Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 05:36 AM EDT

PDB ID	:	6V9U
Title	:	Crystal structure of human TLR8 ectodomain bound to small molecule antagonist 14c
Authors	:	Critton, D.A.
Deposited on	:	2019-12-16
Resolution	:	2.65 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 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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
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 2.65 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 8 unique types of molecules in this entry. The entry contains 12082 atoms, of which 60 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 Toll-like receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	738	Total	C	N	O	S	0	2	0
			5731	3689	952	1071	19			
1	B	735	Total	C	N	O	S	0	1	0
			5646	3637	927	1063	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ARG	-	expression tag	UNP Q9NR97
A	24	SER	-	expression tag	UNP Q9NR97
A	25	PRO	-	expression tag	UNP Q9NR97
A	26	TRP	-	expression tag	UNP Q9NR97
A	828	GLU	-	expression tag	UNP Q9NR97
A	829	PHE	-	expression tag	UNP Q9NR97
A	830	LEU	-	expression tag	UNP Q9NR97
A	831	VAL	-	expression tag	UNP Q9NR97
A	832	PRO	-	expression tag	UNP Q9NR97
A	833	ARG	-	expression tag	UNP Q9NR97
B	23	ARG	-	expression tag	UNP Q9NR97
B	24	SER	-	expression tag	UNP Q9NR97
B	25	PRO	-	expression tag	UNP Q9NR97
B	26	TRP	-	expression tag	UNP Q9NR97
B	828	GLU	-	expression tag	UNP Q9NR97
B	829	PHE	-	expression tag	UNP Q9NR97
B	830	LEU	-	expression tag	UNP Q9NR97
B	831	VAL	-	expression tag	UNP Q9NR97
B	832	PRO	-	expression tag	UNP Q9NR97
B	833	ARG	-	expression tag	UNP Q9NR97

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	C	5	Total C N O 61 34 2 25	0	0	0
2	E	5	Total C N O 61 34 2 25	0	0	0
2	F	5	Total C N O 61 34 2 25	0	0	0

- Molecule 3 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
3	D	2	Total C N O 28 16 2 10	0	0	0

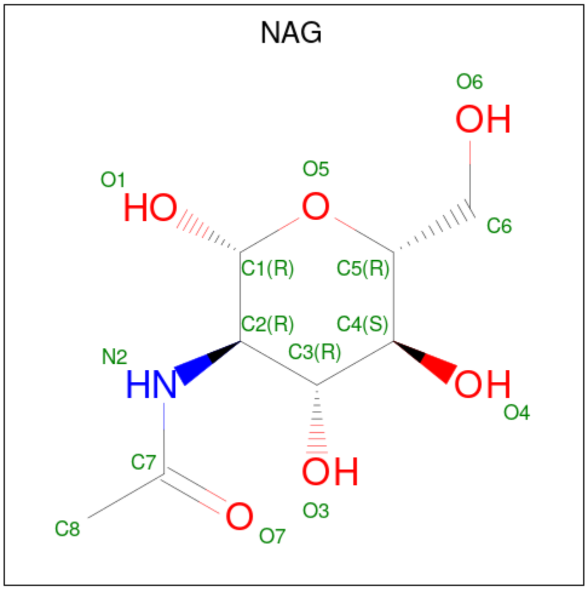
- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	G	3	Total C N O 39 22 2 15	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	H	5	Total C N O 61 34 2 25	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



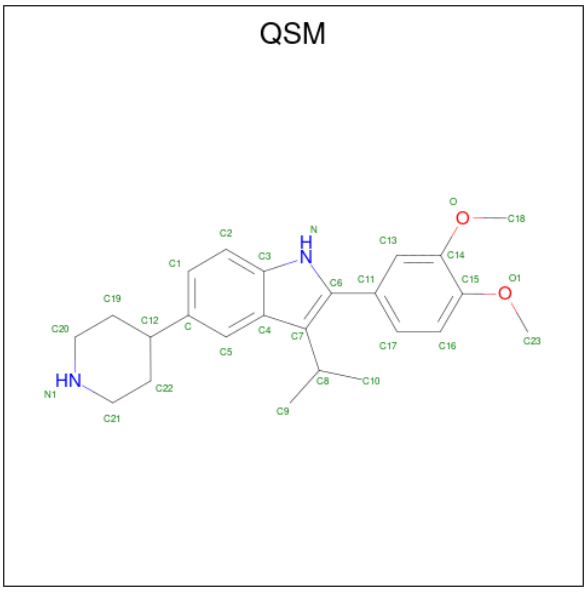
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	A	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0
6	B	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is 2-(3,4-dimethoxyphenyl)-5-(piperidin-4-yl)-3-(propan-2-yl)-1H-indole (three-letter code: QSM) (formula: $C_{24}H_{30}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H N O 58 24 30 2 2	30	0
7	B	1	Total C H N O 58 24 30 2 2	30	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	23	Total O 23 23	0	0
8	B	17	Total O 17 17	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 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	163.59Å 86.75Å 151.40Å 90.00° 119.80° 90.00°	Depositor
Resolution (Å)	131.37 – 2.65	Depositor
% Data completeness (in resolution range)	99.3 (131.37-2.65)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.296 , 0.306	Depositor
Wilson B-factor (Å^2)	57.8	Xtriage
Anisotropy	0.517	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
Total number of atoms	12082	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

25 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	NAG	C	1	2,1	14,14,15	0.32	0	17,19,21	0.83	1 (5%)
2	NAG	C	2	2	14,14,15	0.31	0	17,19,21	0.85	1 (5%)
2	BMA	C	3	2	11,11,12	0.35	0	15,15,17	0.66	0
2	MAN	C	4	2	11,11,12	0.39	0	15,15,17	0.82	1 (6%)
2	MAN	C	5	2	11,11,12	0.39	0	15,15,17	0.85	1 (6%)
3	NAG	D	1	3,1	14,14,15	0.30	0	17,19,21	0.60	0
3	NAG	D	2	3	14,14,15	0.30	0	17,19,21	0.62	1 (5%)
2	NAG	E	1	2,1	14,14,15	0.27	0	17,19,21	0.60	0
2	NAG	E	2	2	14,14,15	0.28	0	17,19,21	0.52	0
2	BMA	E	3	2	11,11,12	0.32	0	15,15,17	0.48	0
2	MAN	E	4	2	11,11,12	0.37	0	15,15,17	0.80	1 (6%)
2	MAN	E	5	2	11,11,12	0.41	0	15,15,17	0.97	2 (13%)
2	NAG	F	1	2,1	14,14,15	0.29	0	17,19,21	0.83	1 (5%)
2	NAG	F	2	2	14,14,15	0.27	0	17,19,21	0.64	0
2	BMA	F	3	2	11,11,12	0.31	0	15,15,17	0.65	0
2	MAN	F	4	2	11,11,12	0.37	0	15,15,17	0.95	1 (6%)
2	MAN	F	5	2	11,11,12	0.42	0	15,15,17	1.10	1 (6%)
4	NAG	G	1	1,4	14,14,15	0.30	0	17,19,21	0.60	0
4	NAG	G	2	4	14,14,15	0.32	0	17,19,21	0.66	1 (5%)
4	BMA	G	3	4	11,11,12	0.35	0	15,15,17	0.53	0
5	NAG	H	1	5,1	14,14,15	0.26	0	17,19,21	0.60	0
5	NAG	H	2	5	14,14,15	0.28	0	17,19,21	0.54	0
5	BMA	H	3	5	11,11,12	0.30	0	15,15,17	0.47	0
5	MAN	H	4	5	11,11,12	0.41	0	15,15,17	0.94	2 (13%)
5	MAN	H	5	5	11,11,12	0.35	0	15,15,17	0.76	1 (6%)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	MAN	E	5	2	-	1/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3	2	-	0/2/19/22	0/1/1/1
2	MAN	F	4	2	-	0/2/19/22	0/1/1/1
2	MAN	F	5	2	-	1/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	1/2/19/22	0/1/1/1
5	MAN	H	5	5	-	1/2/19/22	1/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	5	MAN	C1-O5-C5	3.67	117.16	112.19
2	F	4	MAN	C1-O5-C5	3.36	116.75	112.19
2	E	5	MAN	C1-O5-C5	2.92	116.14	112.19
2	C	5	MAN	C1-O5-C5	2.58	115.69	112.19
2	E	4	MAN	C1-O5-C5	2.57	115.68	112.19
2	C	2	NAG	O5-C1-C2	-2.57	107.23	111.29
5	H	5	MAN	C1-O5-C5	2.53	115.62	112.19
2	F	1	NAG	O5-C1-C2	-2.46	107.41	111.29
5	H	4	MAN	C1-O5-C5	2.46	115.52	112.19
2	C	1	NAG	O5-C1-C2	-2.44	107.43	111.29
4	G	2	NAG	C1-O5-C5	2.37	115.41	112.19
5	H	4	MAN	C1-C2-C3	2.36	112.57	109.67
2	C	4	MAN	C1-O5-C5	2.34	115.37	112.19
3	D	2	NAG	C1-O5-C5	2.19	115.17	112.19
2	E	5	MAN	C1-C2-C3	2.01	112.13	109.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

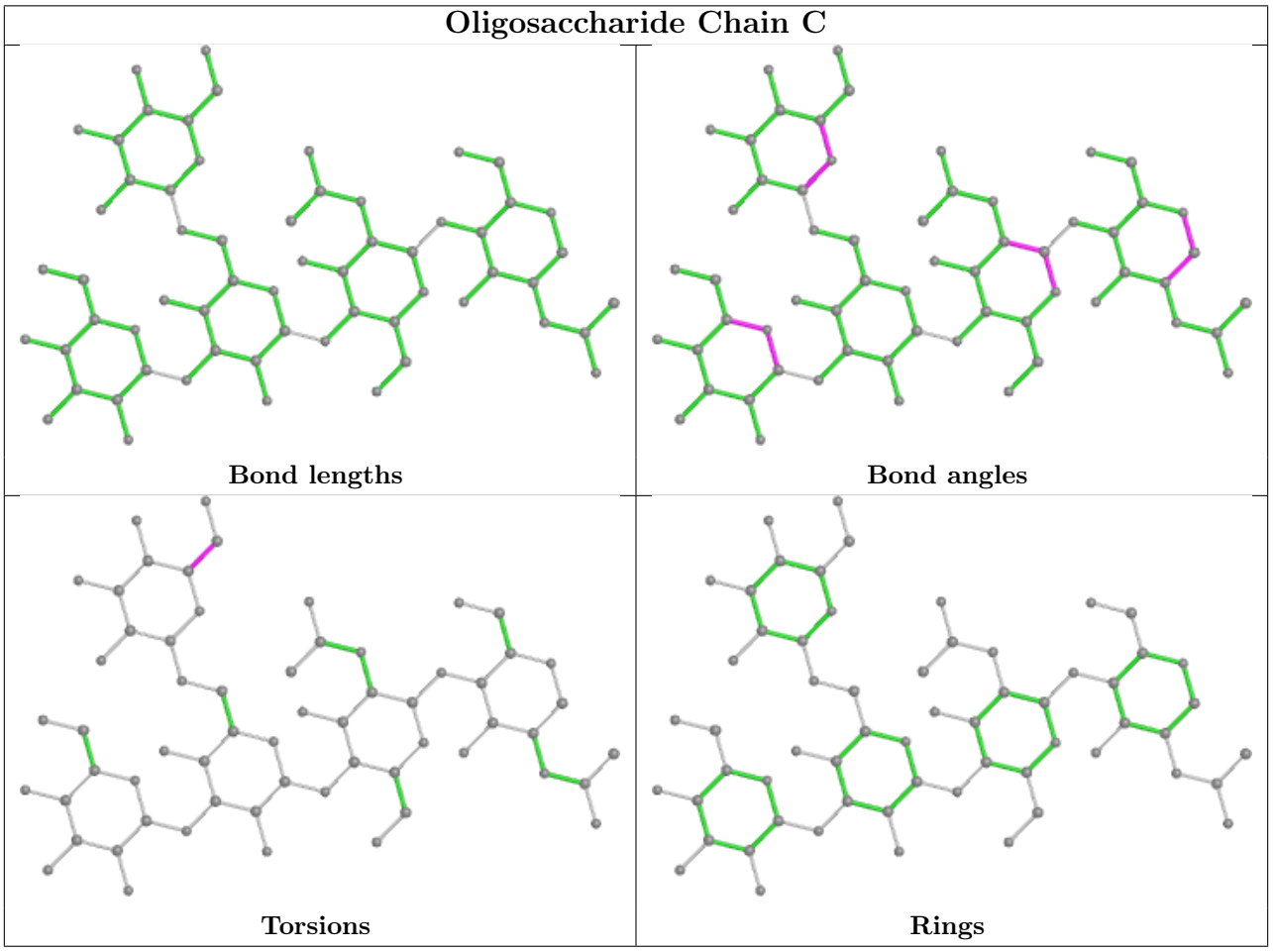
Mol	Chain	Res	Type	Atoms
5	H	4	MAN	O5-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6
2	F	5	MAN	O5-C5-C6-O6
2	E	5	MAN	O5-C5-C6-O6
5	H	5	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

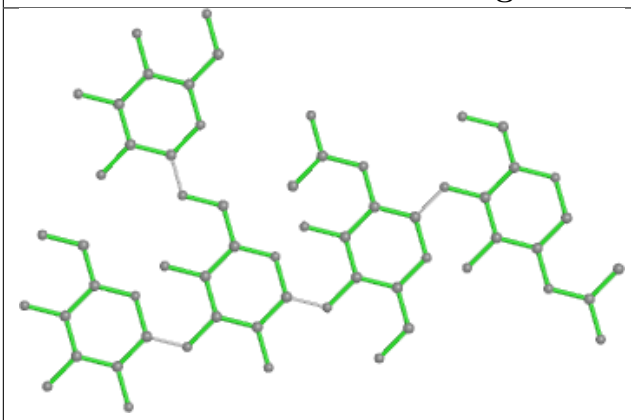
Mol	Chain	Res	Type	Atoms
5	H	5	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

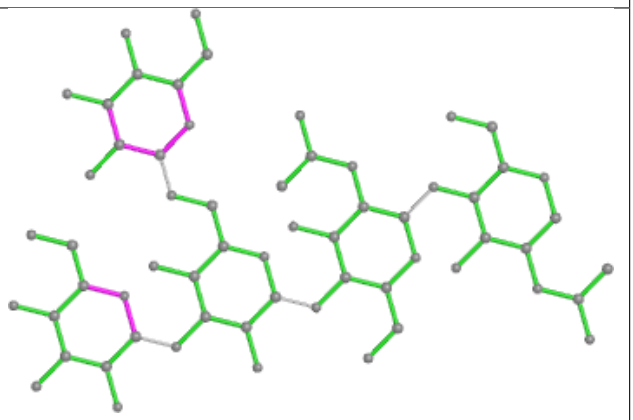
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



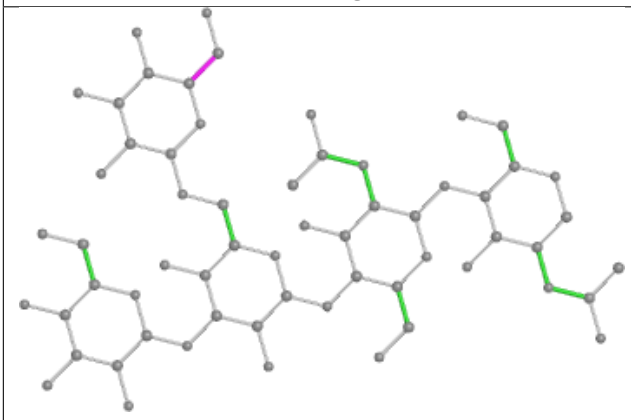
Oligosaccharide Chain E



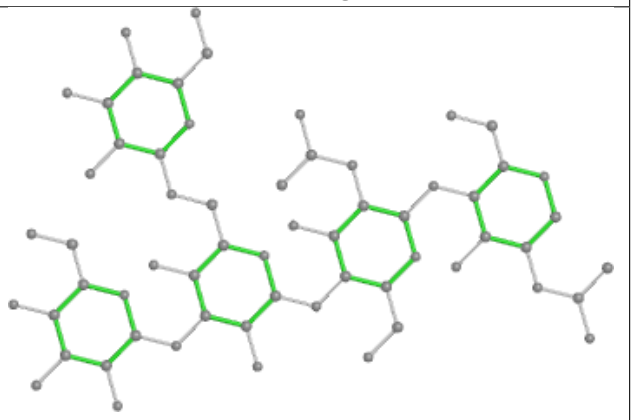
Bond lengths



Bond angles

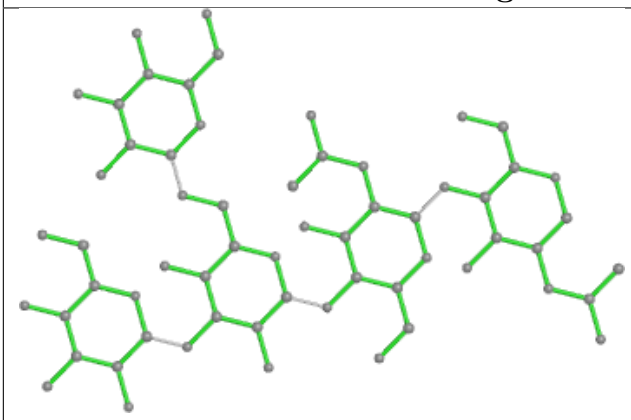


Torsions

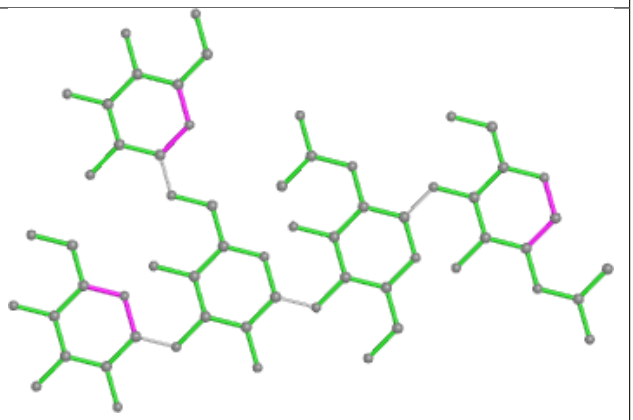


Rings

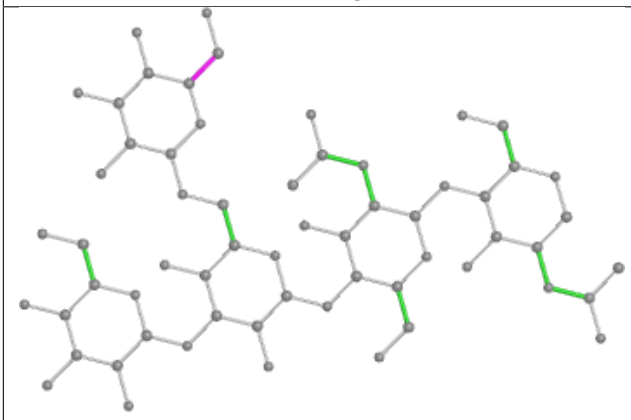
Oligosaccharide Chain F



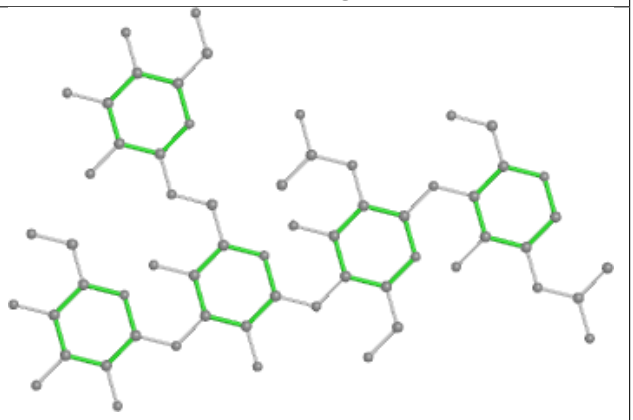
Bond lengths



Bond angles

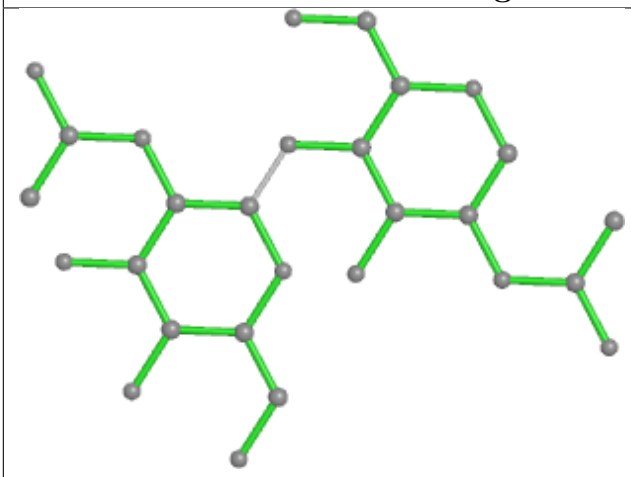


Torsions

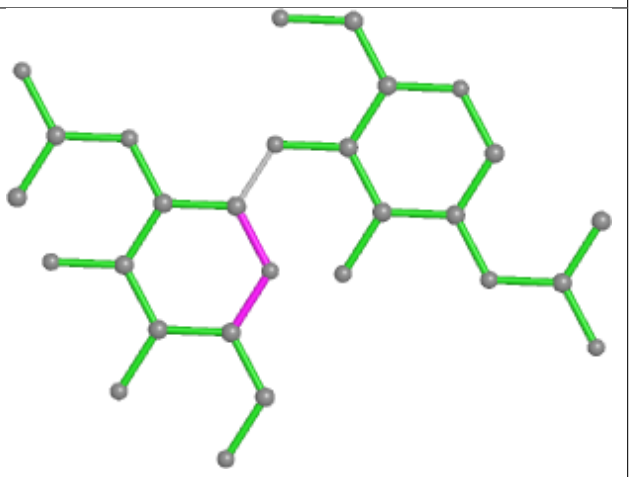


Rings

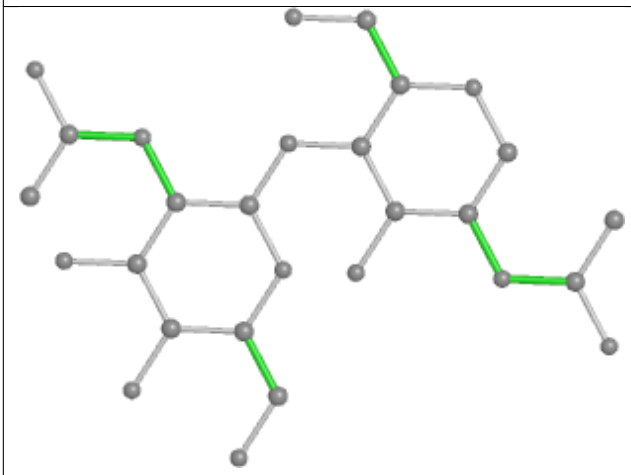
Oligosaccharide Chain D



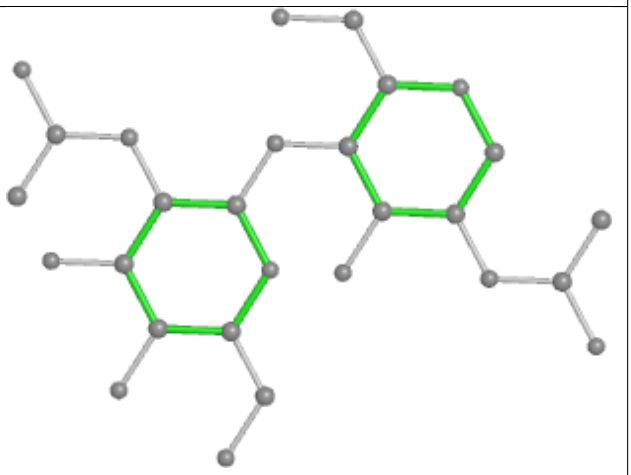
Bond lengths



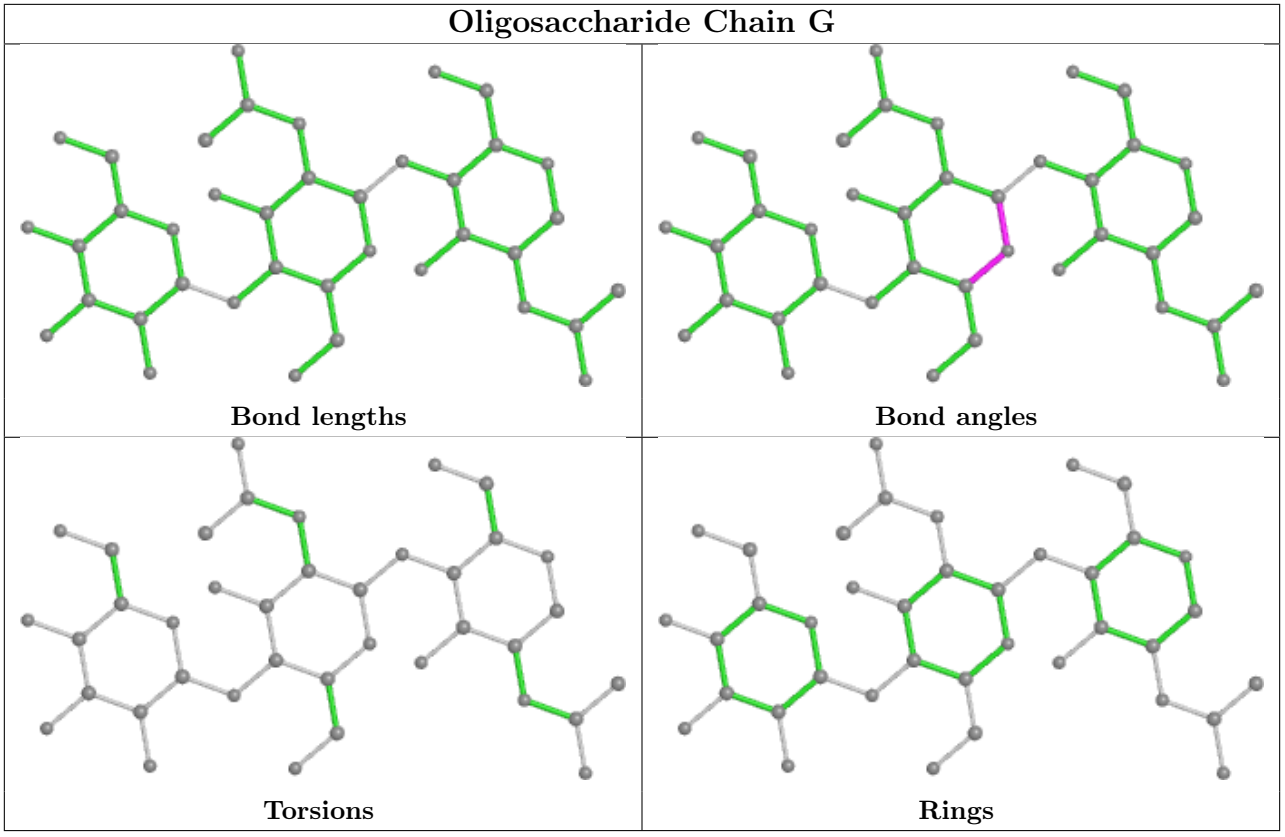
Bond angles

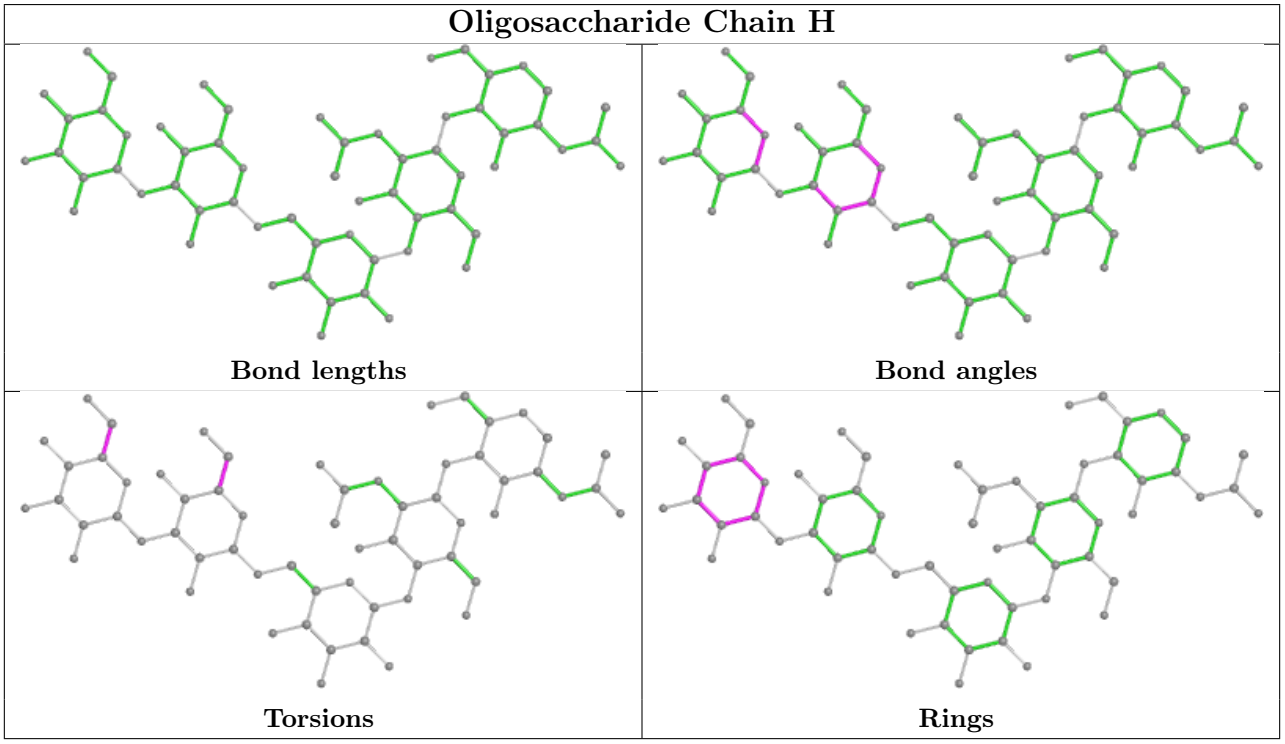


Torsions



Rings





4.6 Ligand geometry (i)

19 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	$\#\|Z\| > 2$
6	NAG	A	919	1	14,14,15	0.30	0	17,19,21	0.66	1 (5%)
6	NAG	B	920	1	14,14,15	0.29	0	17,19,21	0.67	1 (5%)
6	NAG	B	919	1	14,14,15	0.30	0	17,19,21	0.50	0
6	NAG	B	913	1	14,14,15	0.28	0	17,19,21	0.51	0
6	NAG	A	918	1	14,14,15	0.28	0	17,19,21	0.46	0
6	NAG	A	912	1	14,14,15	0.34	0	17,19,21	0.49	0
6	NAG	B	908	1	14,14,15	0.30	0	17,19,21	0.42	0
6	NAG	A	901	1	14,14,15	0.44	0	17,19,21	1.60	2 (11%)
6	NAG	B	909	1	14,14,15	0.28	0	17,19,21	0.54	0
6	NAG	A	921	1	14,14,15	0.29	0	17,19,21	0.55	0
6	NAG	B	901	1	14,14,15	0.30	0	17,19,21	0.55	0
6	NAG	B	902	1	14,14,15	0.31	0	17,19,21	0.45	0
6	NAG	A	908	1	14,14,15	0.31	0	17,19,21	0.40	0
6	NAG	A	920	1	14,14,15	0.32	0	17,19,21	0.66	1 (5%)
6	NAG	B	921	1	14,14,15	0.31	0	17,19,21	0.74	1 (5%)
7	QSM	B	922	-	31,31,31	0.96	1 (3%)	35,44,44	0.91	2 (5%)
7	QSM	A	922	-	31,31,31	0.97	1 (3%)	35,44,44	0.91	2 (5%)
6	NAG	A	902	1	14,14,15	0.30	0	17,19,21	0.59	0
6	NAG	A	909	1	14,14,15	0.34	0	17,19,21	1.13	3 (17%)

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
6	NAG	A	919	1	-	0/6/23/26	0/1/1/1
6	NAG	B	920	1	-	0/6/23/26	0/1/1/1
6	NAG	B	919	1	-	1/6/23/26	0/1/1/1
6	NAG	B	913	1	-	0/6/23/26	0/1/1/1
6	NAG	A	918	1	-	1/6/23/26	0/1/1/1
6	NAG	A	912	1	-	2/6/23/26	0/1/1/1
6	NAG	B	908	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	901	1	-	3/6/23/26	0/1/1/1
6	NAG	B	909	1	-	0/6/23/26	0/1/1/1
6	NAG	A	921	1	-	1/6/23/26	0/1/1/1
6	NAG	B	901	1	-	1/6/23/26	0/1/1/1
6	NAG	B	902	1	-	0/6/23/26	0/1/1/1
6	NAG	A	908	1	-	2/6/23/26	0/1/1/1
6	NAG	A	920	1	-	0/6/23/26	0/1/1/1
6	NAG	B	921	1	-	0/6/23/26	0/1/1/1
7	QSM	B	922	-	-	2/16/24/24	0/4/4/4
7	QSM	A	922	-	-	2/16/24/24	0/4/4/4
6	NAG	A	902	1	-	0/6/23/26	0/1/1/1
6	NAG	A	909	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	922	QSM	C7-C4	4.27	1.45	1.40
7	B	922	QSM	C7-C4	4.22	1.45	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	901	NAG	C1-C2-N2	4.91	118.87	110.49
6	A	901	NAG	C2-N2-C7	4.23	128.93	122.90
6	A	909	NAG	C1-O5-C5	3.13	116.43	112.19
7	A	922	QSM	C-C5-C4	-3.09	119.94	122.00
7	B	922	QSM	C-C5-C4	-3.08	119.95	122.00
7	B	922	QSM	C6-N-C3	2.71	109.46	103.90
7	A	922	QSM	C6-N-C3	2.68	109.42	103.90
6	A	909	NAG	C2-N2-C7	2.33	126.22	122.90
6	A	920	NAG	C1-O5-C5	2.33	115.35	112.19
6	B	920	NAG	C1-O5-C5	2.19	115.16	112.19
6	B	921	NAG	C1-O5-C5	2.18	115.15	112.19
6	A	919	NAG	C1-O5-C5	2.16	115.12	112.19
6	A	909	NAG	C1-C2-N2	2.10	114.08	110.49

There are no chirality outliers.

All (18) torsion outliers are listed below:

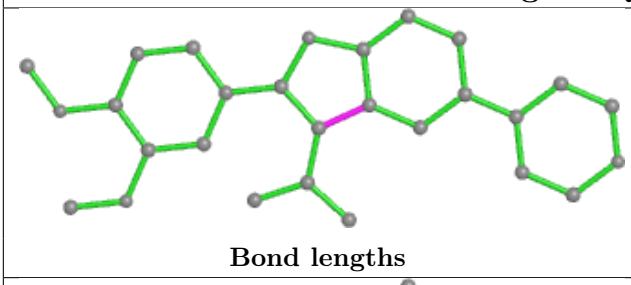
Mol	Chain	Res	Type	Atoms
7	A	922	QSM	C13-C11-C6-N
7	B	922	QSM	C13-C11-C6-N
7	B	922	QSM	C17-C11-C6-N
6	A	908	NAG	O5-C5-C6-O6
6	B	908	NAG	O5-C5-C6-O6
6	B	908	NAG	C4-C5-C6-O6
6	A	912	NAG	O5-C5-C6-O6
6	A	908	NAG	C4-C5-C6-O6
6	A	901	NAG	O5-C5-C6-O6
6	B	901	NAG	O5-C5-C6-O6
6	A	912	NAG	C4-C5-C6-O6
6	A	918	NAG	O5-C5-C6-O6
6	B	919	NAG	O5-C5-C6-O6
7	A	922	QSM	C17-C11-C6-N
6	A	921	NAG	O5-C5-C6-O6
6	A	909	NAG	C3-C2-N2-C7
6	A	901	NAG	C1-C2-N2-C7
6	A	901	NAG	C3-C2-N2-C7

There are no ring outliers.

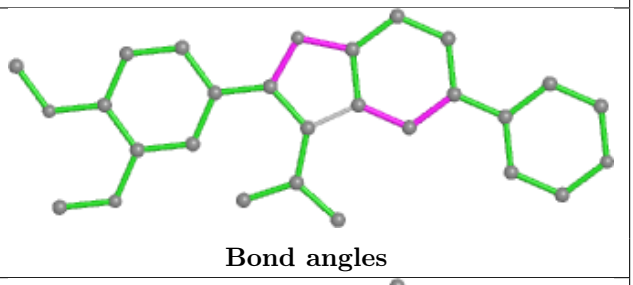
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

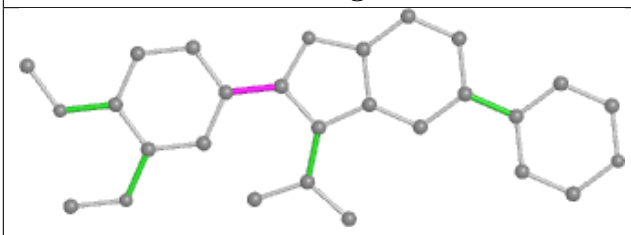
Ligand QSM B 922



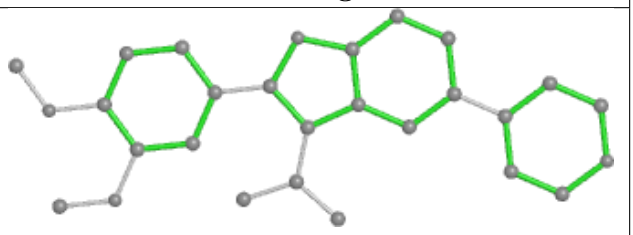
Bond lengths



Bond angles

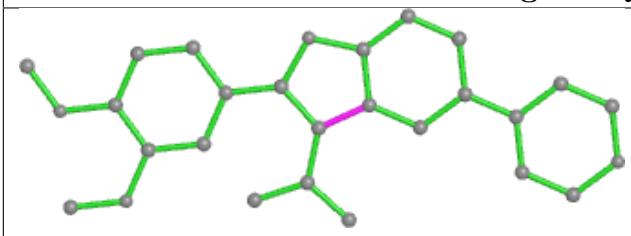


Torsions

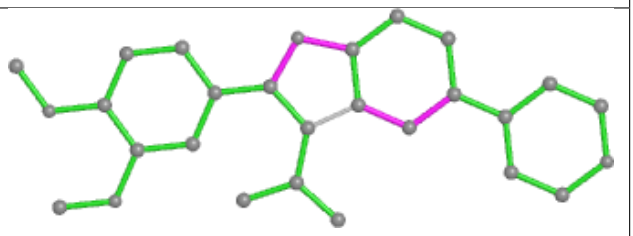


Rings

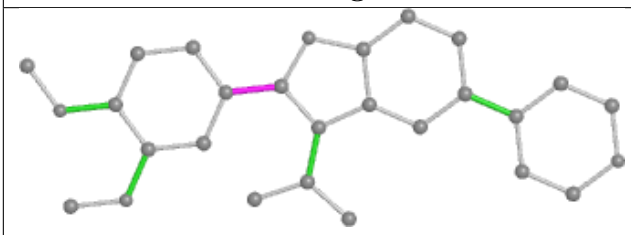
Ligand QSM A 922



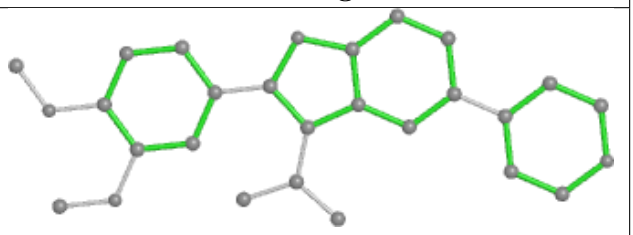
Bond lengths



Bond angles



Torsions



Rings

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

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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