



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:16 PM UTC

PDB ID : 1LTE / pdb_00001lte
Title : STRUCTURE OF A LEGUME LECTIN WITH AN ORDERED N-LINKED CARBOHYDRATE IN COMPLEX WITH LACTOSE
Authors : Shaanan, B.; Lis, H.; Sharon, N.
Deposited on : 1991-06-25
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

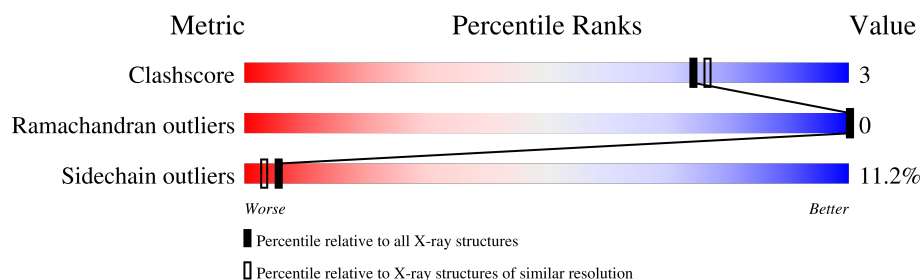
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

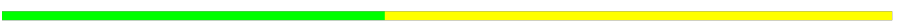
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	239	 71% 25% ..
2	B	7	 43% 57%
3	C	2	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2062 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 CORAL TREE LECTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1857	1188	302	364	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	SER	ALA	conflict	UNP P16404
A	114	GLN	ASN	conflict	UNP P16404
A	178	LEU	ILE	conflict	UNP P16404

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	0	0	0
			80	45	2	33			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Ca 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	100	Total 100	O 100	0	0

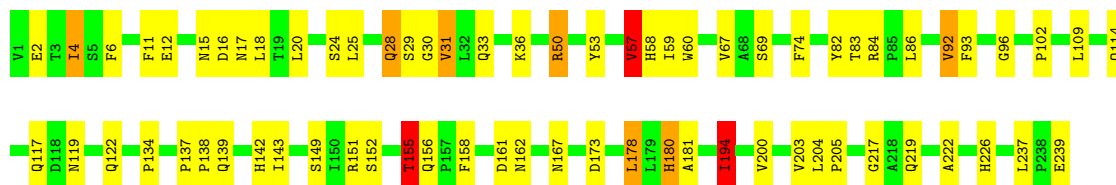
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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 was not executed.

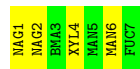
• Molecule 1: CORAL TREE LECTIN

Chain A: 

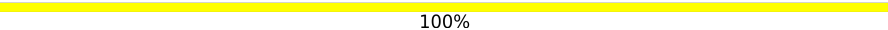


• Molecule 2: Xylitol-(1-2)-[alpha-D-mannopyranose-(1-3)][alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 



• Molecule 3: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain C: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	84.40Å 73.05Å 71.40Å 90.00° 113.42° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2062	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XYL, GAL, BMA, MN, FUC, CA, MAN, BGC, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.92	9/1908 (0.5%)	1.79	44/2606 (1.7%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	VAL	CA-CB	6.27	1.63	1.54
1	A	142	HIS	CD2-NE2	-5.74	1.31	1.37
1	A	57	VAL	CA-CB	5.47	1.62	1.54
1	A	226	HIS	CD2-NE2	-5.43	1.31	1.37
1	A	58	HIS	CD2-NE2	-5.37	1.31	1.37
1	A	142	HIS	CG-ND1	-5.32	1.32	1.38
1	A	180	HIS	CD2-NE2	-5.19	1.32	1.37
1	A	219	GLN	CD-OE1	5.14	1.33	1.23
1	A	58	HIS	CG-ND1	-5.02	1.32	1.38

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	HIS	CA-CB-CG	12.56	126.36	113.80
1	A	92	VAL	CB-CA-C	-8.96	94.66	110.71
1	A	203	VAL	N-CA-C	8.46	118.84	111.56
1	A	50	ARG	CB-CG-CD	-8.42	91.93	111.30
1	A	158	PHE	CA-CB-CG	8.34	122.14	113.80
1	A	162	ASN	OD1-CG-ND2	-8.09	114.51	122.60
1	A	93	PHE	N-CA-C	-8.09	96.06	109.24
1	A	6	PHE	CA-CB-CG	7.96	121.76	113.80
1	A	36	LYS	N-CA-C	7.58	121.22	110.23
1	A	226	HIS	ND1-CG-CD2	7.45	113.55	106.10
1	A	151	ARG	N-CA-CB	-7.39	99.56	110.49
1	A	50	ARG	NE-CZ-NH2	-7.25	112.67	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ILE	CB-CA-C	-7.15	98.07	111.30
1	A	16	ASP	CA-CB-CG	7.04	119.64	112.60
1	A	161	ASP	N-CA-C	-6.58	94.66	107.62
1	A	173	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	178	LEU	N-CA-CB	-6.43	99.94	110.42
1	A	217	GLY	N-CA-C	6.40	122.30	112.51
1	A	2	GLU	CA-CB-CG	6.37	126.84	114.10
1	A	119	ASN	CA-CB-CG	6.37	118.97	112.60
1	A	33	GLN	OE1-CD-NE2	-6.19	116.41	122.60
1	A	28	GLN	OE1-CD-NE2	-6.10	116.50	122.60
1	A	222	ALA	N-CA-C	-6.03	96.65	107.98
1	A	119	ASN	OD1-CG-ND2	-6.02	116.58	122.60
1	A	226	HIS	CG-CD2-NE2	-5.97	101.23	107.20
1	A	156	GLN	OE1-CD-NE2	-5.96	116.64	122.60
1	A	69	SER	N-CA-C	-5.92	100.63	110.17
1	A	74	PHE	CA-CB-CG	5.88	119.69	113.80
1	A	155	THR	N-CA-CB	-5.86	100.70	111.37
1	A	180	HIS	ND1-CG-CD2	5.85	111.95	106.10
1	A	109	LEU	N-CA-C	5.76	119.62	112.24
1	A	33	GLN	CG-CD-NE2	5.76	125.04	116.40
1	A	194	ILE	N-CA-CB	5.69	120.70	111.36
1	A	204	LEU	N-CA-C	5.60	118.02	110.29
1	A	167	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	A	4	ILE	N-CA-C	-5.46	100.37	108.45
1	A	17	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	A	53	TYR	N-CA-C	-5.30	102.44	110.28
1	A	152	SER	N-CA-C	5.25	117.64	110.24
1	A	84	ARG	CG-CD-NE	-5.19	100.58	112.00
1	A	96	GLY	CA-C-N	5.13	125.14	119.90
1	A	96	GLY	C-N-CA	5.13	125.14	119.90
1	A	226	HIS	CB-CG-CD2	-5.11	124.55	131.20
1	A	60	TRP	CA-CB-CG	5.07	123.23	113.60

There are no chirality outliers.

There are no planarity outliers.

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	1857	0	1789	12	0
2	B	80	0	68	0	0
3	C	23	0	21	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	100	0	0	1	0
All	All	2062	0	1878	12	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.

All (12) 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:A:134:PRO:HD3	6:A:814:HOH:O	1.96	0.64
1:A:137:PRO:HG3	1:A:155:THR:HG21	1.90	0.54
1:A:50:ARG:HD2	1:A:102:PRO:HG3	1.92	0.52
1:A:4:ILE:HD13	1:A:57:VAL:HG12	1.90	0.52
1:A:122:GLN:HB3	1:A:205:PRO:HD3	1.93	0.51
1:A:117:GLN:HG3	1:A:149:SER:HB2	1.94	0.50
1:A:181:ALA:HB3	1:A:194:ILE:CD1	2.42	0.50
1:A:138:PRO:HD2	1:A:139:GLN:OE1	2.13	0.48
1:A:181:ALA:HB3	1:A:194:ILE:HD13	1.95	0.47
1:A:11:PHE:O	1:A:30:GLY:HA2	2.15	0.46
1:A:59:ILE:HD12	1:A:59:ILE:HA	1.92	0.42
1:A:143:ILE:HG21	1:A:194:ILE:HD11	2.04	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	237/239 (99%)	232 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/205 (100%)	182 (89%)	23 (11%)	6	3

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	15	ASN
1	A	18	LEU
1	A	20	LEU
1	A	24	SER
1	A	25	LEU
1	A	28	GLN
1	A	29	SER
1	A	31	VAL
1	A	57	VAL
1	A	67	VAL
1	A	82	TYR
1	A	83	THR
1	A	86	LEU
1	A	92	VAL
1	A	114	GLN
1	A	155	THR
1	A	178	LEU
1	A	180	HIS
1	A	194	ILE
1	A	200	VAL
1	A	237	LEU
1	A	239	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

9 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	B	1	2,1	14,14,15	0.70	0	17,19,21	1.57	3 (17%)
2	NAG	B	2	2	14,14,15	0.49	0	17,19,21	0.91	1 (5%)
2	BMA	B	3	2	11,11,12	0.51	0	15,15,17	0.83	0
2	XYL	B	4	2	8,8,9	0.55	0	10,10,11	1.39	2 (20%)
2	MAN	B	5	2	11,11,12	0.78	0	15,15,17	0.86	0
2	MAN	B	6	2	11,11,12	0.59	0	15,15,17	1.03	1 (6%)
2	FUC	B	7	2	10,10,11	0.54	0	14,14,16	0.88	0
3	BGC	C	1	3	12,12,12	0.86	0	17,17,17	1.24	1 (5%)
3	GAL	C	2	3	11,11,12	0.67	0	15,15,17	1.17	3 (20%)

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	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	XYL	B	4	2	-	0/10/10/12	-
2	MAN	B	5	2	-	0/2/19/22	0/1/1/1
2	MAN	B	6	2	-	0/2/19/22	0/1/1/1
2	FUC	B	7	2	-	-	0/1/1/1
3	BGC	C	1	3	-	2/2/22/22	0/1/1/1
3	GAL	C	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	4.31	117.96	112.19
3	C	2	GAL	C1-O5-C5	2.87	116.04	112.19
2	B	1	NAG	C8-C7-N2	2.70	120.59	116.12
3	C	1	BGC	C1-O5-C5	2.63	118.74	113.65
2	B	4	XYL	C4-C3-C2	-2.54	108.56	112.48
2	B	1	NAG	O3-C3-C2	-2.28	104.67	109.40
2	B	4	XYL	O3-C3-C2	2.26	113.45	109.14
2	B	6	MAN	C1-O5-C5	2.18	115.10	112.19
2	B	2	NAG	C3-C4-C5	2.13	114.09	110.23
3	C	2	GAL	C2-C3-C4	-2.06	107.23	110.86
3	C	2	GAL	O2-C2-C1	2.04	113.89	109.22

There are no chirality outliers.

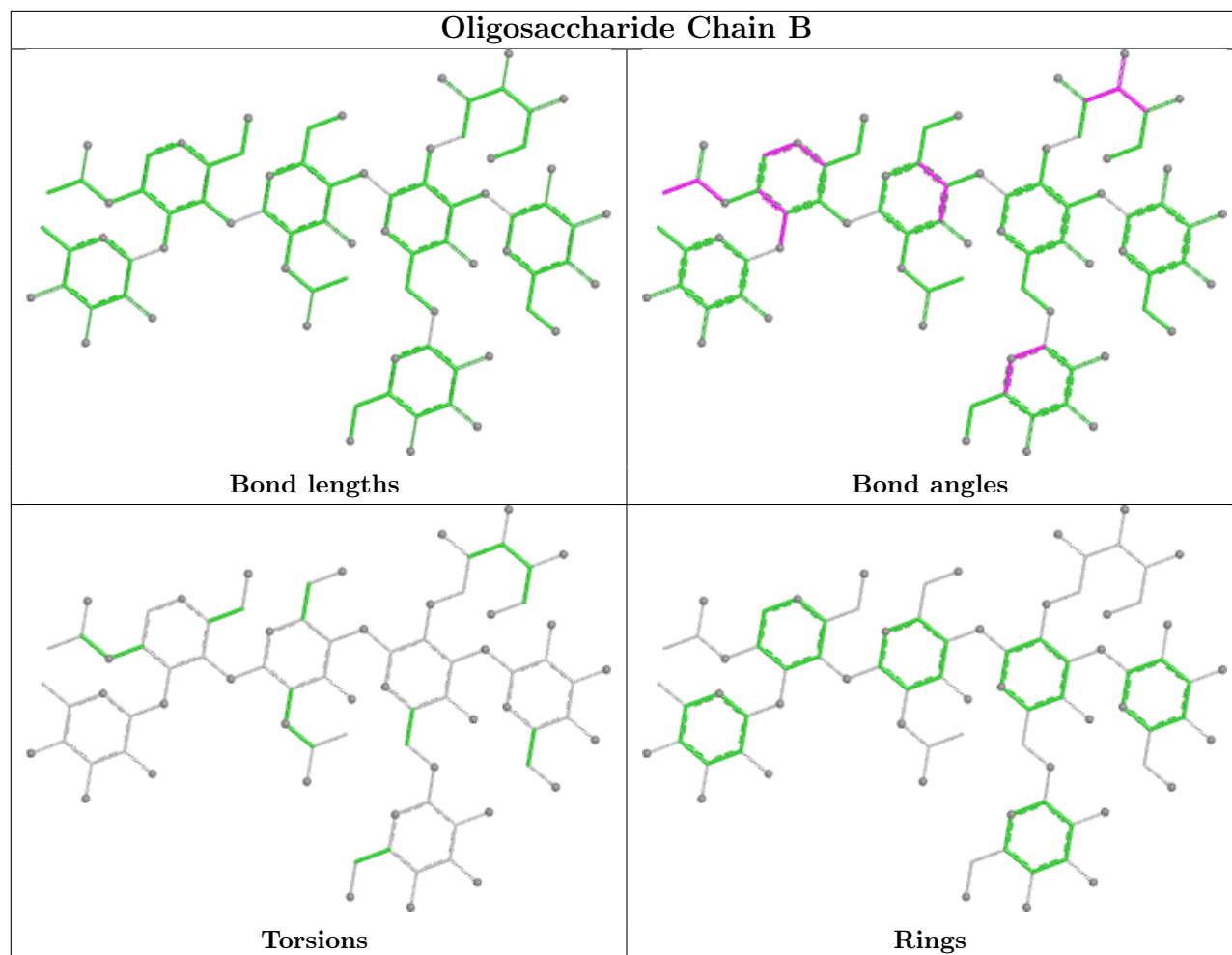
All (2) torsion outliers are listed below:

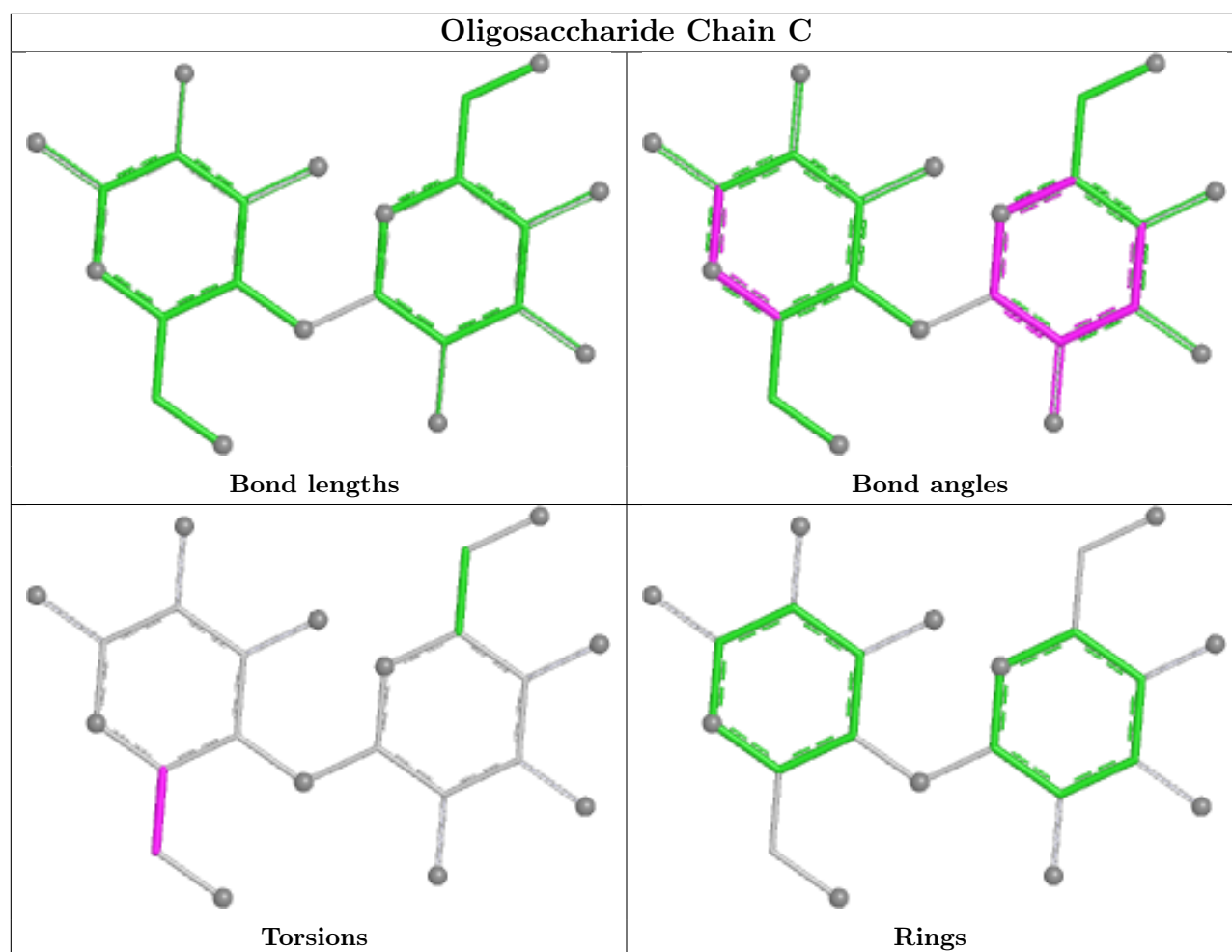
Mol	Chain	Res	Type	Atoms
3	C	1	BGC	C4-C5-C6-O6
3	C	1	BGC	O5-C5-C6-O6

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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.