



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:38 PM UTC

PDB ID : 1BHG / pdb_00001bhg
Title : HUMAN BETA-GLUCURONIDASE AT 2.6 Å RESOLUTION
Authors : Jain, S.; Drendel, W.B.
Deposited on : 1996-03-04
Resolution : 2.53 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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

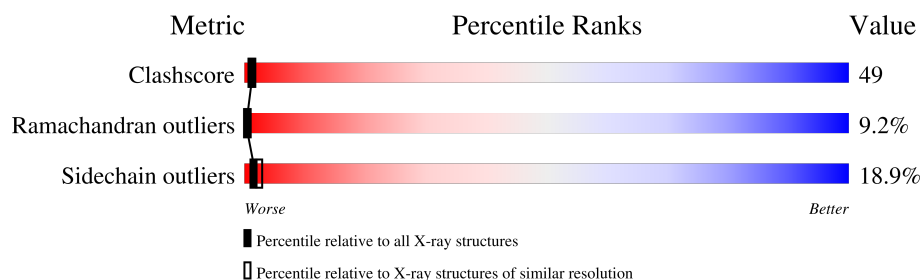
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)

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	613	28% 47% 19% 5%
1	B	613	25% 48% 23% .
2	C	9	33% 56% 11%
2	D	9	22% 44% 33%

2 Entry composition [i](#)

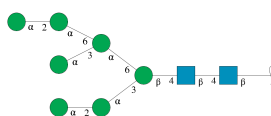
There are 2 unique types of molecules in this entry. The entry contains 10190 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BETA-GLUCURONIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4990	3216	848	911	15			
1	B	611	Total	C	N	O	S	0	0	0
			4990	3216	848	911	15			

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



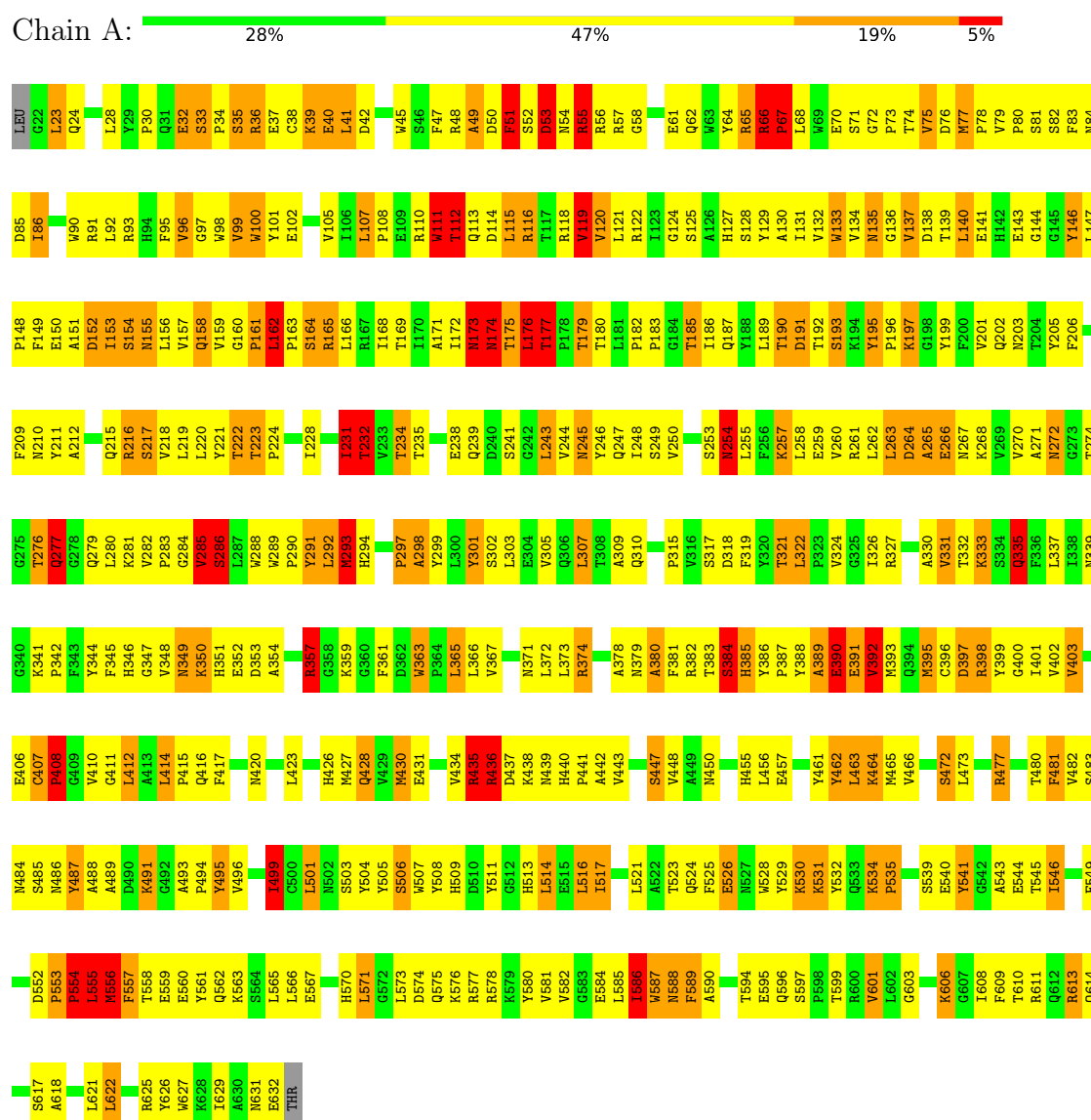
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			105	58	2	45			
2	D	9	Total	C	N	O	0	0	0
			105	58	2	45			

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.

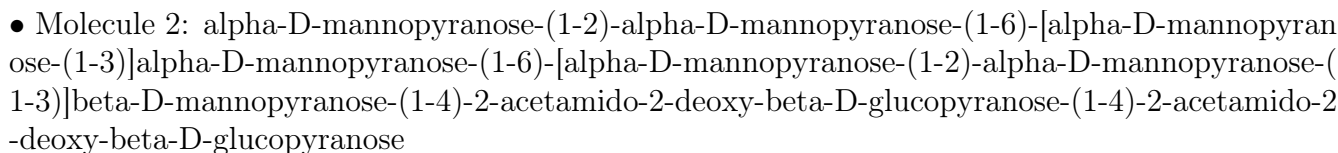
Note EDS was not executed.

• Molecule 1: BETA-GLUCURONIDASE



• Molecule 1: BETA-GLUCURONIDASE





NAG1	NAG2	BMA3	MAN4	MAN5	MAN6	MAN7	MAN8	MAN9
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- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.10Å 124.40Å 134.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.53	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.53)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.231 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10190	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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: BMA, NAG, MAN

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	0.90	4/5139 (0.1%)	1.34	79/7000 (1.1%)
1	B	0.91	3/5139 (0.1%)	1.36	79/7000 (1.1%)
All	All	0.91	7/10278 (0.1%)	1.35	158/14000 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	2
All	All	0	7

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	395	MET	SD-CE	7.86	1.99	1.79
1	B	556	MET	SD-CE	7.11	1.97	1.79
1	A	430	MET	SD-CE	-6.70	1.62	1.79
1	B	393	MET	SD-CE	5.58	1.93	1.79
1	A	177	THR	N-CA	5.38	1.50	1.46

The worst 5 of 158 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	MET	N-CA-C	11.04	127.36	112.68
1	A	36	ARG	N-CA-C	10.80	126.13	109.60
1	A	173	ASN	N-CA-C	10.00	124.84	110.14
1	B	37	GLU	N-CA-C	9.81	122.99	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	472	SER	N-CA-C	-8.93	97.64	110.59

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	TYR	Sidechain
1	A	436	ARG	Sidechain
1	A	462	TYR	Sidechain
1	A	511	TYR	Sidechain
1	A	541	TYR	Sidechain

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	4990	0	4846	439	0
1	B	4990	0	4845	533	0
2	C	105	0	88	4	0
2	D	105	0	88	7	0
All	All	10190	0	9867	975	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 49.

The worst 5 of 975 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ARG:HH21	1:B:153:ILE:HA	1.25	0.99
1:A:107:LEU:HG	1:A:156:LEU:HD21	1.42	0.99
1:A:156:LEU:HD11	1:A:166:LEU:HD13	1.43	0.99
1:B:146:TYR:HB3	1:B:216:ARG:HH22	1.30	0.97
1:B:162:LEU:HB2	1:B:163:PRO:HD3	1.48	0.94

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	609/613 (99%)	462 (76%)	99 (16%)	48 (8%)	1	0
1	B	609/613 (99%)	442 (73%)	103 (17%)	64 (10%)	0	0
All	All	1218/1226 (99%)	904 (74%)	202 (17%)	112 (9%)	0	0

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	SER
1	A	35	SER
1	A	52	SER
1	A	115	LEU
1	A	137	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	540/542 (100%)	440 (82%)	100 (18%)	1	3
1	B	540/542 (100%)	436 (81%)	104 (19%)	1	2
All	All	1080/1084 (100%)	876 (81%)	204 (19%)	1	2

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	92	LEU

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Mol	Chain	Res	Type
1	B	236	SER
1	B	602	LEU
1	B	106	ILE
1	B	172	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	239	GLN
1	B	385	HIS
1	B	279	GLN
1	B	351	HIS
1	B	424	HIS

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 ⓘ

18 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	C	1	1,2	14,14,15	0.87	1 (7%)	17,19,21	1.00	2 (11%)
2	NAG	C	2	2	14,14,15	0.57	0	17,19,21	0.67	0
2	BMA	C	3	2	11,11,12	0.38	0	15,15,17	0.94	1 (6%)
2	MAN	C	4	2	11,11,12	0.86	0	15,15,17	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	C	5	2	11,11,12	0.79	0	15,15,17	0.79	1 (6%)
2	MAN	C	6	2	11,11,12	0.50	0	15,15,17	0.93	1 (6%)
2	MAN	C	7	2	11,11,12	0.67	0	15,15,17	0.84	0
2	MAN	C	8	2	11,11,12	0.59	0	15,15,17	0.60	0
2	MAN	C	9	2	11,11,12	0.62	0	15,15,17	1.47	2 (13%)
2	NAG	D	1	1,2	14,14,15	0.88	1 (7%)	17,19,21	0.52	0
2	NAG	D	2	2	14,14,15	0.58	0	17,19,21	0.76	0
2	BMA	D	3	2	11,11,12	0.70	0	15,15,17	0.74	0
2	MAN	D	4	2	11,11,12	0.56	0	15,15,17	1.23	1 (6%)
2	MAN	D	5	2	11,11,12	0.65	0	15,15,17	0.85	1 (6%)
2	MAN	D	6	2	11,11,12	0.61	0	15,15,17	0.68	1 (6%)
2	MAN	D	7	2	11,11,12	0.57	0	15,15,17	1.00	1 (6%)
2	MAN	D	8	2	11,11,12	0.36	0	15,15,17	0.78	1 (6%)
2	MAN	D	9	2	11,11,12	0.51	0	15,15,17	0.94	1 (6%)

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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	1/2/19/22	1/1/1/1
2	MAN	C	7	2	-	1/2/19/22	0/1/1/1
2	MAN	C	8	2	-	1/2/19/22	0/1/1/1
2	MAN	C	9	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	0/2/19/22	0/1/1/1
2	MAN	D	5	2	-	2/2/19/22	0/1/1/1
2	MAN	D	6	2	-	0/2/19/22	1/1/1/1
2	MAN	D	7	2	-	0/2/19/22	0/1/1/1
2	MAN	D	8	2	-	0/2/19/22	0/1/1/1
2	MAN	D	9	2	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	C1-C2	2.58	1.55	1.52
2	D	1	NAG	C1-C2	2.34	1.55	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	9	MAN	C1-C2-C3	4.55	116.27	109.64
2	C	6	MAN	C1-O5-C5	2.97	116.17	112.19
2	D	7	MAN	C1-O5-C5	2.90	116.07	112.19
2	D	4	MAN	C1-O5-C5	2.83	115.98	112.19
2	D	5	MAN	C1-O5-C5	2.54	115.59	112.19

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	D	5	MAN	O5-C5-C6-O6
2	D	5	MAN	C4-C5-C6-O6
2	C	6	MAN	O5-C5-C6-O6

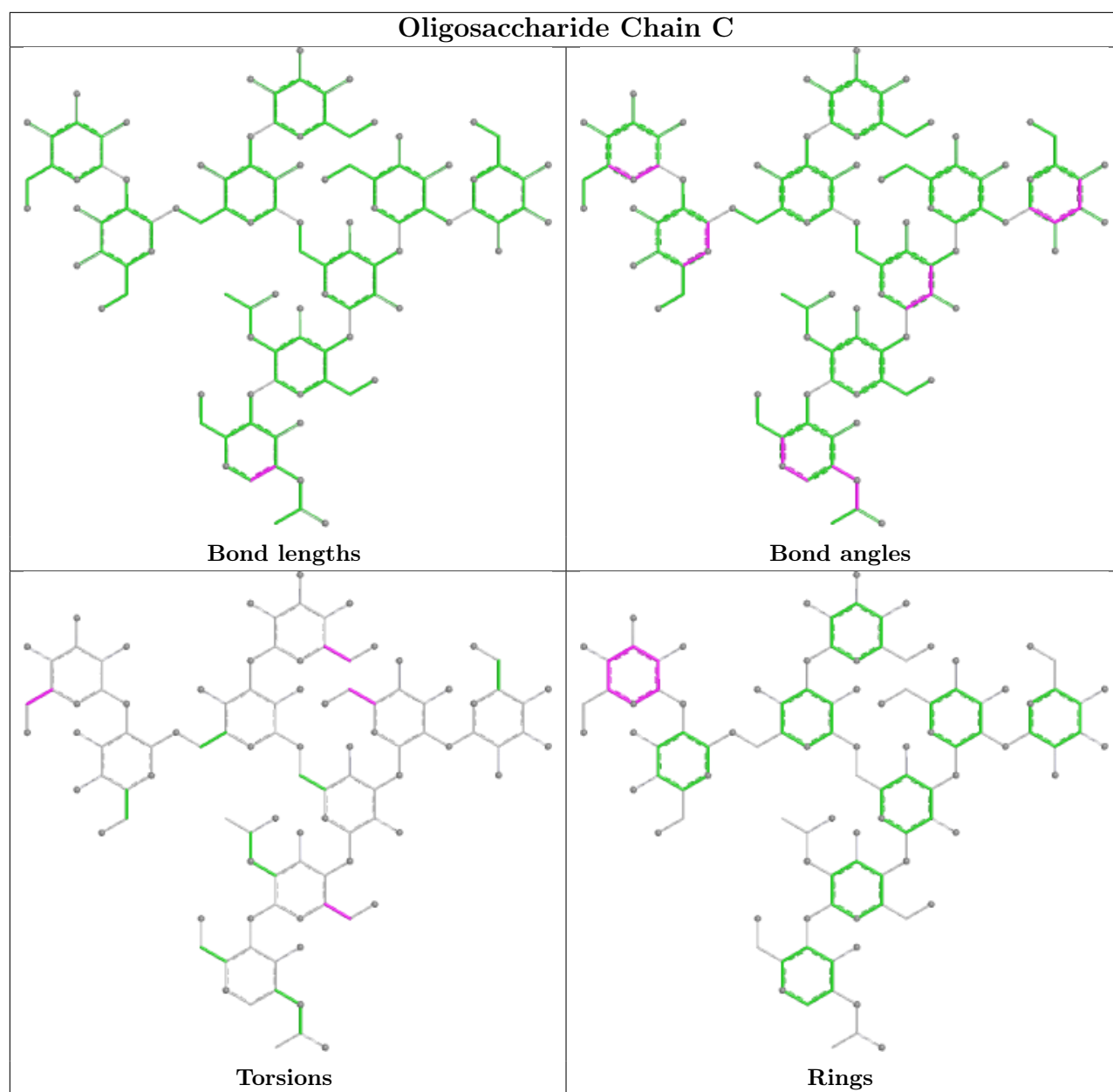
All (2) ring outliers are listed below:

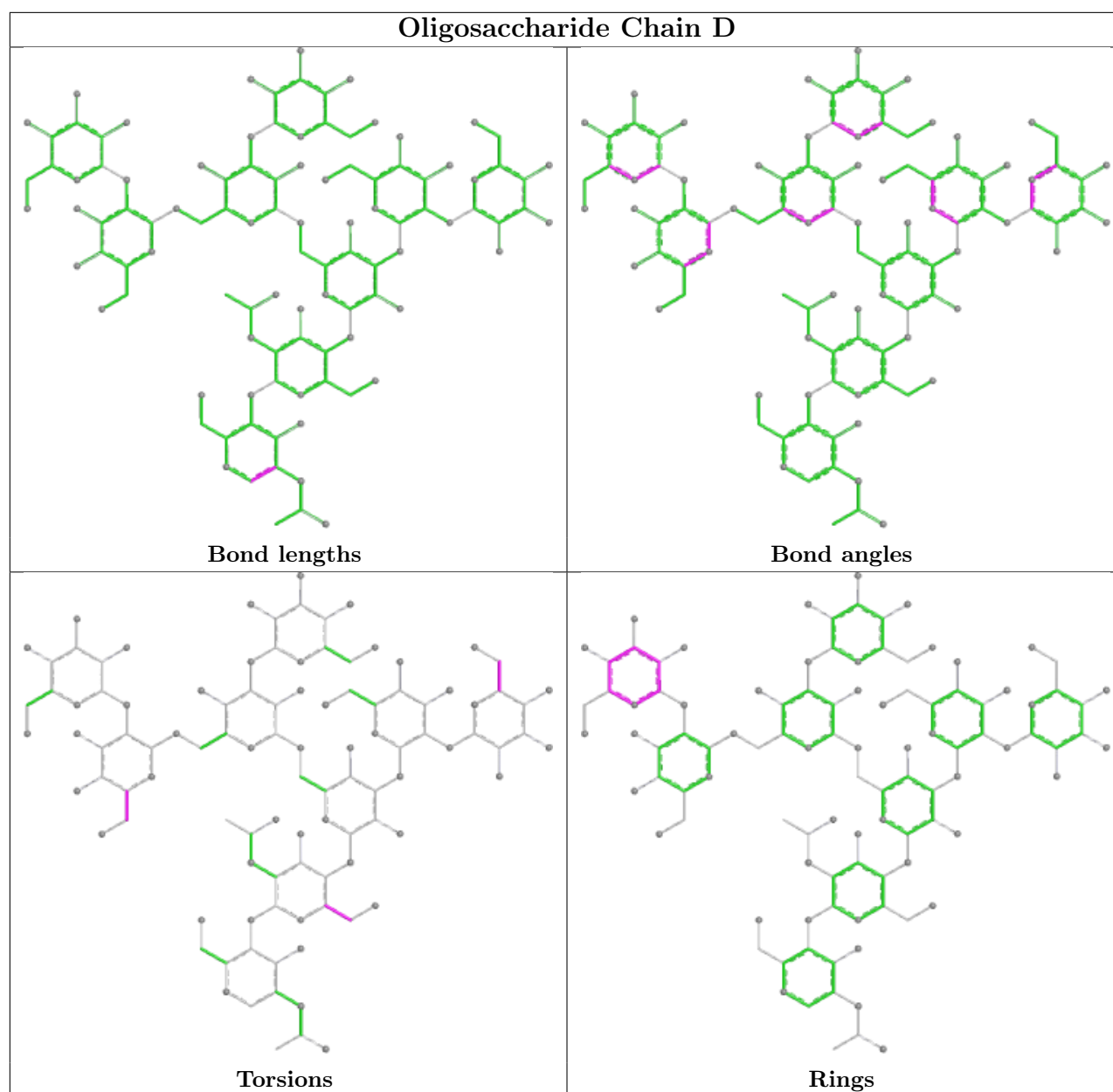
Mol	Chain	Res	Type	Atoms
2	D	6	MAN	C1-C2-C3-C4-C5-O5
2	C	6	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	5	0
2	D	5	MAN	1	0
2	D	8	MAN	1	0
2	C	6	MAN	3	0
2	C	8	MAN	1	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.





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.