



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2023 – 05:09 pm GMT

PDB ID : 2WYF
Title : Crystal structure of PA-IL lectin complexed with aGal12bGal-O-Met at 2.4 Å resolution
Authors : Nurisso, A.; Blanchard, B.; Varrot, A.; Imberty, A.
Deposited on : 2009-11-16
Resolution : 2.40 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

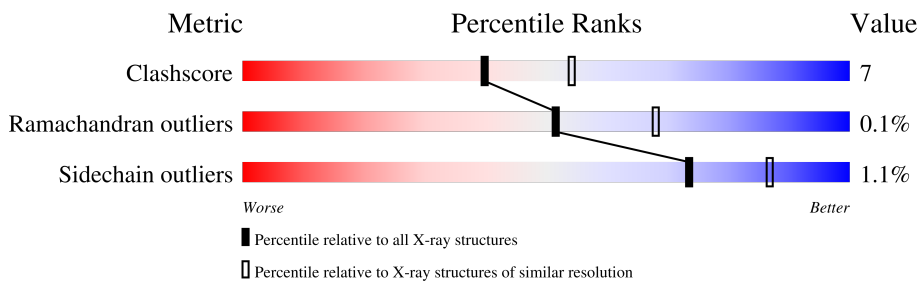
1 Overall quality at a glance i

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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)


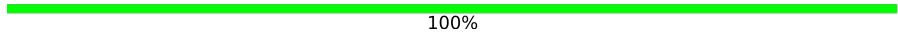
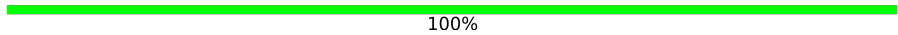
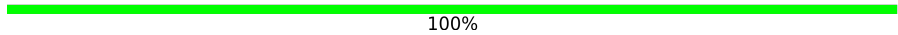
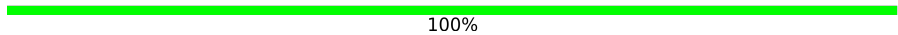
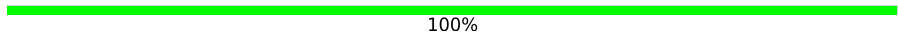
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	121	
1	B	121	
1	C	121	
1	D	121	
1	E	121	
1	F	121	
1	G	121	
1	H	121	

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Mol	Chain	Length	Quality of chain
2	I	2	 50% 50%
2	J	2	 100%
2	K	2	 100%
2	L	2	 100%
2	M	2	 100%
2	N	2	 100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8007 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 PA-I GALACTOPHILIC LECTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	121	Total 900	C 567	N 156	O 174	S 3	0	0	0
1	B	119	Total 885	C 558	N 153	O 171	S 3	0	0	0
1	C	121	Total 900	C 567	N 156	O 174	S 3	0	0	0
1	D	121	Total 900	C 567	N 156	O 174	S 3	0	0	0
1	E	121	Total 900	C 567	N 156	O 174	S 3	0	0	0
1	F	121	Total 900	C 567	N 156	O 174	S 3	0	0	0
1	G	121	Total 900	C 567	N 156	O 174	S 3	0	0	0
1	H	121	Total 900	C 567	N 156	O 174	S 3	0	0	0

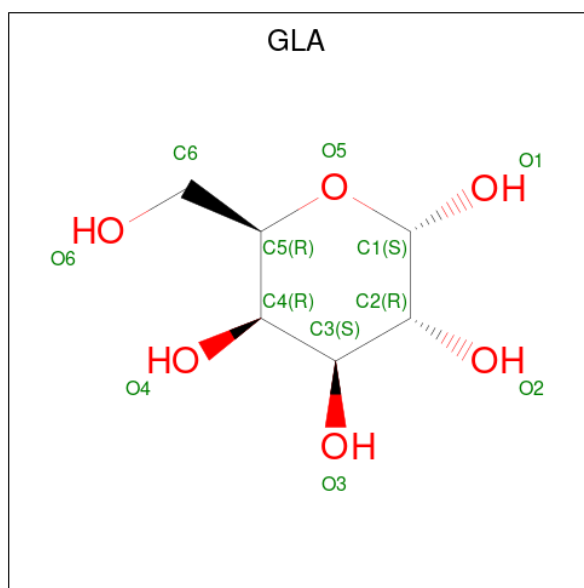
- Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-2)-methyl beta-D-galactopyranoside.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	I	2	Total 24	C 13	O 11	0	0	0
2	J	2	Total 24	C 13	O 11	0	0	0
2	K	2	Total 24	C 13	O 11	0	0	0
2	L	2	Total 24	C 13	O 11	0	0	0
2	M	2	Total 24	C 13	O 11	0	0	0
2	N	2	Total 24	C 13	O 11	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0
3	G	1	Total Ca 1 1	0	0
3	H	1	Total Ca 1 1	0	0

- Molecule 4 is alpha-D-galactopyranose (three-letter code: GLA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 12 6 6	0	0
4	E	1	Total C O 12 6 6	0	0

- Molecule 5 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	91	Total O 91 91	0	0
5	B	75	Total O 75 75	0	0
5	C	85	Total O 85 85	0	0
5	D	88	Total O 88 88	0	0
5	E	76	Total O 76 76	0	0
5	F	68	Total O 68 68	0	0
5	G	89	Total O 89 89	0	0
5	H	74	Total O 74 74	0	0

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. 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. 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.


Note EDS failed to run properly.

- Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain A:  86% 14%




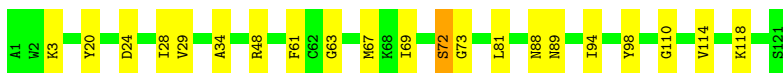
- Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain B:  88% 10% ..




- Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain C:  83% 17%




- Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain D:  79% 21%




- Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain E:  87% 13%



- Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain F:  88% 12%



- Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain G: 91% 9%



- Molecule 1: PA-I GALACTOPHILIC LECTIN

Chain H: 88% 12%



- Molecule 2: alpha-D-galactopyranose-(1-2)-methyl beta-D-galactopyranoside

Chain I: 50% 50%



- Molecule 2: alpha-D-galactopyranose-(1-2)-methyl beta-D-galactopyranoside

Chain J: 100%



- Molecule 2: alpha-D-galactopyranose-(1-2)-methyl beta-D-galactopyranoside

Chain K: 100%



- Molecule 2: alpha-D-galactopyranose-(1-2)-methyl beta-D-galactopyranoside

Chain L: 100%



- Molecule 2: alpha-D-galactopyranose-(1-2)-methyl beta-D-galactopyranoside

Chain M: 100%



- Molecule 2: alpha-D-galactopyranose-(1-2)-methyl beta-D-galactopyranoside

Chain N:  100%

RESIDUE
GLA2

4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.88Å 99.79Å 91.32Å 90.00° 100.77° 90.00°	Depositor
Resolution (Å)	89.80 – 2.40	Depositor
% Data completeness (in resolution range)	99.1 (89.80-2.40)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.166 , 0.259	Depositor
Wilson B-factor (Å ²)	15.4	Xtrriage
Anisotropy	0.427	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8007	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MBG, GLA, CA

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	0.71	0/923	0.76	0/1262
1	B	0.74	0/906	0.73	0/1236
1	C	0.71	0/923	0.77	1/1262 (0.1%)
1	D	0.72	0/923	0.72	0/1262
1	E	0.66	0/923	0.74	0/1262
1	F	0.69	0/923	0.71	0/1262
1	G	0.69	0/923	0.74	1/1262 (0.1%)
1	H	0.68	0/923	0.74	0/1262
All	All	0.70	0/7367	0.74	2/10070 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	24	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	24	ASP	CB-CG-OD1	5.13	122.92	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	900	0	861	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	885	0	847	16	0
1	C	900	0	861	19	0
1	D	900	0	861	20	0
1	E	900	0	861	14	0
1	F	900	0	861	13	0
1	G	900	0	861	6	0
1	H	900	0	861	12	0
2	I	24	0	21	2	0
2	J	24	0	22	0	0
2	K	24	0	21	0	0
2	L	24	0	21	0	0
2	M	24	0	22	0	0
2	N	24	0	22	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	B	12	0	11	0	0
4	E	12	0	11	0	0
5	A	91	0	0	2	0
5	B	75	0	0	2	0
5	C	85	0	0	0	0
5	D	88	0	0	5	0
5	E	76	0	0	1	0
5	F	68	0	0	0	0
5	G	89	0	0	3	0
5	H	74	0	0	2	0
All	All	8007	0	7025	105	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 7.

All (105) 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:C:69:ILE:HG12	1:C:94:ILE:HD12	1.48	0.96
1:E:67:MET:HE2	1:E:94:ILE:HG23	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:MET:HE2	1:F:94:ILE:HG23	1.52	0.92
1:C:67:MET:CE	1:C:94:ILE:HG23	2.06	0.86
1:D:40:GLN:HG3	5:D:2037:HOH:O	1.78	0.83
1:F:1:ALA:CB	5:G:2082:HOH:O	2.26	0.83
1:H:69:ILE:HG12	1:H:94:ILE:HD13	1.59	0.83
1:E:67:MET:HE2	1:E:94:ILE:CG2	2.10	0.81
1:B:15:VAL:HG23	5:B:2009:HOH:O	1.82	0.80
1:F:3:LYS:HG2	1:F:115:ASN:OD1	1.87	0.75
1:C:67:MET:HE2	1:C:94:ILE:HG23	1.70	0.74
1:F:67:MET:HE2	1:F:94:ILE:CG2	2.17	0.74
1:C:67:MET:CE	1:C:94:ILE:CG2	2.68	0.71
1:D:5:GLU:CG	5:D:2006:HOH:O	2.38	0.70
1:C:72:SER:HB3	1:C:73:GLY:O	1.92	0.70
1:A:120:GLN:HG2	5:A:2082:HOH:O	1.89	0.70
1:A:67:MET:CE	1:A:94:ILE:HG23	2.22	0.69
1:B:120:GLN:HG3	1:D:120:GLN:HG3	1.75	0.69
1:C:67:MET:HE3	1:C:94:ILE:CG2	2.23	0.69
1:C:67:MET:HE3	1:C:94:ILE:HG23	1.78	0.64
1:E:121:SER:HB2	1:H:118:LYS:HB2	1.79	0.63
1:A:67:MET:HE2	1:A:94:ILE:HG23	1.80	0.61
1:A:28:ILE:HD12	1:A:81:LEU:HD12	1.85	0.59
1:A:67:MET:CE	1:A:94:ILE:CG2	2.80	0.59
1:D:5:GLU:HG2	5:D:2006:HOH:O	2.02	0.59
1:C:69:ILE:H	1:C:72:SER:HB2	1.69	0.58
1:A:48:ARG:NH2	1:B:41:LYS:HG3	2.19	0.57
1:E:67:MET:CE	1:E:94:ILE:CG2	2.81	0.56
1:F:1:ALA:HB1	5:G:2082:HOH:O	1.98	0.56
1:A:67:MET:HE3	1:A:94:ILE:CG2	2.36	0.55
1:F:1:ALA:HB2	5:G:2082:HOH:O	1.96	0.55
1:H:67:MET:HE2	1:H:94:ILE:HD12	1.89	0.55
1:C:63:GLY:HA2	1:C:98:TYR:CZ	2.41	0.55
1:B:67:MET:HE2	1:B:94:ILE:HG23	1.89	0.55
1:D:24:ASP:OD2	1:D:118:LYS:HE3	2.07	0.55
1:G:79:THR:HB	1:H:79:THR:HB	1.90	0.53
1:A:41:LYS:HB2	1:B:48:ARG:NH1	2.23	0.53
1:C:48:ARG:HG3	1:C:61:PHE:CZ	2.43	0.53
1:A:120:GLN:NE2	5:A:2082:HOH:O	2.40	0.53
1:A:50:HIS:HE1	2:I:1:MBG:H72	1.74	0.53
1:D:11:GLU:OE2	1:G:5:GLU:OE2	2.27	0.53
1:E:28:ILE:O	1:E:80:GLY:HA3	2.09	0.52
1:E:118:LYS:HB2	1:H:121:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:MET:CE	1:H:94:ILE:HD12	2.39	0.52
1:F:3:LYS:CG	1:F:115:ASN:OD1	2.57	0.52
1:B:45:GLN:HB2	5:B:2034:HOH:O	2.10	0.51
1:B:45:GLN:HG3	1:B:79:THR:HG23	1.93	0.51
1:G:28:ILE:HG12	1:G:116:ILE:HG23	1.92	0.51
1:D:52:ASP:OD2	1:D:58:HIS:ND1	2.39	0.50
1:C:20:TYR:HB2	1:C:94:ILE:HD11	1.93	0.49
1:C:34:ALA:HA	1:C:110:GLY:HA3	1.94	0.49
1:D:40:GLN:HB2	1:D:42:TRP:CH2	2.48	0.49
1:D:11:GLU:HG2	1:D:105:TYR:CG	2.48	0.49
1:B:67:MET:CE	1:B:94:ILE:CG2	2.91	0.49
1:G:63:GLY:HA2	1:G:98:TYR:CZ	2.47	0.49
1:C:28:ILE:HD12	1:C:81:LEU:HD12	1.95	0.48
1:F:48:ARG:HG3	1:F:61:PHE:CZ	2.49	0.48
1:G:48:ARG:HD2	1:H:33:TRP:CE3	2.48	0.48
1:E:67:MET:CE	1:E:94:ILE:HG21	2.44	0.48
1:B:96:LEU:C	1:B:97:ILE:HG13	2.33	0.48
1:D:91:GLN:HG2	5:D:2070:HOH:O	2.13	0.48
1:D:28:ILE:HG12	1:D:116:ILE:HG12	1.95	0.48
1:A:79:THR:HB	1:B:79:THR:HB	1.96	0.47
1:C:29:VAL:HG22	1:D:29:VAL:HG22	1.96	0.47
1:A:5:GLU:O	1:A:14:GLN:HG2	2.15	0.47
1:E:40:GLN:HG2	5:E:2032:HOH:O	2.15	0.47
1:H:58:HIS:HB3	5:H:2036:HOH:O	2.15	0.47
1:B:67:MET:CE	1:B:94:ILE:HG23	2.45	0.47
1:E:11:GLU:HG2	1:E:105:TYR:CG	2.51	0.46
1:F:1:ALA:HB2	1:G:121:SER:O	2.15	0.46
1:D:63:GLY:HA2	1:D:98:TYR:CZ	2.50	0.46
1:D:87:PRO:HD2	5:D:2067:HOH:O	2.16	0.46
1:A:48:ARG:HD3	1:B:33:TRP:CE3	2.51	0.45
1:A:50:HIS:CE1	2:I:1:MBG:H72	2.52	0.45
1:E:28:ILE:HG12	1:E:116:ILE:HG12	1.99	0.45
1:A:118:LYS:O	1:D:120:GLN:HA	2.17	0.44
1:F:28:ILE:O	1:F:80:GLY:HA3	2.18	0.44
1:B:120:GLN:OE1	1:D:119:ASP:HB3	2.17	0.44
1:D:45:GLN:HG3	1:D:79:THR:HG23	1.99	0.44
1:A:67:MET:HE3	1:A:94:ILE:HG23	1.93	0.43
1:B:63:GLY:HA2	1:B:98:TYR:CZ	2.54	0.43
1:D:44:PRO:HB2	1:D:78:ASN:O	2.19	0.43
1:B:120:GLN:HA	1:C:118:LYS:O	2.18	0.43
1:D:86:ALA:HA	1:D:87:PRO:HD3	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:GLY:HA2	1:F:98:TYR:CZ	2.54	0.43
1:H:20:TYR:HB2	1:H:94:ILE:HD11	2.00	0.43
1:D:28:ILE:HD12	1:D:81:LEU:HD12	2.01	0.42
1:E:66:VAL:HG12	1:E:76:PRO:HA	2.01	0.42
1:H:48:ARG:HG2	5:H:2031:HOH:O	2.20	0.42
1:C:67:MET:CE	1:C:94:ILE:HG21	2.49	0.42
1:F:7:LEU:HD23	1:F:111:SER:HB3	2.02	0.42
1:A:45:GLN:HG3	1:A:79:THR:HG23	2.01	0.41
1:C:88:ASN:O	1:C:89:ASN:HB2	2.19	0.41
1:E:100:ASP:HB3	1:E:105:TYR:CZ	2.56	0.41
1:H:8:ALA:HB2	1:H:34:ALA:HB1	2.02	0.41
1:E:59:ASP:HB2	1:E:76:PRO:HG3	2.03	0.41
1:E:35:SER:HB2	1:E:41:LYS:HD3	2.02	0.41
1:H:63:GLY:HA2	1:H:98:TYR:CZ	2.56	0.41
1:C:67:MET:HE3	1:C:94:ILE:HG21	1.98	0.41
1:F:67:MET:CE	1:F:94:ILE:CG2	2.94	0.40
1:A:67:MET:HE3	1:A:94:ILE:HG21	2.01	0.40
1:B:67:MET:HE2	1:B:94:ILE:CG2	2.49	0.40
1:A:63:GLY:HA2	1:A:98:TYR:CZ	2.57	0.40
1:A:28:ILE:O	1:A:80:GLY:HA3	2.22	0.40
1:C:3:LYS:HA	1:C:114:VAL:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
1	B	115/121 (95%)	111 (96%)	4 (4%)	0	100	100
1	C	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
1	D	119/121 (98%)	115 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
1	F	119/121 (98%)	113 (95%)	5 (4%)	1 (1%)	19	29
1	G	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
1	H	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
All	All	948/968 (98%)	916 (97%)	31 (3%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	88	ASN

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	94/94 (100%)	93 (99%)	1 (1%)	73	87
1	B	92/94 (98%)	91 (99%)	1 (1%)	73	87
1	C	94/94 (100%)	93 (99%)	1 (1%)	73	87
1	D	94/94 (100%)	93 (99%)	1 (1%)	73	87
1	E	94/94 (100%)	94 (100%)	0	100	100
1	F	94/94 (100%)	93 (99%)	1 (1%)	73	87
1	G	94/94 (100%)	92 (98%)	2 (2%)	53	72
1	H	94/94 (100%)	93 (99%)	1 (1%)	73	87
All	All	750/752 (100%)	742 (99%)	8 (1%)	73	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	B	97	ILE
1	C	72	SER

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Mol	Chain	Res	Type
1	D	94	ILE
1	F	39	THR
1	G	59	ASP
1	G	91	GLN
1	H	41	LYS

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

Mol	Chain	Res	Type
1	A	53	GLN
1	H	115	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](#)

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

5.5 Carbohydrates [i](#)

12 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

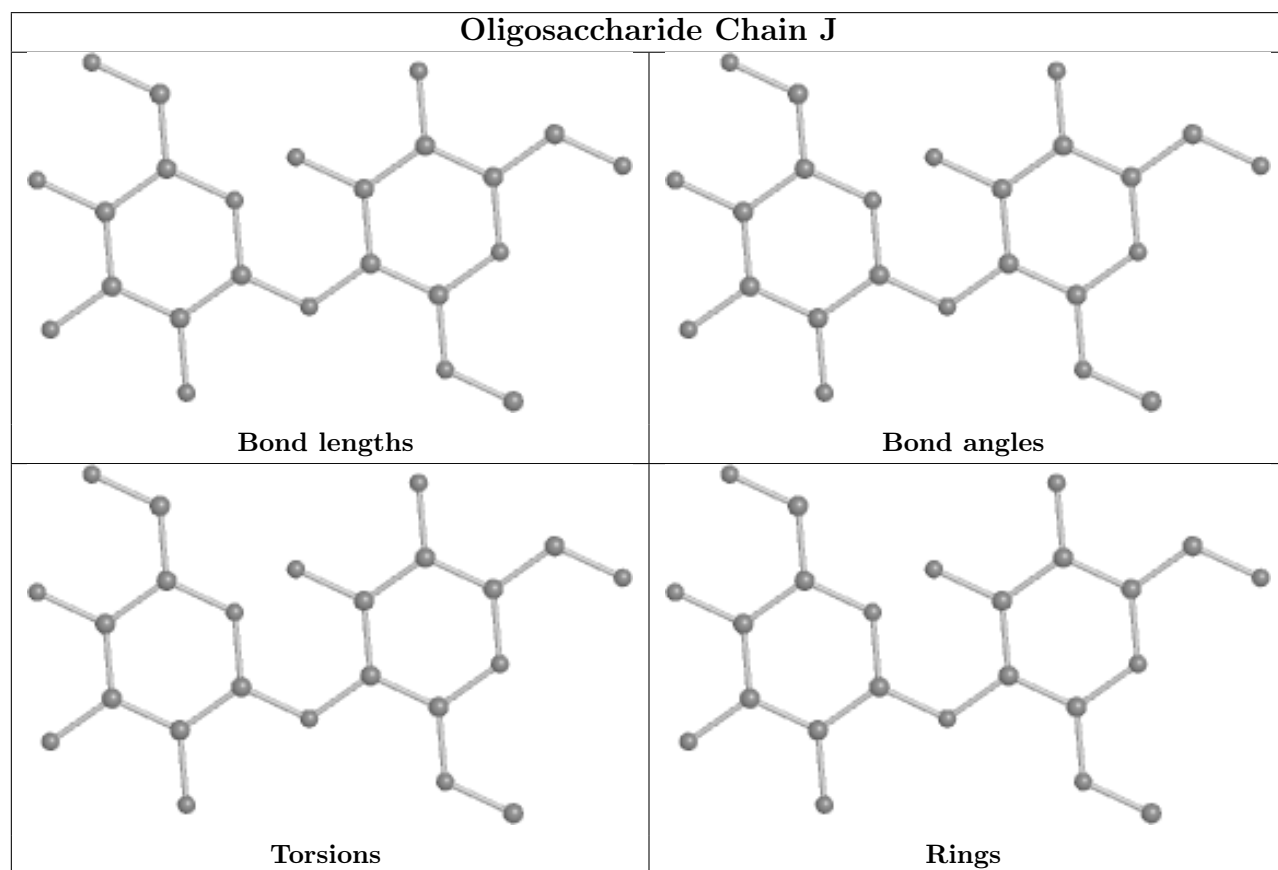
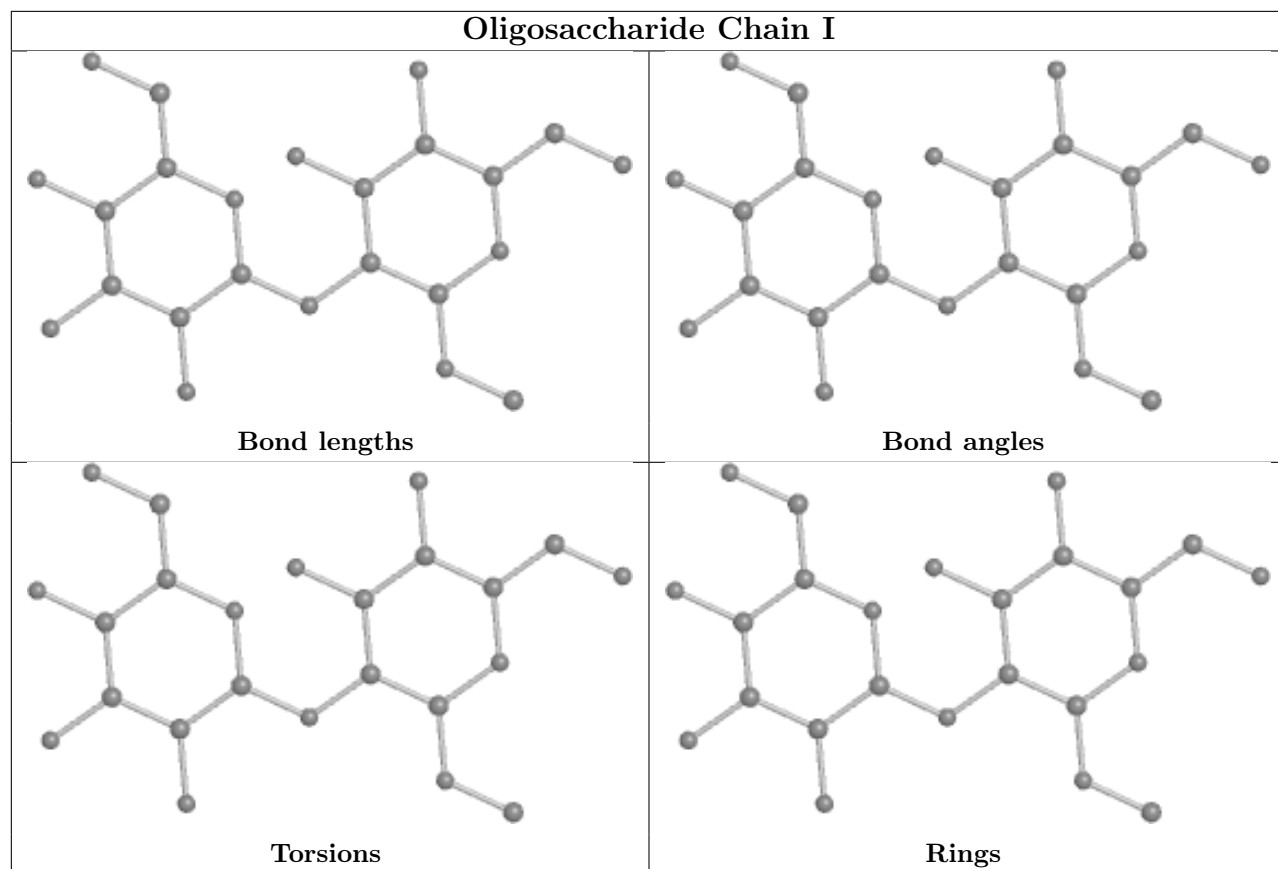
There are no chirality outliers.

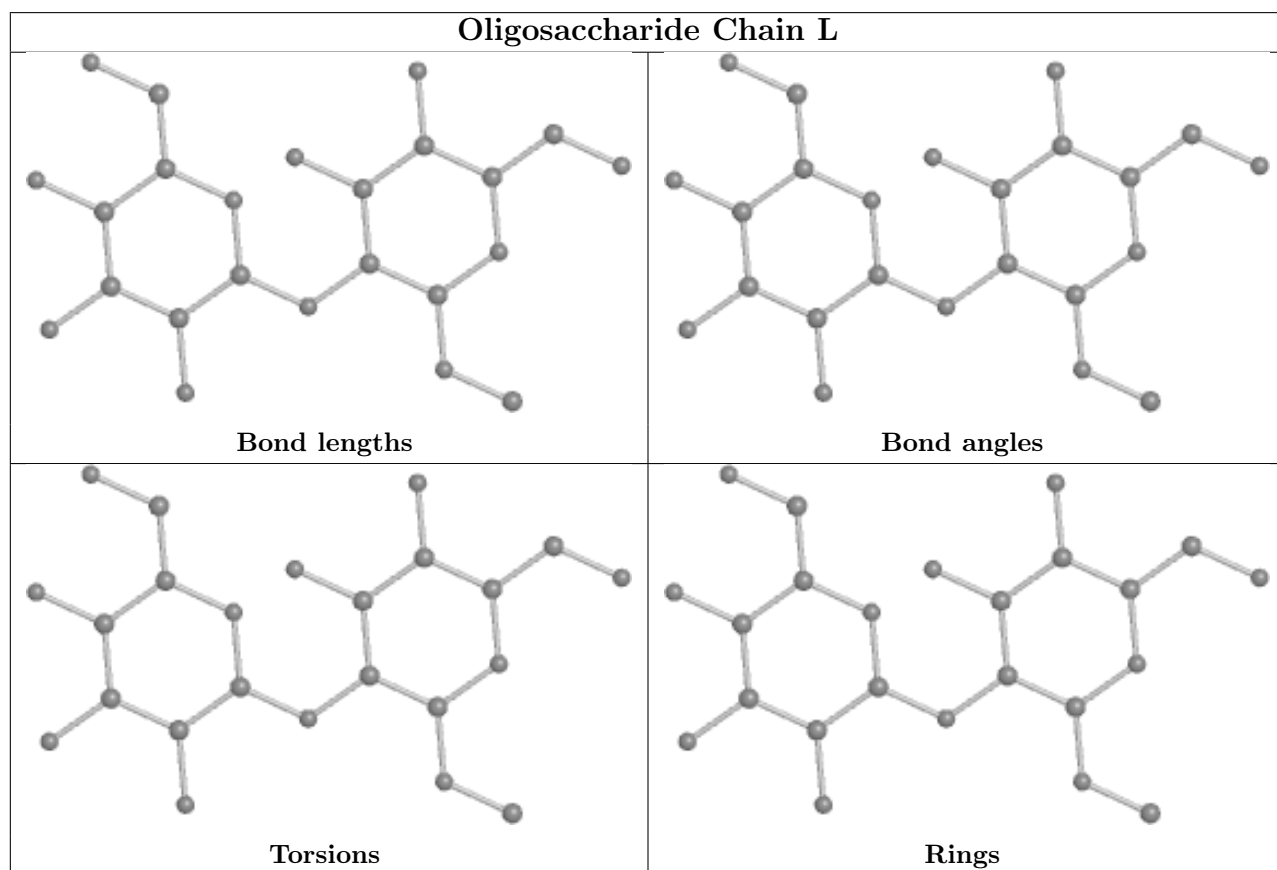
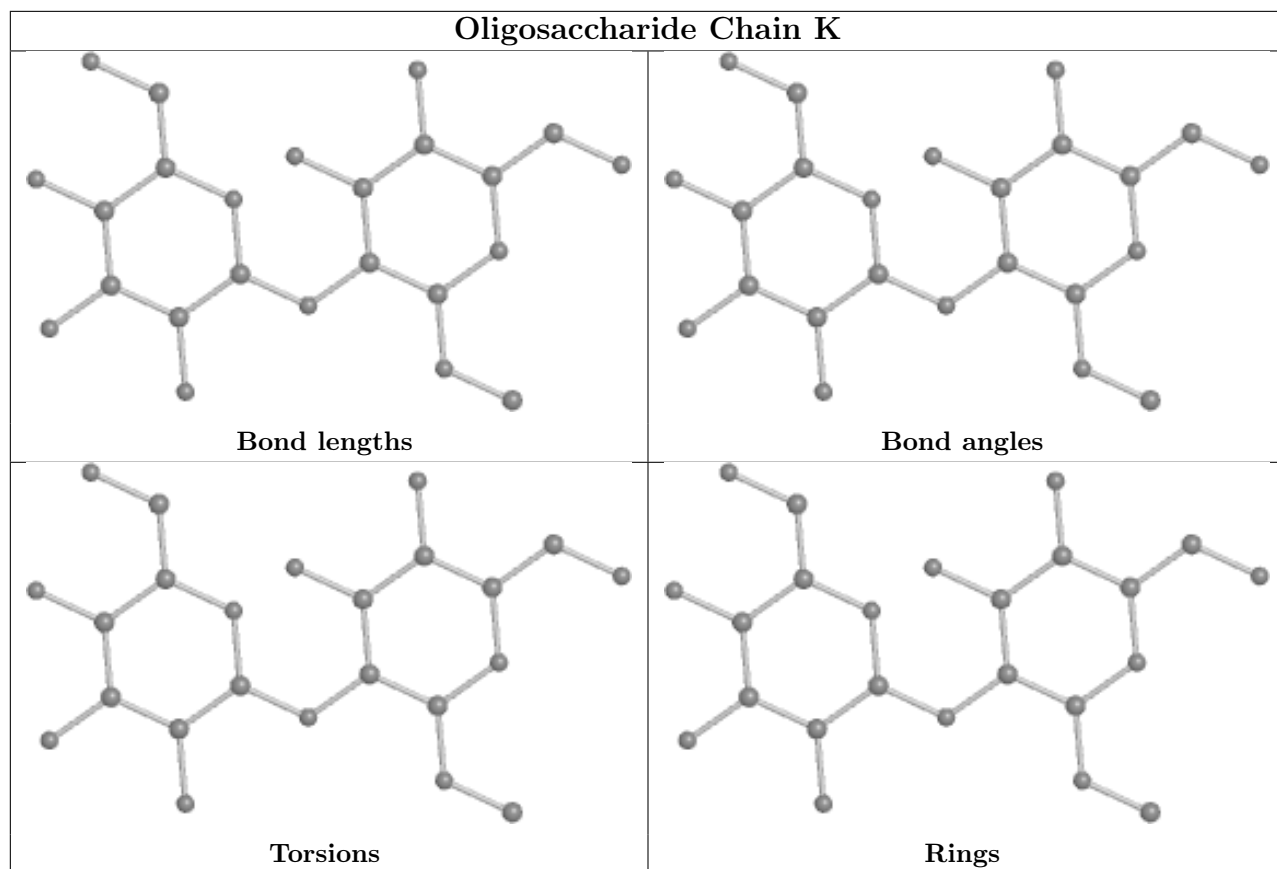
There are no torsion outliers.

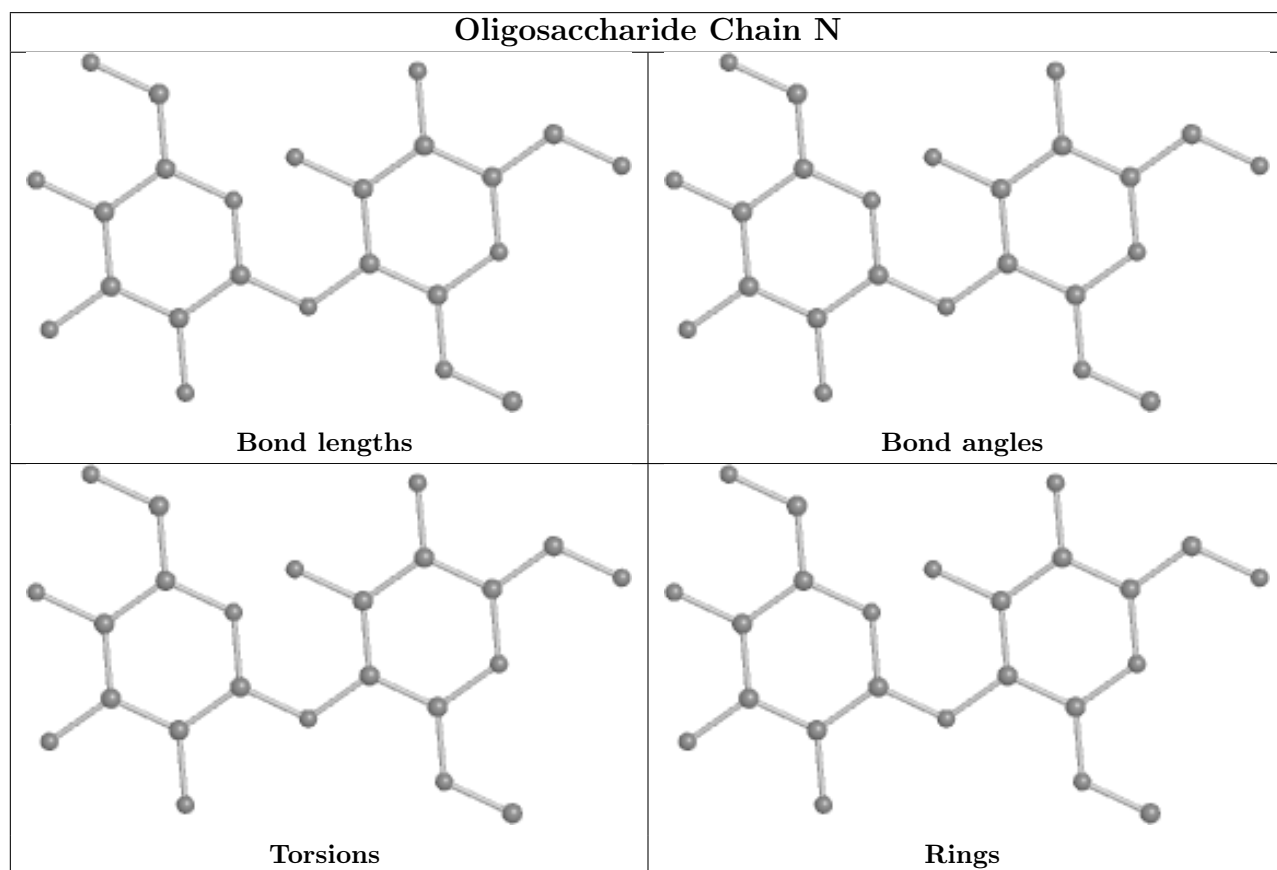
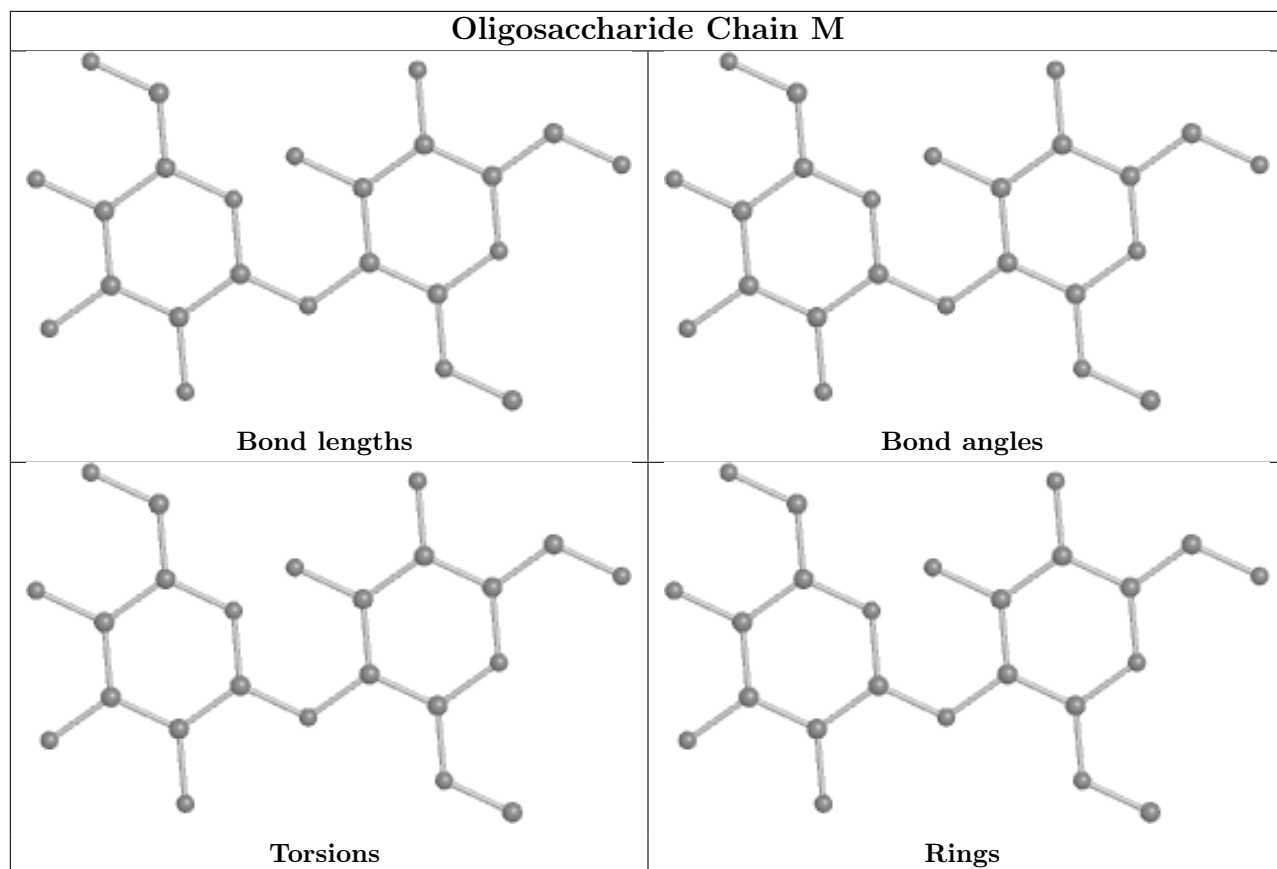
There are no ring outliers.

No monomer is involved in short contacts.

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







5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.