



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2020 – 04:50 PM BST

PDB ID : 3SY0
Title : S25-2- A(2-8)-A(2-4)KDO trisaccharide complex
Authors : Nguyen, H.P.; Seto, N.O.; Mackenzie, C.R.; Brade, L.; Kosma, P.; Brade, H.;
Evans, S.V.
Deposited on : 2011-07-15
Resolution : 1.49 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 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)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
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) : 2.14.6

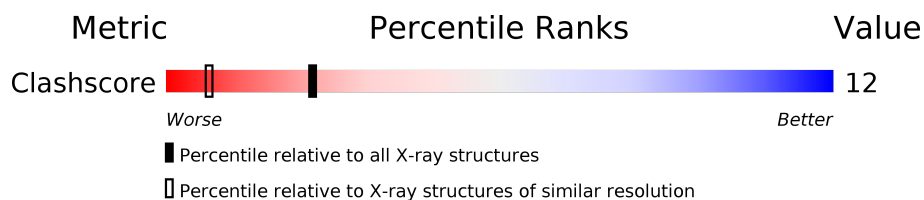
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.49 Å.



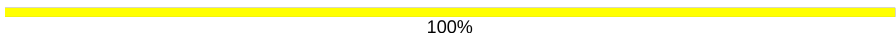
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4955 (1.50-1.46)

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 on 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 failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	219	 78% 21% .
2	B	222	 84% 16%
3	C	3	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4159 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 S25-2 FAB (IGG1K) light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1701	1056	290	347	8			

- Molecule 2 is a protein called S25-2 FAB (IGG1K) heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	222	Total	C	N	O	S	0	0	0
			1698	1075	283	333	7			

- Molecule 3 is an oligosaccharide called 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-8)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-prop-2-en-1-yl 3-deoxy-alpha-D-manno-oct-2-ulopyranosidonic acid.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	3	Total	C	O	0	0	0
			49	27	22			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is water.

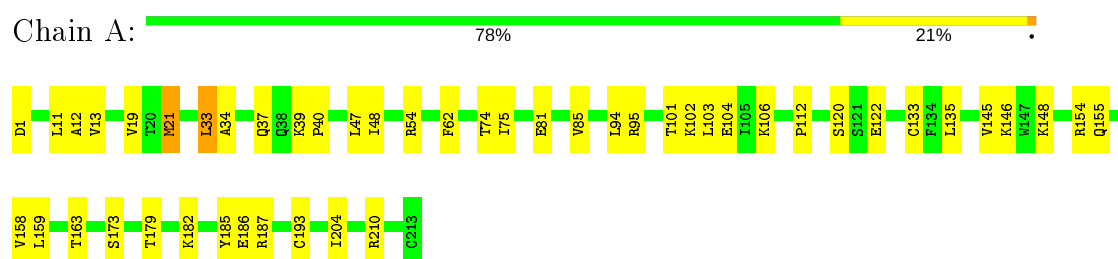
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	376	Total 376	O 376	0	0
6	B	332	Total 332	O 332	0	0

3 Residue-property plots [i](#)

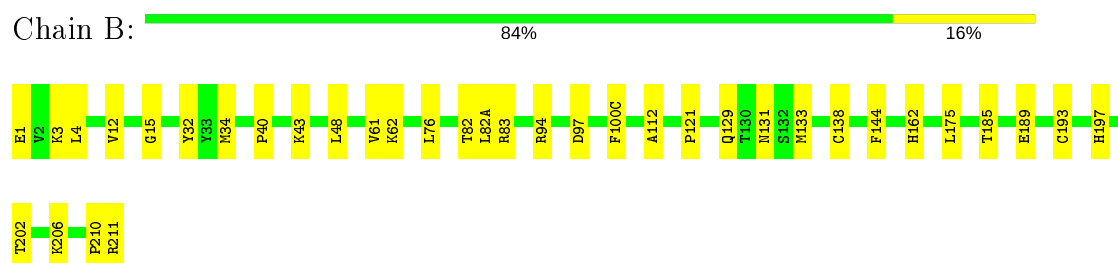
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 failed to run properly.

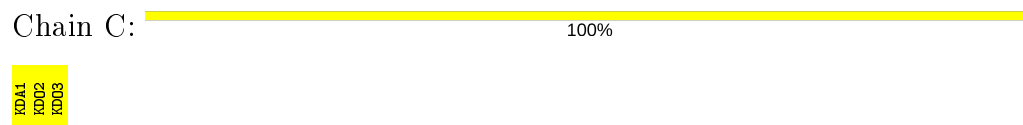
- Molecule 1: S25-2 FAB (IGG1K) light chain



- Molecule 2: S25-2 FAB (IGG1K) heavy chain



- Molecule 3: 3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-8)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid-(2-4)-prop-2-en-1-yl 3-deoxy-alpha-D-manno-oct-2-ulopyranosidonic acid



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	45.60 Å 80.90 Å 130.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.77 – 1.49	Depositor
% Data completeness (in resolution range)	92.1 (19.77-1.49)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 1.49 Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.187 , 0.212	Depositor
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.313	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4159	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: ZN, KDO, MG, KDA

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	0.38	0/1736	0.61	2/2351 (0.1%)
2	B	0.38	0/1744	0.60	0/2381
All	All	0.38	0/3480	0.61	2/4732 (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	A	33	LEU	CA-CB-CG	-7.69	97.61	115.30
1	A	21	MET	CB-CG-SD	-5.18	96.86	112.40

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	1701	0	1648	50	0
2	B	1698	0	1648	30	0
3	C	49	0	39	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
6	A	376	0	0	20	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	332	0	0	7	1
All	All	4159	0	3335	80	1

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.

All (80) 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)
2:B:138:CYS:SG	6:B:437:HOH:O	2.00	1.18
1:A:133:CYS:SG	6:A:439:HOH:O	2.01	1.15
2:B:193:CYS:SG	6:B:437:HOH:O	2.01	1.14
1:A:106:LYS:NZ	6:A:473:HOH:O	1.96	0.96
1:A:62:PHE:CD2	1:A:75:ILE:HD12	2.11	0.86
1:A:133:CYS:CB	6:A:439:HOH:O	2.22	0.81
1:A:21:MET:HG2	6:A:438:HOH:O	1.85	0.77
1:A:12:ALA:HB2	1:A:104:GLU:HG3	1.68	0.75
1:A:186:GLU:OE2	6:A:690:HOH:O	2.05	0.74
2:B:129:GLN:HB2	6:B:638:HOH:O	1.87	0.74
2:B:138:CYS:CB	6:B:437:HOH:O	2.28	0.72
1:A:155:GLN:NE2	6:A:502:HOH:O	2.22	0.72
1:A:163:THR:HG22	1:A:173:SER:H	1.55	0.71
1:A:11:LEU:O	1:A:104:GLU:HG2	1.92	0.68
1:A:1:ASP:O	6:A:388:HOH:O	2.12	0.68
1:A:85:VAL:HG22	1:A:102:LYS:HD3	1.79	0.65
1:A:13:VAL:HG21	1:A:19:VAL:CG2	2.27	0.65
1:A:13:VAL:HG22	1:A:103:LEU:HD11	1.81	0.62
1:A:13:VAL:HG12	6:A:498:HOH:O	1.99	0.62
1:A:13:VAL:HG11	1:A:19:VAL:HG22	1.84	0.60
1:A:33:LEU:HG	1:A:34:ALA:N	2.13	0.60
2:B:3:LYS:C	2:B:4:LEU:HD12	2.23	0.58
1:A:112:PRO:HG2	1:A:204:ILE:HD12	1.84	0.58
2:B:1:GLU:HG3	6:B:245:HOH:O	2.04	0.57
1:A:187:ARG:HD3	6:A:230:HOH:O	2.03	0.57
1:A:146:LYS:NZ	1:A:148:LYS:HE3	2.19	0.57
2:B:62:LYS:HE2	6:B:637:HOH:O	2.05	0.56
1:A:81:GLU:HG2	1:A:81:GLU:O	2.05	0.56
1:A:193:CYS:CB	6:A:439:HOH:O	2.54	0.55
1:A:163:THR:CG2	1:A:173:SER:H	2.19	0.54
1:A:133:CYS:HB2	6:A:439:HOH:O	1.98	0.54
2:B:40:PRO:HB2	2:B:43:LYS:HD3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LYS:NZ	1:A:186:GLU:OE1	2.29	0.53
1:A:62:PHE:HD2	1:A:75:ILE:HD12	1.71	0.52
2:B:129:GLN:C	2:B:131:ASN:H	2.12	0.52
1:A:158:VAL:C	1:A:159:LEU:HD22	2.29	0.52
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.91	0.52
1:A:74:THR:C	1:A:75:ILE:HD13	2.30	0.52
1:A:102:LYS:HD2	6:A:625:HOH:O	2.10	0.52
2:B:3:LYS:NZ	2:B:3:LYS:HB3	2.27	0.50
1:A:135:LEU:HD21	1:A:145:VAL:HG22	1.94	0.49
1:A:146:LYS:HE3	6:A:328:HOH:O	2.12	0.49
2:B:82:THR:HG22	2:B:83:ARG:NH1	2.28	0.49
1:A:193:CYS:HB2	6:A:439:HOH:O	2.11	0.48
1:A:21:MET:HG3	1:A:101:THR:HG21	1.93	0.48
2:B:185:THR:O	2:B:189:GLU:HB2	2.14	0.48
1:A:13:VAL:HG21	1:A:19:VAL:HG22	1.96	0.47
1:A:120:SER:OG	1:A:122:GLU:HG2	2.14	0.47
2:B:131:ASN:O	2:B:133:MET:N	2.41	0.47
1:A:135:LEU:N	1:A:135:LEU:HD12	2.30	0.46
2:B:4:LEU:N	2:B:4:LEU:HD12	2.31	0.46
1:A:185:TYR:CZ	1:A:210:ARG:HD2	2.51	0.46
1:A:122:GLU:HG3	6:A:385:HOH:O	2.16	0.45
1:A:102:LYS:HD2	6:A:623:HOH:O	2.16	0.45
2:B:121:PRO:HD3	2:B:206:LYS:HD3	1.97	0.45
2:B:129:GLN:C	2:B:131:ASN:N	2.70	0.45
2:B:210:PRO:O	2:B:211:ARG:HB2	2.17	0.44
2:B:175:LEU:HD12	2:B:175:LEU:C	2.38	0.44
1:A:85:VAL:CG2	1:A:102:LYS:HD3	2.47	0.44
2:B:34:MET:HB3	2:B:76:LEU:HD22	1.99	0.43
2:B:210:PRO:HG2	2:B:211:ARG:HD2	2.00	0.43
1:A:179:THR:OG1	6:A:493:HOH:O	2.17	0.43
2:B:197:HIS:HB3	2:B:202:THR:HB	2.01	0.43
1:A:81:GLU:HG3	6:A:622:HOH:O	2.18	0.43
2:B:12:VAL:HG11	2:B:82(A):LEU:HD13	2.01	0.42
2:B:131:ASN:C	2:B:133:MET:H	2.19	0.42
1:A:159:LEU:N	1:A:159:LEU:HD22	2.35	0.42
1:A:94:LEU:C	1:A:95:ARG:HD2	2.40	0.42
1:A:48:ILE:HD13	1:A:54:ARG:HA	2.01	0.42
2:B:32:TYR:CE1	2:B:97:ASP:HB3	2.55	0.41
1:A:154:ARG:NH2	6:A:378:HOH:O	2.51	0.41
1:A:104:GLU:HG2	1:A:104:GLU:H	1.73	0.41
2:B:94:ARG:O	2:B:100(C):PHE:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LYS:NZ	1:A:81:GLU:CG	2.84	0.41
2:B:15:GLY:HA2	2:B:83:ARG:HH12	1.86	0.41
1:A:40:PRO:HG2	6:A:471:HOH:O	2.21	0.40
2:B:162:HIS:CD2	6:B:687:HOH:O	2.74	0.40
2:B:82:THR:HG22	2:B:83:ARG:HH12	1.85	0.40
2:B:48:LEU:HD22	2:B:61:VAL:HG11	2.03	0.40
2:B:112:ALA:HB3	2:B:144:PHE:CE2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:628:HOH:O	6:B:634:HOH:O[3_546]	1.86	0.34

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

3 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
3	KDA	C	1	3	15,19,19	1.97	5 (33%)	19,27,27	1.38	4 (21%)
3	KDO	C	2	3	12,15,16	2.01	4 (33%)	16,21,24	1.22	2 (12%)
3	KDO	C	3	3	12,15,16	1.71	3 (25%)	16,21,24	1.27	2 (12%)

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
3	KDA	C	1	3	-	1/11/35/35	0/1/1/1
3	KDO	C	2	3	-	0/6/26/30	0/1/1/1
3	KDO	C	3	3	-	0/6/26/30	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	KDO	C4-C5	-4.59	1.45	1.52
3	C	3	KDO	C4-C5	-3.73	1.47	1.52
3	C	1	KDA	O6-C6	3.39	1.49	1.44
3	C	1	KDA	O6-C2	3.29	1.46	1.42
3	C	2	KDO	O6-C6	3.05	1.48	1.44
3	C	1	KDA	C4-C5	-3.03	1.48	1.52
3	C	1	KDA	O7-C7	-2.96	1.37	1.43
3	C	3	KDO	O7-C7	-2.63	1.37	1.43
3	C	2	KDO	O7-C7	-2.55	1.37	1.43
3	C	3	KDO	O6-C6	2.49	1.47	1.44
3	C	1	KDA	C3-C4	-2.31	1.49	1.53
3	C	2	KDO	C3-C4	-2.02	1.49	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	KDO	C7-C6-C5	2.50	118.18	114.03
3	C	1	KDA	O8-C8-C7	2.45	116.40	111.07
3	C	2	KDO	O8-C8-C7	2.34	116.18	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	KDA	C3-C2-C1	-2.31	110.11	114.12
3	C	1	KDA	O6-C6-C5	2.23	111.69	108.52
3	C	3	KDO	O8-C8-C7	2.22	115.91	111.07
3	C	1	KDA	C8-C7-C6	-2.07	107.97	112.17
3	C	3	KDO	O6-C2-C3	2.03	113.43	109.87

There are no chirality outliers.

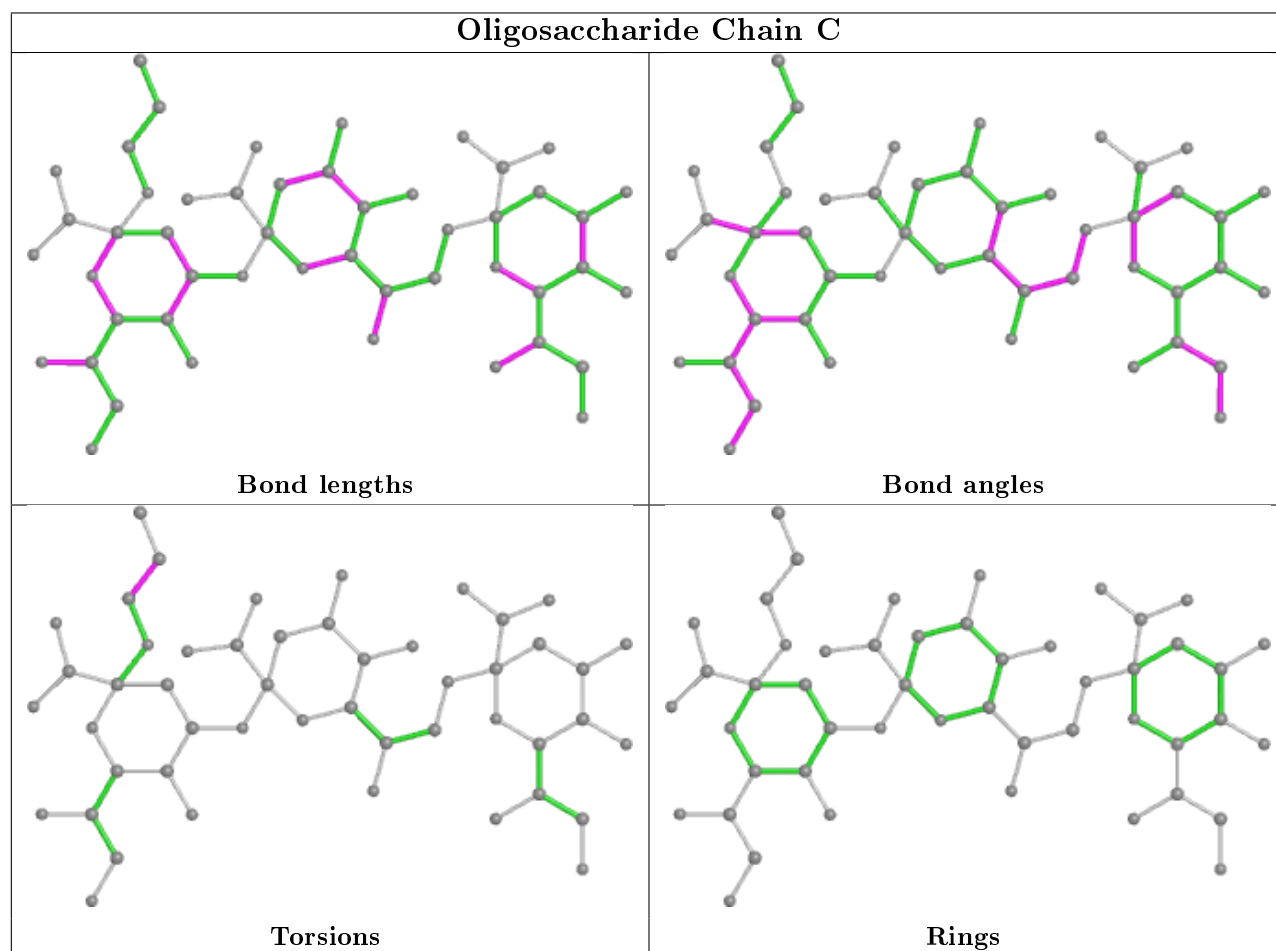
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	KDA	C11-C10-C9-O2

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

Of 3 ligands modelled in this entry, 3 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

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 [i](#)

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.