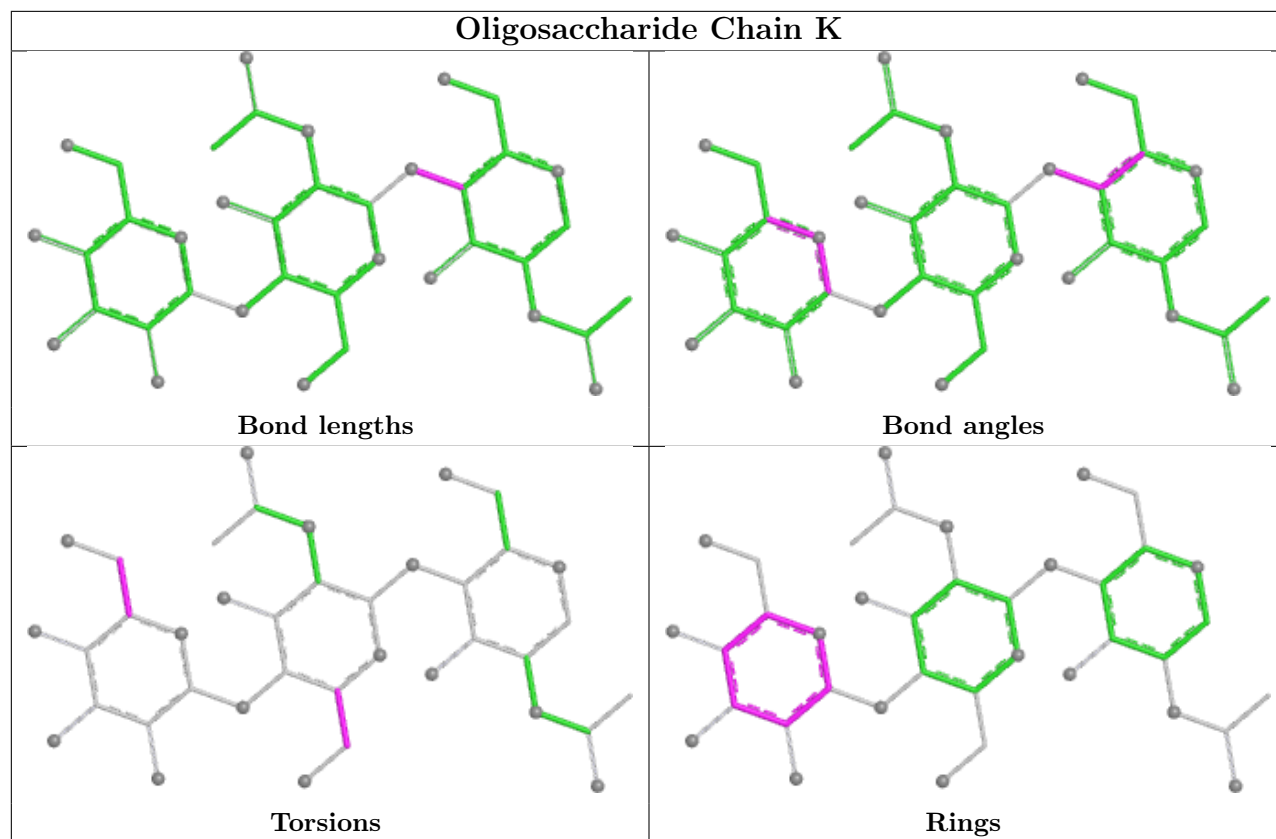
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

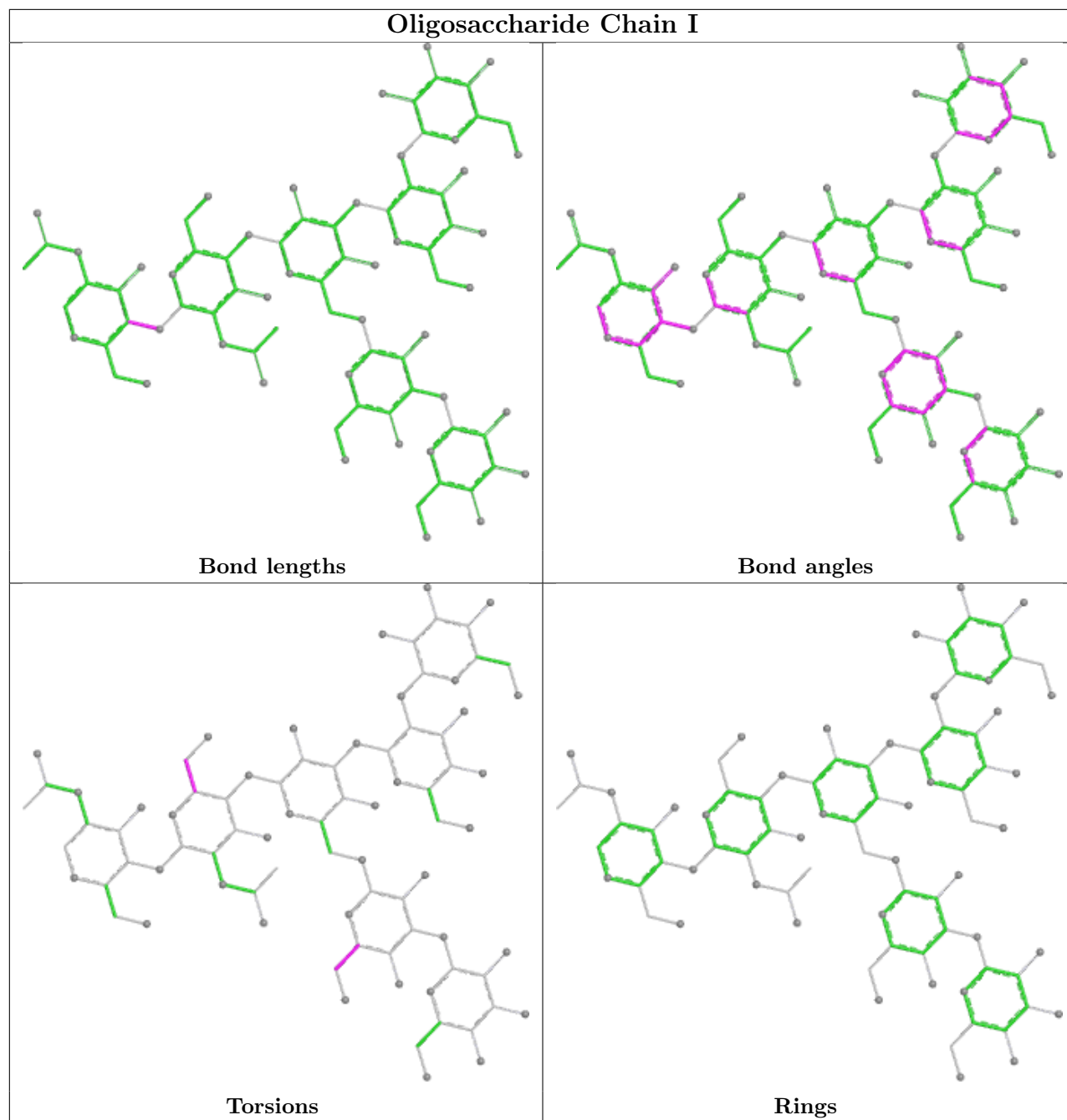


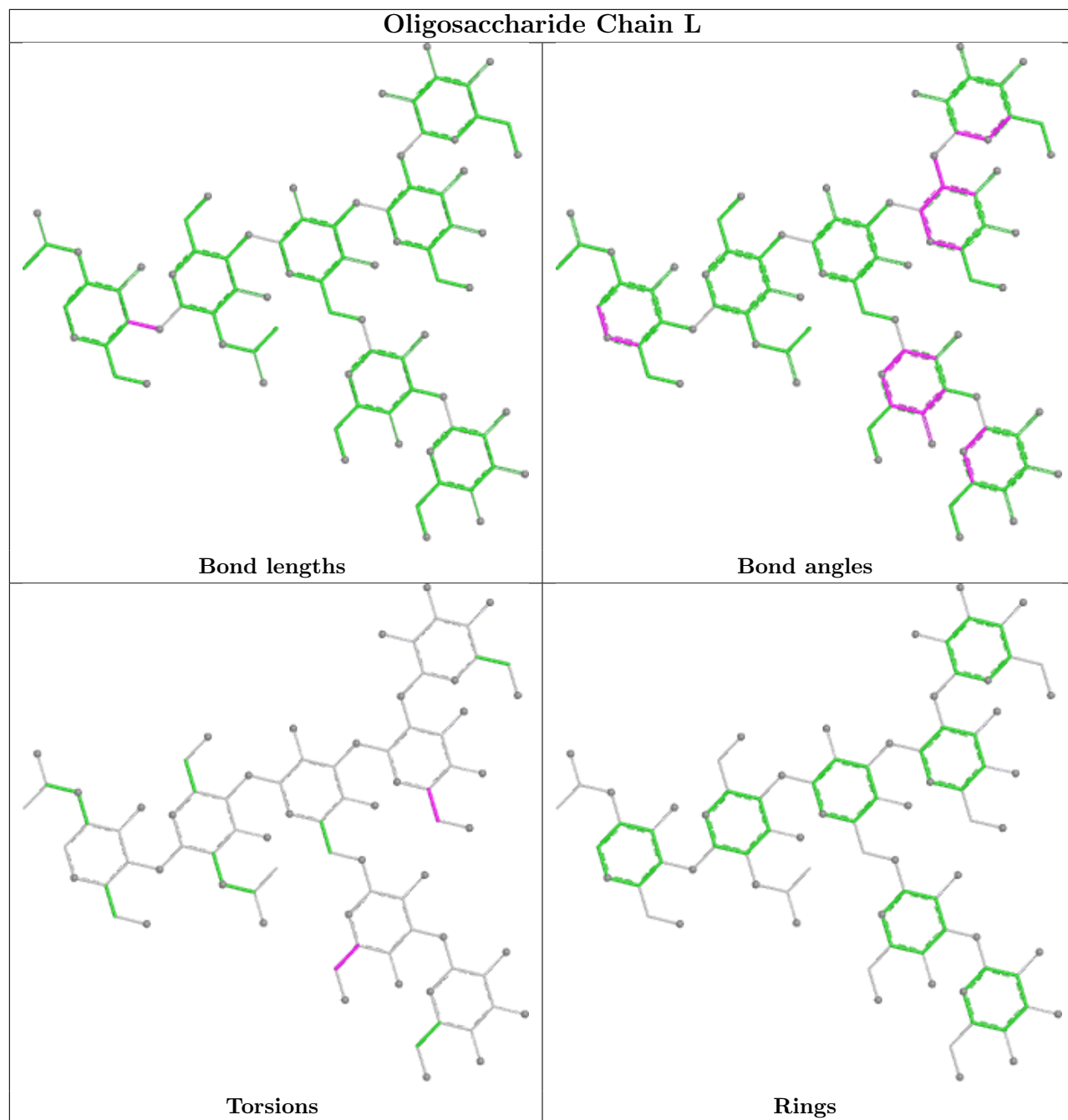


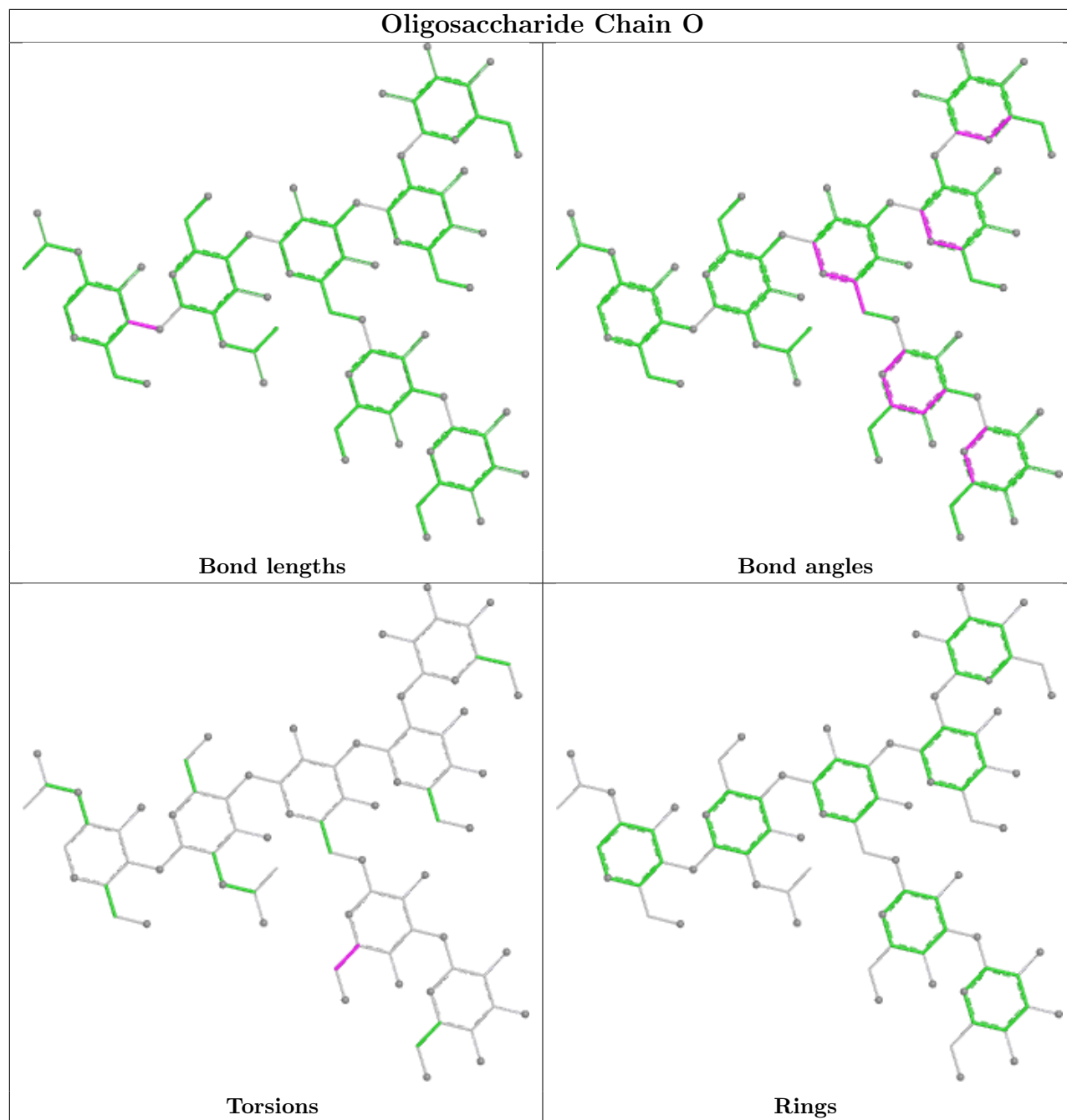


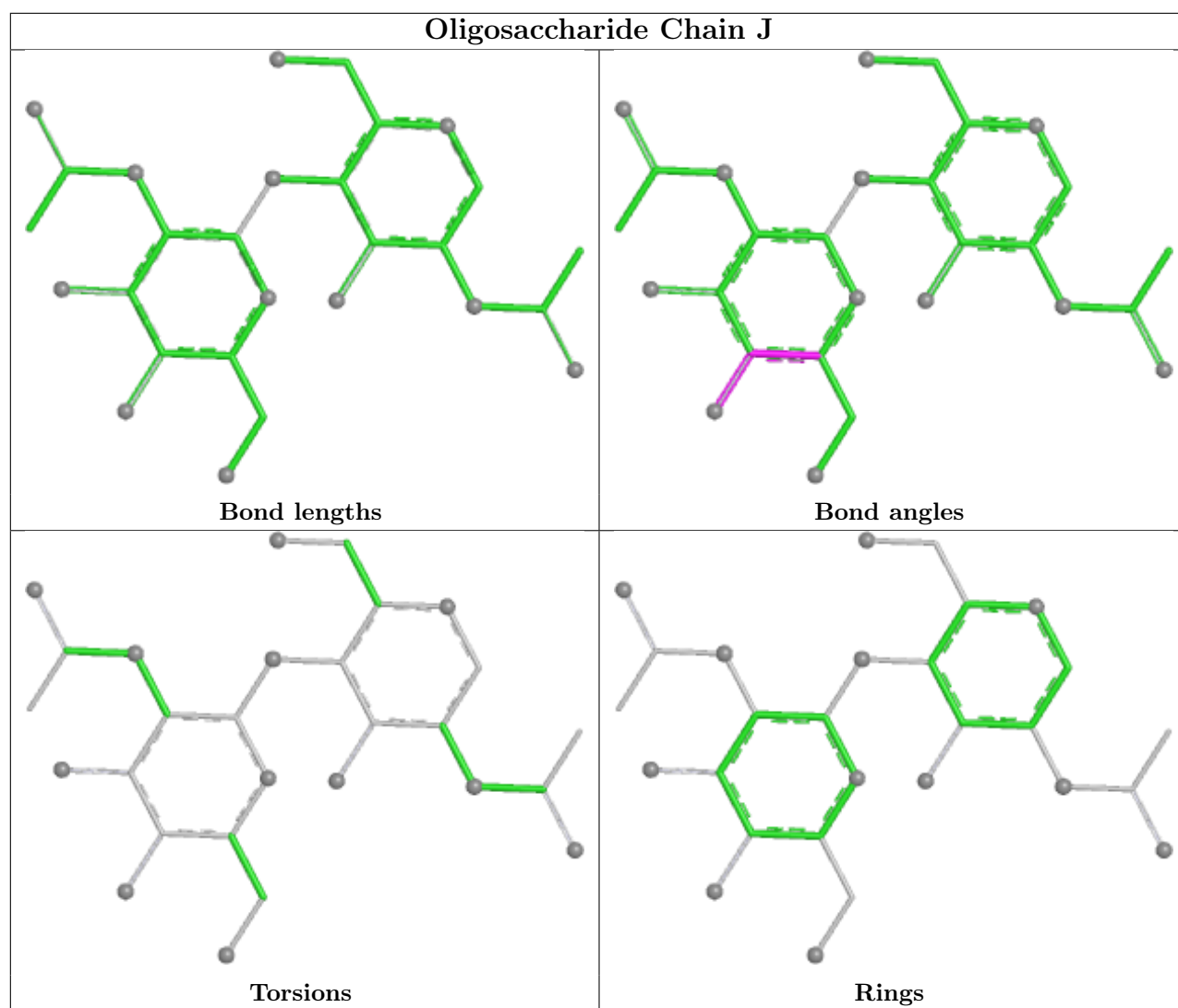


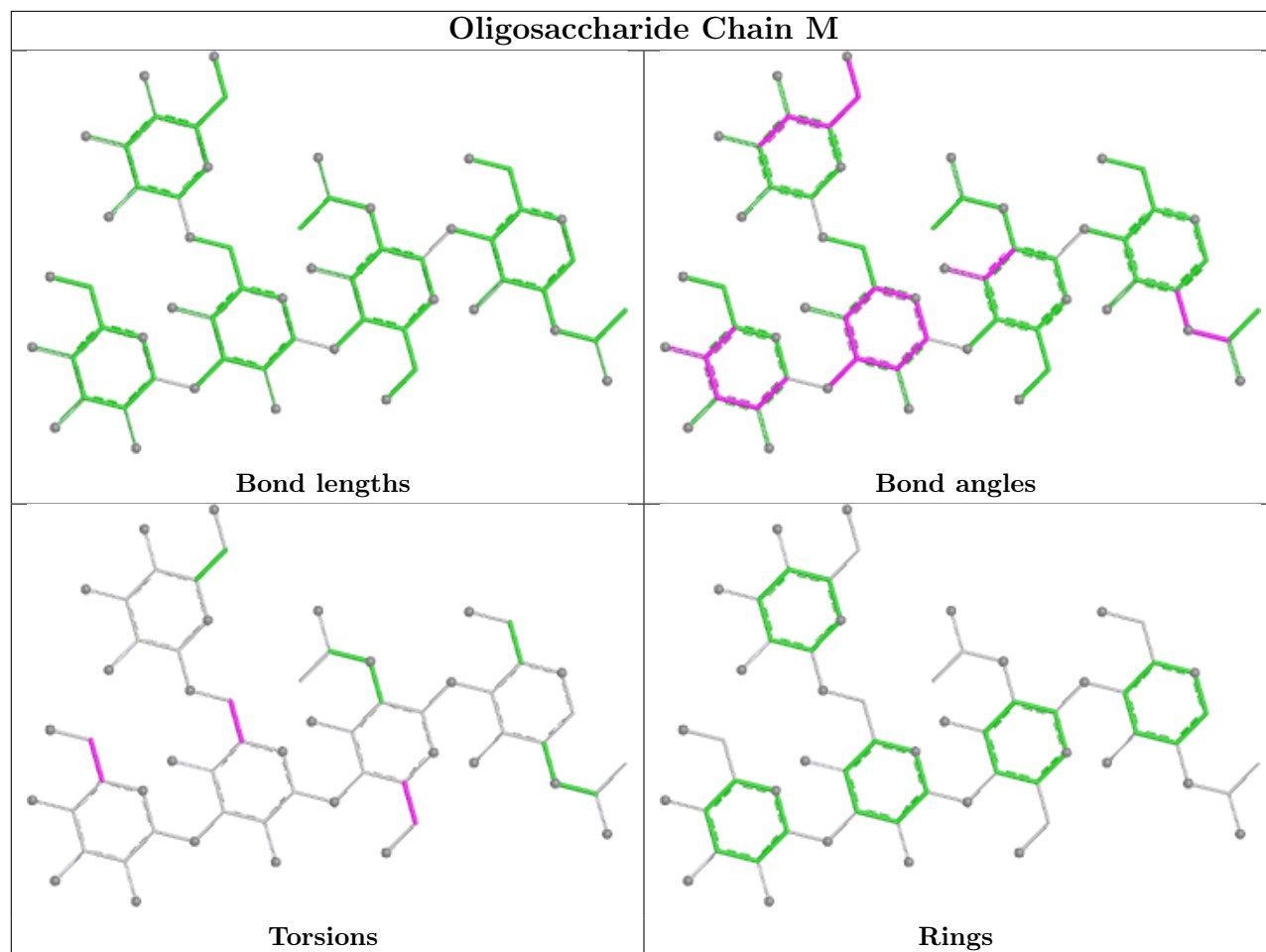


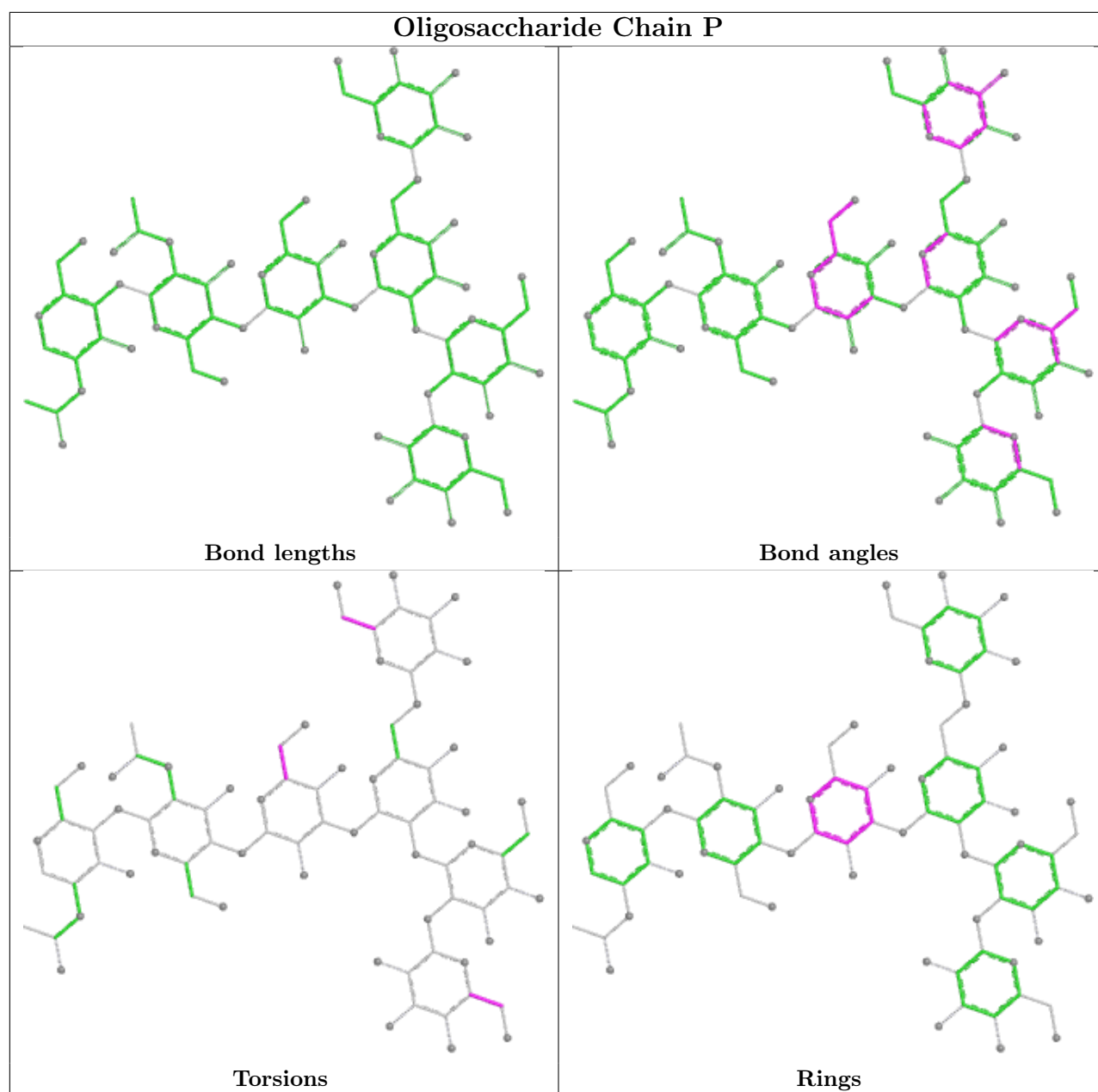












5.6 Ligand geometry [i](#)

20 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
11	TRS	C	920	-	7,7,7	0.67	0	9,9,9	1.21	1 (11%)
10	NAG	B	915	1	14,14,15	0.57	0	17,19,21	1.02	1 (5%)
11	TRS	B	917	-	7,7,7	0.51	0	9,9,9	0.90	0
10	NAG	A	920	1	14,14,15	0.47	0	17,19,21	1.41	2 (11%)
10	NAG	D	920	1	14,14,15	0.46	0	17,19,21	0.75	0
11	TRS	D	922	-	7,7,7	0.54	0	9,9,9	1.31	2 (22%)
10	NAG	D	911	1	14,14,15	0.37	0	17,19,21	1.10	0
10	NAG	A	912	1	13,13,15	0.93	1 (7%)	15,17,21	1.86	3 (20%)
10	NAG	A	919	1	14,14,15	0.34	0	17,19,21	0.94	1 (5%)
10	NAG	D	912	1	13,13,15	0.83	1 (7%)	15,17,21	1.92	3 (20%)
11	TRS	A	921	-	7,7,7	0.59	0	9,9,9	1.20	1 (11%)
10	NAG	C	918	1	14,14,15	0.32	0	17,19,21	0.76	0
10	NAG	B	911	1	14,14,15	0.50	0	17,19,21	2.20	6 (35%)
10	NAG	A	911	1	14,14,15	0.36	0	17,19,21	0.86	1 (5%)
10	NAG	B	912	1	13,13,15	0.69	0	15,17,21	1.82	6 (40%)
10	NAG	C	911	1	14,14,15	0.39	0	17,19,21	1.89	3 (17%)
10	NAG	D	921	1	14,14,15	0.38	0	17,19,21	0.91	1 (5%)
10	NAG	C	919	1	14,14,15	0.36	0	17,19,21	1.44	2 (11%)
10	NAG	C	912	1	13,13,15	0.93	1 (7%)	15,17,21	1.73	3 (20%)
10	NAG	B	916	1	14,14,15	0.52	0	17,19,21	2.52	3 (17%)

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
11	TRS	C	920	-	-	3/9/9/9	-
10	NAG	B	915	1	-	0/6/23/26	0/1/1/1
11	TRS	B	917	-	-	6/9/9/9	-
10	NAG	A	920	1	-	0/6/23/26	0/1/1/1
10	NAG	D	920	1	-	0/6/23/26	0/1/1/1
11	TRS	D	922	-	-	1/9/9/9	-
10	NAG	D	911	1	-	0/6/23/26	0/1/1/1
10	NAG	A	912	1	-	0/6/19/26	0/1/1/1
10	NAG	A	919	1	-	0/6/23/26	0/1/1/1
10	NAG	D	912	1	-	4/6/19/26	0/1/1/1
11	TRS	A	921	-	-	7/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	C	918	1	-	0/6/23/26	0/1/1/1
10	NAG	B	911	1	-	3/6/23/26	0/1/1/1
10	NAG	A	911	1	-	2/6/23/26	0/1/1/1
10	NAG	B	912	1	-	1/6/19/26	0/1/1/1
10	NAG	C	911	1	-	2/6/23/26	0/1/1/1
10	NAG	D	921	1	-	0/6/23/26	0/1/1/1
10	NAG	C	919	1	-	0/6/23/26	0/1/1/1
10	NAG	C	912	1	-	0/6/19/26	0/1/1/1
10	NAG	B	916	1	-	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)
10	A	912	NAG	C1-C2	2.92	1.54	1.51
10	C	912	NAG	C1-C2	2.88	1.54	1.51
10	D	912	NAG	C1-C2	2.41	1.54	1.51

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	916	NAG	C1-O5-C5	8.66	123.79	112.19
10	C	911	NAG	C1-O5-C5	6.29	120.62	112.19
10	B	911	NAG	C2-N2-C7	5.41	130.15	122.90
10	B	911	NAG	C8-C7-N2	4.66	123.85	116.12
10	A	912	NAG	C3-C2-C1	4.59	113.72	109.50

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	911	NAG	C3-C2-N2-C7
11	A	921	TRS	C2-C-C1-O1
11	A	921	TRS	C3-C-C1-O1
11	A	921	TRS	N-C-C1-O1
11	A	921	TRS	C1-C-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	921	TRS	2	0
10	B	911	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	762/809 (94%)	-0.46	3 (0%) 88 86	20, 30, 42, 80	1 (0%)
1	B	761/809 (94%)	-0.19	6 (0%) 82 80	26, 36, 57, 103	0
1	C	761/809 (94%)	-0.33	10 (1%) 75 71	24, 31, 44, 99	0
1	D	761/809 (94%)	-0.38	5 (0%) 84 81	24, 32, 45, 81	0
All	All	3045/3236 (94%)	-0.34	24 (0%) 82 80	20, 32, 49, 103	1 (0%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	224	ILE	7.0
1	B	44	SER	5.2
1	C	44	SER	5.0
1	D	44	SER	4.9
1	A	43	GLU	4.8

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAN	H	3	11/12	0.55	0.15	73,77,84,89	0
2	BMA	N	3	11/12	0.57	0.15	69,73,76,78	0

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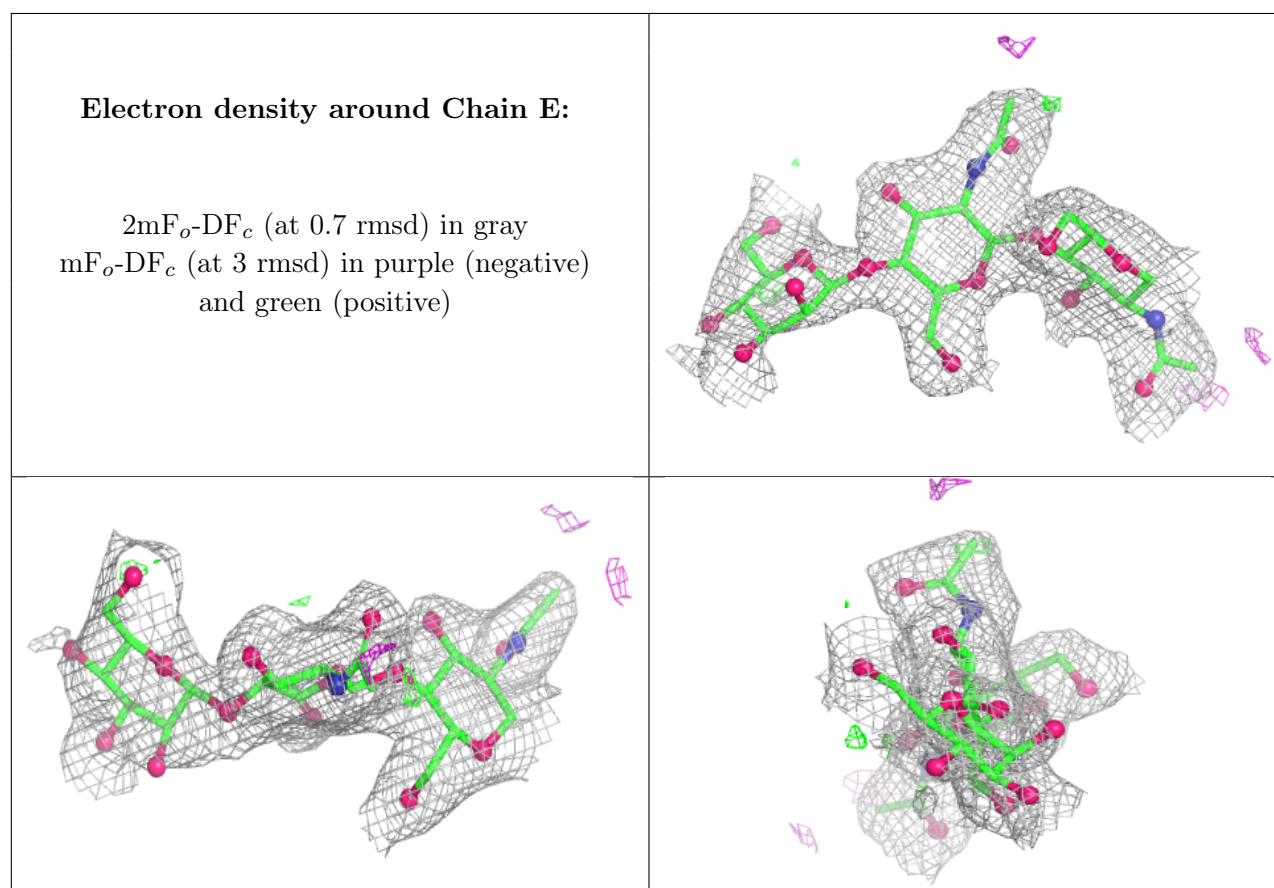
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MAN	I	5	11/12	0.57	0.15	69,73,83,83	0
3	MAN	F	6	11/12	0.62	0.15	46,48,52,53	0
6	MAN	I	6	11/12	0.63	0.14	54,57,57,59	0
4	MAN	G	5	11/12	0.64	0.14	86,91,95,102	0
3	MAN	F	5	11/12	0.66	0.15	68,75,78,79	0
5	MAN	K	3	11/12	0.66	0.13	69,76,80,82	0
8	MAN	M	5	11/12	0.66	0.15	51,54,57,61	0
2	BMA	E	3	11/12	0.67	0.14	73,76,79,80	0
4	MAN	G	3	11/12	0.67	0.15	71,74,78,79	0
3	BMA	F	4	11/12	0.72	0.13	62,66,70,71	0
4	MAN	G	6	11/12	0.73	0.20	100,106,111,112	0
6	MAN	O	4	11/12	0.74	0.13	60,63,67,67	0
6	MAN	O	5	11/12	0.75	0.12	54,61,69,71	0
6	MAN	L	6	11/12	0.75	0.12	44,46,48,49	0
6	MAN	O	6	11/12	0.76	0.11	47,48,52,52	0
8	BMA	M	4	11/12	0.79	0.13	55,58,62,63	0
4	MAN	G	4	11/12	0.81	0.14	56,67,74,81	0
6	MAN	L	4	11/12	0.82	0.10	51,55,57,63	0
6	MAN	I	4	11/12	0.83	0.10	65,67,74,76	0
6	MAN	L	5	11/12	0.83	0.09	56,62,66,67	0
9	MAN	P	3	11/12	0.83	0.10	42,43,45,46	0
9	MAN	P	5	11/12	0.84	0.11	52,54,55,57	0
7	NAG	J	2	14/15	0.85	0.10	38,41,46,47	0
6	MAN	I	7	11/12	0.87	0.09	52,55,56,59	0
9	MAN	P	7	11/12	0.87	0.10	46,52,56,56	0
6	BMA	I	3	11/12	0.88	0.09	52,55,57,63	0
8	MAN	M	3	11/12	0.89	0.08	45,51,54,56	0
5	NAG	K	2	14/15	0.89	0.10	40,49,59,69	0
2	NAG	E	2	14/15	0.89	0.09	43,46,55,66	0
5	NAG	H	2	14/15	0.90	0.09	50,53,59,67	0
6	NAG	L	2	14/15	0.91	0.08	37,39,41,41	0
6	MAN	O	7	11/12	0.91	0.08	44,45,46,46	0
9	MAN	P	6	11/12	0.91	0.09	44,50,52,54	0
4	NAG	G	2	14/15	0.91	0.09	38,43,52,65	0
6	BMA	L	3	11/12	0.92	0.07	40,43,45,50	0
9	MAN	P	4	11/12	0.92	0.07	39,44,49,51	0
6	NAG	I	2	14/15	0.92	0.09	48,51,56,56	0
6	MAN	L	7	11/12	0.92	0.08	41,43,48,51	0
6	NAG	O	2	14/15	0.92	0.09	40,41,44,44	0
6	NAG	I	1	14/15	0.93	0.08	39,43,45,50	0
3	MAN	F	7	11/12	0.93	0.07	41,43,45,45	0
3	BMA	F	3	11/12	0.93	0.07	42,44,47,54	0

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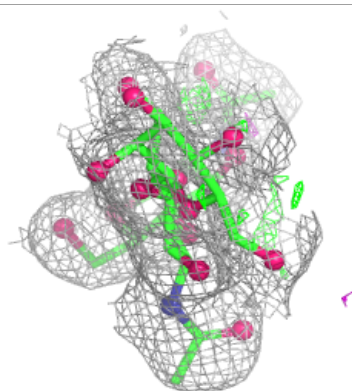
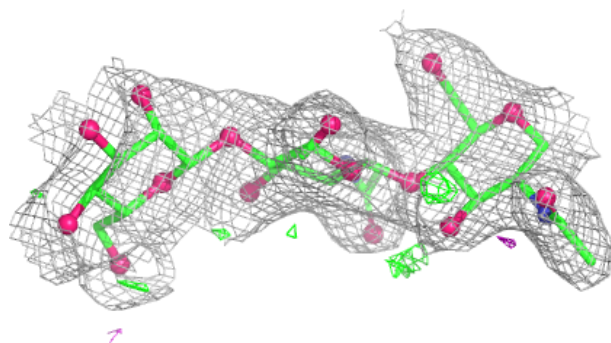
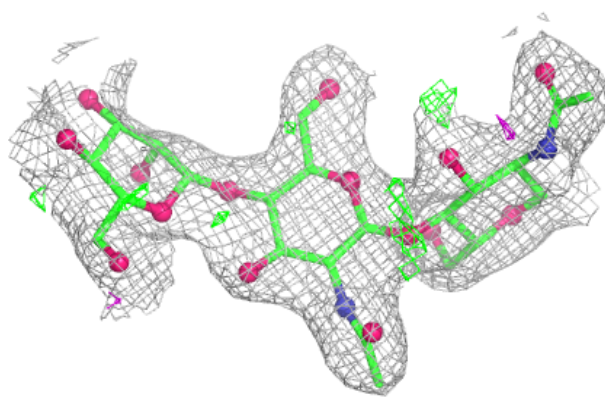
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	N	2	14/15	0.93	0.08	41,46,52,62	0
6	BMA	O	3	11/12	0.93	0.07	40,45,48,57	0
5	NAG	H	1	14/15	0.93	0.09	42,43,47,50	0
9	NAG	P	2	14/15	0.94	0.07	33,35,36,40	0
2	NAG	N	1	14/15	0.94	0.07	27,31,34,41	0
6	NAG	L	1	14/15	0.94	0.07	30,31,35,35	0
4	NAG	G	1	14/15	0.94	0.07	29,32,35,37	0
3	NAG	F	2	14/15	0.94	0.07	35,38,39,41	0
6	NAG	O	1	14/15	0.94	0.07	36,39,41,42	0
8	NAG	M	2	14/15	0.95	0.07	35,37,42,45	0
5	NAG	K	1	14/15	0.95	0.06	32,35,39,43	0
9	NAG	P	1	14/15	0.95	0.06	30,32,33,33	0
8	NAG	M	1	14/15	0.96	0.06	28,29,30,32	0
2	NAG	E	1	14/15	0.96	0.05	31,33,35,40	0
3	NAG	F	1	14/15	0.96	0.06	28,29,31,34	0
7	NAG	J	1	14/15	0.97	0.05	30,33,34,36	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.



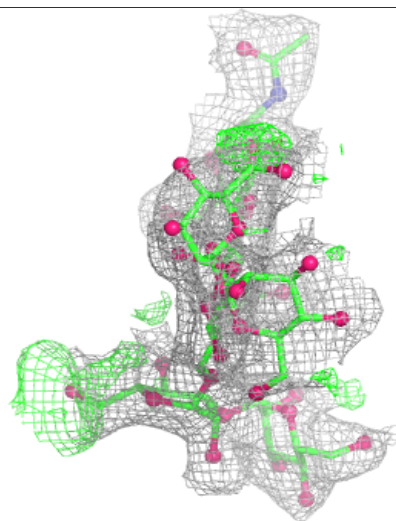
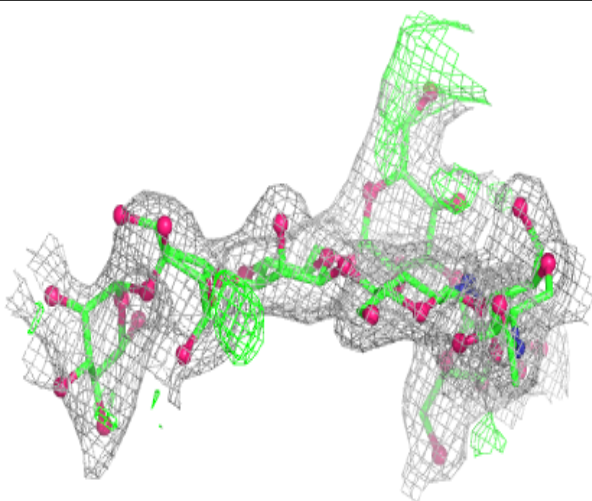
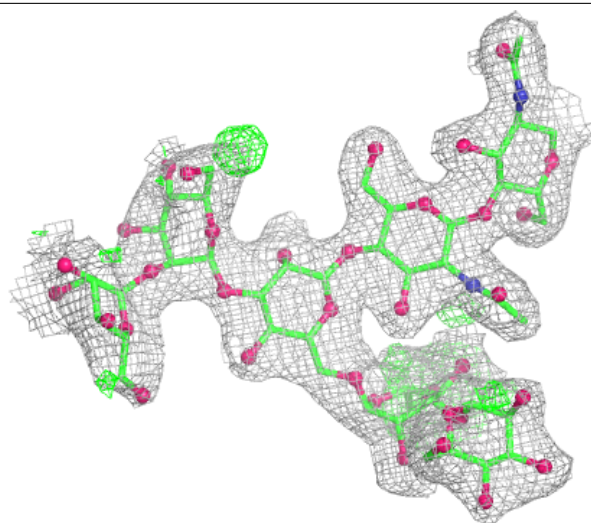
Electron density around Chain N:

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



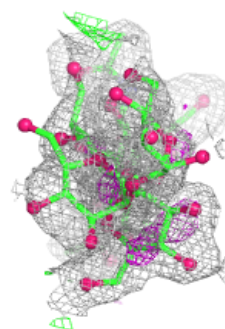
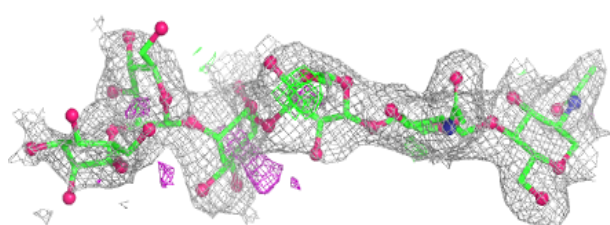
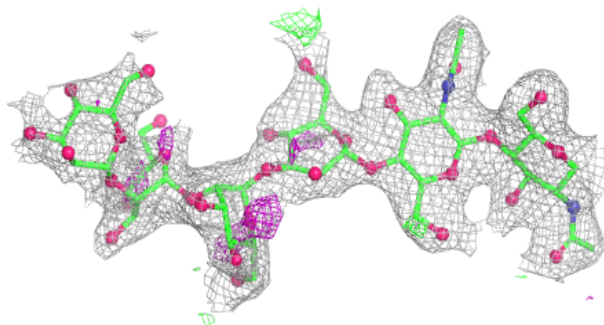
Electron density around Chain F:

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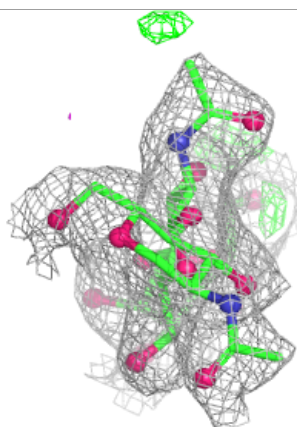
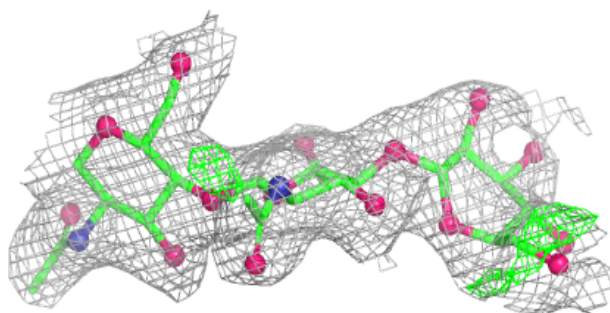
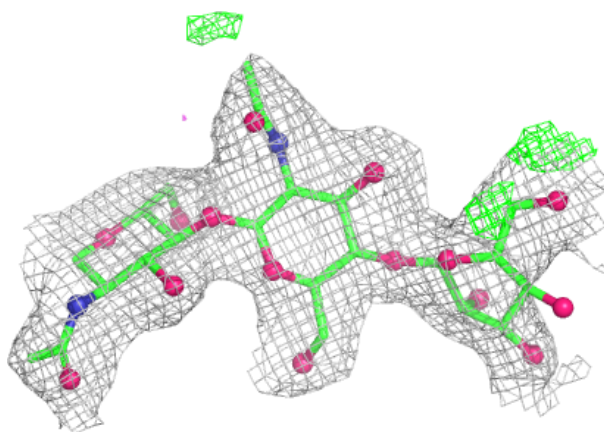


Electron density around Chain G:

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and green (positive)

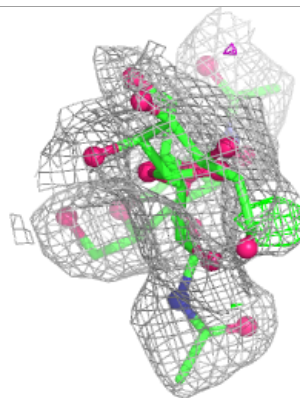
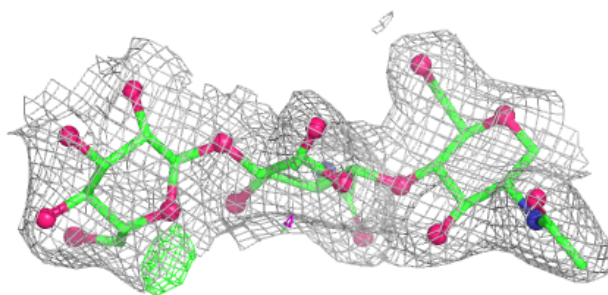
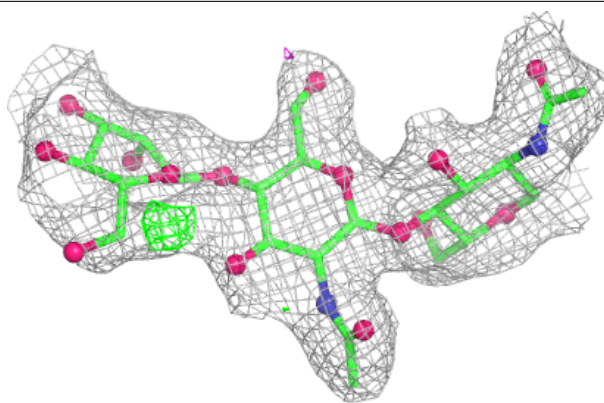
**Electron density around Chain H:**

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and green (positive)



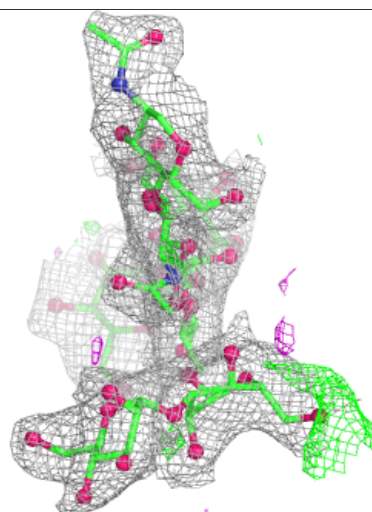
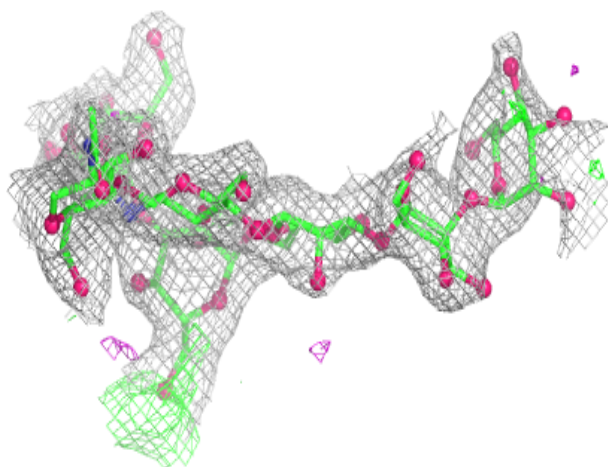
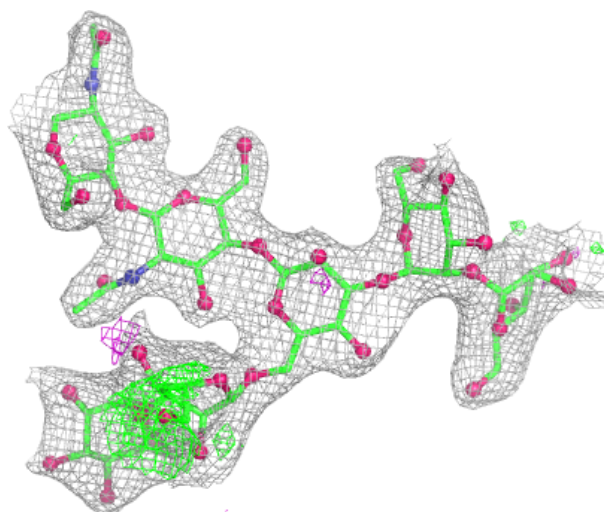
Electron density around Chain K:

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and green (positive)



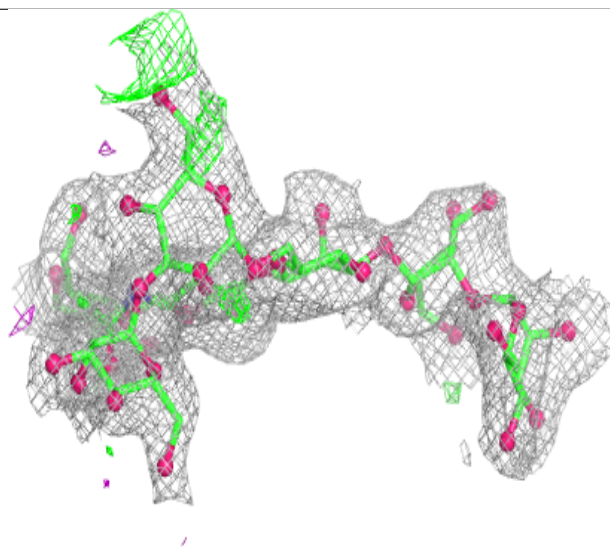
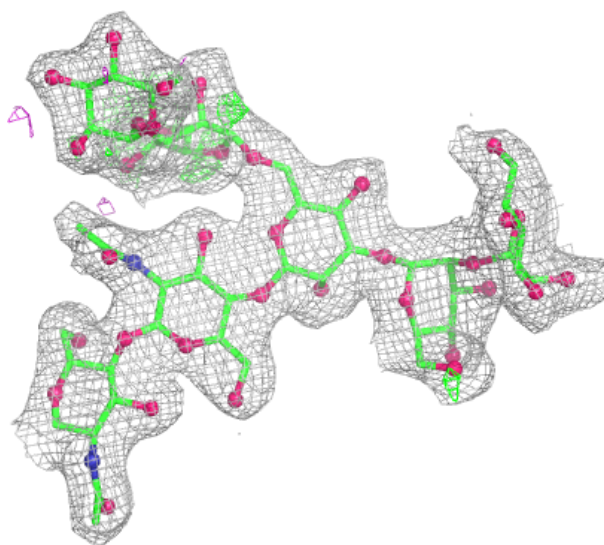
Electron density around Chain I:

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and green (positive)



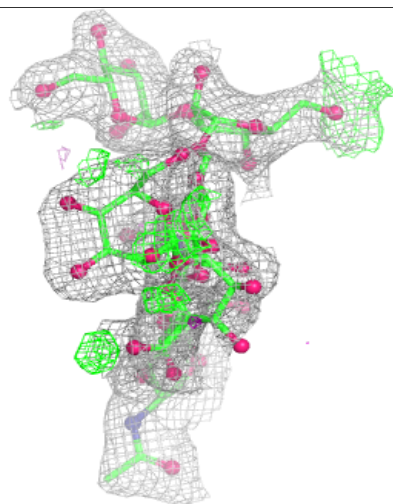
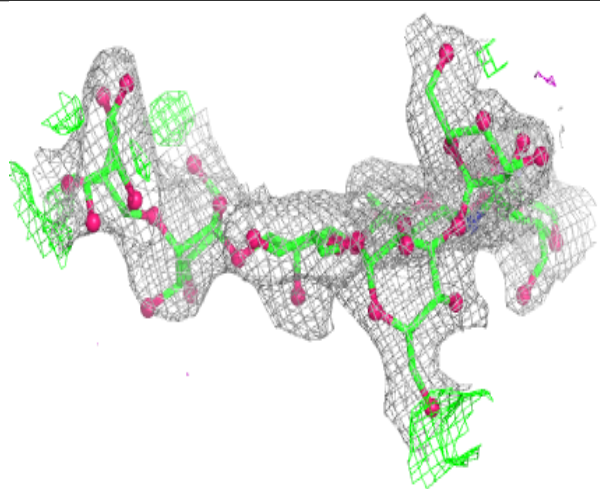
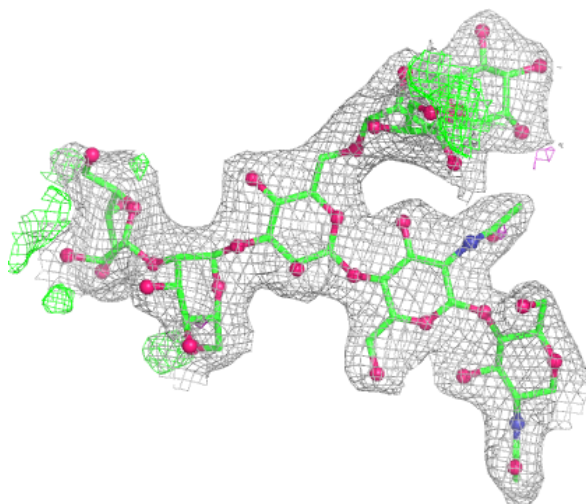
Electron density around Chain L:

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and green (positive)



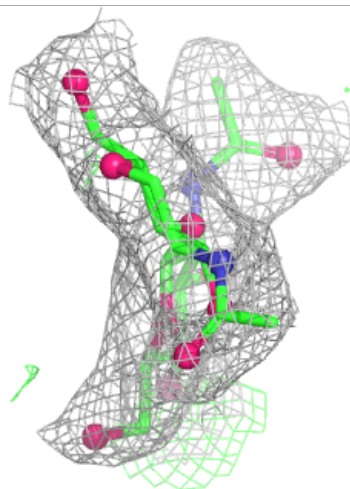
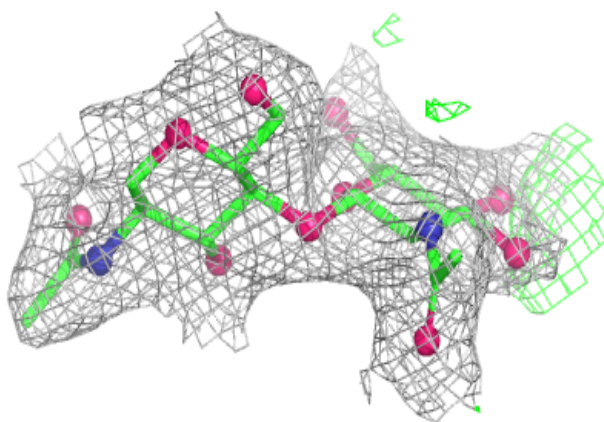
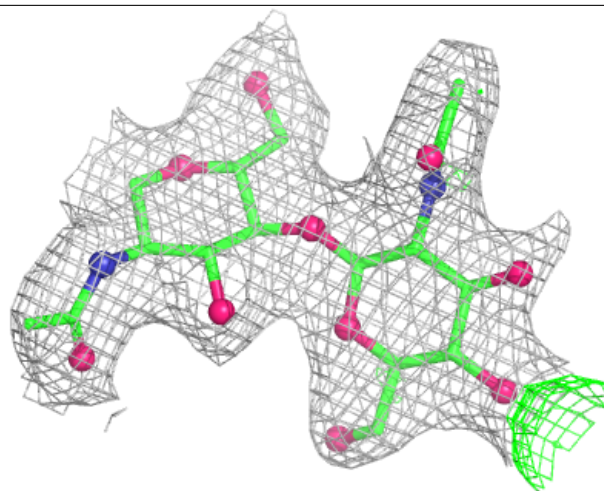
Electron density around Chain O:

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and green (positive)



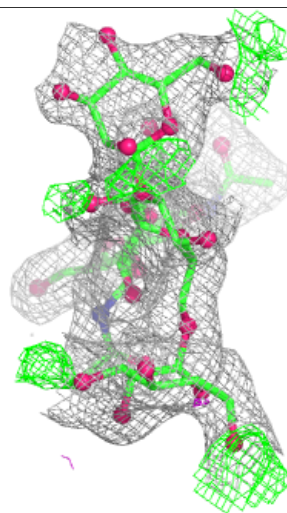
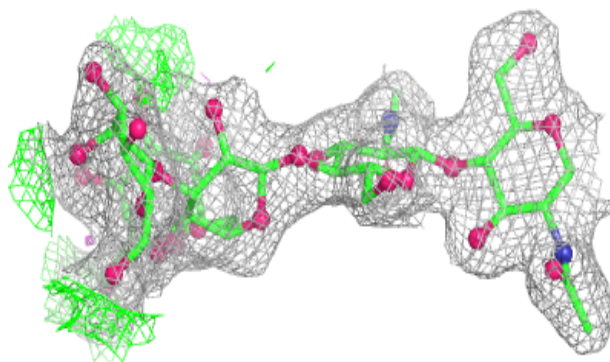
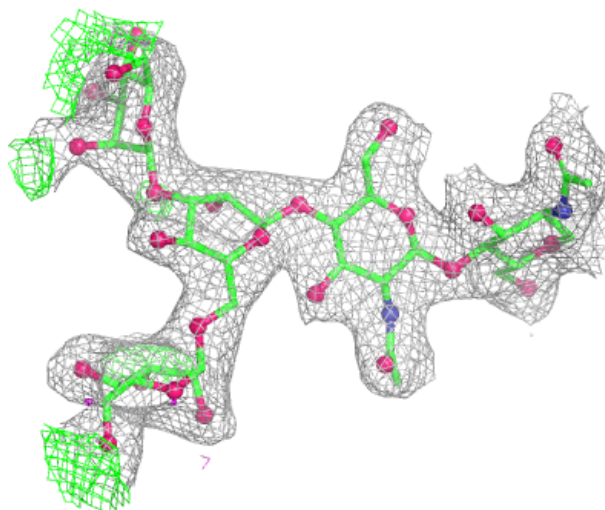
Electron density around Chain J:

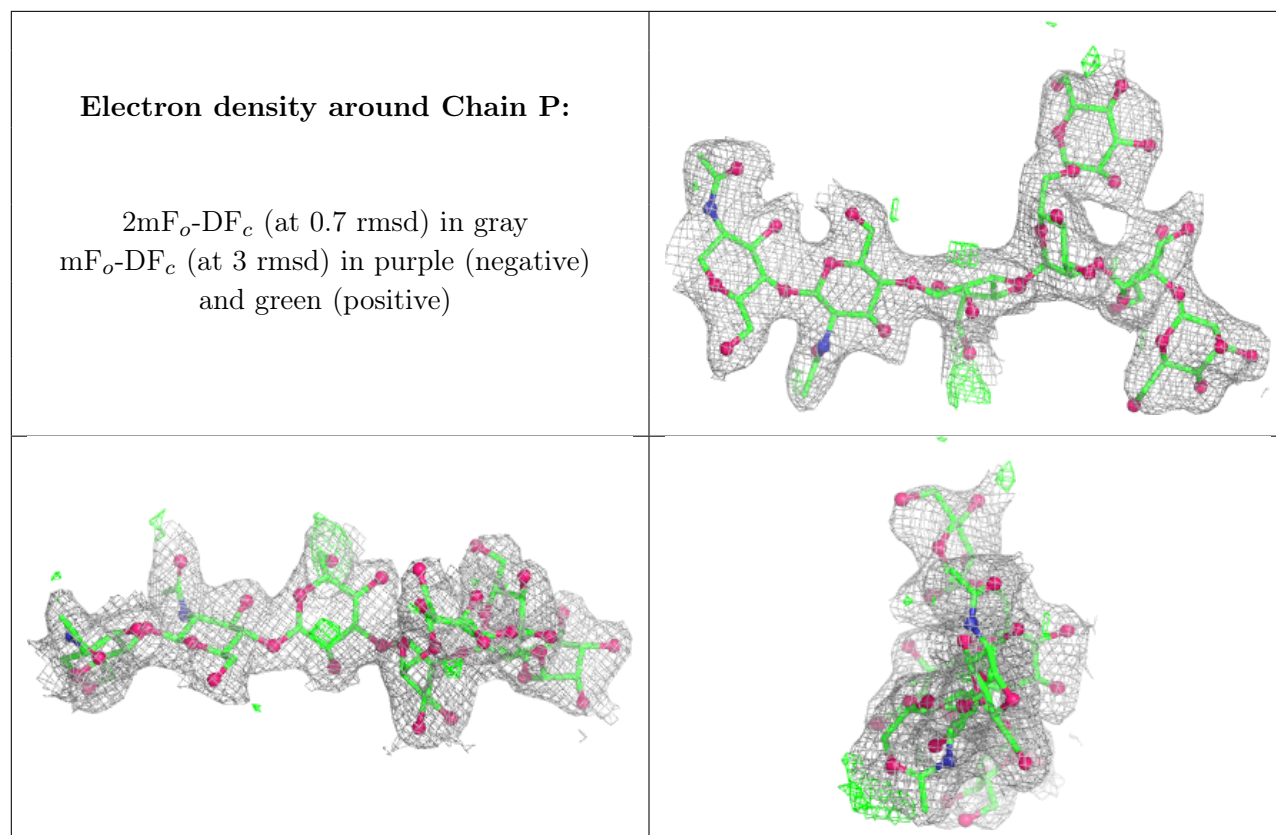
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and green (positive)



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)





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
10	NAG	A	920	14/15	0.65	0.18	61,77,82,85	0
10	NAG	B	916	14/15	0.69	0.15	70,75,79,83	0
10	NAG	B	911	14/15	0.75	0.11	62,67,69,69	0
10	NAG	C	919	14/15	0.77	0.12	58,64,65,66	0
10	NAG	D	921	14/15	0.78	0.14	48,53,54,55	0
10	NAG	A	911	14/15	0.79	0.12	54,60,68,69	0
10	NAG	D	912	13/15	0.81	0.11	46,47,51,52	0
10	NAG	A	912	13/15	0.81	0.10	43,47,50,51	0
10	NAG	C	912	13/15	0.82	0.10	43,46,49,50	0
10	NAG	C	911	14/15	0.82	0.11	46,50,59,60	0
10	NAG	B	912	13/15	0.85	0.10	47,57,62,67	0
11	TRS	A	921	8/8	0.85	0.14	37,41,47,49	0
11	TRS	C	920	8/8	0.85	0.14	40,43,45,45	0
11	TRS	D	922	8/8	0.86	0.13	35,40,41,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	NAG	D	911	14/15	0.87	0.10	47,54,69,69	0
11	TRS	B	917	8/8	0.87	0.12	38,42,44,44	0
10	NAG	D	920	14/15	0.91	0.07	34,35,38,39	0
10	NAG	A	919	14/15	0.94	0.06	32,36,39,41	0
10	NAG	B	915	14/15	0.94	0.07	35,42,43,43	0
10	NAG	C	918	14/15	0.95	0.06	34,38,39,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.