Full wwPDB X-ray Structure Validation Report (i)

Sep 21, 2020 – 04:45 PM BST

PDB ID	:	1JFH
Title	:	STRUCTURE OF A PANCREATIC ALPHA-AMYLASE BOUND TO A SUBSTRATE ANALOGUE AT 2.03 ANGSTROM RESOLUTION
Authors	:	Qian, M.; Payan, F.
Deposited on	:	1997-09-19
Resolution	:	2.03 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 (i) symbol.

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

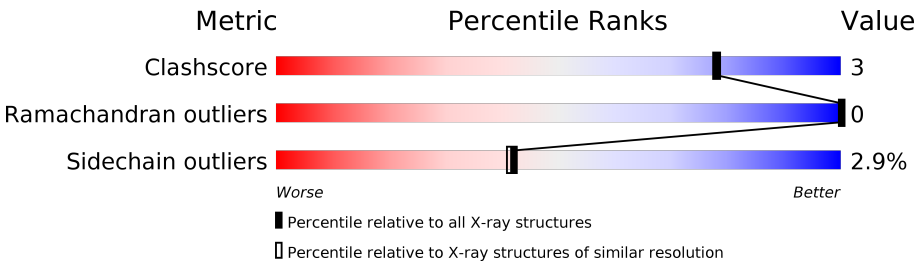
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	496	92% 8%
2	B	2	100%
3	C	2	100%
3	D	2	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4365 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 ALPHA-AMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	496	3908	2470	686	731	21	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	VAL	ILE	conflict	UNP P00690
A	243	LYS	GLN	conflict	UNP P00690
A	310	SER	ALA	conflict	UNP P00690
A	323	ILE	VAL	conflict	UNP P00690

- Molecule 2 is an oligosaccharide called 4-S-methyl-4-thio-alpha-D-glucopyranose-(1-4)-methyl 4-thio-alpha-D-glucopyranoside.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	O	S			
2	B	2	25	14	9	2	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-1,4-dithio-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	O	S			
3	C	2	23	12	9	2	0	0	0
3	D	2	23	12	9	2	0	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0

- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	383	Total O 383 383	0	0

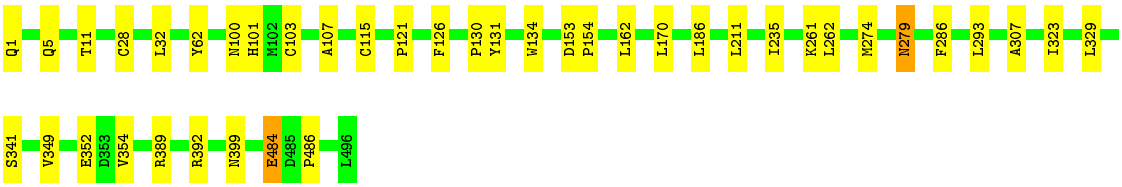
3 Residue-property plots (i)

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: ALPHA-AMYLASE

Chain A: 92% 8%



• Molecule 2: 4-S-methyl-4-thio-alpha-D-glucopyranose-(1-4)-methyl 4-thio-alpha-D-glucopyranoside

Chain B: 100%

• Molecule 3: alpha-D-glucopyranose-(1-4)-1,4-dithio-alpha-D-glucopyranose

Chain C: 100%

• Molecule 3: alpha-D-glucopyranose-(1-4)-1,4-dithio-alpha-D-glucopyranose

Chain D: 100%

4 Data and refinement statistics (i)

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	56.30Å 87.80Å 103.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.03	Depositor
% Data completeness (in resolution range)	(Not available) (35.00-2.03)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.160 , 0.185	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4365	wwPDB-VP
Average B, all atoms (Å^2)	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: MA1, MA3, MA2, CL, CA, GLC, PCA, HG

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	0.33	0/4011	0.59	0/5451

There are no bond length outliers.

There are no bond angle outliers.

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	3908	0	3683	22	0
2	B	25	0	25	0	0
3	C	23	0	21	0	0
3	D	23	0	21	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	383	0	0	1	0
All	All	4365	0	3750	22	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 3.

All (22) 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:279:ASN:H	1:A:279:ASN:HD22	1.39	0.71
1:A:100:ASN:HD22	1:A:101:HIS:HD2	1.39	0.69
1:A:5:GLN:HE21	1:A:5:GLN:HA	1.66	0.59
1:A:349:VAL:O	1:A:352:GLU:HG2	2.07	0.54
1:A:11:THR:H	1:A:399:ASN:HD21	1.57	0.52
1:A:235:ILE:HG21	1:A:307:ALA:HB2	1.94	0.48
1:A:279:ASN:HD22	1:A:279:ASN:N	2.04	0.46
1:A:323:ILE:HD11	1:A:486:PRO:HG2	1.97	0.46
1:A:274:MET:HG3	7:A:561:HOH:O	2.16	0.45
1:A:126:PHE:HB2	1:A:131:TYR:HB2	1.98	0.45
1:A:126:PHE:O	1:A:130:PRO:HA	2.17	0.45
1:A:484:GLU:H	1:A:484:GLU:CD	2.20	0.44
1:A:28:CYS:HA	1:A:32:LEU:HB2	1.98	0.44
1:A:103:CYS:SG	1:A:121:PRO:HG3	2.59	0.43
1:A:62:TYR:O	1:A:101:HIS:HE1	2.03	0.42
1:A:5:GLN:NE2	1:A:5:GLN:HA	2.32	0.42
1:A:279:ASN:H	1:A:279:ASN:ND2	2.11	0.42
1:A:349:VAL:HG22	1:A:354:VAL:HG13	2.02	0.42
1:A:107:ALA:HB3	1:A:121:PRO:HG2	2.02	0.40
1:A:261:LYS:HD2	1:A:286:PHE:HE1	1.85	0.40
1:A:389:ARG:HA	1:A:392:ARG:HG2	2.04	0.40
1:A:153:ASP:HA	1:A:154:PRO:HD2	1.96	0.40

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	494/496 (100%)	481 (97%)	13 (3%)	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	A	412/412 (100%)	400 (97%)	12 (3%)	42 41

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	CYS
1	A	134	TRP
1	A	162	LEU
1	A	170	LEU
1	A	186	LEU
1	A	211	LEU
1	A	262	LEU
1	A	279	ASN
1	A	293	LEU
1	A	329	LEU
1	A	341	SER
1	A	484	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	75	ASN
1	A	77	ASN
1	A	101	HIS
1	A	161	GLN
1	A	279	ASN
1	A	350	ASN
1	A	363	ASN
1	A	399	ASN
1	A	476	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	PCA	A	1	1	7,8,9	0.88	1 (14%)	9,10,12	3.46	5 (55%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CG-CD	2.08	1.56	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	PCA	OE-CD-N	7.14	141.50	124.86
1	A	1	PCA	CG-CD-N	-4.21	97.47	108.39
1	A	1	PCA	CB-CG-CD	3.81	110.54	104.40
1	A	1	PCA	OE-CD-CG	-3.29	121.02	126.76
1	A	1	PCA	CA-N-CD	2.87	123.40	113.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

6 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	MA3	B	1	2	12,13,13	0.67	0	14,18,18	0.69	0
2	MA2	B	2	2	12,12,13	0.70	0	11,16,18	0.52	0
3	MA1	C	1	3	10,12,12	0.56	0	11,17,17	0.46	0
3	GLC	C	2	3	11,11,12	0.35	0	15,15,17	0.61	0
3	MA1	D	1	3	10,12,12	0.50	0	11,17,17	0.44	0
3	GLC	D	2	3	11,11,12	0.44	0	15,15,17	0.58	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	MA3	B	1	2	-	0/4/24/24	0/1/1/1
2	MA2	B	2	2	-	0/4/21/24	0/1/1/1
3	MA1	C	1	3	-	0/2/22/22	0/1/1/1
3	GLC	C	2	3	-	0/2/19/22	0/1/1/1
3	MA1	D	1	3	-	0/2/22/22	0/1/1/1
3	GLC	D	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

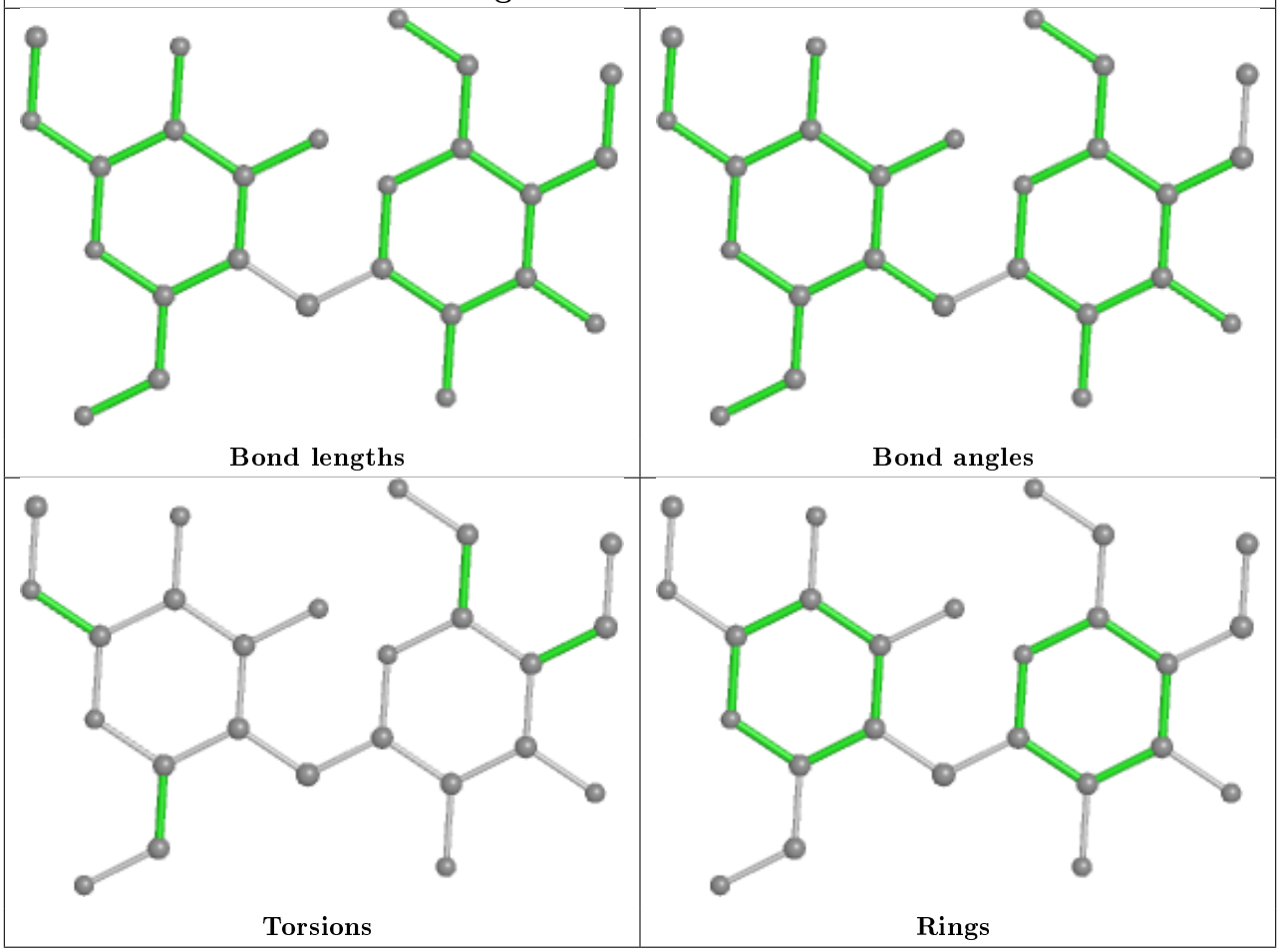
There are no torsion outliers.

There are no ring outliers.

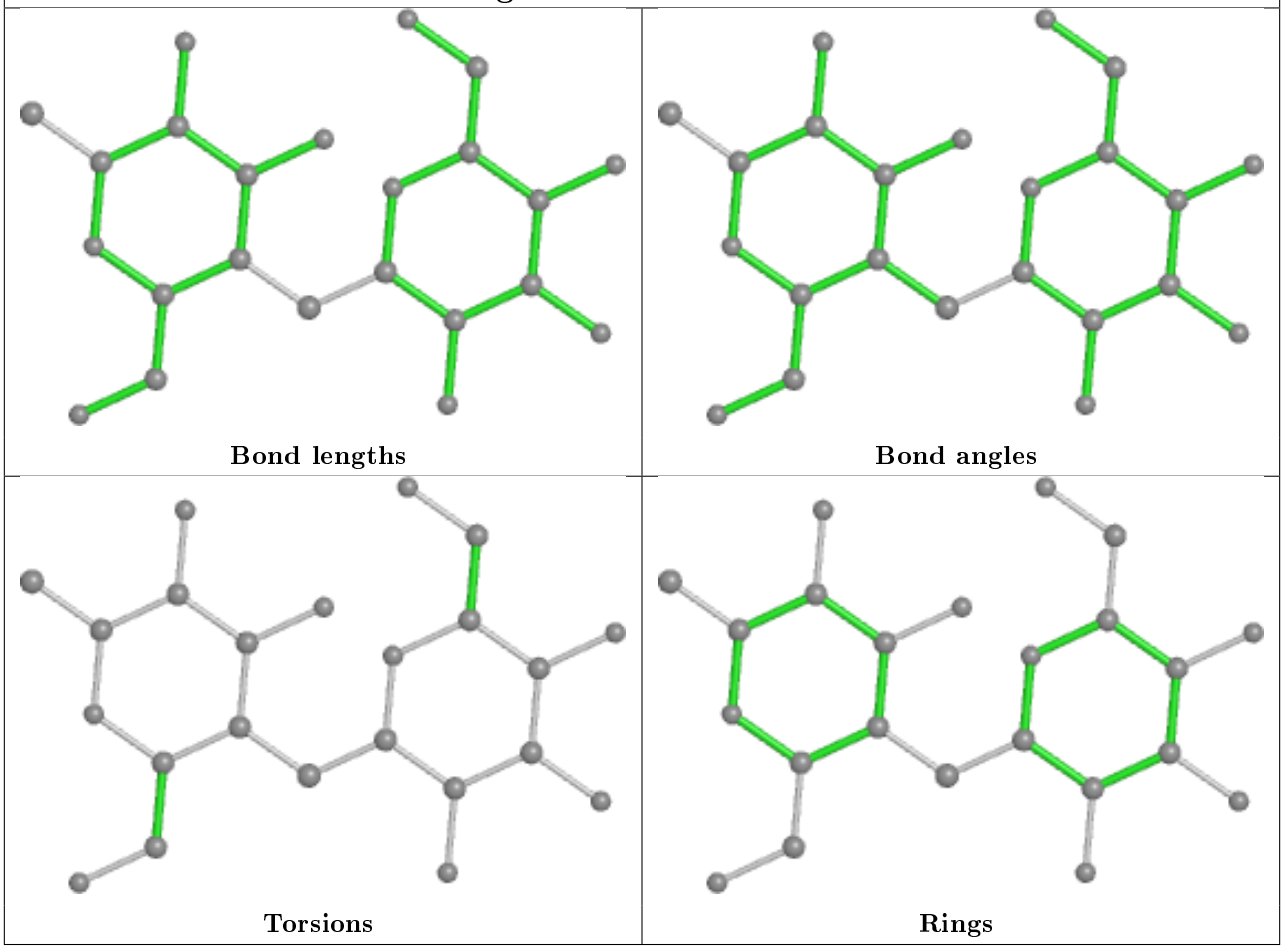
No monomer is involved in short contacts.

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

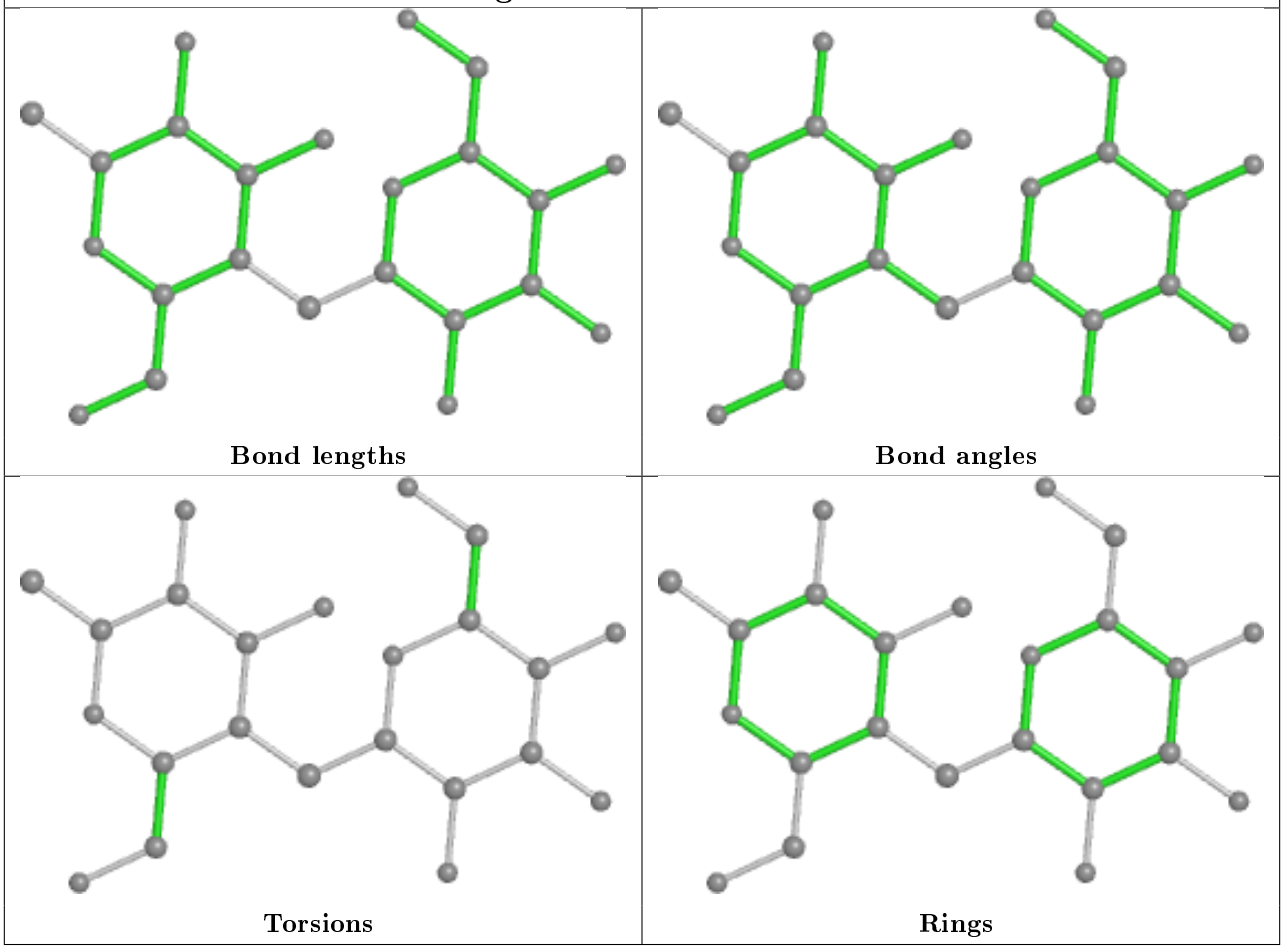
Oligosaccharide Chain B



Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry (i)

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 (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.