



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2024 – 01:10 PM JST

PDB ID : 5AZ5
Title : Crystal structure of human TLR8 in complex with MB-343
Authors : Tanji, H.; Ohto, U.; Shimizu, T.
Deposited on : 2015-09-27
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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

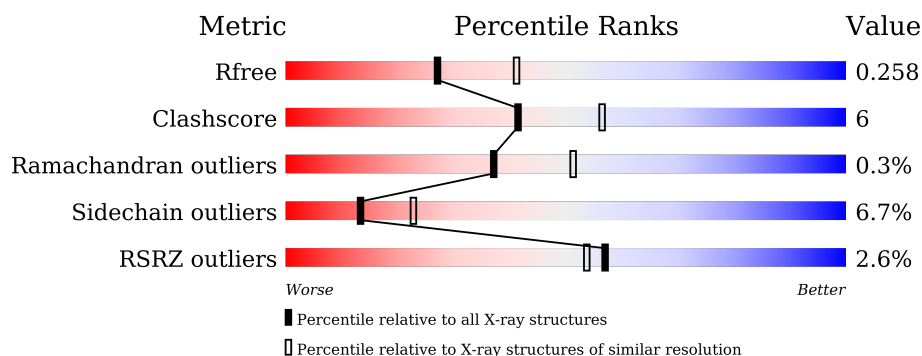
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



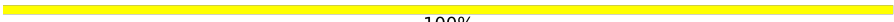
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	811	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> % 77% 13% • 8% </div> </div>
1	B	811	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> % 77% 14% • 8% </div> </div>
1	C	811	<div> <div style="width: 4%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> 4% 75% 16% • 8% </div> </div>
1	D	811	<div> <div style="width: 3%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> 3% 73% 16% • 8% </div> </div>
2	E	4	<div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: yellow; position: relative;"> 100% </div> </div>
2	G	4	<div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: yellow; position: relative;"> 100% </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	4	 100%
3	F	2	 100%
3	I	2	 100%
3	L	2	 100%
3	O	2	 100%
4	J	3	 100%
4	K	3	 67%  33%
4	N	3	 67%  33%
4	P	3	 100%
5	M	4	 100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 25117 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 Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	748	Total	C	N	O	S	0	0	0
			6029	3857	1023	1130	19			
1	B	749	Total	C	N	O	S	0	0	0
			6033	3859	1024	1131	19			
1	C	748	Total	C	N	O	S	0	0	0
			6024	3854	1023	1128	19			
1	D	746	Total	C	N	O	S	0	0	0
			6008	3844	1019	1126	19			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP Q9NR97
A	24	SER	-	expression tag	UNP Q9NR97
A	25	PRO	-	expression tag	UNP Q9NR97
A	26	TRP	-	expression tag	UNP Q9NR97
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97
B	23	ARG	-	expression tag	UNP Q9NR97
B	24	SER	-	expression tag	UNP Q9NR97
B	25	PRO	-	expression tag	UNP Q9NR97
B	26	TRP	-	expression tag	UNP Q9NR97
B	828	GLU	-	expression tag	UNP Q9NR97
B	829	PHE	-	expression tag	UNP Q9NR97
B	830	LEU	-	expression tag	UNP Q9NR97
B	831	VAL	-	expression tag	UNP Q9NR97
B	832	PRO	-	expression tag	UNP Q9NR97
B	833	ARG	-	expression tag	UNP Q9NR97
C	23	ARG	-	expression tag	UNP Q9NR97

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Chain	Residue	Modelled	Actual	Comment	Reference
C	24	SER	-	expression tag	UNP Q9NR97
C	25	PRO	-	expression tag	UNP Q9NR97
C	26	TRP	-	expression tag	UNP Q9NR97
C	828	GLU	-	expression tag	UNP Q9NR97
C	829	PHE	-	expression tag	UNP Q9NR97
C	830	LEU	-	expression tag	UNP Q9NR97
C	831	VAL	-	expression tag	UNP Q9NR97
C	832	PRO	-	expression tag	UNP Q9NR97
C	833	ARG	-	expression tag	UNP Q9NR97
D	23	ARG	-	expression tag	UNP Q9NR97
D	24	SER	-	expression tag	UNP Q9NR97
D	25	PRO	-	expression tag	UNP Q9NR97
D	26	TRP	-	expression tag	UNP Q9NR97
D	828	GLU	-	expression tag	UNP Q9NR97
D	829	PHE	-	expression tag	UNP Q9NR97
D	830	LEU	-	expression tag	UNP Q9NR97
D	831	VAL	-	expression tag	UNP Q9NR97
D	832	PRO	-	expression tag	UNP Q9NR97
D	833	ARG	-	expression tag	UNP Q9NR97

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



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

- Molecule 3 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
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	O	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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.



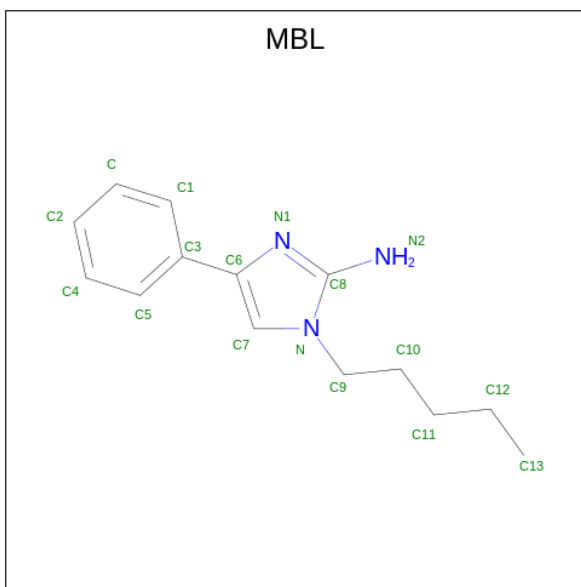
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	N	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	P	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 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.



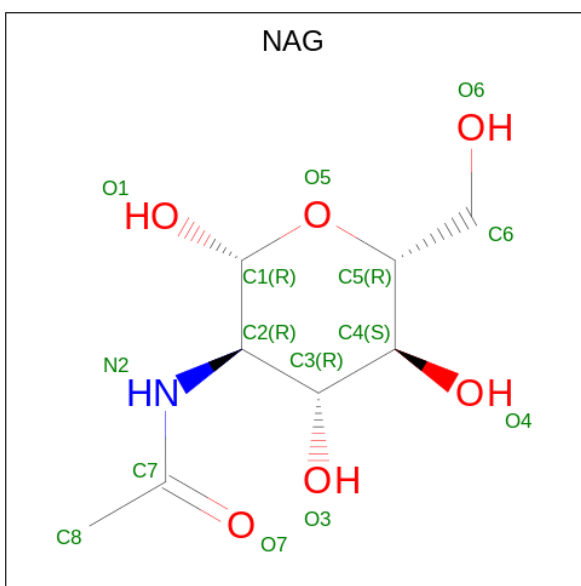
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	M	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is 1-pentyl-4-phenyl-imidazol-2-amine (three-letter code: MBL) (formula: C₁₄H₁₉N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			17	14	3		
6	A	1	Total	C	N	0	0
			17	14	3		
6	C	1	Total	C	N	0	0
			17	14	3		
6	C	1	Total	C	N	0	0
			17	14	3		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

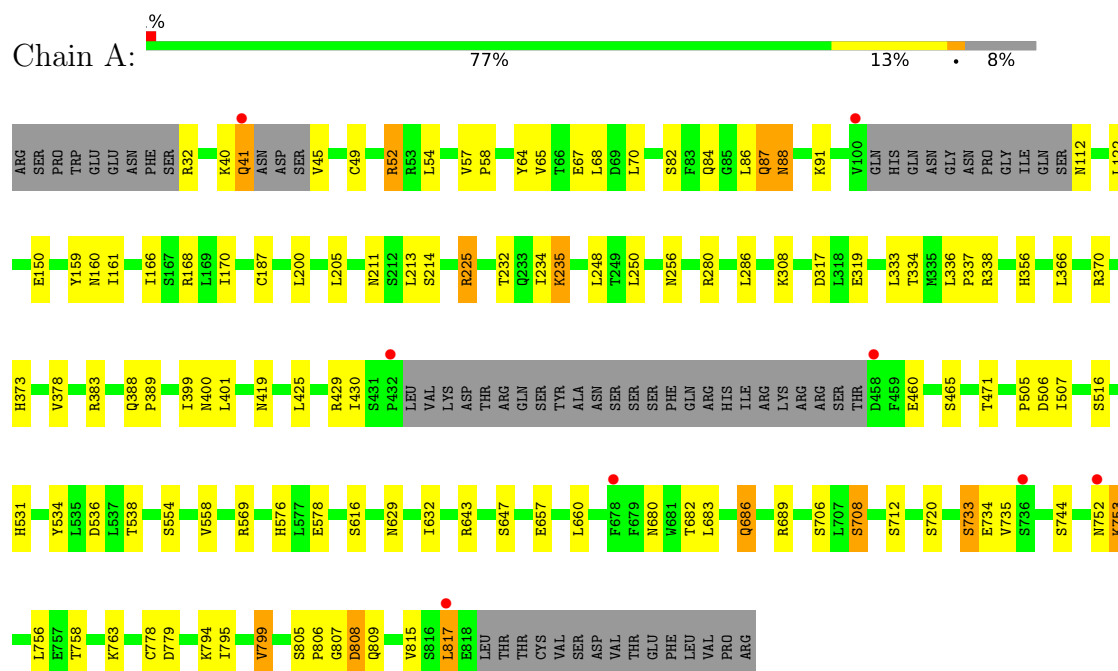
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	98	Total	O	0	0
			98	98		
8	B	83	Total	O	0	0
			83	83		
8	C	57	Total	O	0	0
			57	57		
8	D	53	Total	O	0	0
			53	53		

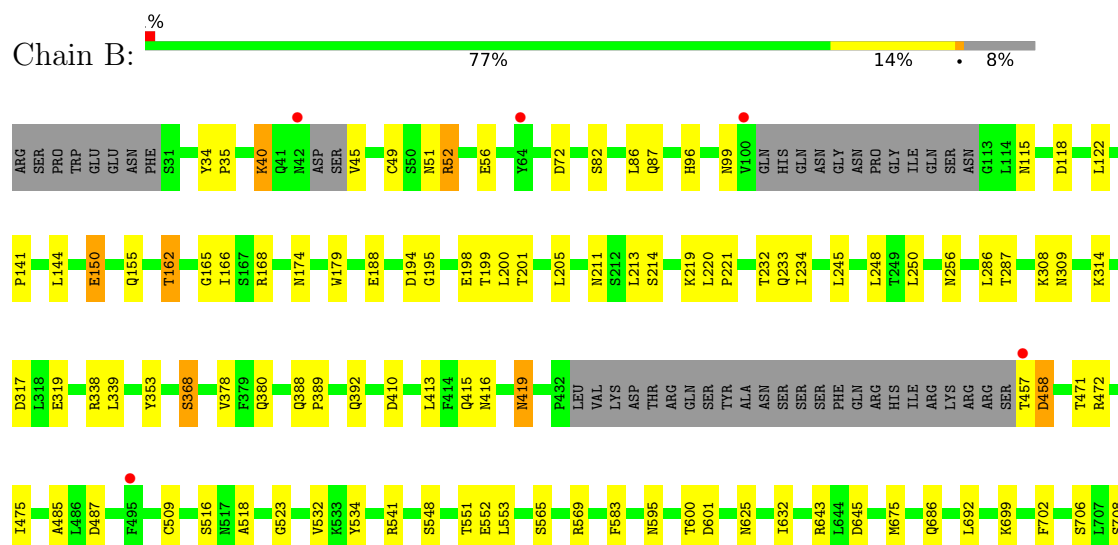
3 Residue-property plots [i](#)

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: Toll-like receptor 8

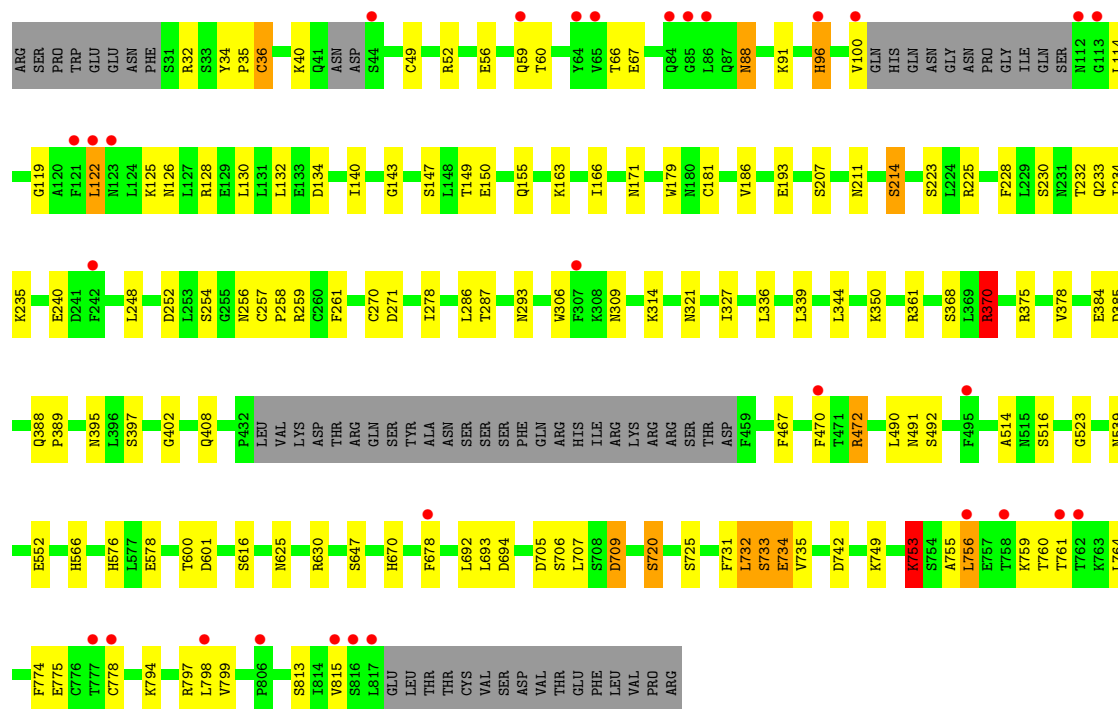
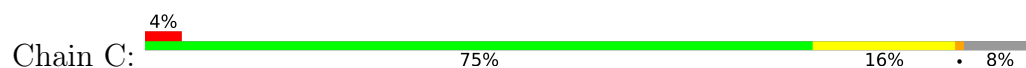


• Molecule 1: Toll-like receptor 8

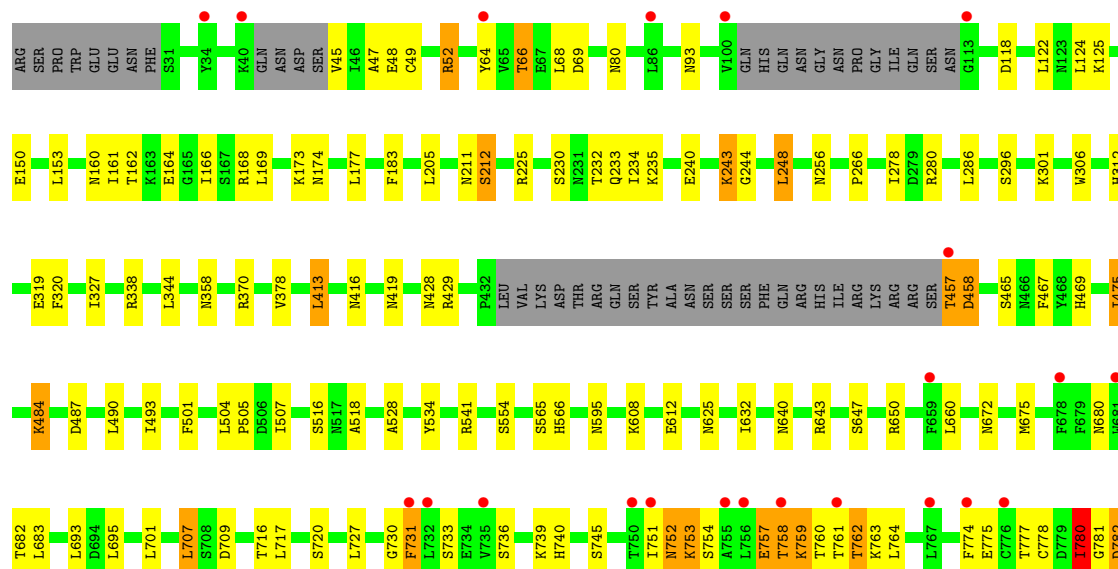
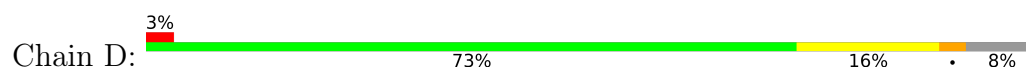




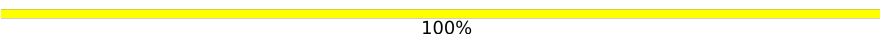
• Molecule 1: Toll-like receptor 8



• Molecule 1: Toll-like receptor 8

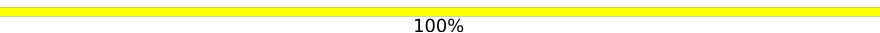


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%

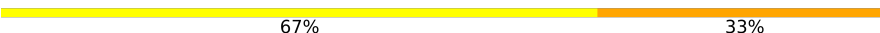
MAG1
MAG2

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

Chain J:  100%

MAG1
MAG2
BMA3

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

Chain K:  67% 33%

MAG1
MAG2
BMA3

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

Chain N:  67% 33%

MAG1
MAG2
BMA3

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

Chain P:  100%

MAG1
MAG2
BMA3

- Molecule 5: 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 M:  100%

MAG1
MAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.63Å 141.12Å 170.97Å 90.00° 90.32° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.5 (50.00-2.40) 95.8 (50.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.196 , 0.259 0.200 , 0.258	Depositor DCC
R_{free} test set	7732 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	53.3	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 24.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25117	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: NAG, MAN, MBL, BMA

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	0.64	0/6153	0.75	2/8343 (0.0%)
1	B	0.58	0/6157	0.73	2/8349 (0.0%)
1	C	0.57	0/6148	0.72	2/8336 (0.0%)
1	D	0.57	0/6132	0.73	4/8315 (0.0%)
All	All	0.59	0/24590	0.73	10/33343 (0.0%)

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	1
1	D	0	2
All	All	0	3

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	D	338	ARG	NE-CZ-NH1	-5.83	117.38	120.30
1	B	645	ASP	CB-CG-OD1	5.76	123.48	118.30
1	C	630	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	370	ARG	NE-CZ-NH1	5.69	123.15	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	753	LYS	Peptide
1	D	762	THR	Peptide
1	D	780	ILE	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	6029	0	6016	53	0
1	B	6033	0	6021	55	0
1	C	6024	0	6015	81	0
1	D	6008	0	5997	126	0
2	E	50	0	43	0	0
2	G	50	0	43	0	0
2	H	50	0	43	0	0
3	F	28	0	25	0	0
3	I	28	0	25	0	0
3	L	28	0	25	0	0
3	O	28	0	25	0	0
4	J	39	0	34	0	0
4	K	39	0	34	1	0
4	N	39	0	34	2	0
4	P	39	0	34	0	0
5	M	50	0	43	0	0
6	A	34	0	0	0	0
6	C	34	0	0	0	0
7	A	42	0	39	3	0
7	B	56	0	52	0	0
7	C	56	0	52	0	0
7	D	42	0	39	2	0
8	A	98	0	0	2	0
8	B	83	0	0	2	0
8	C	57	0	0	2	0
8	D	53	0	0	2	0
All	All	25117	0	24639	313	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 6.

The worst 5 of 313 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:D:243:LYS:HB3	1:D:244:GLY:HA3	1.20	1.17
1:D:759:LYS:HD2	1:D:760:THR:H	1.09	1.09
1:D:758:THR:HB	1:D:760:THR:HG23	1.32	1.08
1:D:759:LYS:HD2	1:D:760:THR:N	1.79	0.97
1:D:751:ILE:HD12	1:D:783:PHE:CD1	2.01	0.96

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	740/811 (91%)	692 (94%)	47 (6%)	1 (0%)	48	65
1	B	741/811 (91%)	694 (94%)	45 (6%)	2 (0%)	37	51
1	C	740/811 (91%)	680 (92%)	56 (8%)	4 (0%)	25	38
1	D	738/811 (91%)	677 (92%)	58 (8%)	3 (0%)	30	44
All	All	2959/3244 (91%)	2743 (93%)	206 (7%)	10 (0%)	37	51

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	806	PRO
1	B	458	ASP
1	D	709	ASP
1	C	378	VAL
1	B	378	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	695/755 (92%)	646 (93%)	49 (7%)	12	20
1	B	696/755 (92%)	654 (94%)	42 (6%)	16	27
1	C	695/755 (92%)	652 (94%)	43 (6%)	15	26
1	D	693/755 (92%)	642 (93%)	51 (7%)	11	19
All	All	2779/3020 (92%)	2594 (93%)	185 (7%)	13	23

5 of 185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	470	PHE
1	D	173	LYS
1	C	705	ASP
1	C	775	GLU
1	D	286	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	123	ASN
1	D	233	GLN
1	D	358	ASN
1	B	55	GLN
1	B	51	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

42 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
7	NAG	C	913	1	14,14,15	0.93	1 (7%)	17,19,21	1.30	4 (23%)
4	NAG	N	2	4	14,14,15	0.61	0	17,19,21	1.42	2 (11%)
4	NAG	P	1	1,4	14,14,15	0.65	0	17,19,21	1.43	1 (5%)
7	NAG	A	914	1	14,14,15	0.72	0	17,19,21	2.19	6 (35%)
4	NAG	P	2	4	14,14,15	0.75	0	17,19,21	1.27	2 (11%)
2	NAG	G	2	2	14,14,15	1.07	1 (7%)	17,19,21	1.23	2 (11%)
3	NAG	F	2	3	14,14,15	0.85	1 (7%)	17,19,21	1.77	4 (23%)
7	NAG	B	1010	1	14,14,15	0.78	1 (7%)	17,19,21	1.75	3 (17%)
4	NAG	K	1	1,4	14,14,15	0.74	0	17,19,21	1.46	4 (23%)
4	NAG	K	2	4	14,14,15	0.67	0	17,19,21	2.03	9 (52%)
4	NAG	N	1	1,4	14,14,15	0.96	1 (7%)	17,19,21	1.49	2 (11%)
7	NAG	C	914	1	14,14,15	0.86	1 (7%)	17,19,21	0.98	2 (11%)
2	MAN	E	4	2	11,11,12	0.81	0	15,15,17	1.31	3 (20%)
4	NAG	J	2	4	14,14,15	1.14	2 (14%)	17,19,21	1.75	5 (29%)
7	NAG	D	1006	1	14,14,15	0.53	0	17,19,21	1.60	3 (17%)
7	NAG	B	1013	1	14,14,15	0.72	0	17,19,21	1.85	4 (23%)
5	NAG	M	1	5,1	14,14,15	0.54	0	17,19,21	1.23	3 (17%)
5	MAN	M	4	5	11,11,12	0.98	1 (9%)	15,15,17	1.46	3 (20%)
3	NAG	O	2	3	14,14,15	0.74	0	17,19,21	1.51	4 (23%)
2	NAG	G	1	2,1	14,14,15	0.63	0	17,19,21	1.50	4 (23%)
7	NAG	B	1012	1	14,14,15	0.90	1 (7%)	17,19,21	1.40	2 (11%)
3	NAG	I	2	3	14,14,15	0.89	1 (7%)	17,19,21	1.84	5 (29%)
7	NAG	C	907	1	14,14,15	0.87	0	17,19,21	1.48	2 (11%)
7	NAG	C	912	1	14,14,15	0.71	0	17,19,21	1.69	2 (11%)
2	NAG	E	1	2,1	14,14,15	0.89	0	17,19,21	1.35	2 (11%)
3	NAG	O	1	3,1	14,14,15	0.73	1 (7%)	17,19,21	1.58	2 (11%)
3	NAG	I	1	3,1	14,14,15	0.91	0	17,19,21	1.59	3 (17%)
2	MAN	H	4	2	11,11,12	0.87	0	15,15,17	1.90	7 (46%)
3	NAG	L	1	3,1	14,14,15	0.70	0	17,19,21	1.48	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	M	2	5	14,14,15	0.95	1 (7%)	17,19,21	0.96	1 (5%)
7	NAG	B	1011	1	14,14,15	0.67	0	17,19,21	1.05	0
7	NAG	D	1010	1	14,14,15	0.75	0	17,19,21	1.20	3 (17%)
3	NAG	F	1	3,1	14,14,15	0.64	0	17,19,21	1.51	4 (23%)
2	NAG	E	2	2	14,14,15	0.84	0	17,19,21	1.66	7 (41%)
2	MAN	G	4	2	11,11,12	0.55	0	15,15,17	1.42	3 (20%)
7	NAG	A	913	1	14,14,15	0.73	0	17,19,21	1.51	3 (17%)
7	NAG	D	1011	1	14,14,15	0.67	0	17,19,21	1.87	5 (29%)
2	NAG	H	1	2,1	14,14,15	0.78	0	17,19,21	1.79	4 (23%)
2	NAG	H	2	2	14,14,15	0.53	0	17,19,21	1.31	3 (17%)
3	NAG	L	2	3	14,14,15	0.60	0	17,19,21	1.41	4 (23%)
7	NAG	A	912	1	14,14,15	0.59	0	17,19,21	2.41	4 (23%)
4	NAG	J	1	1,4	14,14,15	0.90	0	17,19,21	1.24	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	913	1	-	3/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
7	NAG	A	914	1	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
7	NAG	B	1010	1	-	0/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
7	NAG	C	914	1	-	2/6/23/26	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
7	NAG	D	1006	1	-	4/6/23/26	0/1/1/1
7	NAG	B	1013	1	-	4/6/23/26	0/1/1/1
5	NAG	M	1	5,1	-	0/6/23/26	0/1/1/1
5	MAN	M	4	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
7	NAG	B	1012	1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
7	NAG	C	907	1	-	4/6/23/26	0/1/1/1
7	NAG	C	912	1	-	0/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
2	MAN	H	4	2	-	0/2/19/22	0/1/1/1
3	NAG	L	1	3,1	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
7	NAG	B	1011	1	-	0/6/23/26	0/1/1/1
7	NAG	D	1010	1	-	0/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	MAN	G	4	2	-	0/2/19/22	0/1/1/1
7	NAG	A	913	1	-	1/6/23/26	0/1/1/1
7	NAG	D	1011	1	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
7	NAG	A	912	1	-	0/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2	NAG	O5-C1	-3.20	1.38	1.43
2	G	2	NAG	O5-C1	-2.97	1.39	1.43
4	N	1	NAG	O5-C1	-2.72	1.39	1.43
5	M	2	NAG	O5-C1	-2.71	1.39	1.43
7	B	1012	NAG	O5-C1	-2.60	1.39	1.43

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	912	NAG	O5-C1-C2	5.74	120.35	111.29
7	C	912	NAG	C1-O5-C5	5.54	119.70	112.19
7	A	914	NAG	O5-C1-C2	-5.38	102.80	111.29
7	A	912	NAG	C1-O5-C5	5.08	119.07	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1010	NAG	C1-O5-C5	4.79	118.68	112.19

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1013	NAG	O5-C5-C6-O6
5	M	4	MAN	O5-C5-C6-O6
7	C	907	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
7	B	1013	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	914	NAG	1	0
4	K	1	NAG	1	0
4	N	1	NAG	2	0
7	D	1010	NAG	1	0
7	A	913	NAG	2	0
7	D	1011	NAG	1	0

5.5 Carbohydrates [i](#)

36 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	0.89	0	17,19,21	1.35	2 (11%)
2	NAG	E	2	2	14,14,15	0.84	0	17,19,21	1.66	7 (41%)
2	BMA	E	3	2	11,11,12	0.78	0	15,15,17	1.92	5 (33%)
2	MAN	E	4	2	11,11,12	0.81	0	15,15,17	1.31	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	1	3,1	14,14,15	0.64	0	17,19,21	1.51	4 (23%)
3	NAG	F	2	3	14,14,15	0.85	1 (7%)	17,19,21	1.77	4 (23%)
2	NAG	G	1	2,1	14,14,15	0.63	0	17,19,21	1.50	4 (23%)
2	NAG	G	2	2	14,14,15	1.07	1 (7%)	17,19,21	1.23	2 (11%)
2	BMA	G	3	2	11,11,12	0.58	0	15,15,17	1.69	4 (26%)
2	MAN	G	4	2	11,11,12	0.55	0	15,15,17	1.42	3 (20%)
2	NAG	H	1	2,1	14,14,15	0.78	0	17,19,21	1.79	4 (23%)
2	NAG	H	2	2	14,14,15	0.53	0	17,19,21	1.31	3 (17%)
2	BMA	H	3	2	11,11,12	0.69	0	15,15,17	1.84	4 (26%)
2	MAN	H	4	2	11,11,12	0.87	0	15,15,17	1.90	7 (46%)
3	NAG	I	1	3,1	14,14,15	0.91	0	17,19,21	1.59	3 (17%)
3	NAG	I	2	3	14,14,15	0.89	1 (7%)	17,19,21	1.84	5 (29%)
4	NAG	J	1	1,4	14,14,15	0.90	0	17,19,21	1.24	2 (11%)
4	NAG	J	2	4	14,14,15	1.14	2 (14%)	17,19,21	1.75	5 (29%)
4	BMA	J	3	4	11,11,12	0.58	0	15,15,17	1.75	4 (26%)
4	NAG	K	1	1,4	14,14,15	0.74	0	17,19,21	1.46	4 (23%)
4	NAG	K	2	4	14,14,15	0.67	0	17,19,21	2.03	9 (52%)
4	BMA	K	3	4	11,11,12	0.74	0	15,15,17	1.46	3 (20%)
3	NAG	L	1	3,1	14,14,15	0.70	0	17,19,21	1.48	2 (11%)
3	NAG	L	2	3	14,14,15	0.60	0	17,19,21	1.41	4 (23%)
5	NAG	M	1	5,1	14,14,15	0.54	0	17,19,21	1.23	3 (17%)
5	NAG	M	2	5	14,14,15	0.95	1 (7%)	17,19,21	0.96	1 (5%)
5	BMA	M	3	5	11,11,12	0.70	0	15,15,17	1.61	4 (26%)
5	MAN	M	4	5	11,11,12	0.98	1 (9%)	15,15,17	1.46	3 (20%)
4	NAG	N	1	1,4	14,14,15	0.96	1 (7%)	17,19,21	1.49	2 (11%)
4	NAG	N	2	4	14,14,15	0.61	0	17,19,21	1.42	2 (11%)
4	BMA	N	3	4	11,11,12	1.21	1 (9%)	15,15,17	1.96	5 (33%)
3	NAG	O	1	3,1	14,14,15	0.73	1 (7%)	17,19,21	1.58	2 (11%)
3	NAG	O	2	3	14,14,15	0.74	0	17,19,21	1.51	4 (23%)
4	NAG	P	1	1,4	14,14,15	0.65	0	17,19,21	1.43	1 (5%)
4	NAG	P	2	4	14,14,15	0.75	0	17,19,21	1.27	2 (11%)
4	BMA	P	3	4	11,11,12	0.59	0	15,15,17	1.52	2 (13%)

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

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2	NAG	O5-C1	-3.20	1.38	1.43
2	G	2	NAG	O5-C1	-2.97	1.39	1.43
4	N	1	NAG	O5-C1	-2.72	1.39	1.43
5	M	2	NAG	O5-C1	-2.71	1.39	1.43
4	N	3	BMA	O3-C3	2.59	1.49	1.43

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	3	BMA	C1-C2-C3	5.07	115.90	109.67
4	P	1	NAG	C1-O5-C5	4.73	118.60	112.19
4	N	3	BMA	C1-C2-C3	4.57	115.28	109.67
4	J	2	NAG	O5-C1-C2	-4.54	104.12	111.29
4	J	3	BMA	C1-O5-C5	4.46	118.24	112.19

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	3	BMA	C4-C5-C6-O6
5	M	4	MAN	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
5	M	4	MAN	C4-C5-C6-O6

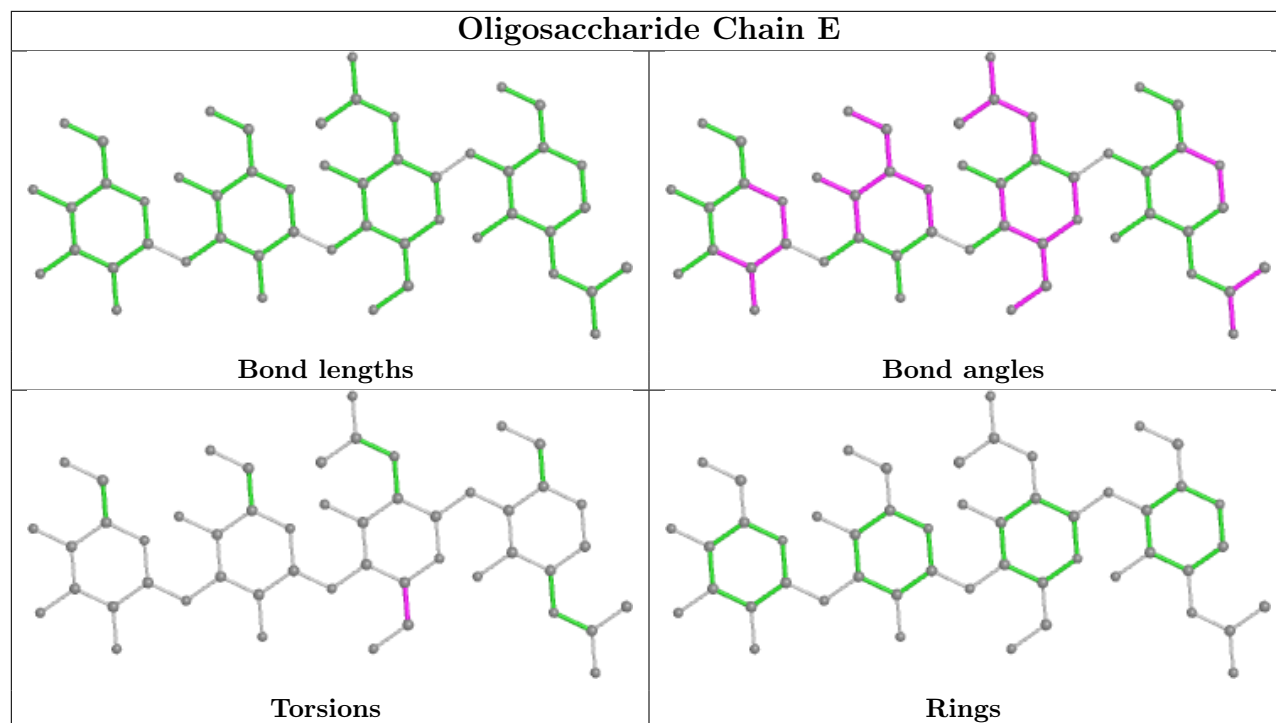
There are no ring outliers.

2 monomers are involved in 3 short contacts:

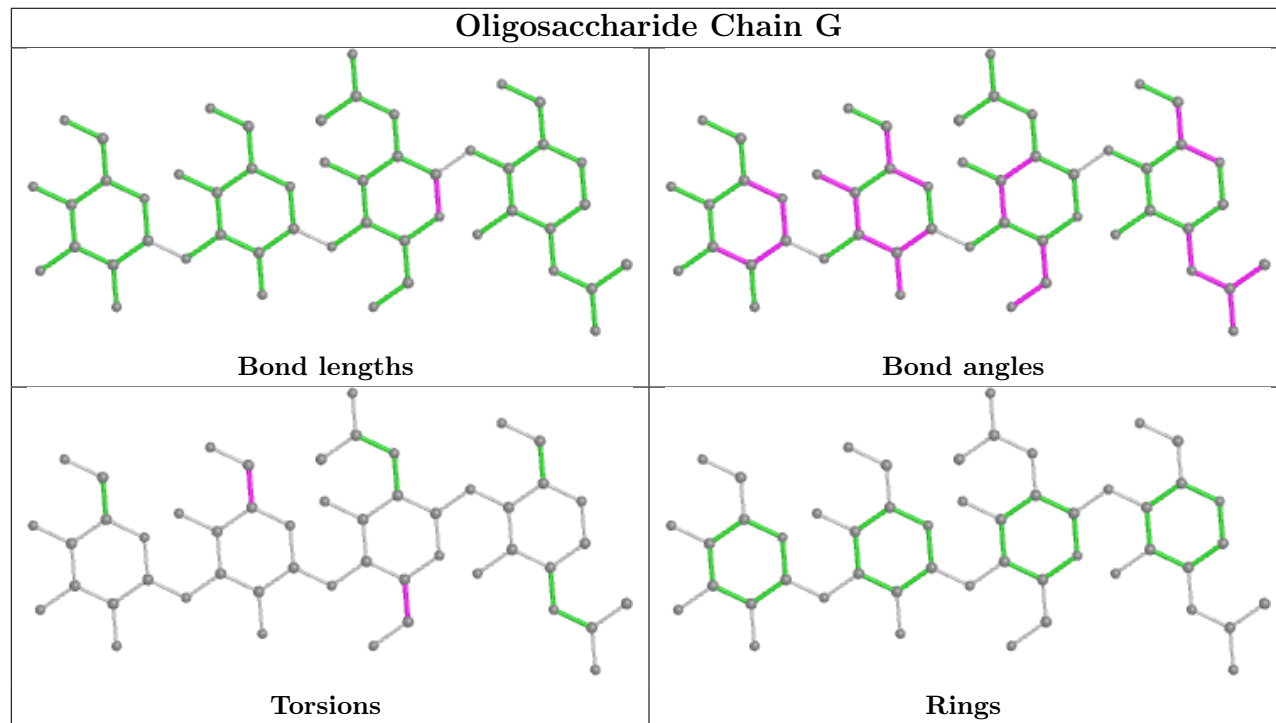
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	NAG	1	0
4	N	1	NAG	2	0

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

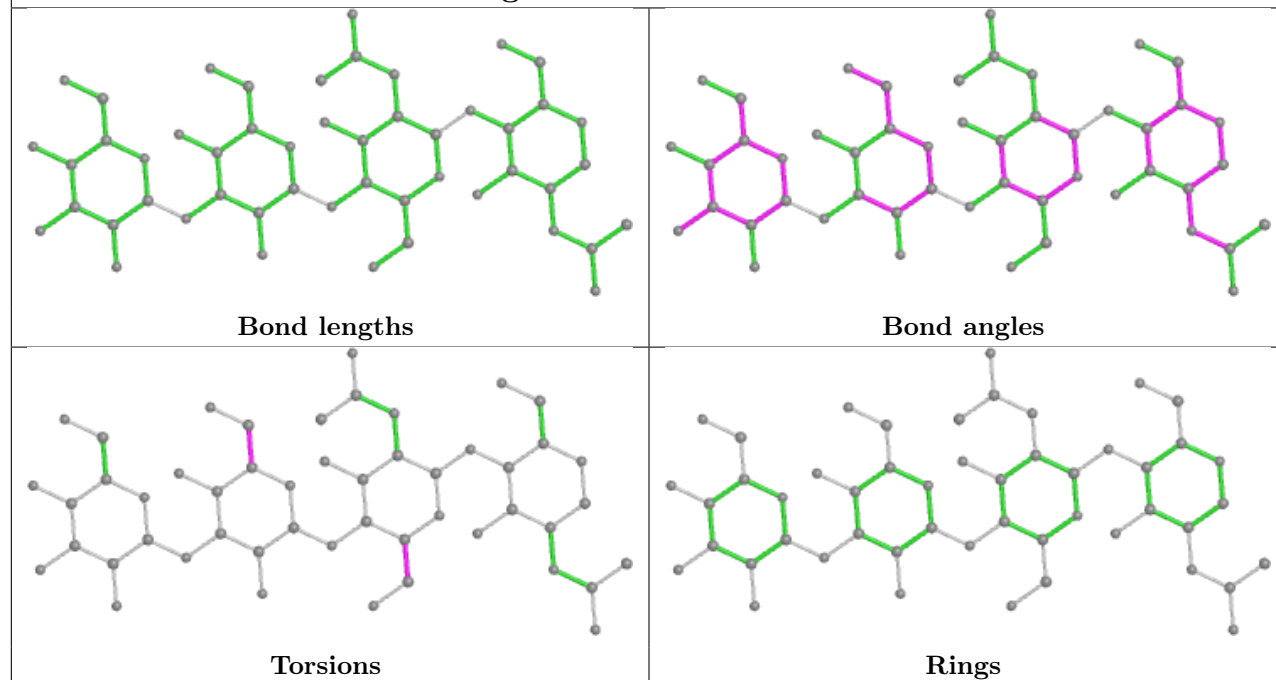
Oligosaccharide Chain E



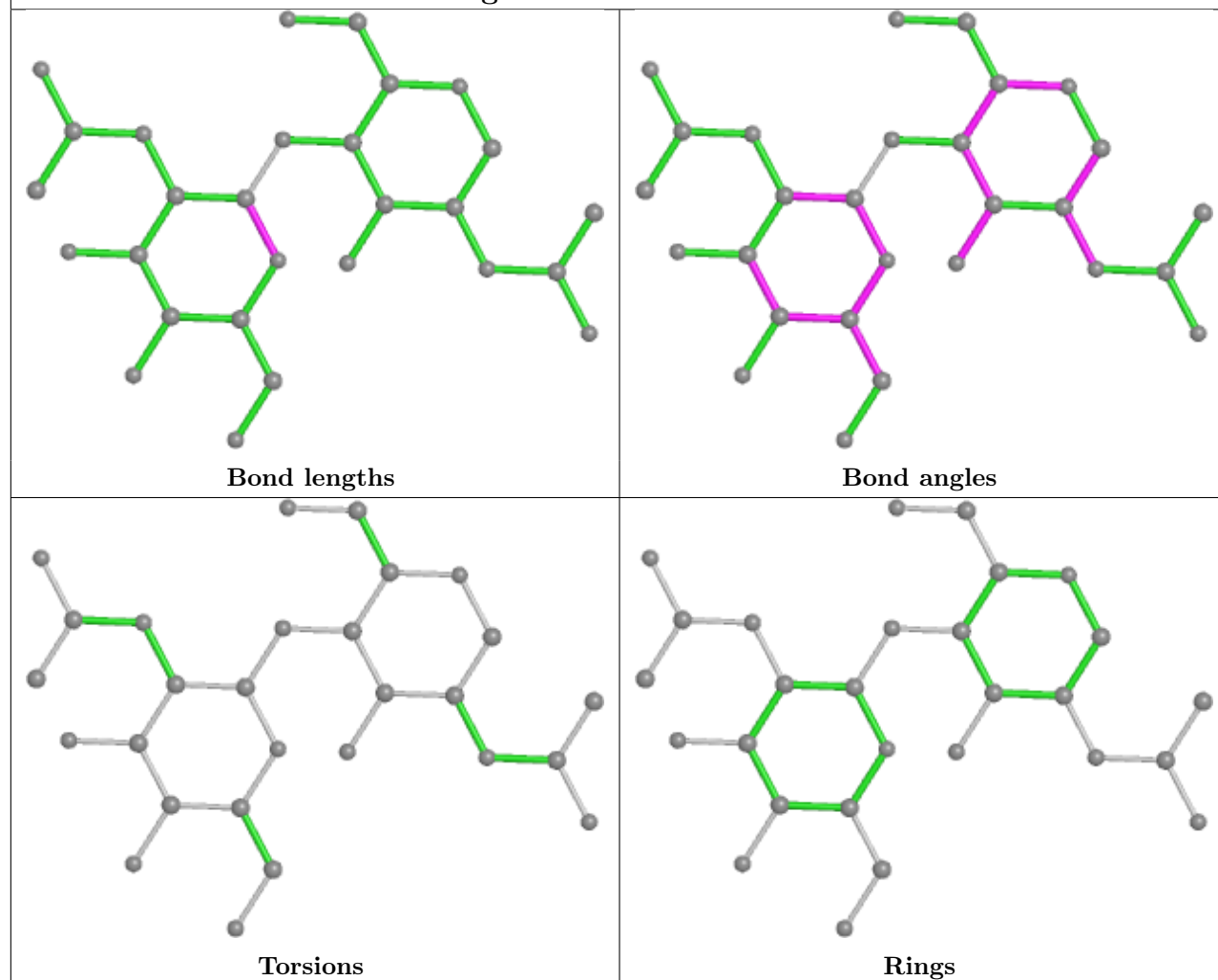
Oligosaccharide Chain G

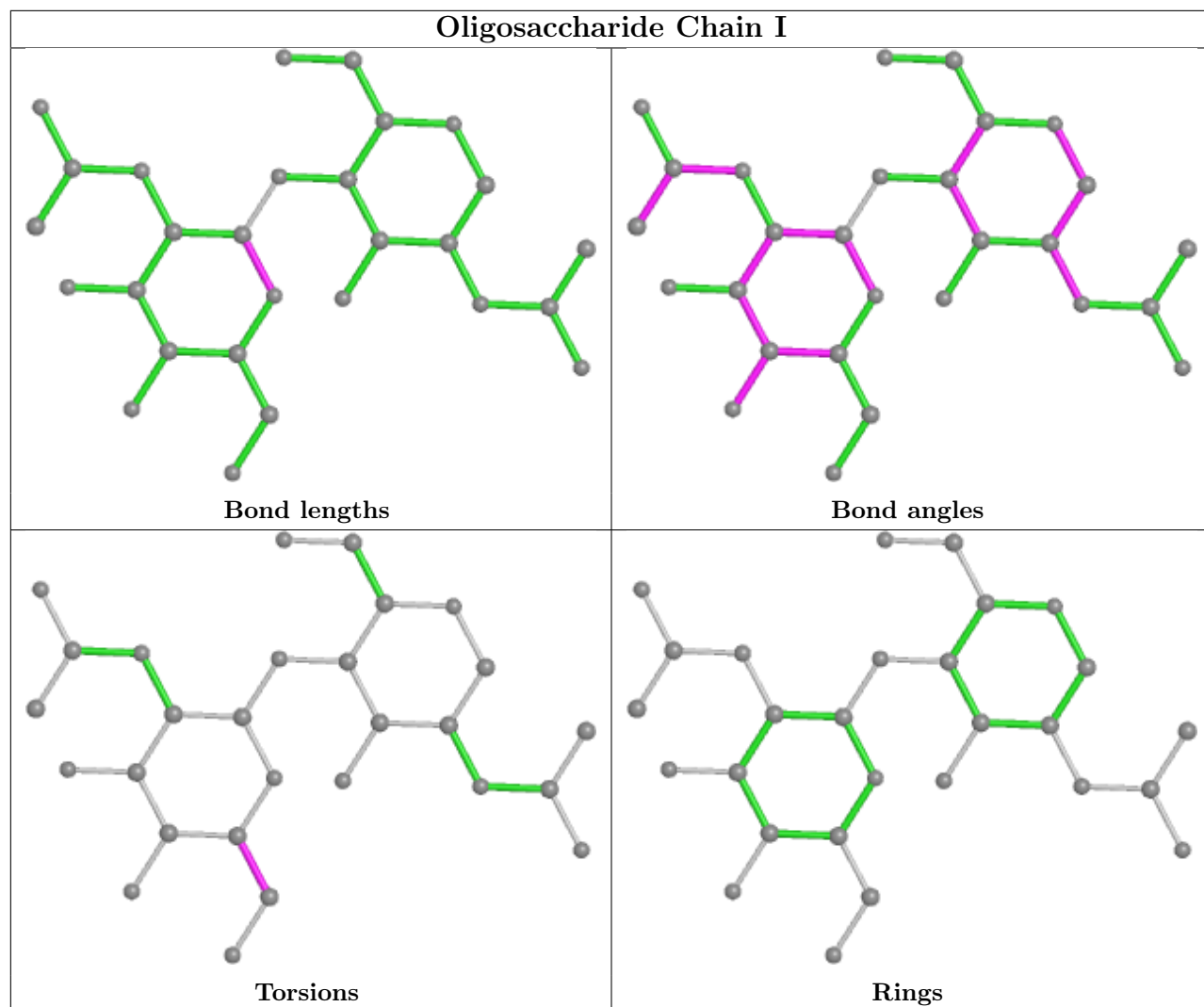


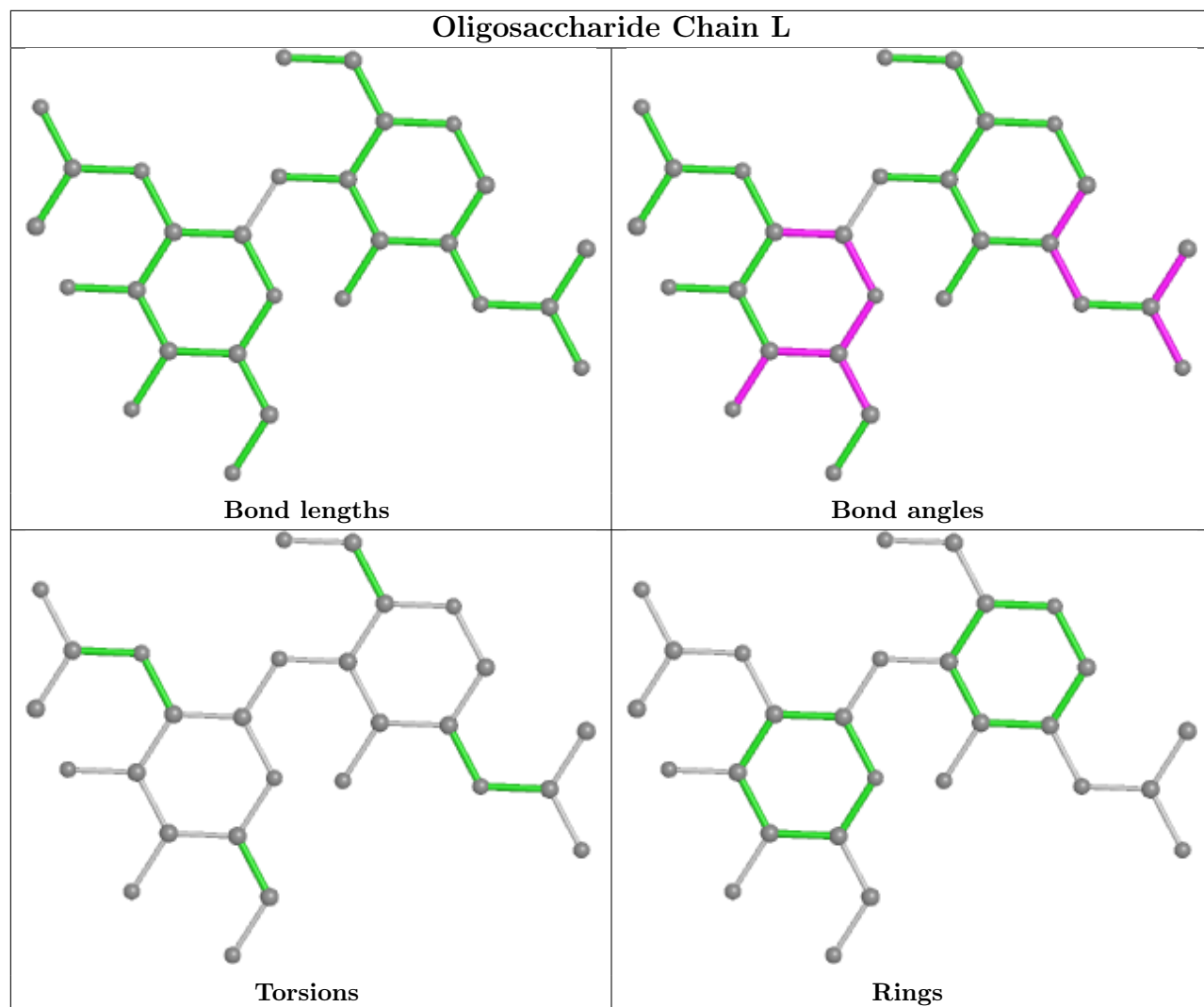
Oligosaccharide Chain H

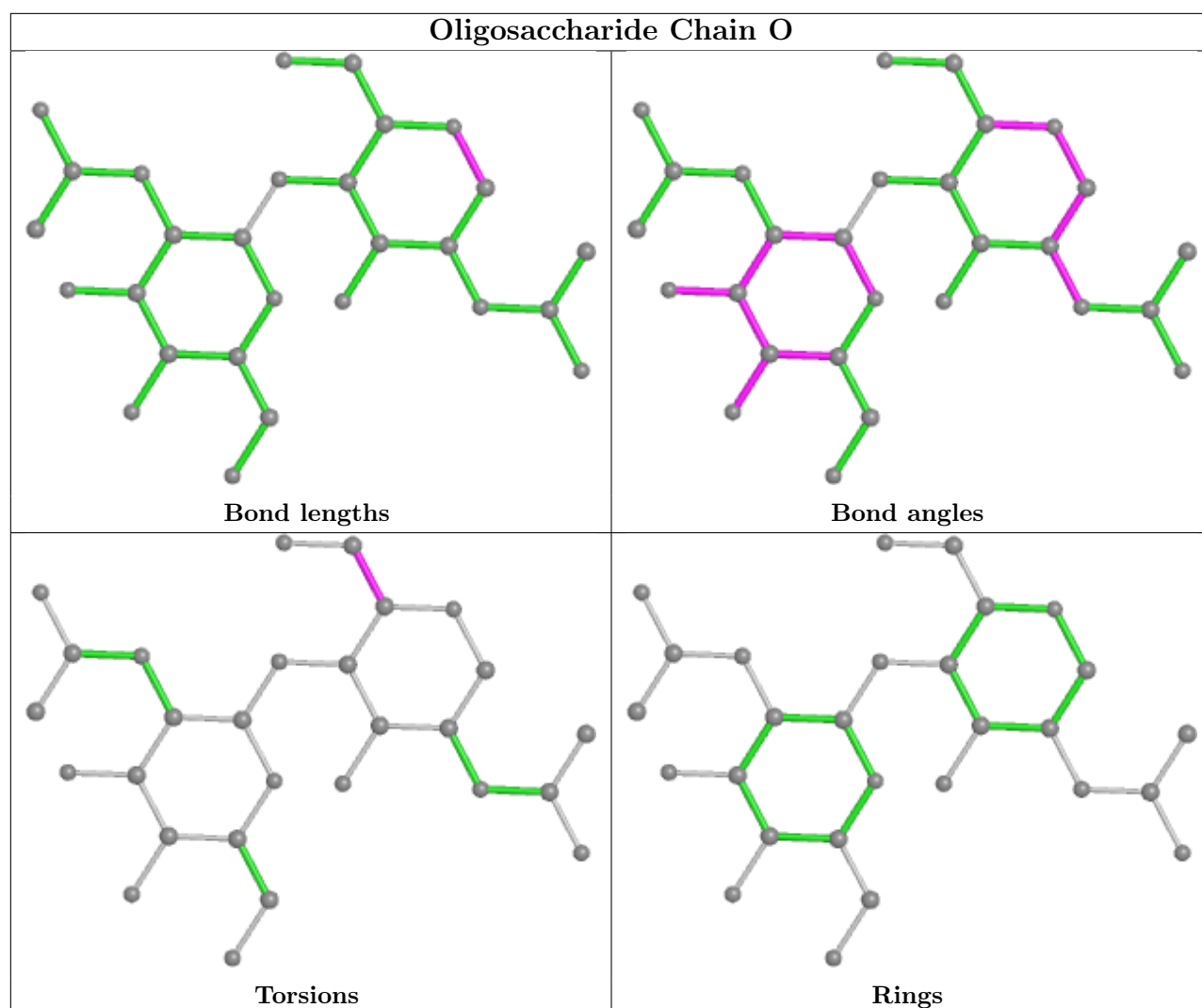


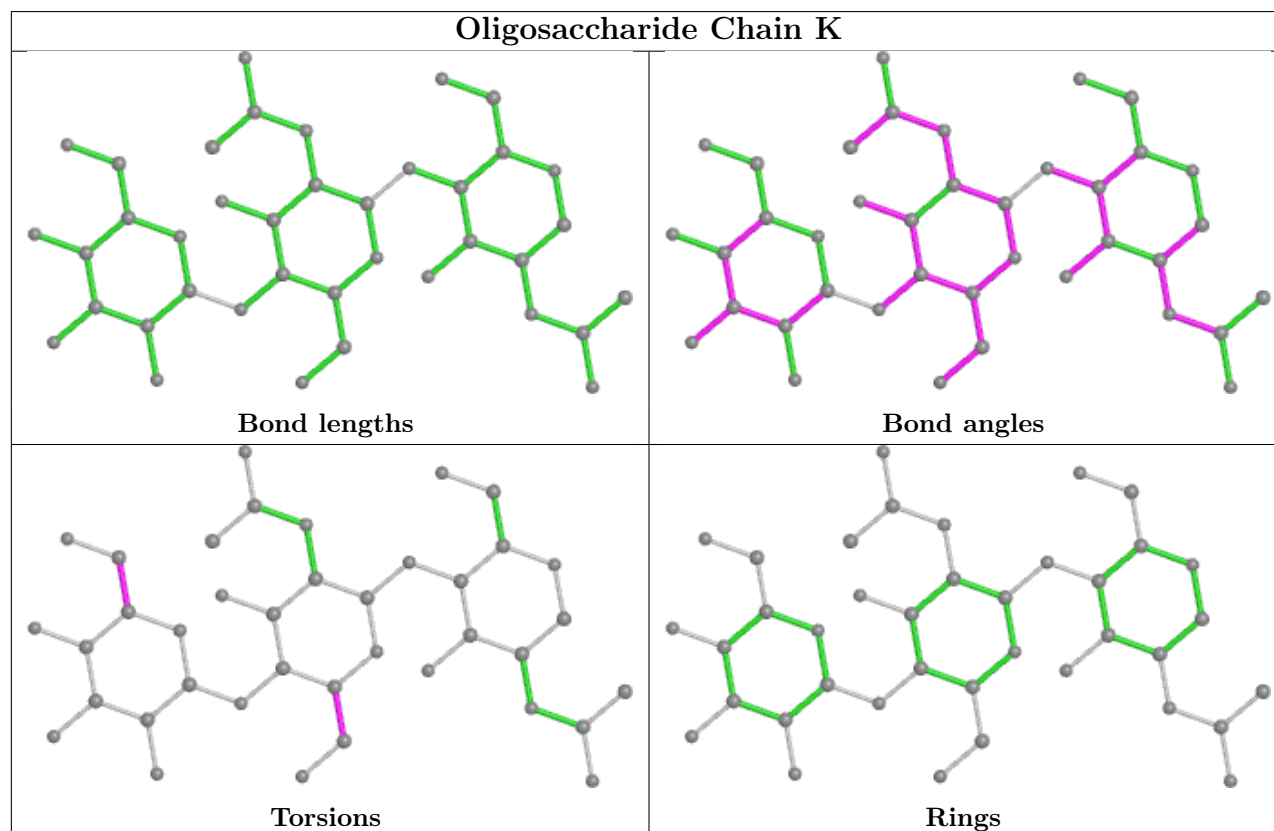
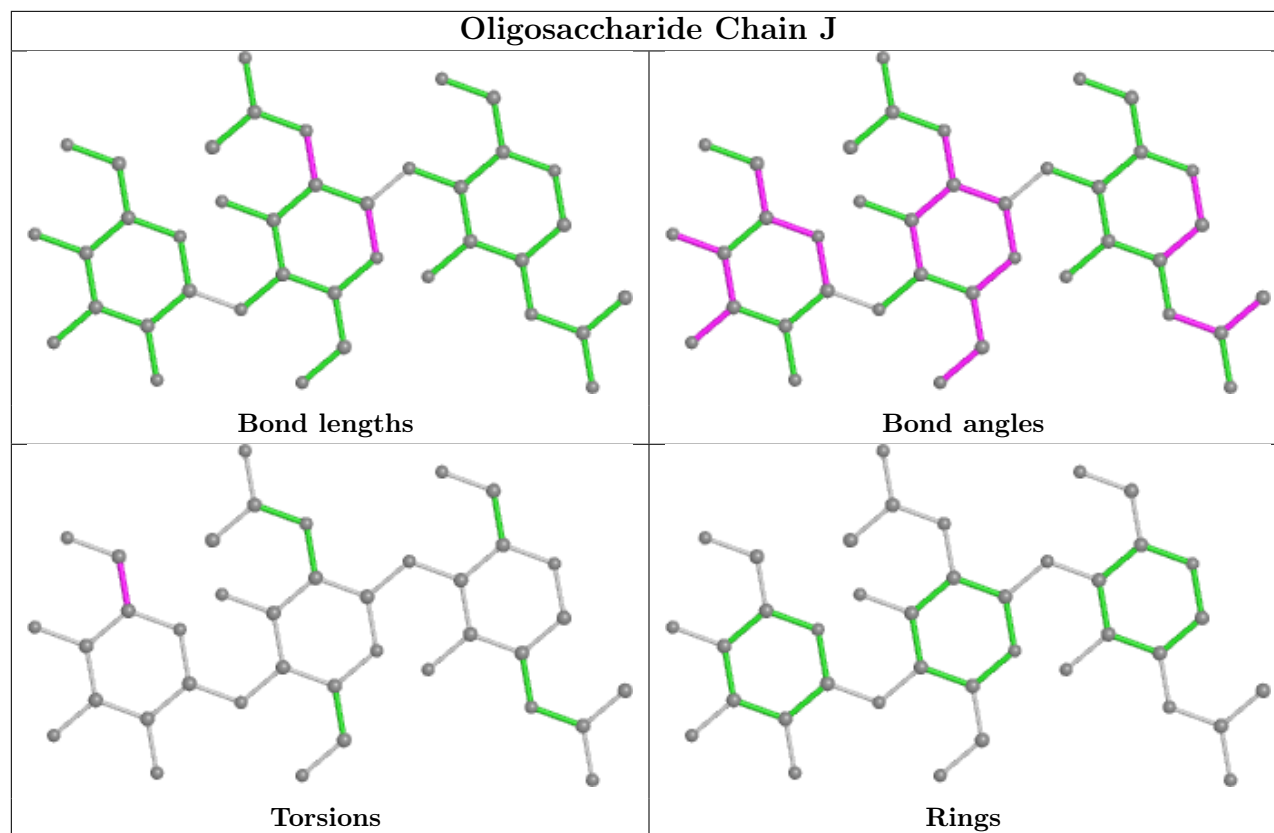
Oligosaccharide Chain F

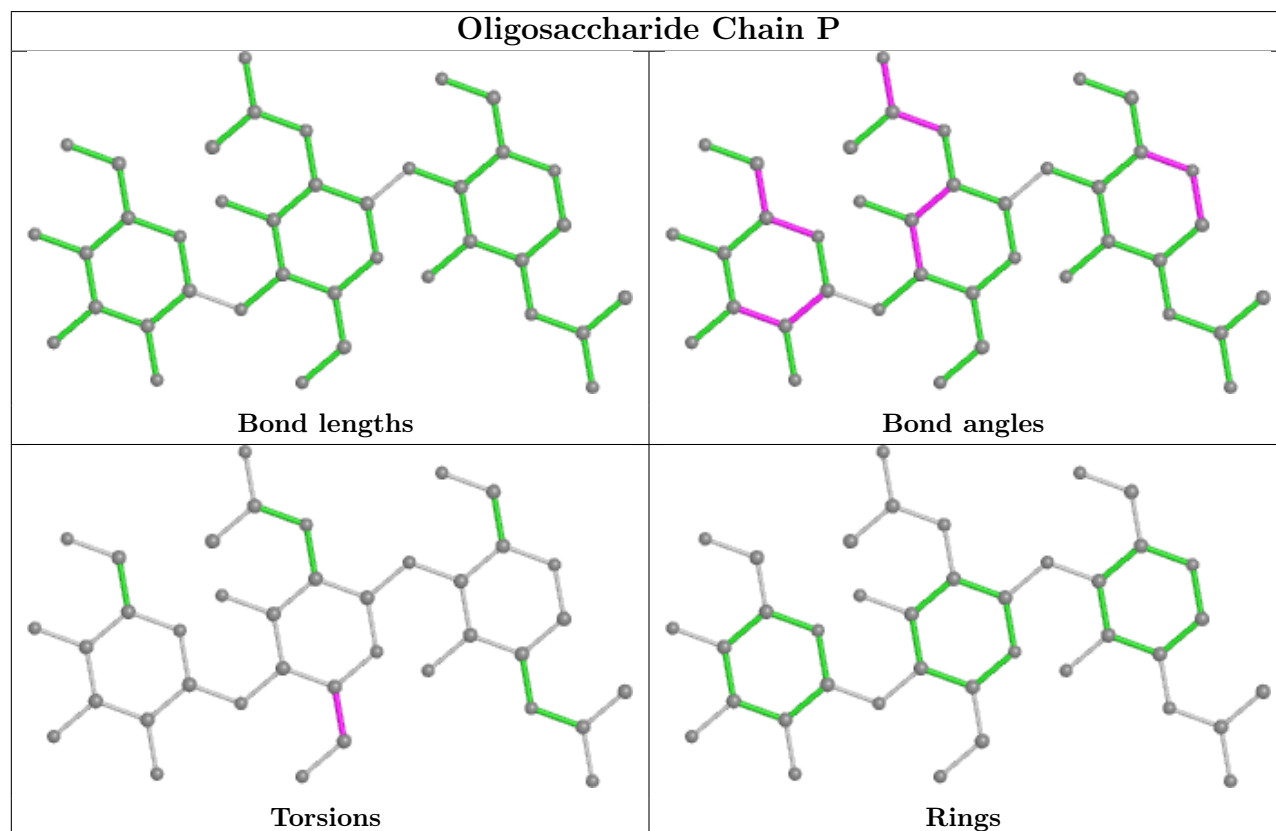
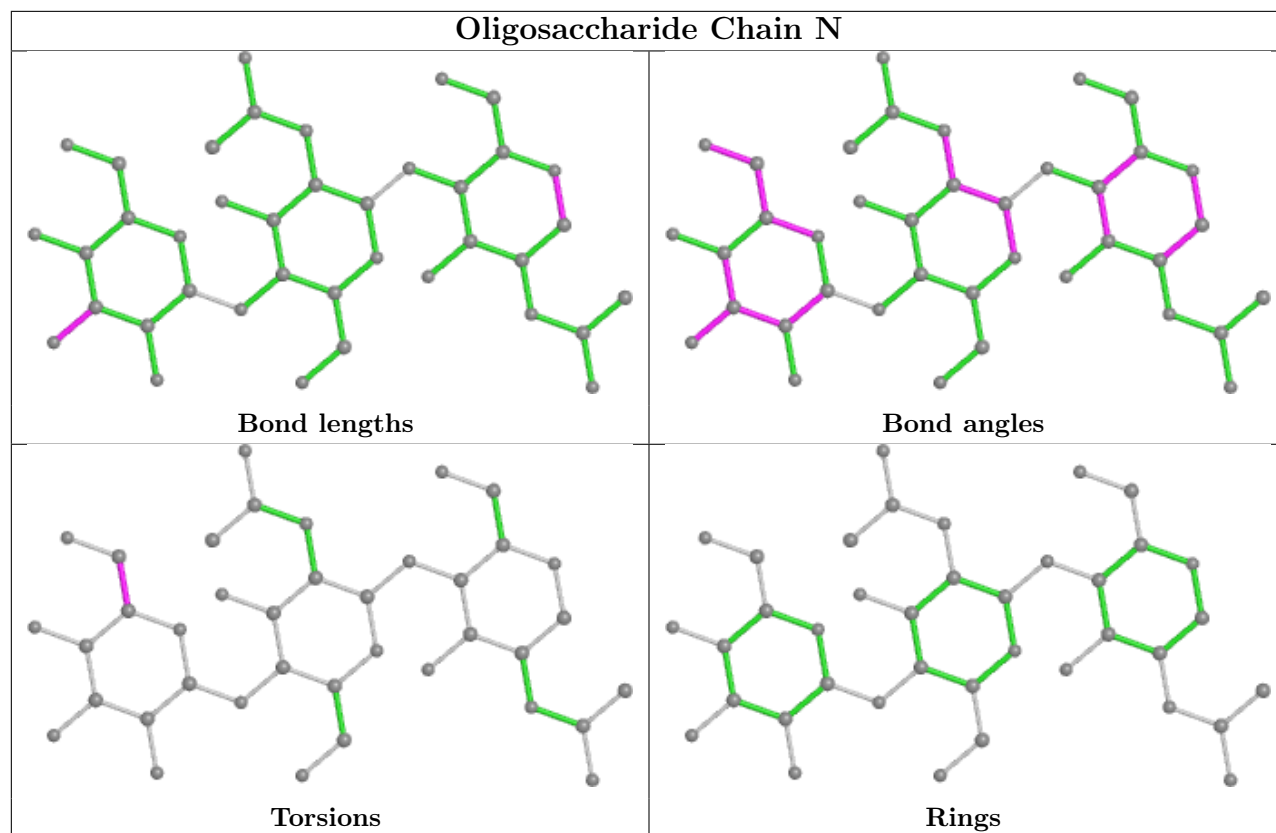


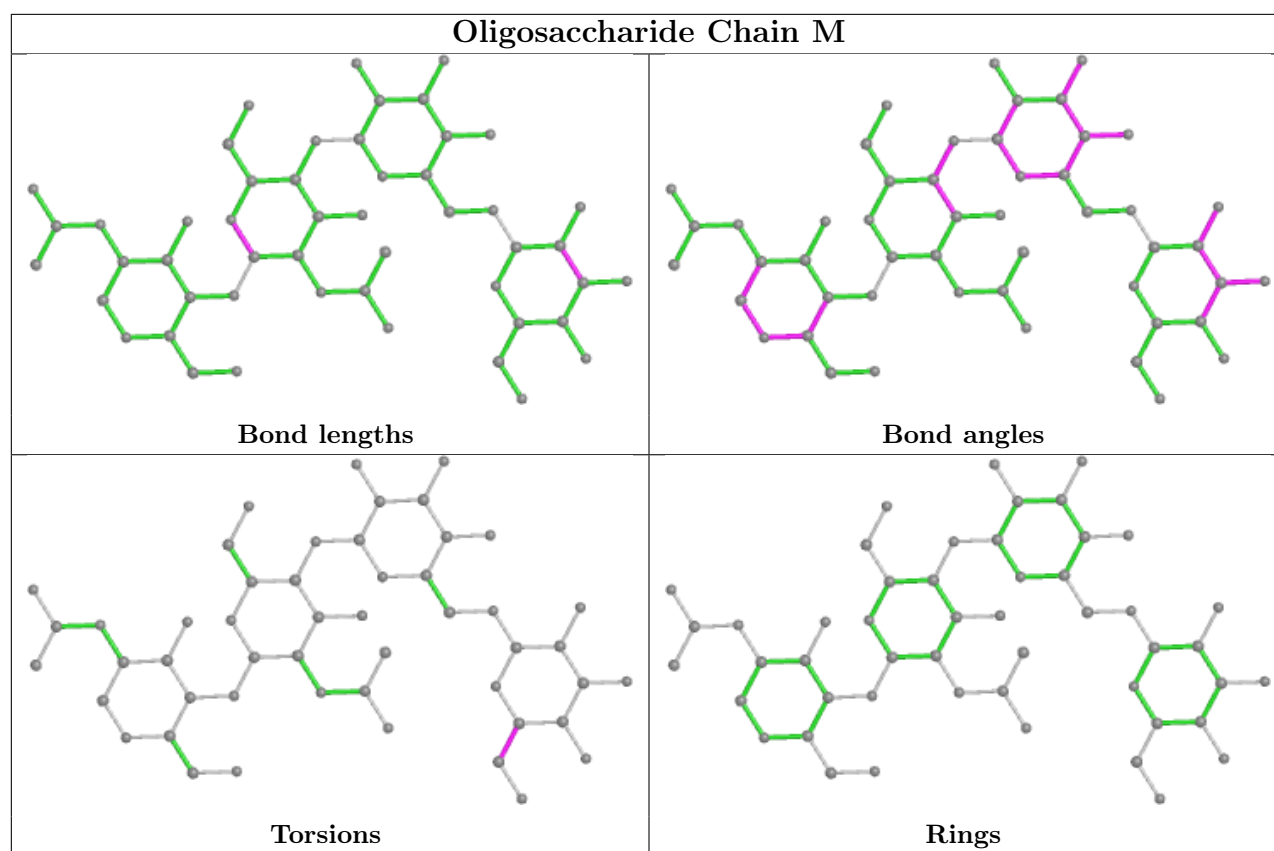












5.6 Ligand geometry [i](#)

18 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	$\# Z > 2$
7	NAG	D	1010	1	14,14,15	0.75	0	17,19,21	1.20	3 (17%)
7	NAG	C	913	1	14,14,15	0.93	1 (7%)	17,19,21	1.30	4 (23%)
6	MBL	A	915	-	16,18,18	0.92	1 (6%)	18,23,23	1.44	3 (16%)
7	NAG	D	1006	1	14,14,15	0.53	0	17,19,21	1.60	3 (17%)
7	NAG	A	914	1	14,14,15	0.72	0	17,19,21	2.19	6 (35%)
7	NAG	B	1013	1	14,14,15	0.72	0	17,19,21	1.85	4 (23%)
6	MBL	C	915	-	16,18,18	1.57	1 (6%)	18,23,23	1.51	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MBL	A	901	-	16,18,18	1.13	1 (6%)	18,23,23	0.95	0
7	NAG	A	913	1	14,14,15	0.73	0	17,19,21	1.51	3 (17%)
7	NAG	B	1012	1	14,14,15	0.90	1 (7%)	17,19,21	1.40	2 (11%)
7	NAG	B	1010	1	14,14,15	0.78	1 (7%)	17,19,21	1.75	3 (17%)
7	NAG	D	1011	1	14,14,15	0.67	0	17,19,21	1.87	5 (29%)
7	NAG	C	907	1	14,14,15	0.87	0	17,19,21	1.48	2 (11%)
7	NAG	B	1011	1	14,14,15	0.67	0	17,19,21	1.05	0
7	NAG	A	912	1	14,14,15	0.59	0	17,19,21	2.41	4 (23%)
7	NAG	C	912	1	14,14,15	0.71	0	17,19,21	1.69	2 (11%)
6	MBL	C	901	-	16,18,18	0.96	1 (6%)	18,23,23	1.19	1 (5%)
7	NAG	C	914	1	14,14,15	0.86	1 (7%)	17,19,21	0.98	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	D	1010	1	-	0/6/23/26	0/1/1/1
7	NAG	C	913	1	-	3/6/23/26	0/1/1/1
6	MBL	A	915	-	-	0/9/9/9	0/2/2/2
7	NAG	D	1006	1	-	4/6/23/26	0/1/1/1
7	NAG	A	914	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1013	1	-	4/6/23/26	0/1/1/1
6	MBL	C	915	-	-	0/9/9/9	0/2/2/2
6	MBL	A	901	-	-	0/9/9/9	0/2/2/2
7	NAG	A	913	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1012	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1010	1	-	0/6/23/26	0/1/1/1
7	NAG	D	1011	1	-	2/6/23/26	0/1/1/1
7	NAG	C	907	1	-	4/6/23/26	0/1/1/1
7	NAG	B	1011	1	-	0/6/23/26	0/1/1/1
7	NAG	A	912	1	-	0/6/23/26	0/1/1/1
7	NAG	C	912	1	-	0/6/23/26	0/1/1/1
6	MBL	C	901	-	-	0/9/9/9	0/2/2/2
7	NAG	C	914	1	-	2/6/23/26	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)
6	C	915	MBL	C7-N	-5.23	1.31	1.38
6	A	901	MBL	C7-N	-3.62	1.33	1.38
6	C	901	MBL	C7-N	-3.12	1.34	1.38
7	B	1012	NAG	O5-C1	-2.60	1.39	1.43
6	A	915	MBL	C7-N	-2.56	1.35	1.38

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	912	NAG	O5-C1-C2	5.74	120.35	111.29
7	C	912	NAG	C1-O5-C5	5.54	119.70	112.19
7	A	914	NAG	O5-C1-C2	-5.38	102.80	111.29
7	A	912	NAG	C1-O5-C5	5.08	119.07	112.19
7	B	1010	NAG	C1-O5-C5	4.79	118.68	112.19

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1013	NAG	O5-C5-C6-O6
7	C	907	NAG	O5-C5-C6-O6
7	B	1013	NAG	C4-C5-C6-O6
7	A	914	NAG	C8-C7-N2-C2
7	A	914	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1010	NAG	1	0
7	A	914	NAG	1	0
7	A	913	NAG	2	0
7	D	1011	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	748/811 (92%)	-0.35	8 (1%) 77 75	34, 50, 80, 110	0
1	B	749/811 (92%)	-0.22	12 (1%) 70 67	33, 55, 99, 145	0
1	C	748/811 (92%)	0.07	30 (4%) 43 40	34, 64, 105, 168	0
1	D	746/811 (91%)	0.02	27 (3%) 46 43	36, 63, 121, 169	0
All	All	2991/3244 (92%)	-0.12	77 (2%) 57 54	33, 57, 104, 169	0

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	100	VAL	6.8
1	C	817	LEU	6.7
1	A	100	VAL	6.2
1	D	732	LEU	5.8
1	B	100	VAL	5.6

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	MAN	G	4	11/12	0.71	0.13	78,91,95,96	0
7	NAG	A	914	14/15	0.74	0.12	61,68,72,78	0
5	MAN	M	4	11/12	0.76	0.14	76,93,101,102	0
7	NAG	D	1011	14/15	0.79	0.10	79,87,95,106	0
3	NAG	O	2	14/15	0.80	0.12	65,75,87,88	0
7	NAG	D	1006	14/15	0.82	0.12	73,83,92,96	0
2	MAN	H	4	11/12	0.83	0.12	57,75,79,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	L	2	14/15	0.84	0.14	70,82,92,93	0
7	NAG	B	1013	14/15	0.85	0.10	66,73,78,78	0
2	MAN	E	4	11/12	0.85	0.11	55,63,68,69	0
7	NAG	A	912	14/15	0.85	0.12	76,83,94,96	0
7	NAG	B	1011	14/15	0.86	0.10	74,88,92,95	0
7	NAG	C	907	14/15	0.86	0.11	66,77,87,95	0
3	NAG	F	2	14/15	0.88	0.12	48,66,70,70	0
7	NAG	C	914	14/15	0.90	0.09	59,64,67,70	0
3	NAG	I	2	14/15	0.90	0.10	54,64,70,71	0
7	NAG	B	1012	14/15	0.90	0.09	56,65,75,78	0
7	NAG	B	1010	14/15	0.90	0.08	50,57,64,72	0
7	NAG	C	912	14/15	0.91	0.10	56,66,74,82	0
4	NAG	K	2	14/15	0.92	0.08	53,57,64,66	0
2	NAG	G	2	14/15	0.93	0.12	33,45,49,58	0
4	NAG	P	1	14/15	0.93	0.08	42,49,54,54	0
7	NAG	C	913	14/15	0.93	0.10	61,76,82,85	0
2	NAG	H	1	14/15	0.94	0.09	35,42,48,50	0
4	NAG	N	2	14/15	0.95	0.06	42,50,58,58	0
2	NAG	H	2	14/15	0.95	0.06	45,49,58,63	0
4	NAG	J	2	14/15	0.95	0.07	36,44,51,52	0
2	NAG	G	1	14/15	0.95	0.07	38,41,46,49	0
7	NAG	D	1010	14/15	0.95	0.08	51,54,64,65	0
5	NAG	M	2	14/15	0.95	0.06	38,42,51,55	0
5	NAG	M	1	14/15	0.96	0.06	35,38,41,46	0
3	NAG	L	1	14/15	0.96	0.06	40,46,50,54	0
4	NAG	P	2	14/15	0.96	0.07	47,55,63,63	0
4	NAG	K	1	14/15	0.96	0.06	44,47,56,57	0
7	NAG	A	913	14/15	0.96	0.06	56,60,64,64	0
3	NAG	I	1	14/15	0.97	0.06	34,41,45,49	0
2	NAG	E	2	14/15	0.97	0.05	35,40,48,52	0
4	NAG	J	1	14/15	0.97	0.05	29,38,41,43	0
4	NAG	N	1	14/15	0.97	0.06	39,43,45,47	0
2	NAG	E	1	14/15	0.97	0.05	29,35,37,38	0
3	NAG	O	1	14/15	0.97	0.06	45,50,54,61	0
3	NAG	F	1	14/15	0.98	0.05	36,40,47,48	0

6.3 Carbohydrates

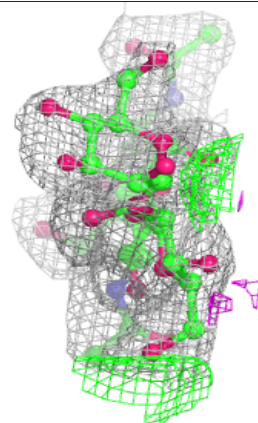
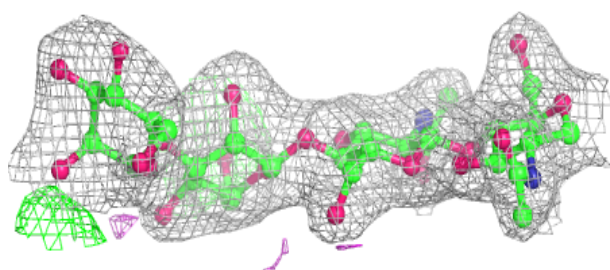
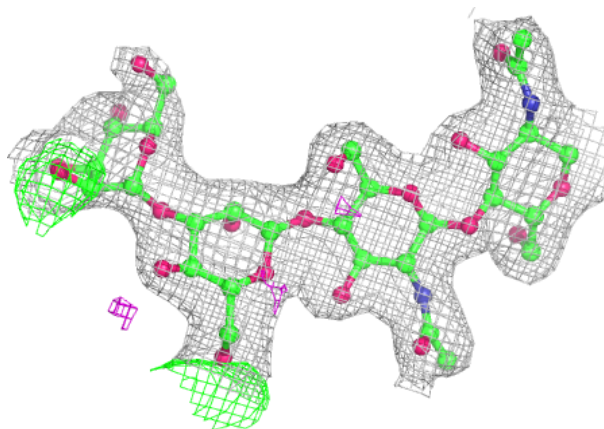
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	G	4	11/12	0.71	0.13	78,91,95,96	0
4	BMA	P	3	11/12	0.71	0.12	69,73,80,81	0
4	BMA	K	3	11/12	0.76	0.13	64,70,79,83	0
5	MAN	M	4	11/12	0.76	0.14	76,93,101,102	0
4	BMA	N	3	11/12	0.78	0.12	50,63,71,72	0
4	BMA	J	3	11/12	0.79	0.12	53,66,72,72	0
3	NAG	O	2	14/15	0.80	0.12	65,75,87,88	0
2	BMA	E	3	11/12	0.82	0.09	50,59,62,62	0
2	BMA	G	3	11/12	0.83	0.10	55,68,79,85	0
2	MAN	H	4	11/12	0.83	0.12	57,75,79,81	0
3	NAG	L	2	14/15	0.84	0.14	70,82,92,93	0
2	MAN	E	4	11/12	0.85	0.11	55,63,68,69	0
2	BMA	H	3	11/12	0.85	0.10	55,66,72,82	0
5	BMA	M	3	11/12	0.87	0.09	57,65,69,84	0
3	NAG	F	2	14/15	0.88	0.12	48,66,70,70	0
3	NAG	I	2	14/15	0.90	0.10	54,64,70,71	0
4	NAG	K	2	14/15	0.92	0.08	53,57,64,66	0
4	NAG	P	1	14/15	0.93	0.08	42,49,54,54	0
2	NAG	G	2	14/15	0.93	0.12	33,45,49,58	0
2	NAG	H	1	14/15	0.94	0.09	35,42,48,50	0
2	NAG	H	2	14/15	0.95	0.06	45,49,58,63	0
4	NAG	J	2	14/15	0.95	0.07	36,44,51,52	0
5	NAG	M	2	14/15	0.95	0.06	38,42,51,55	0
4	NAG	N	2	14/15	0.95	0.06	42,50,58,58	0
2	NAG	G	1	14/15	0.95	0.07	38,41,46,49	0
5	NAG	M	1	14/15	0.96	0.06	35,38,41,46	0
3	NAG	L	1	14/15	0.96	0.06	40,46,50,54	0
4	NAG	P	2	14/15	0.96	0.07	47,55,63,63	0
4	NAG	K	1	14/15	0.96	0.06	44,47,56,57	0
2	NAG	E	2	14/15	0.97	0.05	35,40,48,52	0
4	NAG	J	1	14/15	0.97	0.05	29,38,41,43	0
4	NAG	N	1	14/15	0.97	0.06	39,43,45,47	0
2	NAG	E	1	14/15	0.97	0.05	29,35,37,38	0
3	NAG	I	1	14/15	0.97	0.06	34,41,45,49	0
3	NAG	O	1	14/15	0.97	0.06	45,50,54,61	0
3	NAG	F	1	14/15	0.98	0.05	36,40,47,48	0

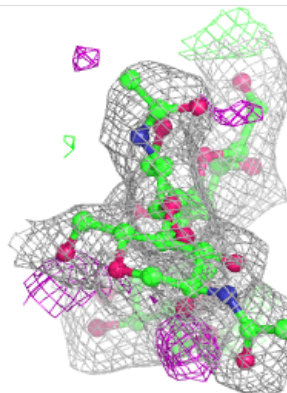
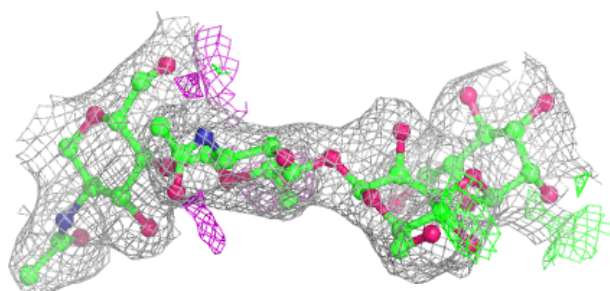
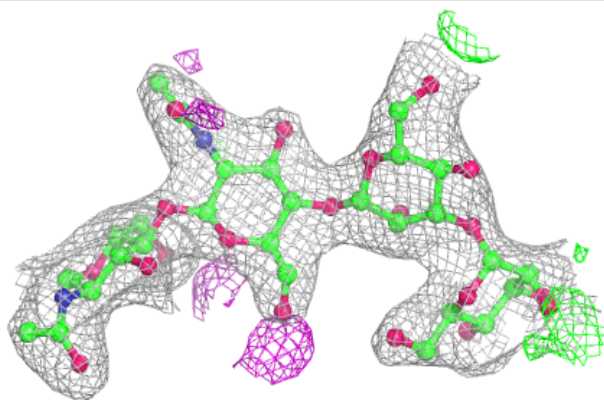
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

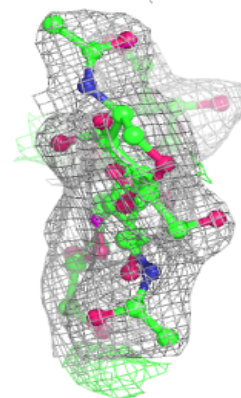
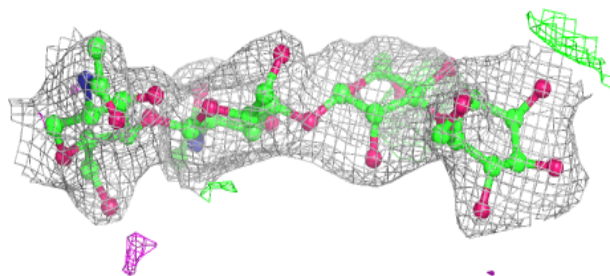
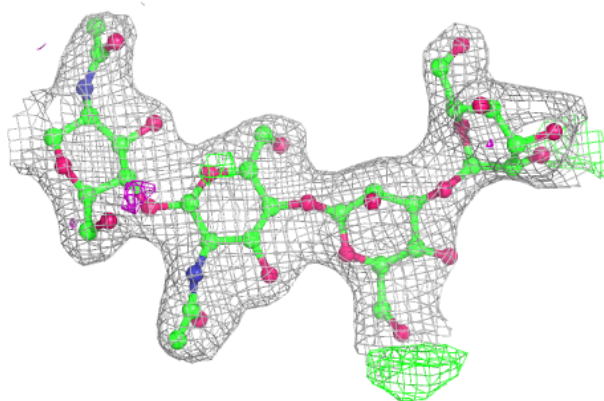
**Electron density around Chain G:**

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

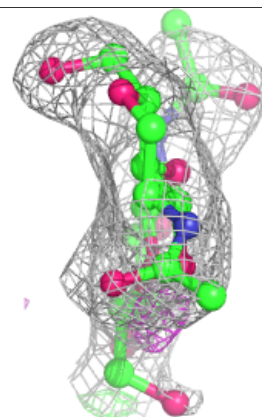
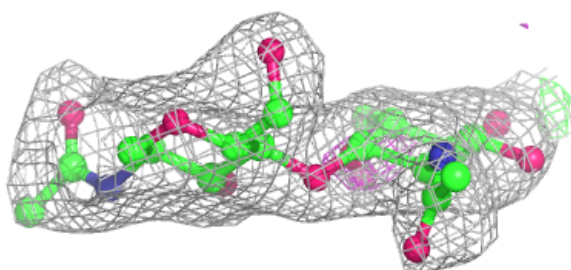
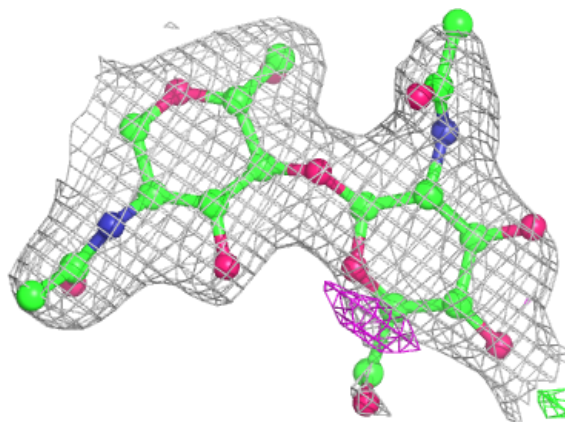


Electron density around Chain H:

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

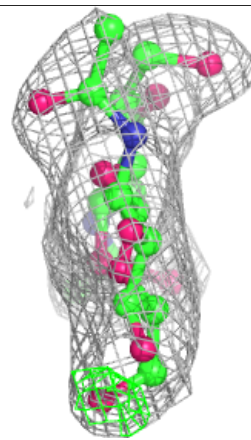
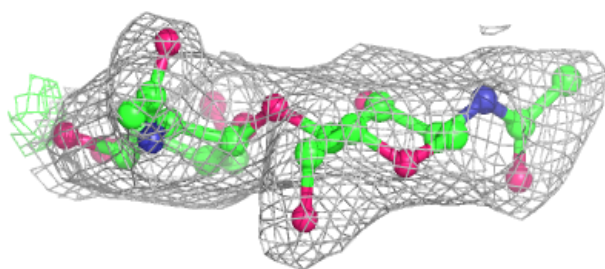
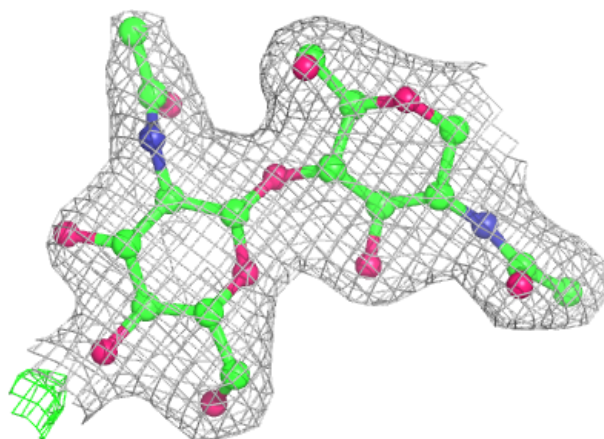
**Electron density around Chain F:**

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



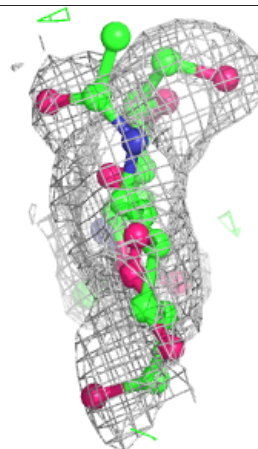
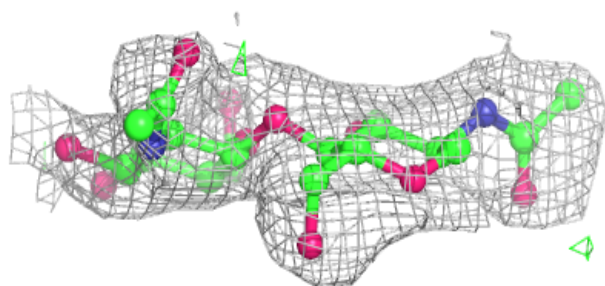
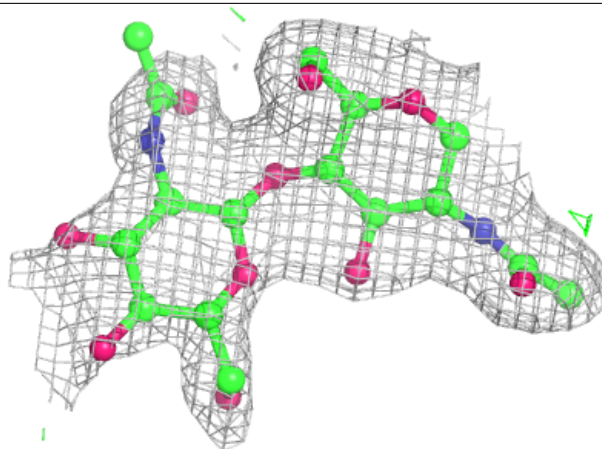
Electron density around Chain I:

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



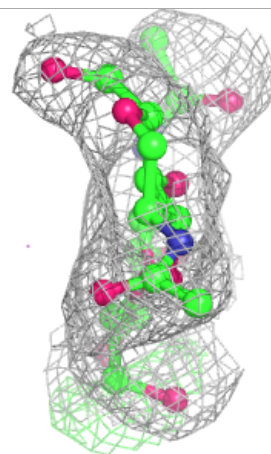
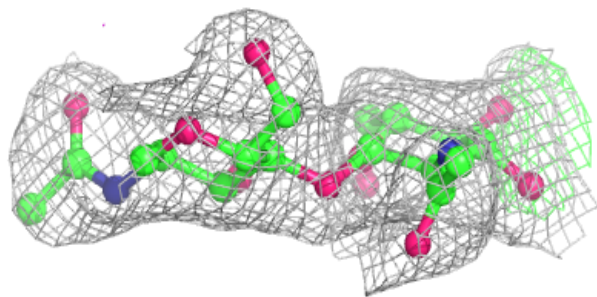
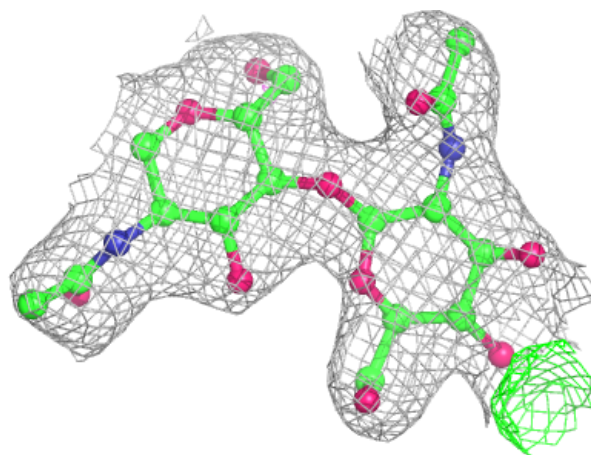
Electron density around Chain L:

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



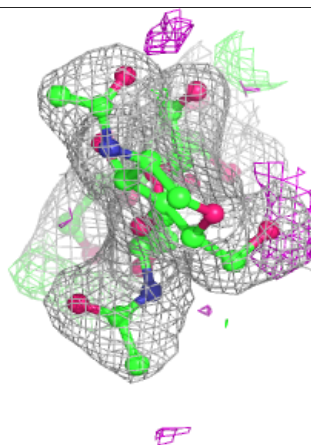
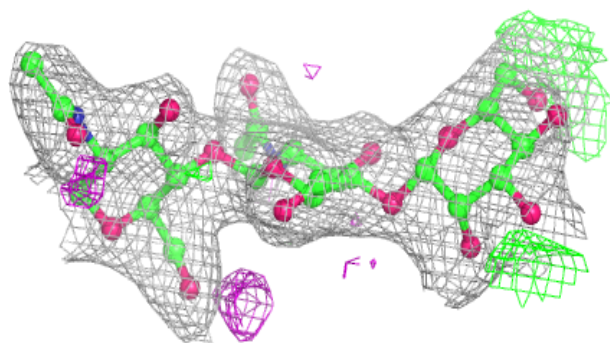
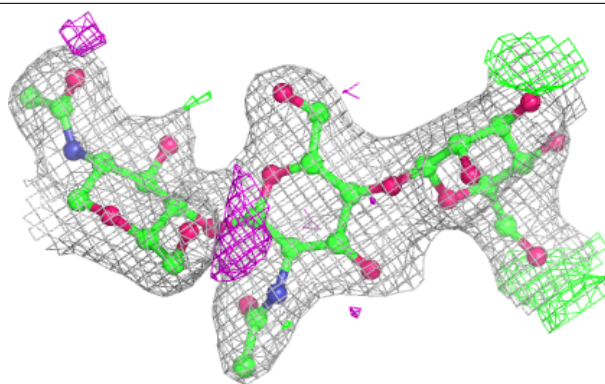
Electron density around Chain O:

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



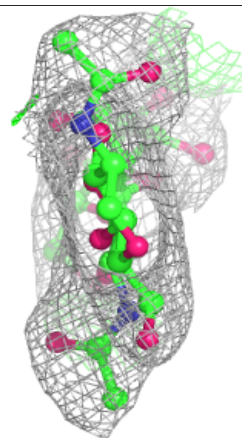
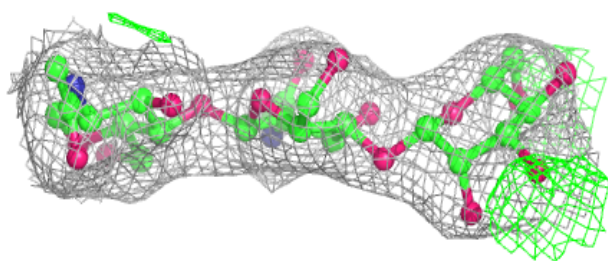
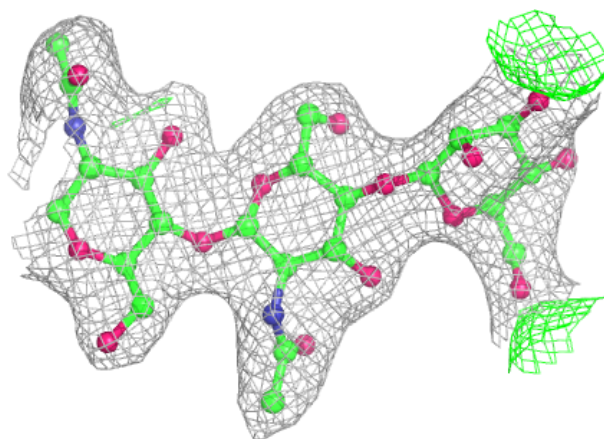
Electron density around Chain J:

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

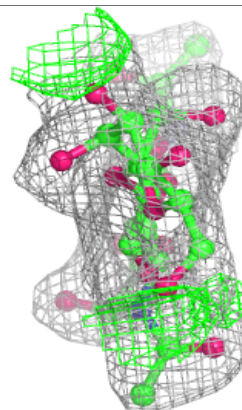
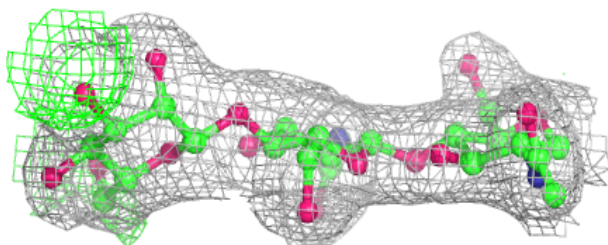
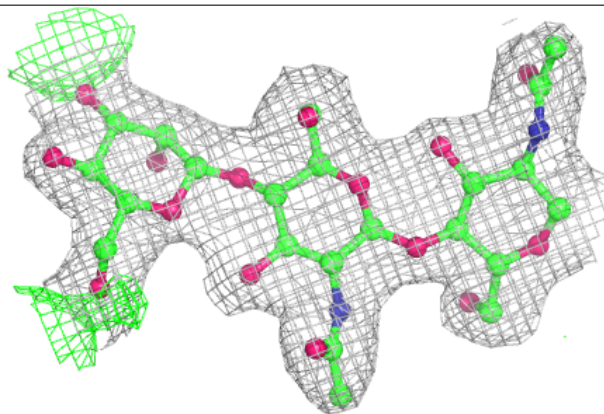


Electron density around Chain K:

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

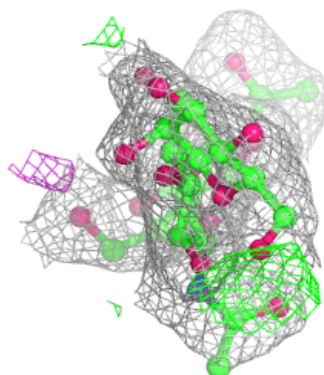
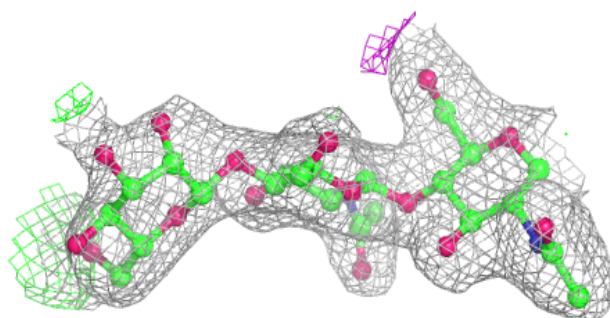
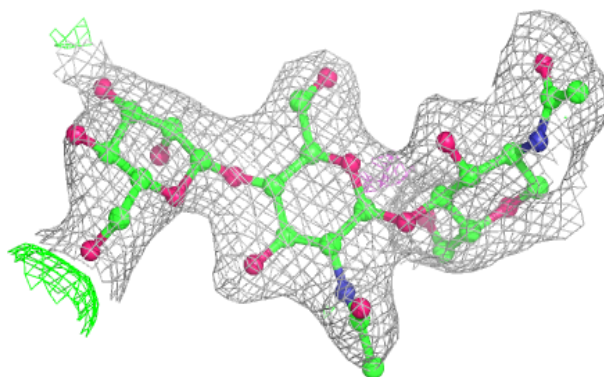
**Electron density around Chain N:**

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

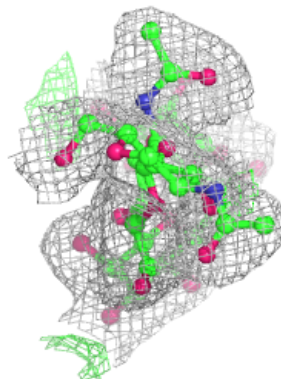
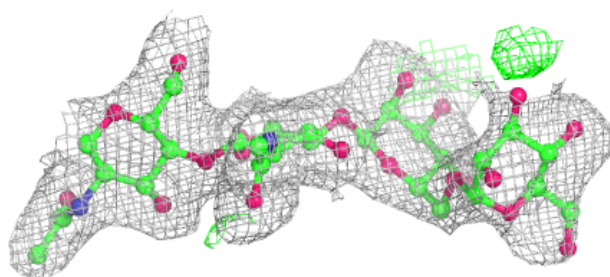
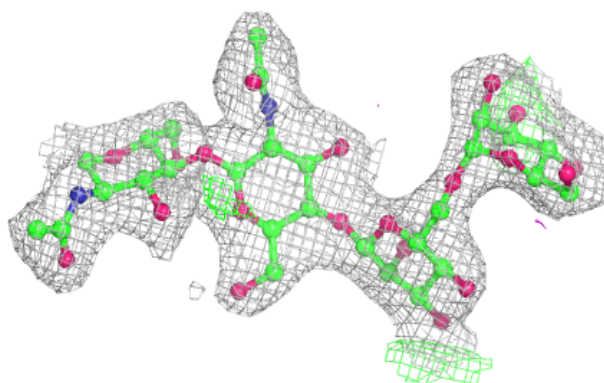


Electron density around Chain P:

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

**Electron density around Chain 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

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(\AA^2)	Q<0.9
7	NAG	A	914	14/15	0.74	0.12	61,68,72,78	0
7	NAG	D	1011	14/15	0.79	0.10	79,87,95,106	0
7	NAG	D	1006	14/15	0.82	0.12	73,83,92,96	0
7	NAG	A	912	14/15	0.85	0.12	76,83,94,96	0
7	NAG	B	1013	14/15	0.85	0.10	66,73,78,78	0
7	NAG	B	1011	14/15	0.86	0.10	74,88,92,95	0
7	NAG	C	907	14/15	0.86	0.11	66,77,87,95	0
7	NAG	C	914	14/15	0.90	0.09	59,64,67,70	0
7	NAG	B	1010	14/15	0.90	0.08	50,57,64,72	0
7	NAG	B	1012	14/15	0.90	0.09	56,65,75,78	0
7	NAG	C	912	14/15	0.91	0.10	56,66,74,82	0
7	NAG	C	913	14/15	0.93	0.10	61,76,82,85	0
7	NAG	D	1010	14/15	0.95	0.08	51,54,64,65	0
6	MBL	C	901	17/17	0.95	0.10	50,57,61,63	0
6	MBL	A	901	17/17	0.96	0.08	43,48,54,54	0
6	MBL	A	915	17/17	0.96	0.08	39,44,49,49	0
7	NAG	A	913	14/15	0.96	0.06	56,60,64,64	0
6	MBL	C	915	17/17	0.97	0.07	44,47,55,56	0

6.5 Other polymers

There are no such residues in this entry.