



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2024 – 11:47 PM EDT

PDB ID : 1SLC
Title : X-RAY CRYSTALLOGRAPHY REVEALS CROSSLINKING OF MAMMALIAN LECTIN (GALECTIN-1) BY BIAN TENNARY COMPLEX TYPE SACCHARIDES
Authors : Bourne, Y.; Cambillau, C.
Deposited on : 1994-03-12
Resolution : 2.15 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

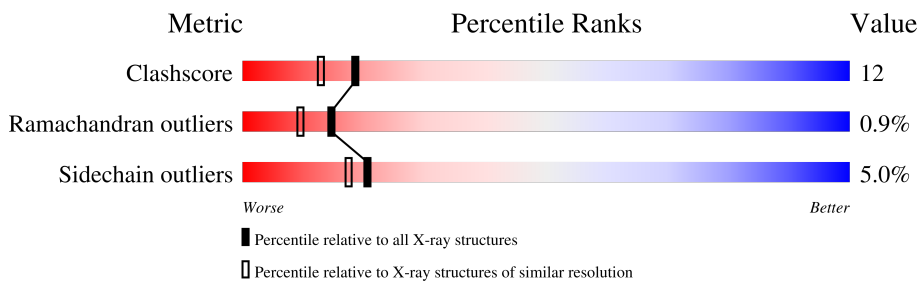
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)

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	134	<div> <div>74%</div> <div>24%</div> <div>.</div> </div>
1	B	134	<div> <div>72%</div> <div>26%</div> <div>..</div> </div>
1	C	134	<div> <div>70%</div> <div>26%</div> <div>...</div> </div>
1	D	134	<div> <div>75%</div> <div>22%</div> <div>..</div> </div>
2	E	8	<div> <div>62%</div> <div>38%</div> </div>
3	F	8	<div> <div>38%</div> <div>62%</div> </div>

2 Entry composition [i](#)

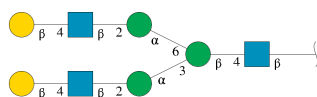
There are 4 unique types of molecules in this entry. The entry contains 4744 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BOVINE GALECTIN-1.

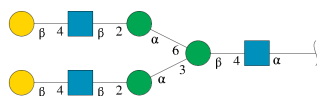
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	0	0
			1028	649	178	195	6			
1	B	134	Total	C	N	O	S	0	0	0
			1028	649	178	195	6			
1	C	133	Total	C	N	O	S	0	0	0
			1022	646	177	194	5			
1	D	134	Total	C	N	O	S	0	0	0
			1028	649	178	195	6			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	0	0	0
			98	54	3	41			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	8	Total	C	N	O	0	0	0
			98	54	3	41			

- Molecule 4 is water.

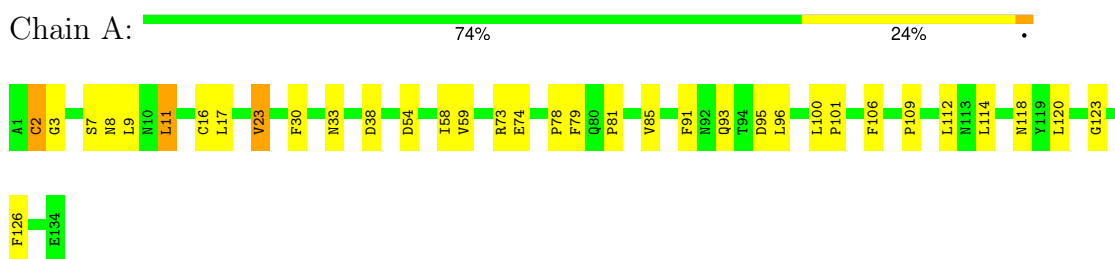
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total	O	0	0
			140	140		
4	B	115	Total	O	0	0
			115	115		
4	C	92	Total	O	0	0
			92	92		
4	D	95	Total	O	0	0
			95	95		

3 Residue-property plots [i](#)

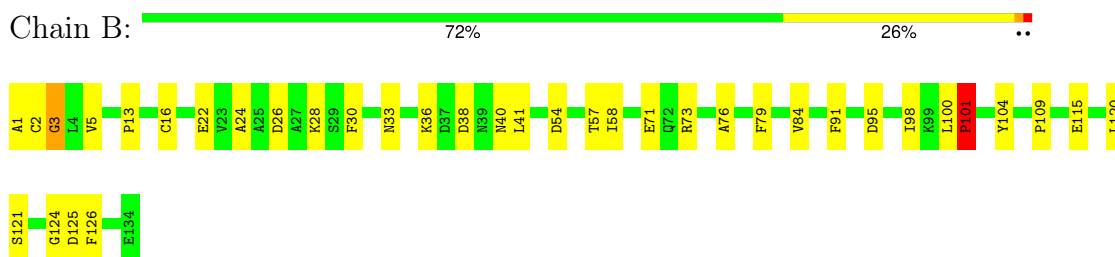
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

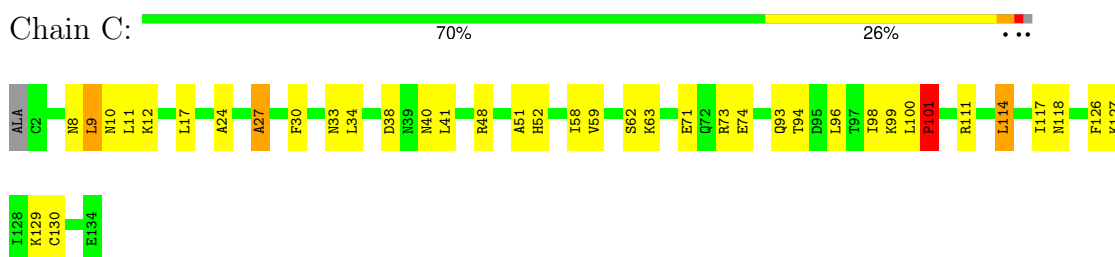
• Molecule 1: BOVINE GALECTIN-1



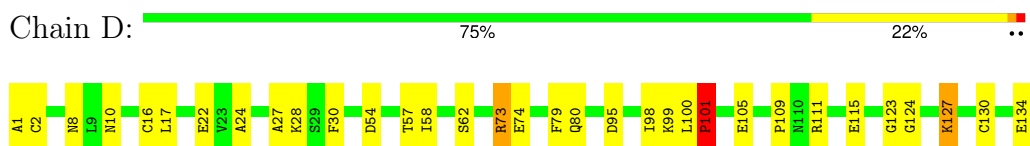
• Molecule 1: BOVINE GALECTIN-1



• Molecule 1: BOVINE GALECTIN-1



• Molecule 1: BOVINE GALECTIN-1



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

Chain E:  62% 38%

MAN1	MAN2	MAN3	MAN4	MAN5	MAN6	MAN7	MAN8
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- Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose

Chain F:  38% 62%

MAN1	MAN2	MAN3	MAN4	MAN5	MAN6	MAN7	MAN8
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	77.80Å 77.80Å 85.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.15	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.15)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4744	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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: MAN, NAG, GAL, NDG, 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	0.42	0/1049	0.67	0/1418
1	B	0.41	0/1049	0.69	1/1418 (0.1%)
1	C	0.41	0/1043	0.71	0/1410
1	D	0.39	0/1049	0.69	1/1418 (0.1%)
All	All	0.41	0/4190	0.69	2/5664 (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	B	3	GLY	N-CA-C	-5.83	98.54	113.10
1	D	101	PRO	N-CA-C	5.23	125.70	112.10

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	1028	0	1001	27	0
1	B	1028	0	1001	24	0
1	C	1022	0	990	29	0
1	D	1028	0	1001	19	0
2	E	98	0	84	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	98	0	81	0	0
4	A	140	0	0	5	0
4	B	115	0	0	3	0
4	C	92	0	0	1	0
4	D	95	0	0	2	0
All	All	4744	0	4158	98	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 12.

The worst 5 of 98 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:16:CYS:SG	1:D:134:GLU:HB2	2.19	0.82
1:A:112:LEU:HB3	1:A:114:LEU:HD13	1.63	0.79
1:D:22:GLU:O	1:D:127:LYS:HD2	1.89	0.73
1:B:36:LYS:HG2	1:B:40:ASN:HB2	1.72	0.71
1:B:100:LEU:HB3	1:B:101:PRO:HD2	1.72	0.71

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	132/134 (98%)	124 (94%)	8 (6%)	0	100	100
1	B	132/134 (98%)	121 (92%)	10 (8%)	1 (1%)	16	11
1	C	131/134 (98%)	123 (94%)	6 (5%)	2 (2%)	8	4
1	D	132/134 (98%)	126 (96%)	4 (3%)	2 (2%)	8	4
All	All	527/536 (98%)	494 (94%)	28 (5%)	5 (1%)	14	9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	PRO
1	C	27	ALA
1	D	27	ALA
1	C	101	PRO
1	D	101	PRO

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	110/110 (100%)	107 (97%)	3 (3%)	40	42
1	B	110/110 (100%)	106 (96%)	4 (4%)	30	29
1	C	109/110 (99%)	103 (94%)	6 (6%)	18	14
1	D	110/110 (100%)	101 (92%)	9 (8%)	9	5
All	All	439/440 (100%)	417 (95%)	22 (5%)	20	17

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	8	ASN
1	D	73	ARG
1	D	17	LEU
1	D	80	GLN
1	B	101	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	50	ASN
1	C	80	GLN
1	D	10	ASN
1	D	8	ASN
1	B	50	ASN

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 ⓘ

16 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	15,15,15	0.47	0	21,21,21	0.71	0
2	BMA	E	2	2	11,11,12	0.64	0	15,15,17	0.55	0
2	MAN	E	3	2	11,11,12	0.42	0	15,15,17	0.71	1 (6%)
2	NAG	E	4	2	14,14,15	0.35	0	17,19,21	0.64	0
2	GAL	E	5	2	11,11,12	0.37	0	15,15,17	0.50	0
2	MAN	E	6	2	11,11,12	0.42	0	15,15,17	1.23	3 (20%)
2	NAG	E	7	2	14,14,15	0.51	0	17,19,21	0.89	1 (5%)
2	GAL	E	8	2	11,11,12	0.33	0	15,15,17	0.38	0
3	NDG	F	1	3	15,15,15	0.96	1 (6%)	21,21,21	1.11	2 (9%)
3	BMA	F	2	3	11,11,12	0.90	1 (9%)	15,15,17	0.79	1 (6%)
3	MAN	F	3	3	11,11,12	0.59	0	15,15,17	0.78	0
3	NAG	F	4	3	14,14,15	0.53	0	17,19,21	1.01	1 (5%)
3	GAL	F	5	3	11,11,12	0.36	0	15,15,17	0.55	0
3	MAN	F	6	3	11,11,12	0.45	0	15,15,17	0.91	1 (6%)
3	NAG	F	7	3	14,14,15	0.55	0	17,19,21	1.04	1 (5%)
3	GAL	F	8	3	11,11,12	0.36	0	15,15,17	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2	-	0/6/26/26	0/1/1/1
2	BMA	E	2	2	-	0/2/19/22	0/1/1/1
2	MAN	E	3	2	-	0/2/19/22	0/1/1/1
2	NAG	E	4	2	-	1/6/23/26	0/1/1/1
2	GAL	E	5	2	-	0/2/19/22	0/1/1/1
2	MAN	E	6	2	-	0/2/19/22	0/1/1/1
2	NAG	E	7	2	-	0/6/23/26	0/1/1/1
2	GAL	E	8	2	-	0/2/19/22	0/1/1/1
3	NDG	F	1	3	-	2/6/26/26	0/1/1/1
3	BMA	F	2	3	-	0/2/19/22	0/1/1/1
3	MAN	F	3	3	-	0/2/19/22	0/1/1/1
3	NAG	F	4	3	-	1/6/23/26	0/1/1/1
3	GAL	F	5	3	-	0/2/19/22	0/1/1/1
3	MAN	F	6	3	-	1/2/19/22	0/1/1/1
3	NAG	F	7	3	-	1/6/23/26	0/1/1/1
3	GAL	F	8	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NDG	C1-C2	2.26	1.55	1.52
3	F	2	BMA	C2-C3	2.07	1.55	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	6	MAN	C1-O5-C5	2.88	116.05	112.19
3	F	4	NAG	C2-N2-C7	-2.84	119.09	122.90
3	F	2	BMA	C1-C2-C3	2.73	113.62	109.64
3	F	7	NAG	C2-N2-C7	-2.73	119.25	122.90
2	E	6	MAN	C1-O5-C5	2.72	115.84	112.19

There are no chirality outliers.

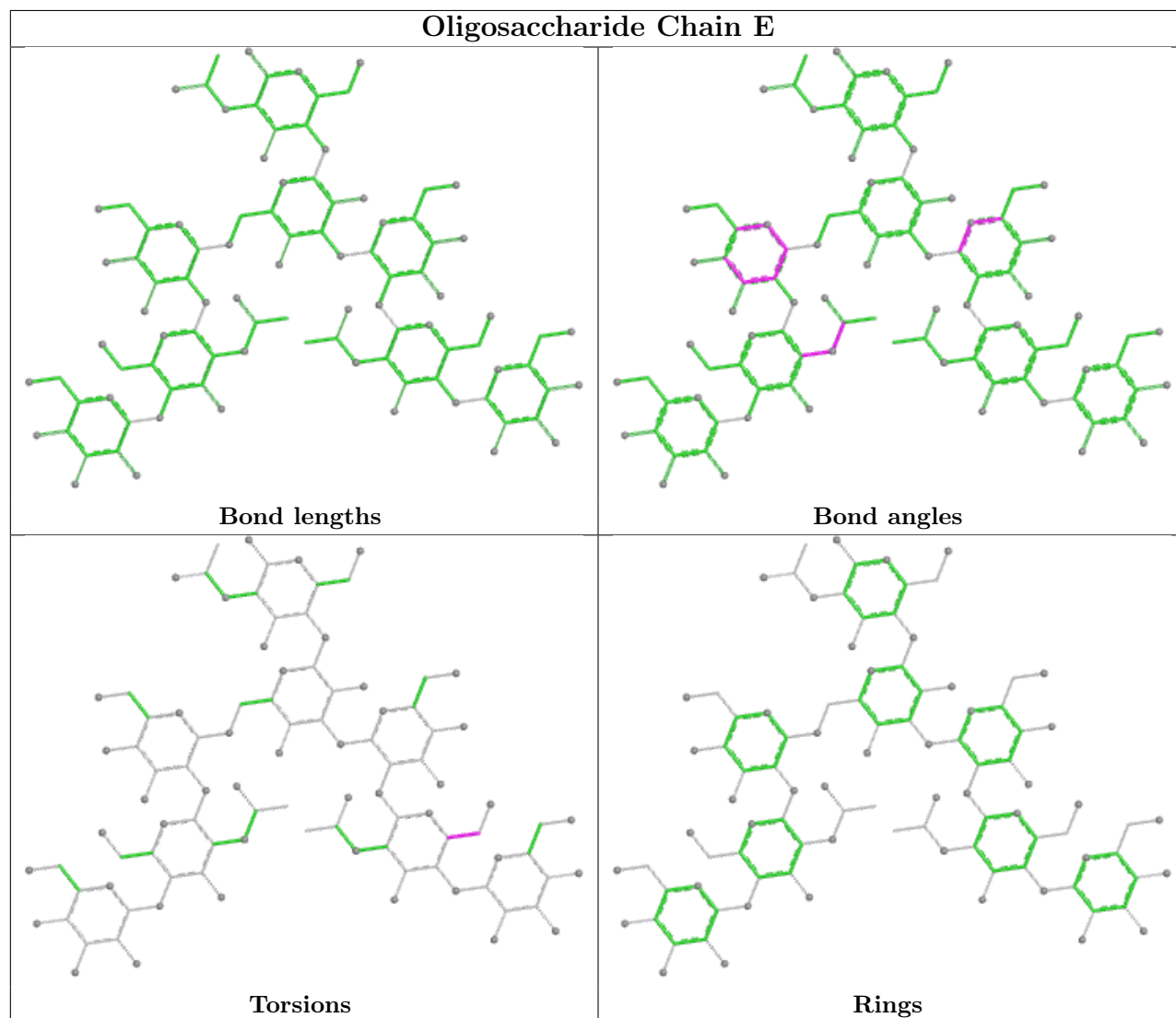
5 of 6 torsion outliers are listed below:

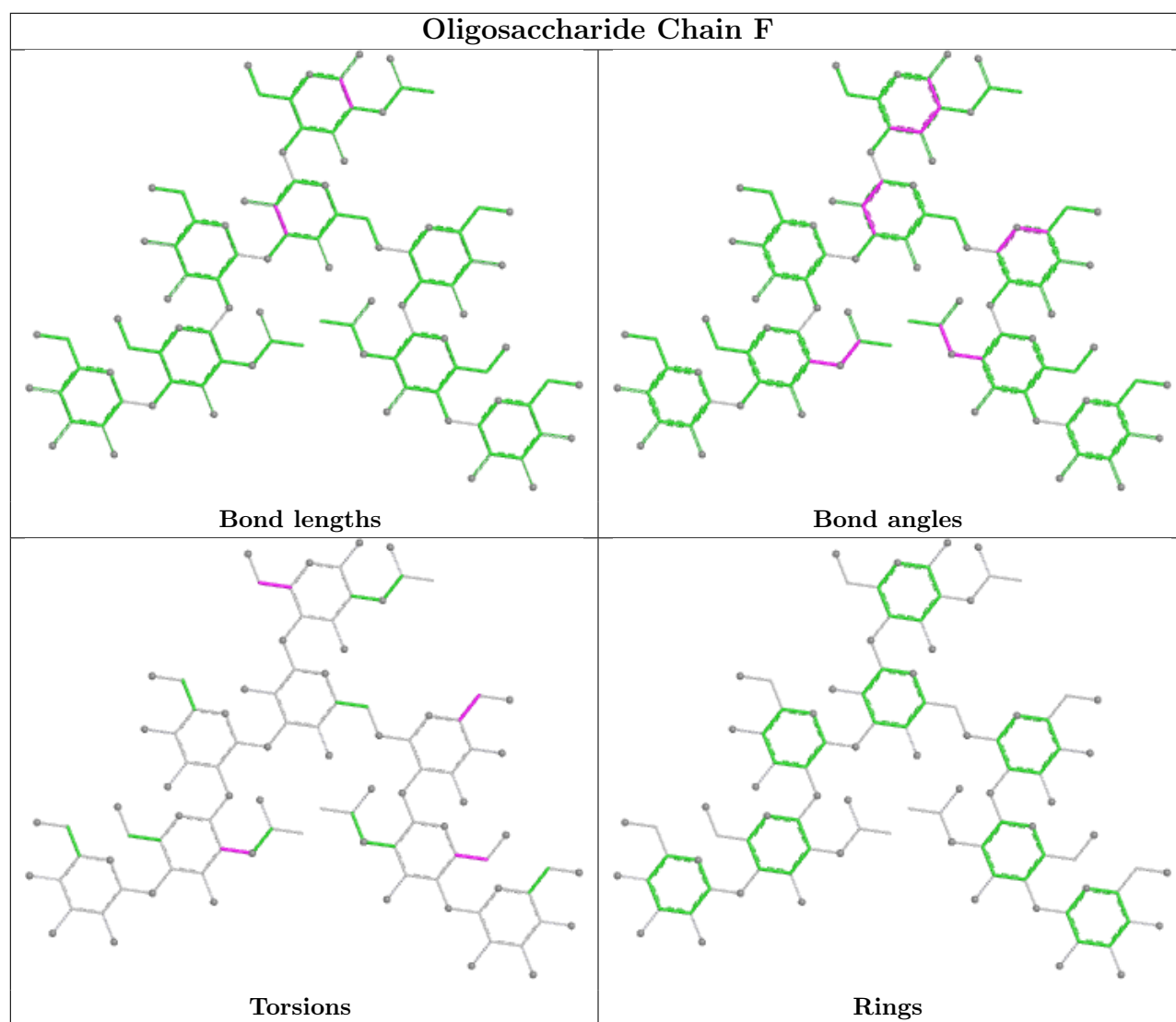
Mol	Chain	Res	Type	Atoms
2	E	4	NAG	O5-C5-C6-O6
3	F	1	NDG	C4-C5-C6-O6
3	F	1	NDG	O5-C5-C6-O6
3	F	7	NAG	C4-C5-C6-O6
3	F	4	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 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.