



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1PV7 / pdb_00001pv7
Title : Crystal structure of lactose permease with TDG
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Deposited on : 2003-06-26
Resolution : 3.60 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

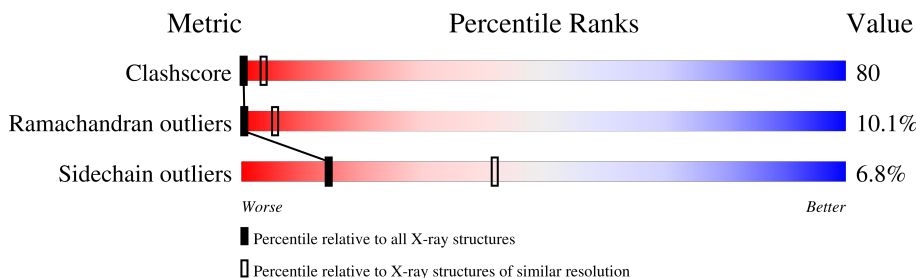
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)

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	417	18% 62% 19% .
1	B	417	20% 62% 17% .
2	E	2	100%
2	F	2	100%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6626 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 Lactose permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3290	2222	506	541	21			
1	B	417	Total	C	N	O	S	0	0	0
			3290	2222	506	541	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	GLY	CYS	engineered mutation	UNP P02920
B	154	GLY	CYS	engineered mutation	UNP P02920

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

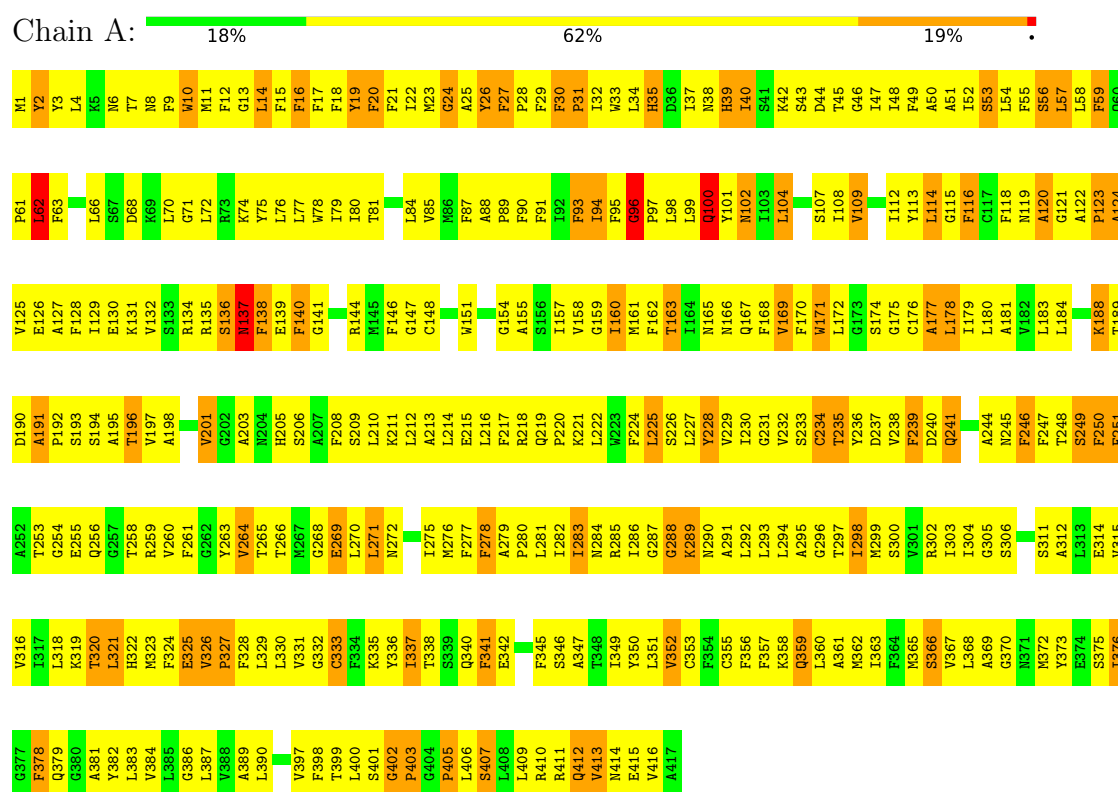
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	S	0	0	0
			23	12	10	1			
2	F	2	Total	C	O	S	0	0	0
			23	12	10	1			

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.

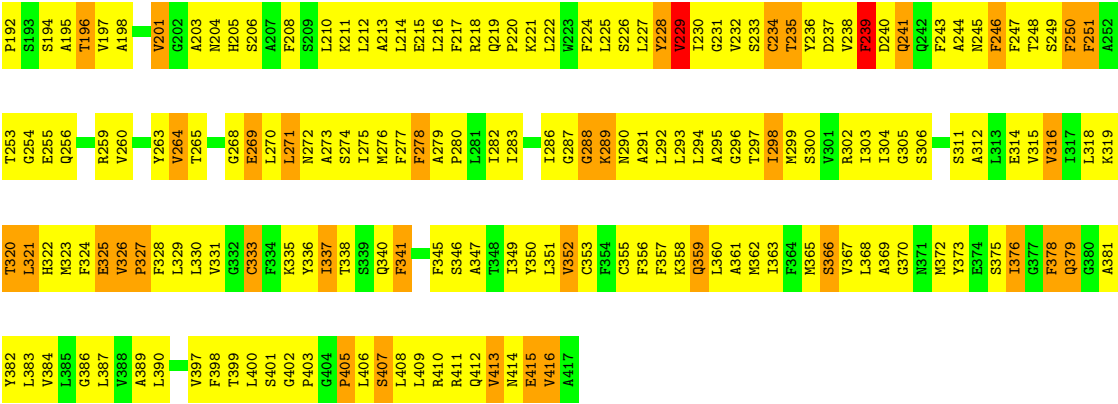
Note EDS was not executed.

- Molecule 1: Lactose permease



- Molecule 1: Lactose permease





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

Chain E: 100%



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

Chain F: 100%



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 21	Depositor
Cell constants a, b, c, α , β , γ	101.35Å 125.84Å 188.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	4.00 – 3.60	Depositor
% Data completeness (in resolution range)	(Not available) (4.00-3.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.271 , 0.296	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6626	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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: YIO, GAL

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	0.83	1/3387 (0.0%)	1.25	39/4588 (0.9%)
1	B	0.79	1/3387 (0.0%)	1.24	35/4588 (0.8%)
All	All	0.81	2/6774 (0.0%)	1.25	74/9176 (0.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	40	ILE	CA-CB	-5.88	1.47	1.54
1	A	40	ILE	CA-CB	-5.81	1.47	1.54

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	LEU	N-CA-C	-12.63	97.18	111.71
1	A	114	LEU	N-CA-C	-12.36	97.49	111.71
1	A	232	VAL	N-CA-C	10.94	121.77	110.72
1	B	232	VAL	N-CA-C	10.94	121.77	110.72
1	A	140	PHE	N-CA-C	-8.33	102.88	112.87

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	3290	0	3333	541	0
1	B	3290	0	3333	527	0
2	E	23	0	21	0	0
2	F	23	0	21	0	0
All	All	6626	0	6708	1064	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 80.

The worst 5 of 1064 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:30:PHE:HB3	1:A:31:PRO:HD3	1.29	1.10
1:B:87:PHE:HB3	1:B:174:SER:HB2	1.36	1.08
1:B:256:GLN:OE1	1:B:259:ARG:HD2	1.54	1.07
1:B:30:PHE:HB3	1:B:31:PRO:HD3	1.31	1.07
1:A:293:LEU:HD13	1:A:397:VAL:HG22	1.36	1.06

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	415/417 (100%)	261 (63%)	114 (28%)	40 (10%)	0	6
1	B	415/417 (100%)	261 (63%)	110 (26%)	44 (11%)	0	5
All	All	830/834 (100%)	522 (63%)	224 (27%)	84 (10%)	0	5

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	HIS

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Mol	Chain	Res	Type
1	A	102	ASN
1	A	160	ILE
1	A	196	THR
1	A	407	SER

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	345/345 (100%)	322 (93%)	23 (7%)	15	42
1	B	345/345 (100%)	321 (93%)	24 (7%)	14	41
All	All	690/690 (100%)	643 (93%)	47 (7%)	14	42

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	59	PHE
1	B	239	PHE
1	B	62	LEU
1	B	136	SER
1	B	246	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	137	ASN
1	B	290	ASN
1	B	272	ASN
1	B	340	GLN
1	A	242	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 ⓘ

4 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	E	1	2	11,12,12	1.63	3 (27%)	15,17,17	0.84	0
2	GAL	E	2	2	11,11,12	2.25	5 (45%)	15,15,17	0.89	0
2	YIO	F	1	2	11,12,12	1.75	4 (36%)	15,17,17	0.84	0
2	GAL	F	2	2	11,11,12	1.79	3 (27%)	15,15,17	0.86	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	YIO	E	1	2	-	0/2/22/22	0/1/1/1
2	GAL	E	2	2	-	0/2/19/22	0/1/1/1
2	YIO	F	1	2	-	0/2/22/22	0/1/1/1
2	GAL	F	2	2	-	1/2/19/22	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	GAL	C4-C5	3.99	1.61	1.53
2	E	2	GAL	C4-C3	3.90	1.62	1.52
2	F	2	GAL	C4-C3	3.41	1.61	1.52
2	F	1	YIO	O5-C1	3.39	1.47	1.42
2	F	2	GAL	C4-C5	3.11	1.59	1.53

There are no bond angle outliers.

There are no chirality outliers.

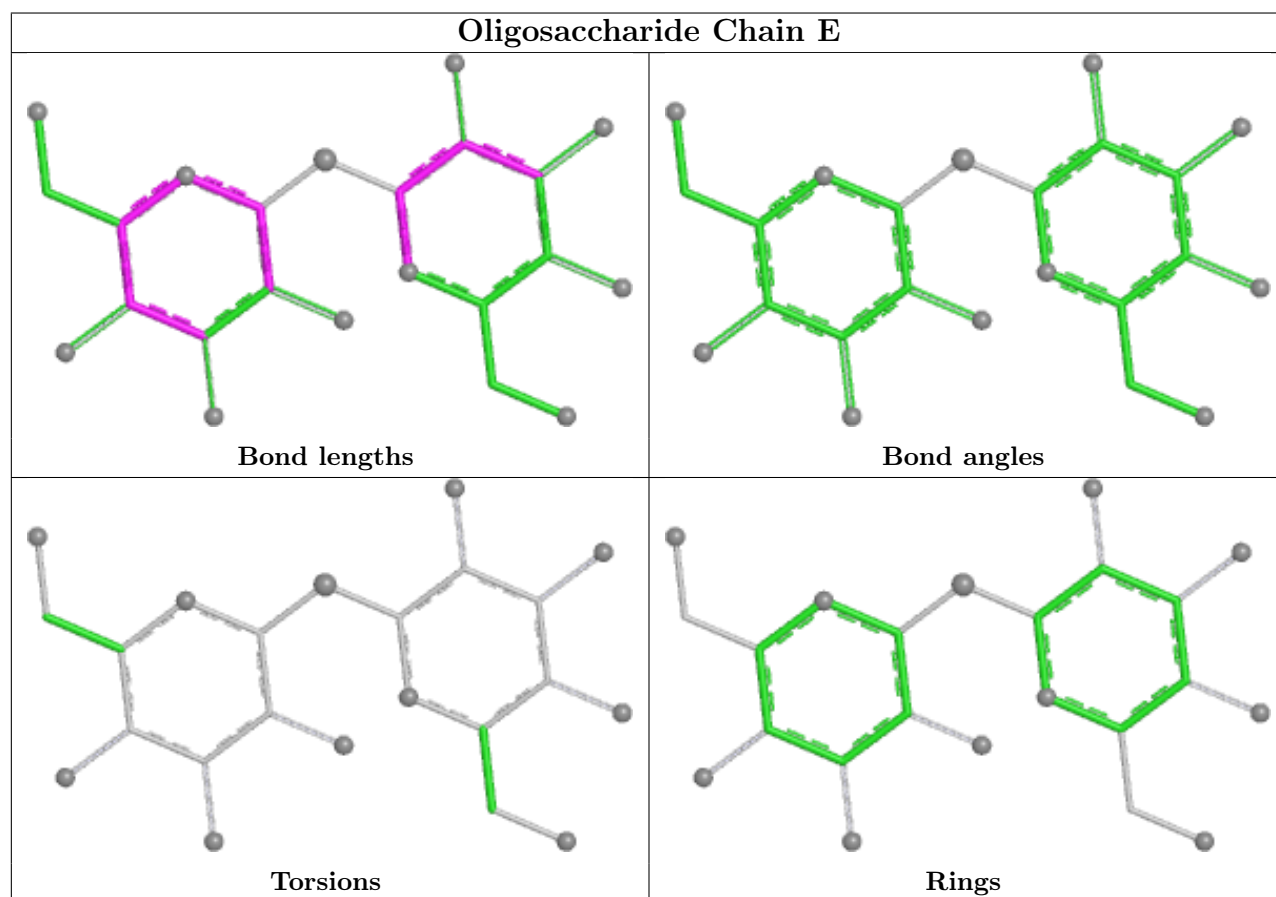
All (1) torsion outliers are listed below:

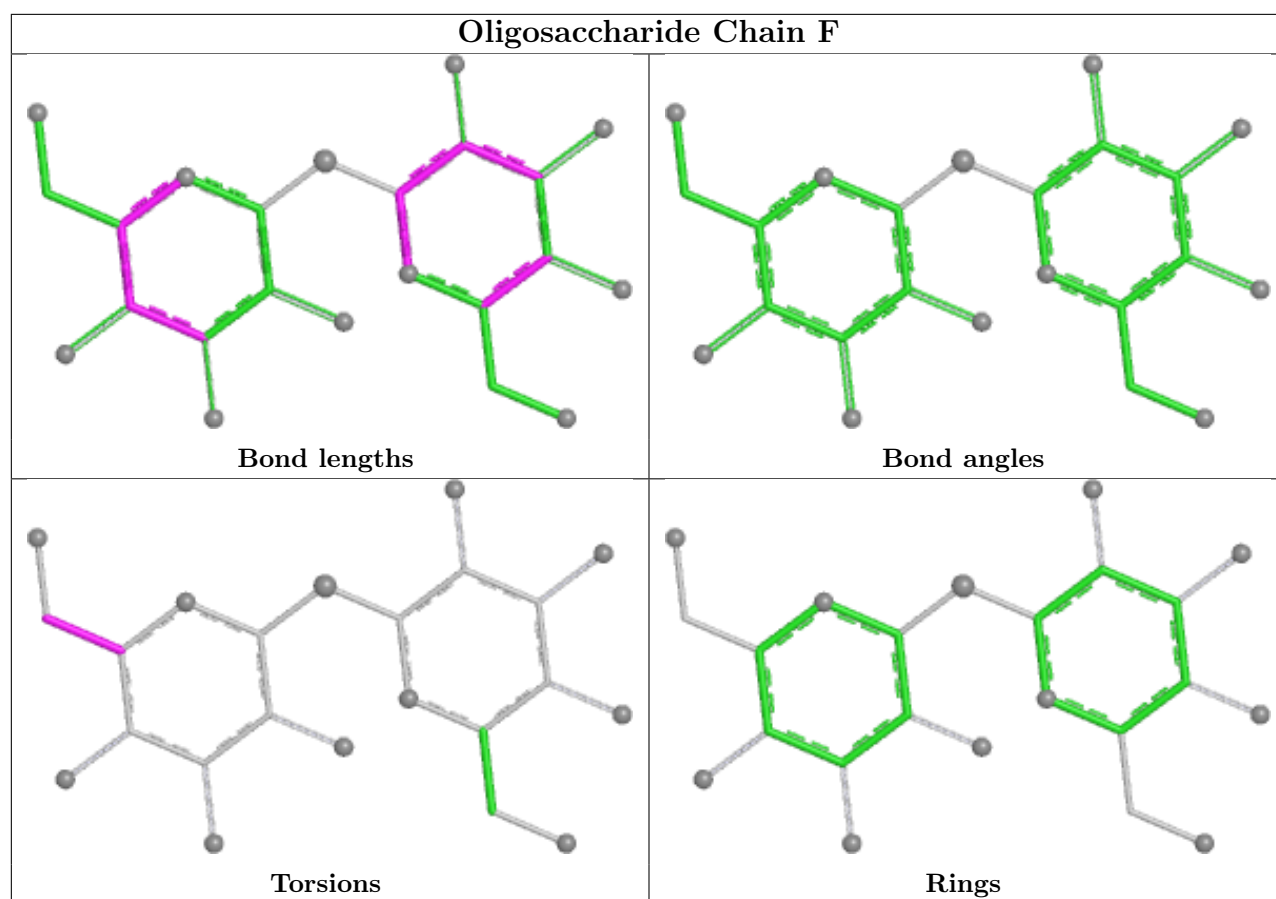
Mol	Chain	Res	Type	Atoms
2	F	2	GAL	C4-C5-C6-O6

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](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.