wwPDB X-ray Structure Validation Summary Report (i)

Oct 1, 2023 – 11:18 PM EDT

PDB ID	:	6MGP
Title	:	Structure of human 4-1BB / 4-1BBL complex
Authors	:	Kimberlin, C.R.; Chin, S.M.; Roe-Zurz, Z.; Xu, A.; Yang, Y.
Deposited on	:	2018-09-14
Resolution	:	2.13 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	FAILED
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)	:	2.35.1

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 2.13 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6717 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 Tumor necrosis factor ligand superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	150	1097	705	195	196	1	0	0	0
			Total	C	N	O	S			
1	B	152	1130	723	205	201	1	0	1	0
			Total	C	N	O				
1	C	152	1123	720	200	203		0	1	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	GLY	-	expression tag	UNP P41273
A	256	SER	-	expression tag	UNP P41273
A	257	HIS	-	expression tag	UNP P41273
A	258	HIS	-	expression tag	UNP P41273
A	259	HIS	-	expression tag	UNP P41273
A	260	HIS	-	expression tag	UNP P41273
A	261	HIS	-	expression tag	UNP P41273
A	262	HIS	-	expression tag	UNP P41273
A	263	HIS	-	expression tag	UNP P41273
A	264	HIS	-	expression tag	UNP P41273
B	255	GLY	-	expression tag	UNP P41273
B	256	SER	-	expression tag	UNP P41273
B	257	HIS	-	expression tag	UNP P41273
B	258	HIS	-	expression tag	UNP P41273
B	259	HIS	-	expression tag	UNP P41273
B	260	HIS	-	expression tag	UNP P41273
B	261	HIS	-	expression tag	UNP P41273
B	262	HIS	-	expression tag	UNP P41273
B	263	HIS	-	expression tag	UNP P41273
B	264	HIS	-	expression tag	UNP P41273
C	255	GLY	-	expression tag	UNP P41273
C	256	SER	-	expression tag	UNP P41273
C	257	HIS	-	expression tag	UNP P41273

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Chain	Residue	Modelled	Actual	Comment	Reference
C	258	HIS	-	expression tag	UNP P41273
C	259	HIS	-	expression tag	UNP P41273
C	260	HIS	-	expression tag	UNP P41273
C	261	HIS	-	expression tag	UNP P41273
C	262	HIS	-	expression tag	UNP P41273
C	263	HIS	-	expression tag	UNP P41273
C	264	HIS	-	expression tag	UNP P41273

- Molecule 2 is a protein called Tumor necrosis factor receptor superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	X	144	1040	612	193	213	22	0	0	0
			Total	C	N	O	S			
2	Y	143	1024	607	185	210	22	0	0	0
			Total	C	N	O	S			
2	Z	144	1027	610	186	209	22	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

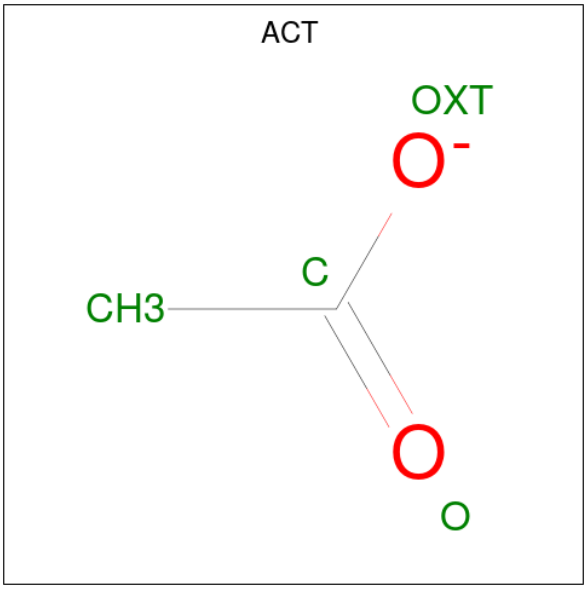
Chain	Residue	Modelled	Actual	Comment	Reference
X	163	GLU	-	expression tag	UNP Q07011
X	164	ASN	-	expression tag	UNP Q07011
X	165	LEU	-	expression tag	UNP Q07011
X	166	TYR	-	expression tag	UNP Q07011
X	167	PHE	-	expression tag	UNP Q07011
X	168	GLN	-	expression tag	UNP Q07011
Y	163	GLU	-	expression tag	UNP Q07011
Y	164	ASN	-	expression tag	UNP Q07011
Y	165	LEU	-	expression tag	UNP Q07011
Y	166	TYR	-	expression tag	UNP Q07011
Y	167	PHE	-	expression tag	UNP Q07011
Y	168	GLN	-	expression tag	UNP Q07011
Z	163	GLU	-	expression tag	UNP Q07011
Z	164	ASN	-	expression tag	UNP Q07011
Z	165	LEU	-	expression tag	UNP Q07011
Z	166	TYR	-	expression tag	UNP Q07011
Z	167	PHE	-	expression tag	UNP Q07011
Z	168	GLN	-	expression tag	UNP Q07011

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyr

anose.

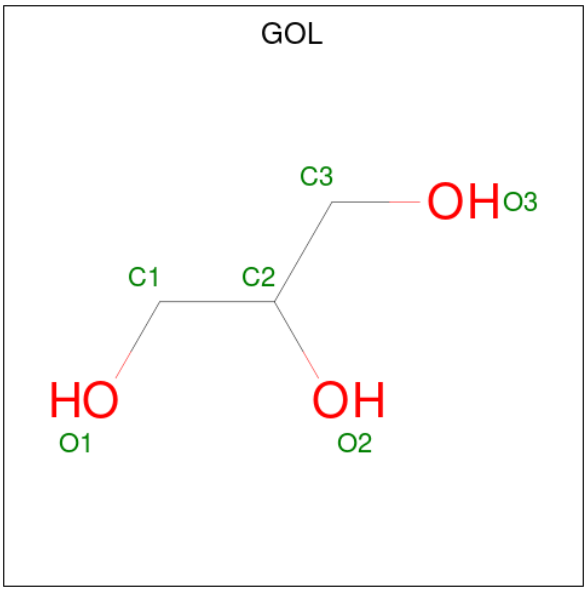
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	4	48	28	2	18	0	0	0
			Total	C	N	O			
3	E	4	48	28	2	18	0	0	0
			Total	C	N	O			
3	F	4	48	28	2	18	0	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0
			Total	C	O		
4	A	1	4	2	2	0	0
			Total	C	O		
4	C	1	4	2	2	0	0
			Total	C	O		
4	X	1	4	2	2	0	0
			Total	C	O		
4	Y	1	4	2	2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	6	3	3	0	0
			Total	C	O		
5	C	1	6	3	3	0	0
			Total	C	O		
5	Z	1	6	3	3	0	0
			Total	C	O		
5	Z	1	6	3	3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	14	14	14	0	0
			Total	O		
6	B	20	20	20	0	0
			Total	O		
6	C	14	14	14	0	0
			Total	O		
6	X	10	10	10	0	0
			Total	O		
6	Y	16	16	16	0	0
			Total	O		
6	Z	14	14	14	0	0

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

3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	102.01Å 229.38Å 114.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.13	Depositor
% Data completeness (in resolution range)	98.9 (48.91-2.13)	Depositor
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.60 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.217 , 0.250	Depositor
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.399	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6717	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains (i)

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

4.3.3 RNA (i)

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

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

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

12 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	D	1	3,2	14,14,15	0.32	0	17,19,21	0.75	0
3	FUC	D	2	3	10,10,11	0.70	0	14,14,16	1.21	2 (14%)
3	NAG	D	3	3	14,14,15	0.37	0	17,19,21	0.41	0
3	FUC	D	4	3	10,10,11	1.22	1 (10%)	14,14,16	1.03	1 (7%)
3	NAG	E	1	3,2	14,14,15	0.69	1 (7%)	17,19,21	0.72	0
3	FUC	E	2	3	10,10,11	0.77	1 (10%)	14,14,16	1.20	1 (7%)
3	NAG	E	3	3	14,14,15	0.46	0	17,19,21	0.33	0
3	FUC	E	4	3	10,10,11	1.06	0	14,14,16	1.05	0
3	NAG	F	1	3,2	14,14,15	0.68	0	17,19,21	1.50	3 (17%)
3	FUC	F	2	3	10,10,11	1.07	1 (10%)	14,14,16	1.61	3 (21%)
3	NAG	F	3	3	14,14,15	0.53	0	17,19,21	0.36	0
3	FUC	F	4	3	10,10,11	2.11	3 (30%)	14,14,16	1.88	3 (21%)

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	D	1	3,2	-	4/6/23/26	0/1/1/1
3	FUC	D	2	3	-	-	0/1/1/1
3	NAG	D	3	3	-	1/6/23/26	0/1/1/1
3	FUC	D	4	3	-	-	0/1/1/1
3	NAG	E	1	3,2	-	2/6/23/26	0/1/1/1
3	FUC	E	2	3	-	-	0/1/1/1
3	NAG	E	3	3	-	2/6/23/26	0/1/1/1
3	FUC	E	4	3	-	-	0/1/1/1
3	NAG	F	1	3,2	-	2/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1
3	NAG	F	3	3	-	0/6/23/26	0/1/1/1
3	FUC	F	4	3	-	-	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)
3	F	4	FUC	C1-C2	4.91	1.63	1.52
3	F	4	FUC	C2-C3	3.02	1.57	1.52
3	F	2	FUC	C1-C2	2.85	1.58	1.52
3	F	4	FUC	O5-C1	2.62	1.47	1.43
3	D	4	FUC	O5-C1	-2.56	1.39	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1	NAG	C1-O5-C5	4.73	118.60	112.19
3	F	4	FUC	C1-C2-C3	4.53	115.23	109.67
3	F	4	FUC	C1-O5-C5	3.66	121.06	112.78
3	F	2	FUC	C1-C2-C3	3.65	114.15	109.67
3	F	2	FUC	C1-O5-C5	3.00	119.58	112.78

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

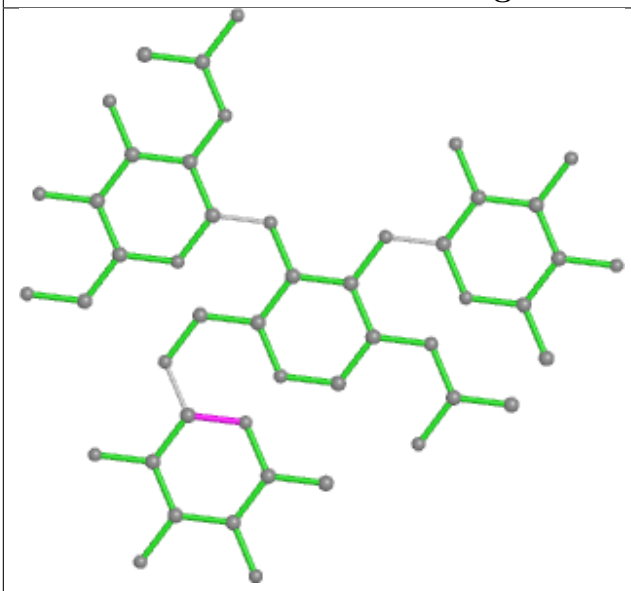
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	3	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6

There are no ring outliers.

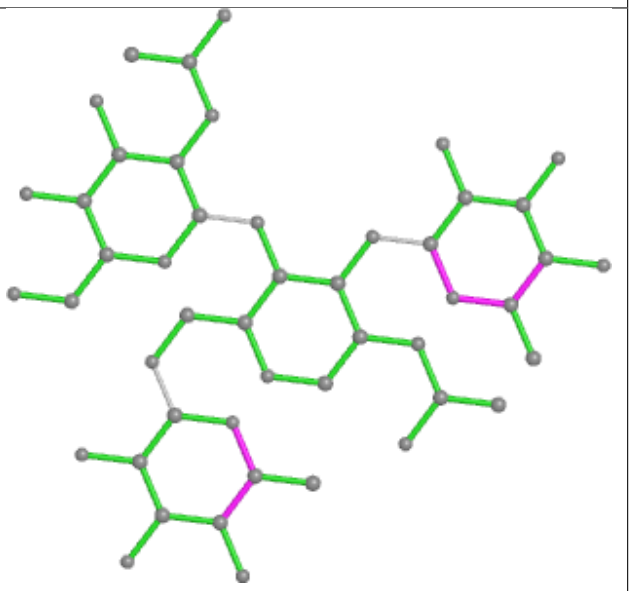
No monomer is involved in short contacts.

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

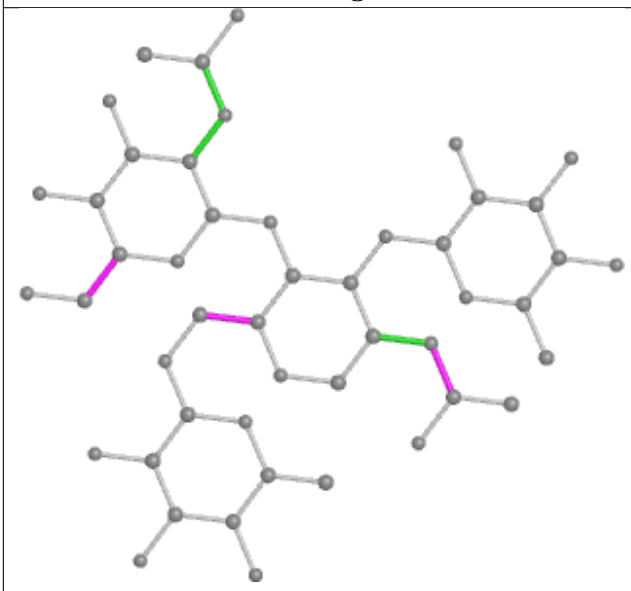
Oligosaccharide Chain D



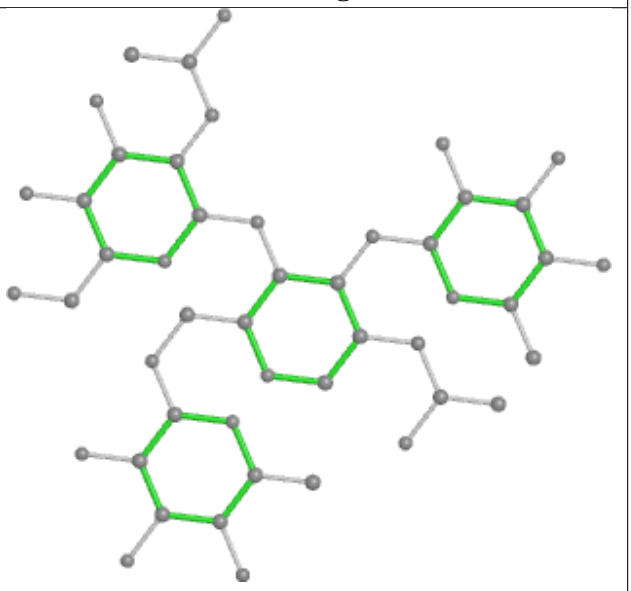
Bond lengths



Bond angles

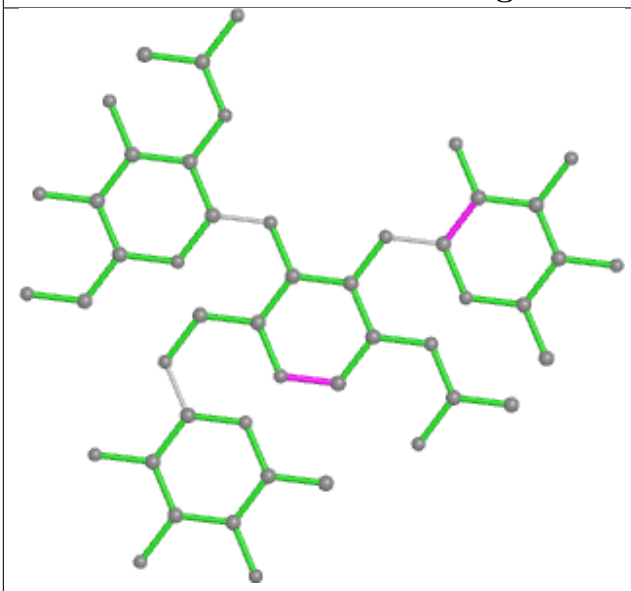


Torsions

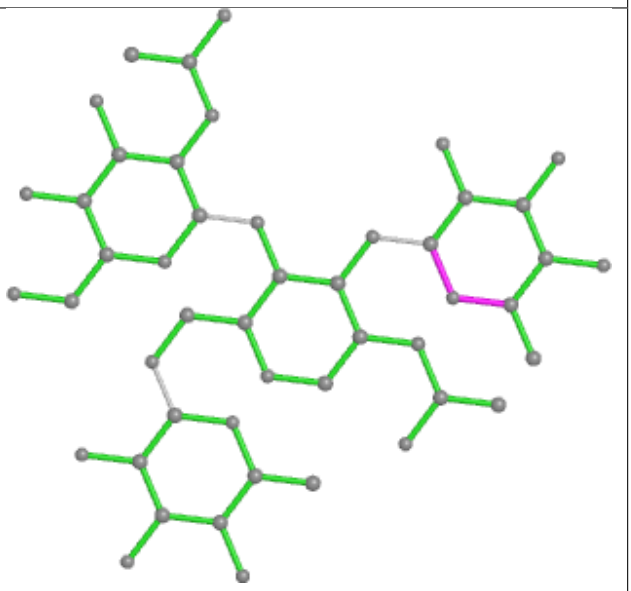


Rings

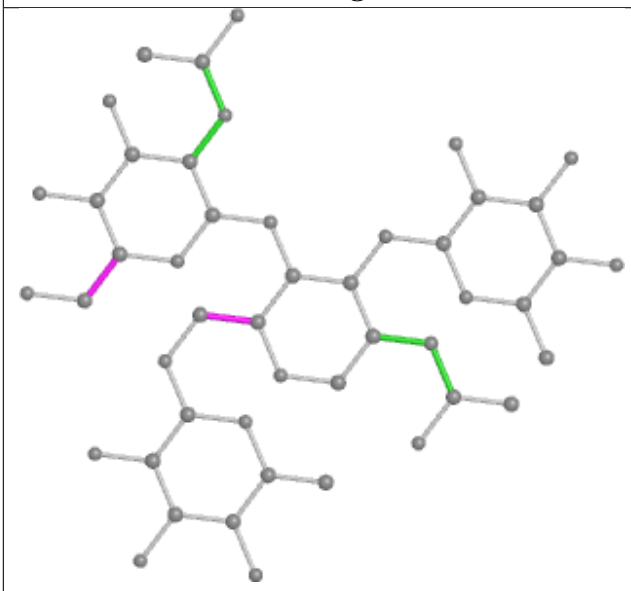
Oligosaccharide Chain E



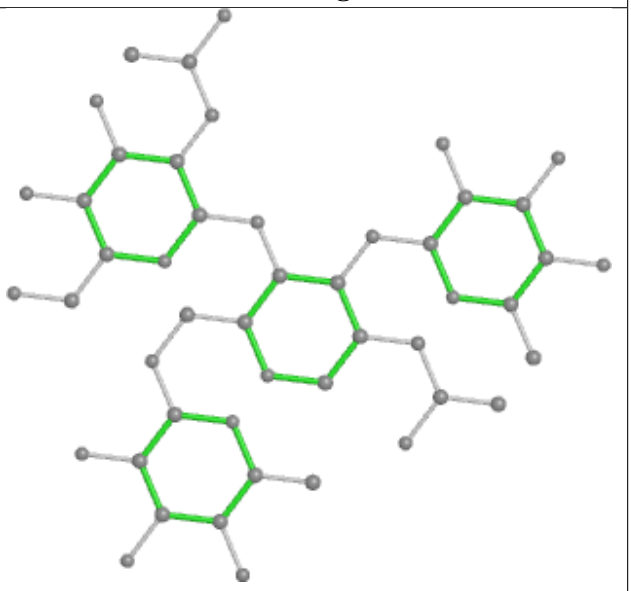
Bond lengths



Bond angles

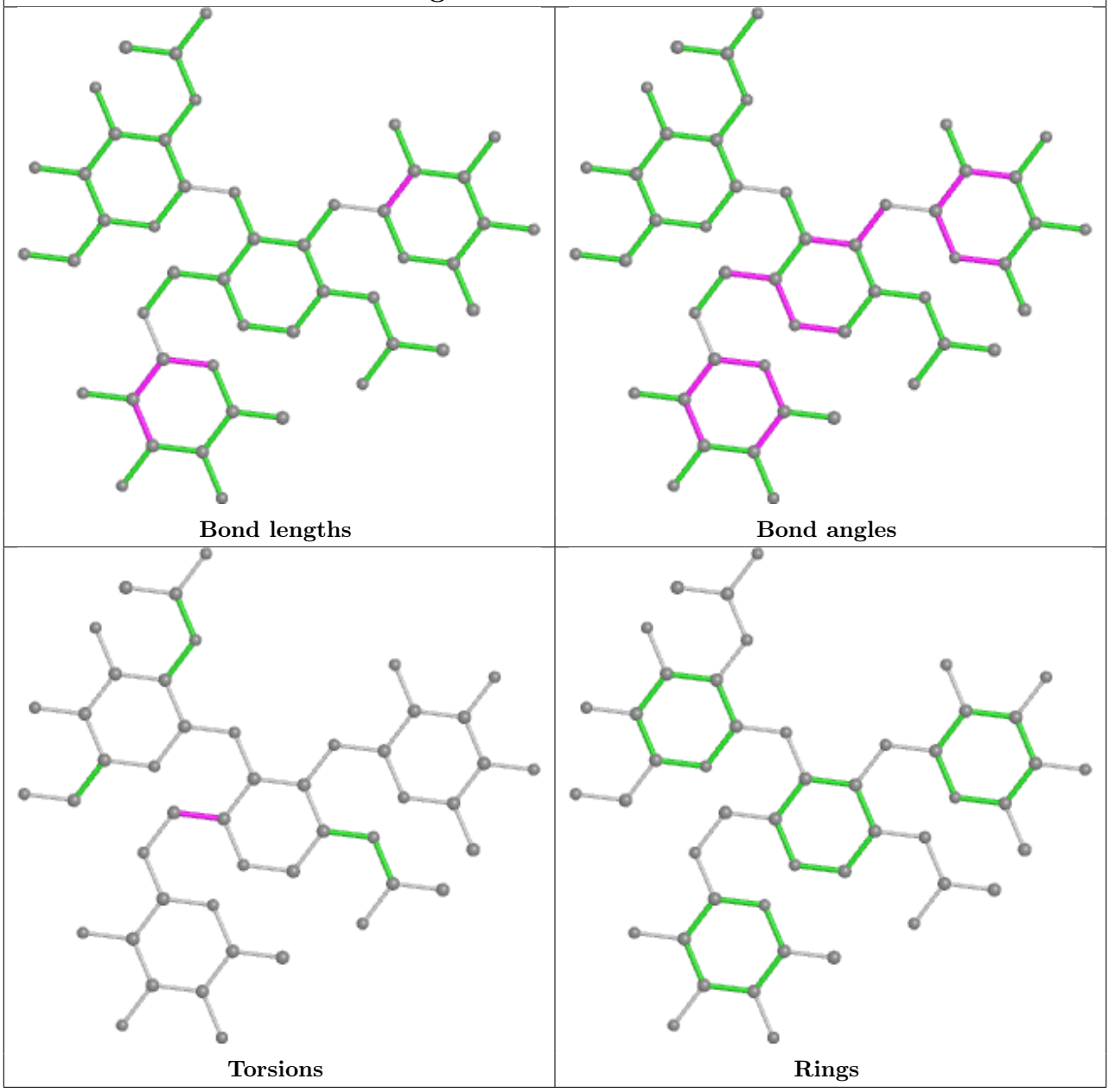


Torsions



Rings

Oligosaccharide Chain F



4.6 Ligand geometry (i)

9 ligands 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	$\#\|Z\| > 2$
4	ACT	A	301	-	3,3,3	0.77	0	3,3,3	1.34	0
5	GOL	C	301	-	5,5,5	0.33	0	5,5,5	0.43	0
4	ACT	C	302	-	3,3,3	0.70	0	3,3,3	1.30	0
4	ACT	Y	205	-	3,3,3	0.79	0	3,3,3	1.30	0
5	GOL	Z	206	-	5,5,5	0.38	0	5,5,5	0.30	0
4	ACT	A	302	-	3,3,3	0.77	0	3,3,3	1.26	0
5	GOL	Z	205	-	5,5,5	0.36	0	5,5,5	0.20	0
4	ACT	X	205	-	3,3,3	0.77	0	3,3,3	1.28	0
5	GOL	B	301	-	5,5,5	0.43	0	5,5,5	0.23	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
5	GOL	Z	206	-	-	4/4/4/4	-
5	GOL	Z	205	-	-	4/4/4/4	-
5	GOL	B	301	-	-	2/4/4/4	-
5	GOL	C	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	301	GOL	O1-C1-C2-C3
5	Z	205	GOL	O1-C1-C2-C3
5	Z	206	GOL	C1-C2-C3-O3
5	Z	206	GOL	O2-C2-C3-O3
5	C	301	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

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

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

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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