wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2020 – 12:36 PM BST

PDB ID	:	3SC2
Title	:	REFINED ATOMIC MODEL OF WHEAT SERINE CARBOXYPEPTIDASE II AT 2.2-ANGSTROMS RESOLUTION
Authors	:	Liao, D.-I.; Remington, S.J.
Deposited on	:	1992-07-01
Resolution	:	2.20 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 (i) symbol.

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

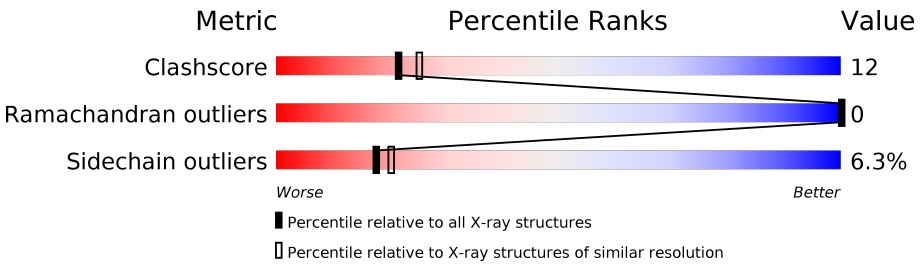
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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	259	63% 30% 5% •
2	B	152	67% 28% • •
3	C	4	50% 50%
3	D	4	25% 75%
4	E	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	C	3	X	-	-	-
3	FUC	C	4	X	-	-	-
3	MAN	D	3	X	-	-	-
4	NAG	E	2	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3533 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 SERINE CARBOXYPEPTIDASE II (CPDW-II).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	254	1997	1277	334	379	7	8	0	0

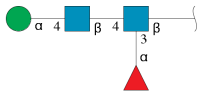
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ALA	ARG	conflict	UNP P08819

- Molecule 2 is a protein called SERINE CARBOXYPEPTIDASE II (CPDW-II).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	152	1213	777	210	220	6	13	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	4	49	28	2	19	0	0	0
3	D	4	49	28	2	19	0	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	2	28	16	2	10	0	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	119	119	119	0	0
			Total	O		
5	B	78	78	78	0	0

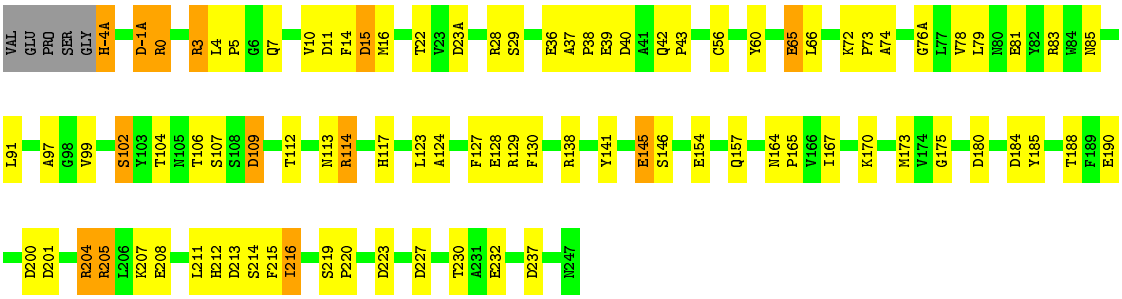
3 Residue-property plots (i)

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.

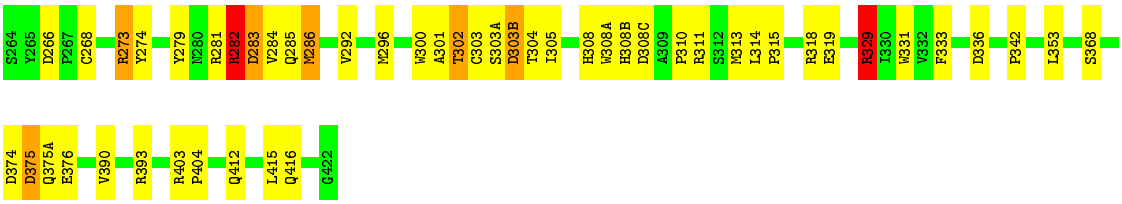
• Molecule 1: SERINE CARBOXYPEPTIDASE II (CPDW-II)

Chain A: 63% 30% 5%



• Molecule 2: SERINE CARBOXYPEPTIDASE II (CPDW-II)

Chain B: 67% 28%



• Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 50% 50%

• Molecule 3: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 25% 75%

• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	98.40Å 98.40Å 209.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3533	wwPDB-VP
Average B, all atoms ($Å^2$)	31.0	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: FUC, 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	1.12	9/2060 (0.4%)	1.58	35/2810 (1.2%)
2	B	1.08	1/1253 (0.1%)	1.66	25/1717 (1.5%)
All	All	1.10	10/3313 (0.3%)	1.61	60/4527 (1.3%)

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
2	B	1	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	GLU	CD-OE2	7.98	1.34	1.25
1	A	208	GLU	CD-OE1	7.95	1.34	1.25
1	A	39	GLU	CD-OE1	7.36	1.33	1.25
1	A	81	GLU	CD-OE1	7.26	1.33	1.25
1	A	128	GLU	CD-OE2	6.52	1.32	1.25

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	114	ARG	NE-CZ-NH1	14.93	127.76	120.30
1	A	205	ARG	NE-CZ-NH1	13.58	127.09	120.30
1	A	114	ARG	NE-CZ-NH2	-12.53	114.04	120.30
2	B	283	ASP	N-CA-CB	-10.76	91.23	110.60
2	B	329	ARG	NE-CZ-NH1	10.45	125.52	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	375	ASP	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	282	ARG	Sidechain

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	1997	0	1854	45	0
2	B	1213	0	1157	36	0
3	C	49	0	42	1	0
3	D	49	0	43	5	0
4	E	28	0	25	4	0
5	A	119	0	0	4	0
5	B	78	0	0	2	0
All	All	3533	0	3121	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 12.

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)
3:D:2:NAG:O5	3:D:4:FUC:H5	1.79	0.83
1:A:5:PRO:HG2	2:B:284:VAL:HG22	1.70	0.73
2:B:281:ARG:O	2:B:285:GLN:HG3	1.88	0.73
2:B:282:ARG:O	2:B:286:MET:HB2	1.92	0.70
1:A:106:THR:O	1:A:109:ASP:HB2	1.92	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	A	252/259 (97%)	240 (95%)	12 (5%)	0	100	100
2	B	150/152 (99%)	141 (94%)	9 (6%)	0	100	100
All	All	402/411 (98%)	381 (95%)	21 (5%)	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	206/210 (98%)	193 (94%)	13 (6%)	18	20
2	B	127/127 (100%)	119 (94%)	8 (6%)	18	20
All	All	333/337 (99%)	312 (94%)	21 (6%)	18	20

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	ARG
1	A	215	PHE
2	B	303(B)	ASP
1	A	204	ARG
2	B	329	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	117	HIS
1	A	233	GLN
2	B	308	HIS
2	B	412	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)

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	$\#\|Z\| > 2$
3	NAG	C	1	1,3	14,14,15	0.75	0	17,19,21	2.78	6 (35%)
3	NAG	C	2	3	14,14,15	1.15	2 (14%)	17,19,21	3.22	6 (35%)
3	MAN	C	3	3	11,11,12	1.09	0	15,15,17	2.44	4 (26%)
3	FUC	C	4	3	10,10,11	3.12	3 (30%)	14,14,16	5.24	7 (50%)
3	NAG	D	1	1,3	14,14,15	0.57	0	17,19,21	1.60	4 (23%)
3	NAG	D	2	3	14,14,15	1.09	0	17,19,21	1.88	3 (17%)
3	MAN	D	3	3	11,11,12	0.82	0	15,15,17	2.06	6 (40%)
3	FUC	D	4	3	10,10,11	3.08	3 (30%)	14,14,16	4.31	10 (71%)
4	NAG	E	1	2,4	14,14,15	0.93	1 (7%)	17,19,21	1.05	1 (5%)
4	NAG	E	2	4	14,14,15	1.19	1 (7%)	17,19,21	2.77	10 (58%)

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	NAG	C	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	MAN	C	3	3	1/1/4/5	2/2/19/22	0/1/1/1
3	FUC	C	4	3	1/1/4/5	-	0/1/1/1
3	NAG	D	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	MAN	D	3	3	2/2/4/5	2/2/19/22	0/1/1/1
3	FUC	D	4	3	-	-	0/1/1/1
4	NAG	E	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	1/1/5/7	3/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4	FUC	O5-C1	8.73	1.57	1.43
3	C	4	FUC	O5-C1	8.53	1.57	1.43
3	C	4	FUC	O5-C5	3.71	1.51	1.43
4	E	2	NAG	C1-C2	3.47	1.57	1.52
3	D	4	FUC	O5-C5	3.29	1.50	1.43

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	4	FUC	O3-C3-C2	11.86	132.70	109.99
3	C	2	NAG	O6-C6-C5	8.74	141.29	111.29
3	C	4	FUC	C2-C3-C4	-8.73	95.78	110.89
3	D	4	FUC	C1-C2-C3	8.48	120.09	109.67
3	D	4	FUC	O3-C3-C2	7.86	125.04	109.99

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	3	MAN	C2
3	D	3	MAN	C1
4	E	2	NAG	C2
3	C	4	FUC	C1
3	C	3	MAN	C1

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	NAG	C8-C7-N2-C2
3	D	1	NAG	O7-C7-N2-C2
3	C	3	MAN	O5-C5-C6-O6
3	D	3	MAN	C4-C5-C6-O6
3	C	3	MAN	C4-C5-C6-O6

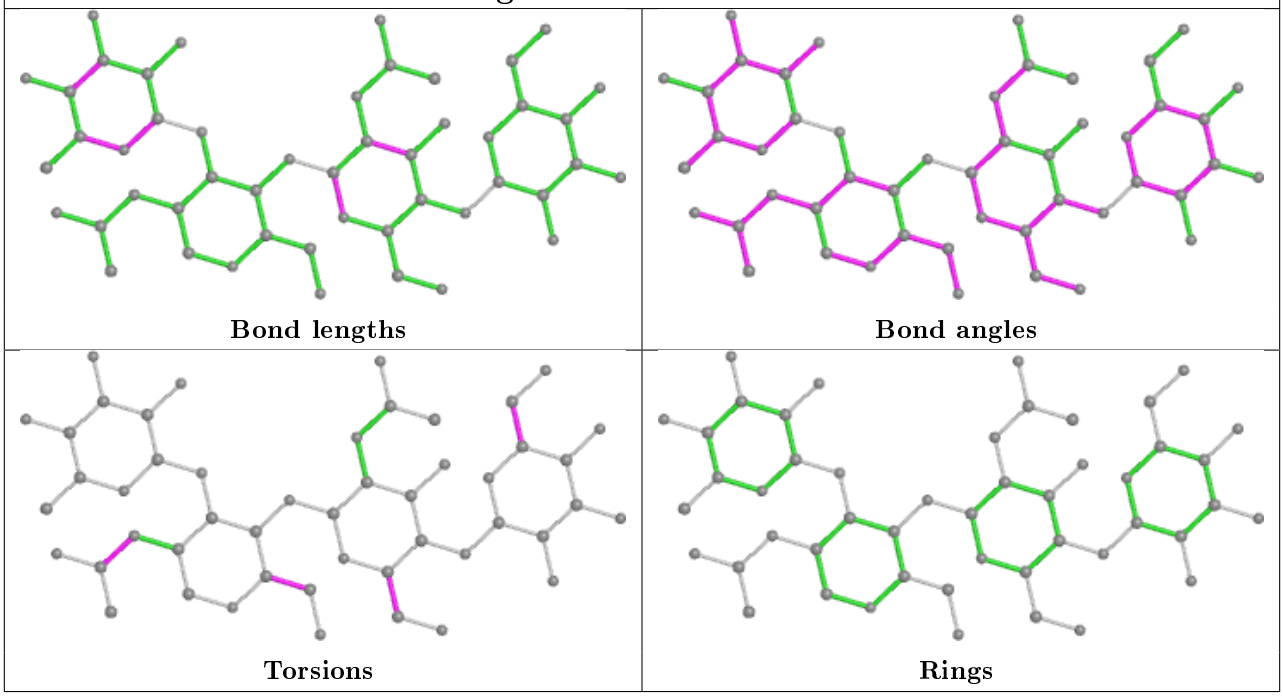
There are no ring outliers.

5 monomers are involved in 10 short contacts:

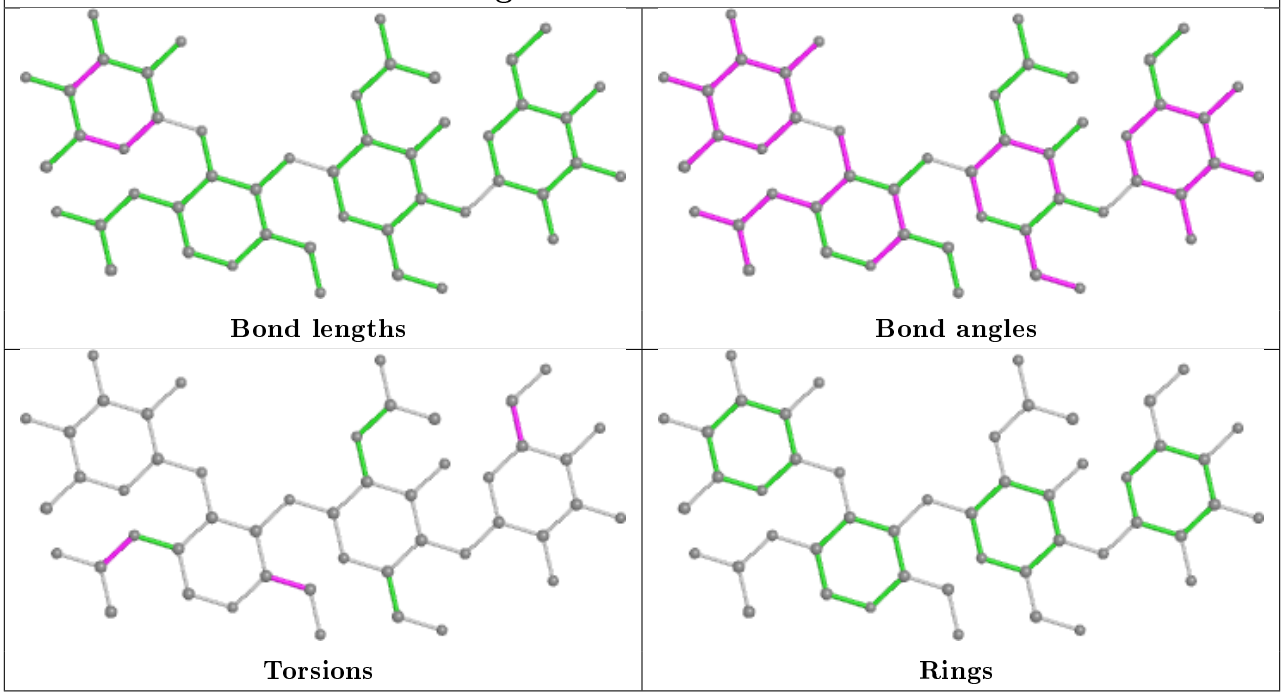
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	4	0
3	D	4	FUC	5	0
3	D	2	NAG	5	0
3	C	4	FUC	1	0
3	C	2	NAG	1	0

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

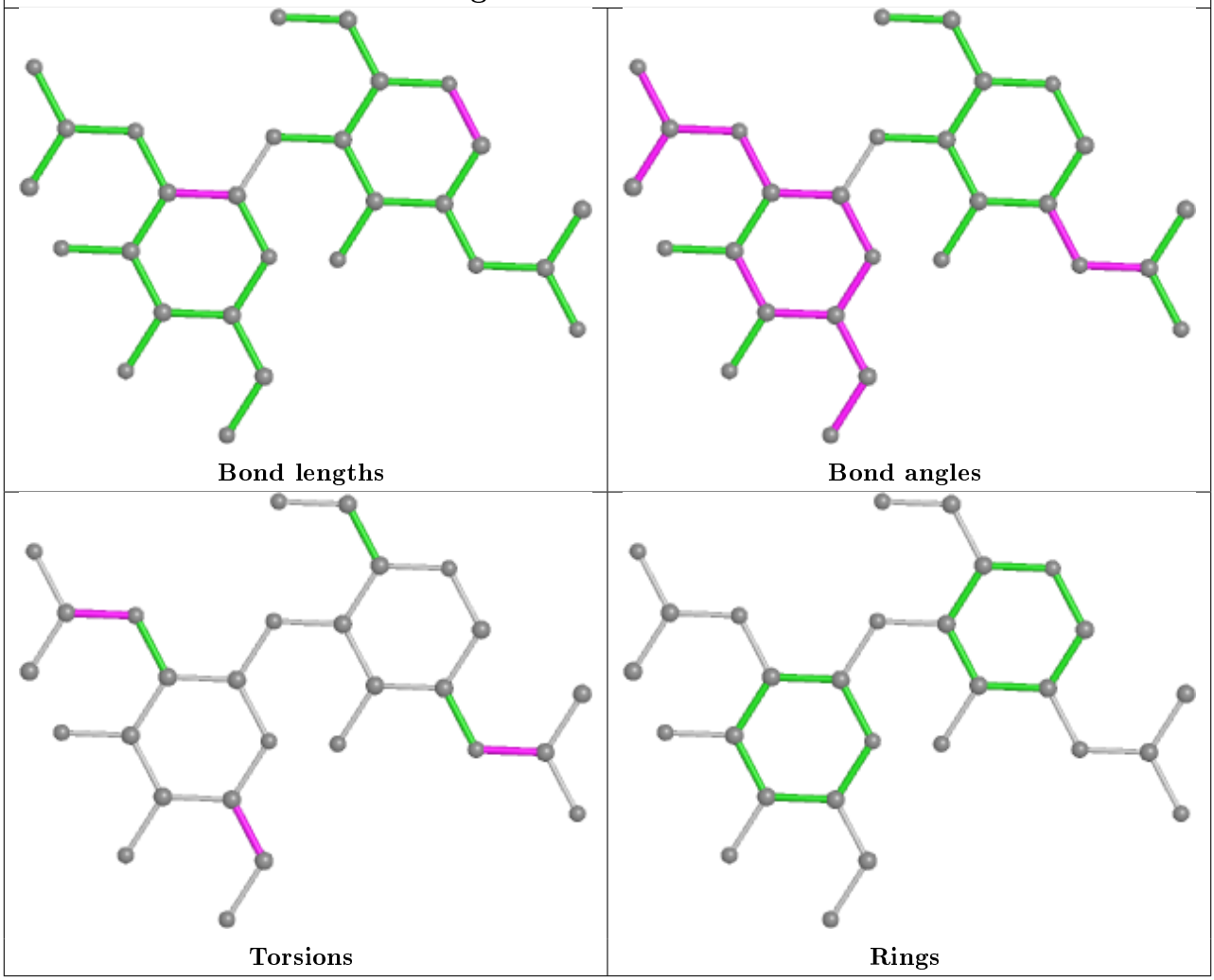
Oligosaccharide Chain C



Oligosaccharide Chain D



Oligosaccharide Chain E



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.