



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 13, 2024 – 11:00 AM EDT

PDB ID : 1LT5  
Title : HEAT-LABILE ENTEROTOXIN B-PENTAMER COMPLEXED WITH  
THIODIGALACTOSIDE  
Authors : Merritt, E.A.; Hol, W.G.J.  
Deposited on : 1997-09-30  
Resolution : 1.70 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](mailto: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>.

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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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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) : 2.36.2

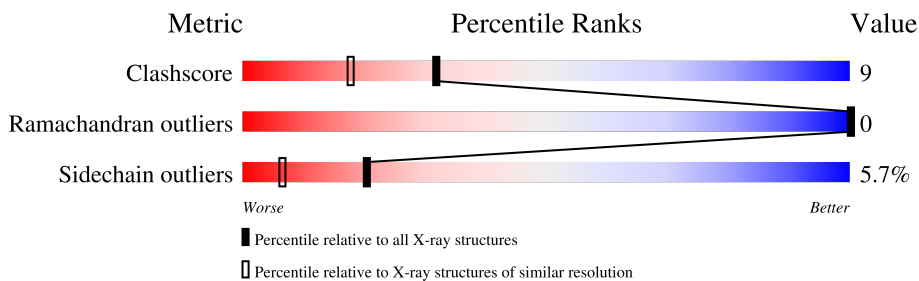
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

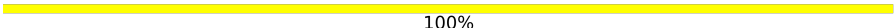

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	D	103	89% 8% .
1	E	103	74% 21% . .
1	F	103	79% 17% .
1	G	103	73% 23% . .
1	H	103	86% 11% .
2	K	2	50% 50%
2	L	2	100%
2	M	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	N	2	 100%
2	O	2	 50% 50%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4650 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 HEAT-LABILE ENTEROTOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	103	824	516	139	163	6	0	0	0
1	E	103	824	516	139	163	6	0	0	0
1	F	103	824	516	139	163	6	0	0	0
1	G	103	824	516	139	163	6	0	0	0
1	H	103	824	516	139	163	6	0	0	0

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-1)-1-thio-beta-D-galactopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	O	S			
2	K	2	23	12	10	1	0	0	0
2	L	2	23	12	10	1	0	0	0
2	M	2	23	12	10	1	0	0	0
2	N	2	23	12	10	1	0	0	0
2	O	2	23	12	10	1	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	D	76	76	76	0	0
3	E	77	77	77	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
3	F	92	Total O 92 92	0	0
3	G	86	Total O 86 86	0	0
3	H	84	Total O 84 84	0	0

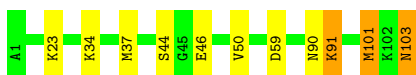
### 3 Residue-property plots [i](#)

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 was not executed.

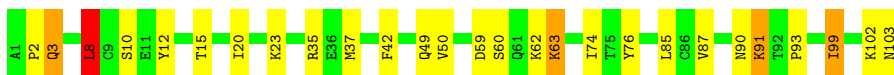
- Molecule 1: HEAT-LABILE ENTEROTOXIN

Chain D:  89% 8%




- Molecule 1: HEAT-LABILE ENTEROTOXIN

Chain E:  74% 21%



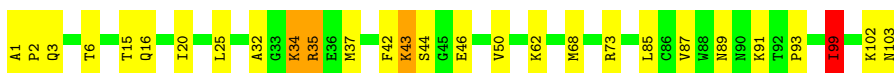
- Molecule 1: HEAT-LABILE ENTEROTOXIN

Chain F:  79% 17%



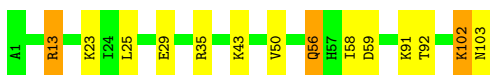
- Molecule 1: HEAT-LABILE ENTEROTOXIN

Chain G:  73% 23%



- Molecule 1: HEAT-LABILE ENTEROTOXIN

Chain H:  86% 11%



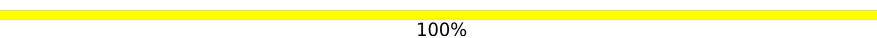
- Molecule 2: beta-D-galactopyranose-(1-1)-1-thio-beta-D-galactopyranose

Chain K:  50% 50%



Y101  
GAL2

- Molecule 2: beta-D-galactopyranose-(1-1)-1-thio-beta-D-galactopyranose

Chain L:  100%



Y101  
GAL2

- Molecule 2: beta-D-galactopyranose-(1-1)-1-thio-beta-D-galactopyranose

Chain M:  50% 50%



Y101  
GAL2

- Molecule 2: beta-D-galactopyranose-(1-1)-1-thio-beta-D-galactopyranose

Chain N:  100%



Y101  
GAL2

- Molecule 2: beta-D-galactopyranose-(1-1)-1-thio-beta-D-galactopyranose

Chain O:  50% 50%



Y101  
GAL2

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.68Å 100.13Å 63.67Å 90.00° 107.66° 90.00°	Depositor
Resolution (Å)	25.00 – 1.70	Depositor
% Data completeness (in resolution range)	73.0 (25.00-1.70)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	4650	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	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: GAL, YIO

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	D	0.45	0/835	0.71	1/1124 (0.1%)
1	E	0.44	0/835	0.74	2/1124 (0.2%)
1	F	0.46	0/835	0.72	1/1124 (0.1%)
1	G	0.54	1/835 (0.1%)	0.79	3/1124 (0.3%)
1	H	0.57	0/835	0.74	1/1124 (0.1%)
All	All	0.49	1/4175 (0.0%)	0.74	8/5620 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	68	MET	CG-SD	-5.11	1.67	1.81

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	50	VAL	N-CA-C	-6.29	94.01	111.00
1	E	50	VAL	N-CA-C	-6.08	94.59	111.00
1	F	50	VAL	N-CA-C	-5.76	95.45	111.00
1	G	50	VAL	N-CA-C	-5.70	95.60	111.00
1	G	99	ILE	CB-CA-C	-5.63	100.34	111.60

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	D	824	0	841	11	0
1	E	824	0	841	22	0
1	F	824	0	841	19	0
1	G	824	0	841	26	0
1	H	824	0	841	14	0
2	K	23	0	21	0	0
2	L	23	0	21	1	0
2	M	23	0	21	1	0
2	N	23	0	21	0	0
2	O	23	0	21	1	0
3	D	76	0	0	4	0
3	E	77	0	0	2	0
3	F	92	0	0	2	0
3	G	86	0	0	6	0
3	H	84	0	0	6	0
All	All	4650	0	4310	76	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 9.

The worst 5 of 76 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:E:3:GLN:HG3	1:F:93:PRO:HG3	1.54	0.89
1:G:1:ALA:HB1	1:H:92:THR:O	1.76	0.85
1:F:71:THR:O	1:F:75:THR:HG23	1.80	0.80
1:G:6:THR:HG23	3:G:139:HOH:O	1.90	0.71
1:D:103:ASN:HB3	1:E:23:LYS:NZ	2.09	0.68

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	D	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
1	E	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
1	F	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
1	G	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
1	H	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
All	All	505/515 (98%)	497 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	D	95/95 (100%)	91 (96%)	4 (4%)	30	12
1	E	95/95 (100%)	88 (93%)	7 (7%)	13	3
1	F	95/95 (100%)	88 (93%)	7 (7%)	13	3
1	G	95/95 (100%)	90 (95%)	5 (5%)	22	7
1	H	95/95 (100%)	91 (96%)	4 (4%)	30	12
All	All	475/475 (100%)	448 (94%)	27 (6%)	20	6

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	63	LYS
1	F	102	LYS
1	H	56	GLN
1	F	92	THR
1	G	34	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	56	GLN
1	H	94	ASN
1	E	94	ASN
1	F	94	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](#)

10 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	YIO	K	1	2	11,12,12	1.21	0	15,17,17	1.42	1 (6%)
2	GAL	K	2	2	11,11,12	0.82	0	15,15,17	0.91	0
2	YIO	L	1	2	11,12,12	0.68	0	15,17,17	0.86	0
2	GAL	L	2	2	11,11,12	1.03	2 (18%)	15,15,17	1.15	0
2	YIO	M	1	2	11,12,12	1.03	1 (9%)	15,17,17	1.12	2 (13%)
2	GAL	M	2	2	11,11,12	0.86	0	15,15,17	1.84	2 (13%)
2	YIO	N	1	2	11,12,12	1.02	1 (9%)	15,17,17	1.38	2 (13%)
2	GAL	N	2	2	11,11,12	1.19	1 (9%)	15,15,17	1.35	1 (6%)
2	YIO	O	1	2	11,12,12	0.63	0	15,17,17	1.05	1 (6%)
2	GAL	O	2	2	11,11,12	1.09	2 (18%)	15,15,17	1.36	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	YIO	K	1	2	-	0/2/22/22	0/1/1/1
2	GAL	K	2	2	-	0/2/19/22	0/1/1/1
2	YIO	L	1	2	-	0/2/22/22	0/1/1/1
2	GAL	L	2	2	-	0/2/19/22	0/1/1/1
2	YIO	M	1	2	-	0/2/22/22	0/1/1/1
2	GAL	M	2	2	-	0/2/19/22	0/1/1/1
2	YIO	N	1	2	-	0/2/22/22	0/1/1/1
2	GAL	N	2	2	-	0/2/19/22	0/1/1/1
2	YIO	O	1	2	-	0/2/22/22	0/1/1/1
2	GAL	O	2	2	-	0/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	2	GAL	C1-C2	3.51	1.60	1.52
2	N	1	YIO	C1-C2	-2.48	1.49	1.53
2	M	1	YIO	O3-C3	-2.30	1.37	1.43
2	L	2	GAL	C4-C3	2.29	1.58	1.52
2	L	2	GAL	C4-C5	2.21	1.57	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	2	GAL	O3-C3-C2	-5.21	100.03	109.99
2	N	2	GAL	O5-C1-C2	-4.18	104.33	110.77
2	K	1	YIO	O5-C1-C2	-3.57	105.82	110.31
2	N	1	YIO	C1-C2-C3	-3.07	104.52	110.59
2	O	2	GAL	C1-O5-C5	-2.74	108.48	112.19

There are no chirality outliers.

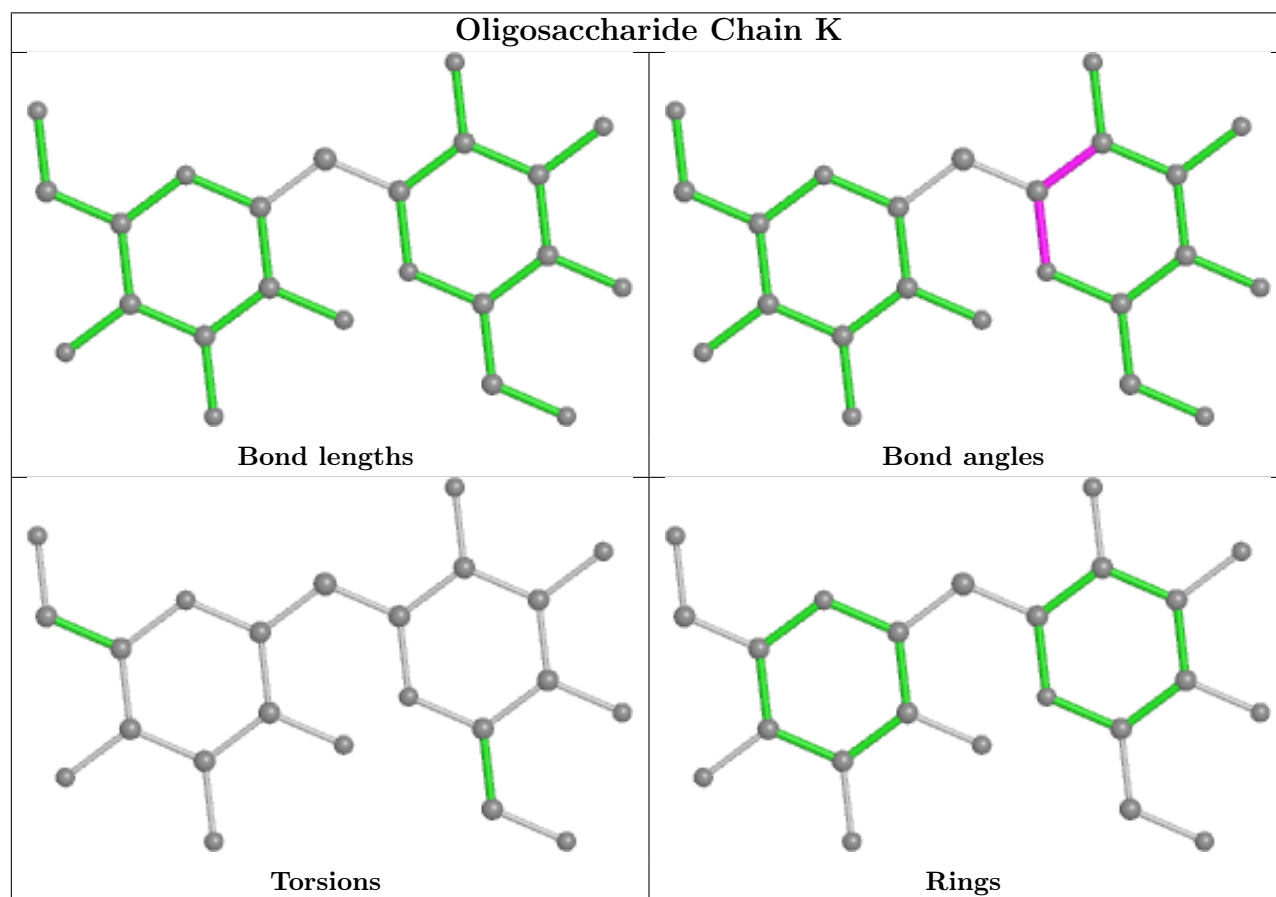
There are no torsion outliers.

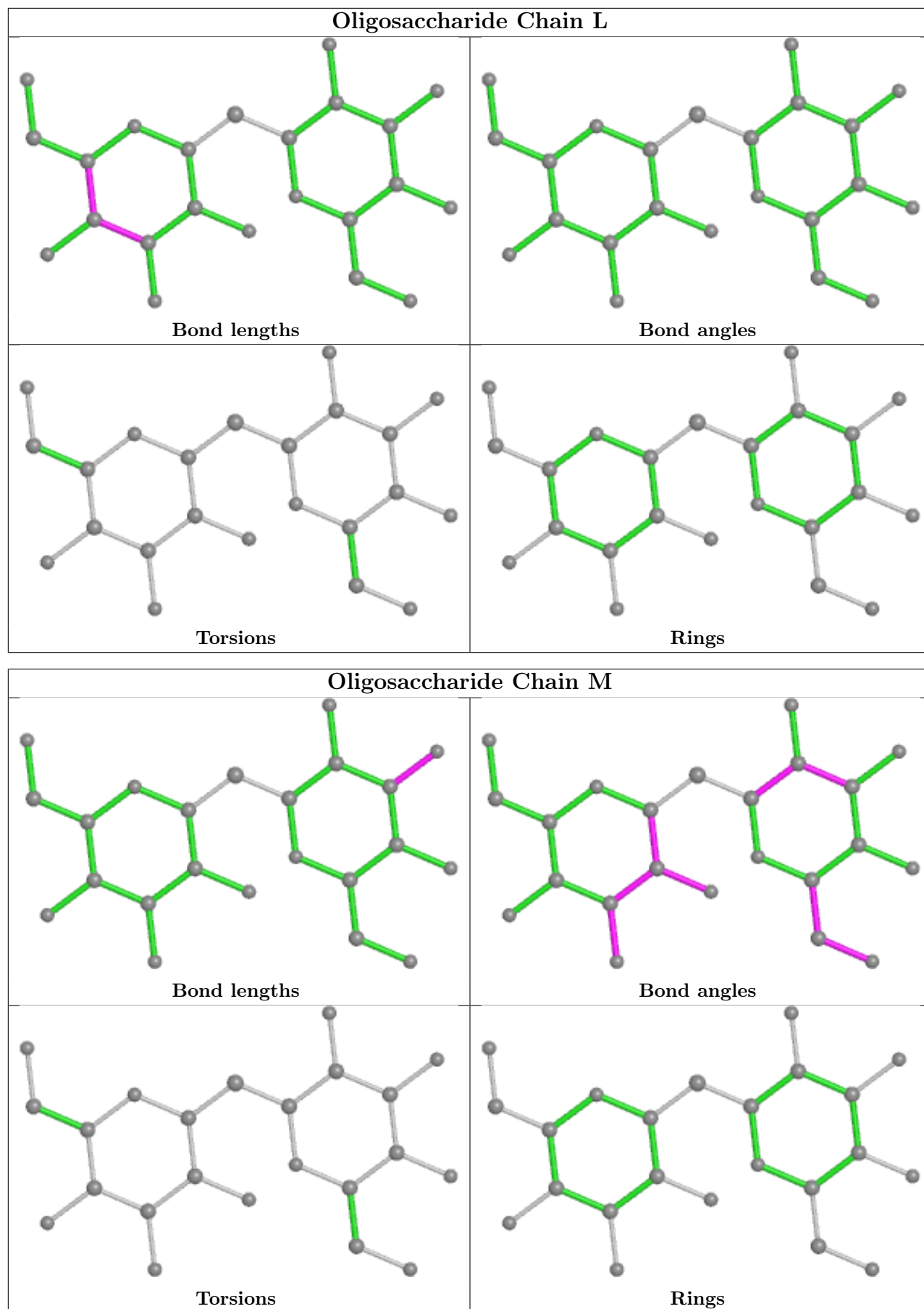
There are no ring outliers.

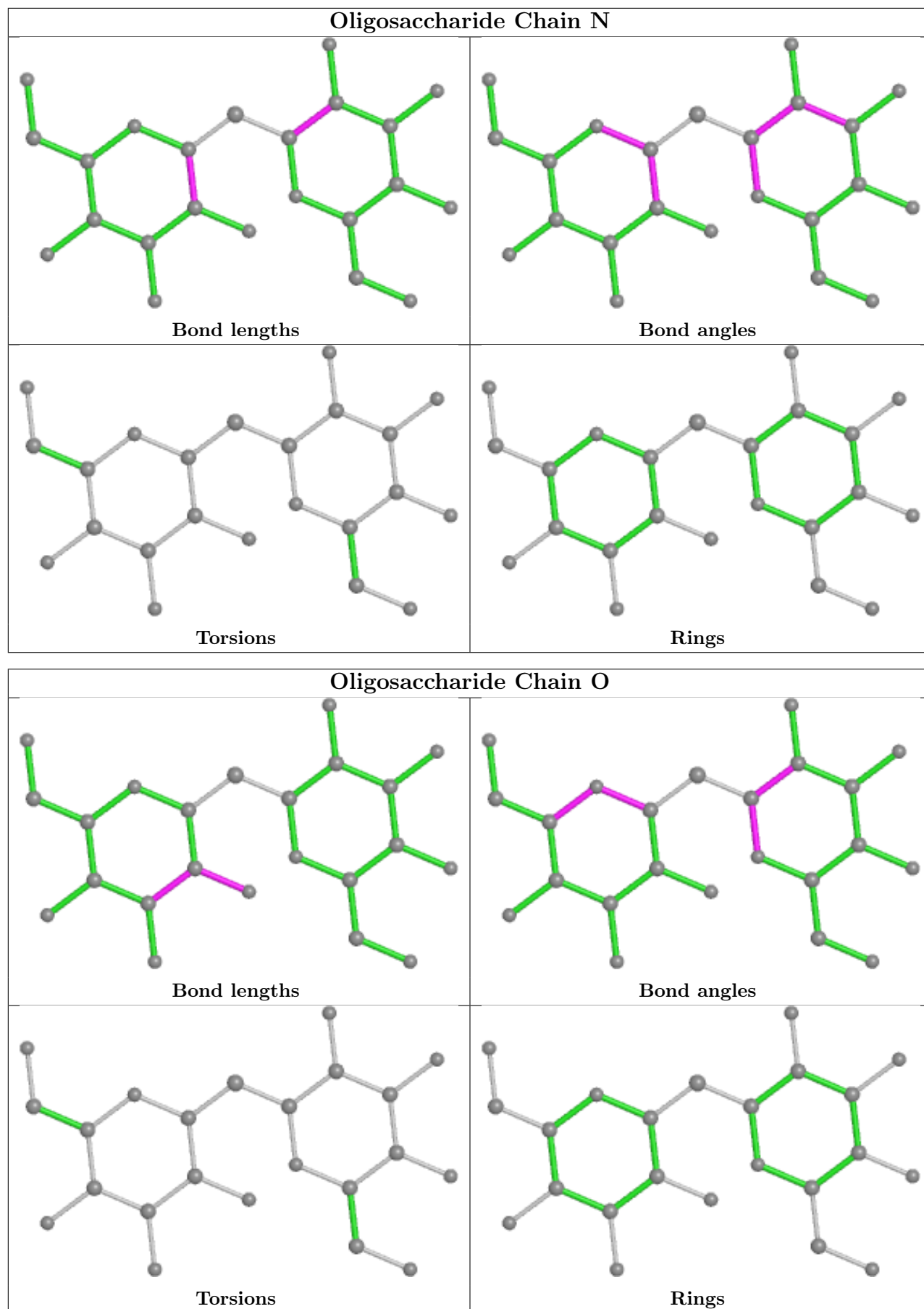
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	1	YIO	1	0
2	O	2	GAL	1	0
2	L	1	YIO	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.