Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2023 – 11:41 PM EDT

PDB ID	:	6MGQ
Title	:	ERAP1 in the open conformation bound to 10mer phosphinic inhibitor DG014
Authors	:	Stern, L.J.; Maben, Z.
Deposited on	:	2018-09-14
Resolution	:	2.92 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
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 2.92 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 20671 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 Endoplasmic reticulum aminopeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	861	Total	C	N	O	S	0	2	0
			6895	4438	1139	1284	34			
1	B	858	Total	C	N	O	S	0	2	0
			6705	4315	1104	1252	34			
1	C	843	Total	C	N	O	S	0	2	0
			6679	4299	1105	1243	32			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	ASP	GLY	conflict	UNP Q9NZ08
A	514	ARG	GLY	conflict	UNP Q9NZ08
A	528	ARG	LYS	conflict	UNP Q9NZ08
A	730	GLU	GLN	conflict	UNP Q9NZ08
A	949	LEU	-	expression tag	UNP Q9NZ08
A	950	GLU	-	expression tag	UNP Q9NZ08
A	951	ARG	-	expression tag	UNP Q9NZ08
A	952	MET	-	expression tag	UNP Q9NZ08
A	953	LEU	-	expression tag	UNP Q9NZ08
A	954	GLU	-	expression tag	UNP Q9NZ08
A	955	SER	-	expression tag	UNP Q9NZ08
A	956	ARG	-	expression tag	UNP Q9NZ08
A	957	GLY	-	expression tag	UNP Q9NZ08
A	958	PRO	-	expression tag	UNP Q9NZ08
A	959	PHE	-	expression tag	UNP Q9NZ08
A	960	GLU	-	expression tag	UNP Q9NZ08
A	961	GLN	-	expression tag	UNP Q9NZ08
A	962	LYS	-	expression tag	UNP Q9NZ08
A	963	LEU	-	expression tag	UNP Q9NZ08
A	964	ILE	-	expression tag	UNP Q9NZ08
A	965	SER	-	expression tag	UNP Q9NZ08
A	966	GLU	-	expression tag	UNP Q9NZ08
A	967	GLU	-	expression tag	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
A	968	ASP	-	expression tag	UNP Q9NZ08
A	969	LEU	-	expression tag	UNP Q9NZ08
A	970	ASN	-	expression tag	UNP Q9NZ08
A	971	MET	-	expression tag	UNP Q9NZ08
A	972	HIS	-	expression tag	UNP Q9NZ08
A	973	THR	-	expression tag	UNP Q9NZ08
A	974	GLU	-	expression tag	UNP Q9NZ08
A	975	HIS	-	expression tag	UNP Q9NZ08
A	976	HIS	-	expression tag	UNP Q9NZ08
A	977	HIS	-	expression tag	UNP Q9NZ08
A	978	HIS	-	expression tag	UNP Q9NZ08
A	979	HIS	-	expression tag	UNP Q9NZ08
A	980	HIS	-	expression tag	UNP Q9NZ08
B	346	ASP	GLY	conflict	UNP Q9NZ08
B	514	ARG	GLY	conflict	UNP Q9NZ08
B	528	ARG	LYS	conflict	UNP Q9NZ08
B	730	GLU	GLN	conflict	UNP Q9NZ08
B	949	LEU	-	expression tag	UNP Q9NZ08
B	950	GLU	-	expression tag	UNP Q9NZ08
B	951	ARG	-	expression tag	UNP Q9NZ08
B	952	MET	-	expression tag	UNP Q9NZ08
B	953	LEU	-	expression tag	UNP Q9NZ08
B	954	GLU	-	expression tag	UNP Q9NZ08
B	955	SER	-	expression tag	UNP Q9NZ08
B	956	ARG	-	expression tag	UNP Q9NZ08
B	957	GLY	-	expression tag	UNP Q9NZ08
B	958	PRO	-	expression tag	UNP Q9NZ08
B	959	PHE	-	expression tag	UNP Q9NZ08
B	960	GLU	-	expression tag	UNP Q9NZ08
B	961	GLN	-	expression tag	UNP Q9NZ08
B	962	LYS	-	expression tag	UNP Q9NZ08
B	963	LEU	-	expression tag	UNP Q9NZ08
B	964	ILE	-	expression tag	UNP Q9NZ08
B	965	SER	-	expression tag	UNP Q9NZ08
B	966	GLU	-	expression tag	UNP Q9NZ08
B	967	GLU	-	expression tag	UNP Q9NZ08
B	968	ASP	-	expression tag	UNP Q9NZ08
B	969	LEU	-	expression tag	UNP Q9NZ08
B	970	ASN	-	expression tag	UNP Q9NZ08
B	971	MET	-	expression tag	UNP Q9NZ08
B	972	HIS	-	expression tag	UNP Q9NZ08
B	973	THR	-	expression tag	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
B	974	GLU	-	expression tag	UNP Q9NZ08
B	975	HIS	-	expression tag	UNP Q9NZ08
B	976	HIS	-	expression tag	UNP Q9NZ08
B	977	HIS	-	expression tag	UNP Q9NZ08
B	978	HIS	-	expression tag	UNP Q9NZ08
B	979	HIS	-	expression tag	UNP Q9NZ08
B	980	HIS	-	expression tag	UNP Q9NZ08
C	346	ASP	GLY	conflict	UNP Q9NZ08
C	514	ARG	GLY	conflict	UNP Q9NZ08
C	528	ARG	LYS	conflict	UNP Q9NZ08
C	730	GLU	GLN	conflict	UNP Q9NZ08
C	949	LEU	-	expression tag	UNP Q9NZ08
C	950	GLU	-	expression tag	UNP Q9NZ08
C	951	ARG	-	expression tag	UNP Q9NZ08
C	952	MET	-	expression tag	UNP Q9NZ08
C	953	LEU	-	expression tag	UNP Q9NZ08
C	954	GLU	-	expression tag	UNP Q9NZ08
C	955	SER	-	expression tag	UNP Q9NZ08
C	956	ARG	-	expression tag	UNP Q9NZ08
C	957	GLY	-	expression tag	UNP Q9NZ08
C	958	PRO	-	expression tag	UNP Q9NZ08
C	959	PHE	-	expression tag	UNP Q9NZ08
C	960	GLU	-	expression tag	UNP Q9NZ08
C	961	GLN	-	expression tag	UNP Q9NZ08
C	962	LYS	-	expression tag	UNP Q9NZ08
C	963	LEU	-	expression tag	UNP Q9NZ08
C	964	ILE	-	expression tag	UNP Q9NZ08
C	965	SER	-	expression tag	UNP Q9NZ08
C	966	GLU	-	expression tag	UNP Q9NZ08
C	967	GLU	-	expression tag	UNP Q9NZ08
C	968	ASP	-	expression tag	UNP Q9NZ08
C	969	LEU	-	expression tag	UNP Q9NZ08
C	970	ASN	-	expression tag	UNP Q9NZ08
C	971	MET	-	expression tag	UNP Q9NZ08
C	972	HIS	-	expression tag	UNP Q9NZ08
C	973	THR	-	expression tag	UNP Q9NZ08
C	974	GLU	-	expression tag	UNP Q9NZ08
C	975	HIS	-	expression tag	UNP Q9NZ08
C	976	HIS	-	expression tag	UNP Q9NZ08
C	977	HIS	-	expression tag	UNP Q9NZ08
C	978	HIS	-	expression tag	UNP Q9NZ08
C	979	HIS	-	expression tag	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
C	980	HIS	-	expression tag	UNP Q9NZ08

- Molecule 2 is a protein called Phosphinic inhibitor DG014.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	5	Total	C	N	O	P	0	0	0
			46	34	4	7	1			
2	E	5	Total	C	N	O	P	0	0	0
			46	34	4	7	1			
2	F	5	Total	C	N	O	P	0	0	0
			46	34	4	7	1			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
3	G	4	Total	C	N	O	0	0	0
			50	28	2	20			

- 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
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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
5	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	J	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0
6	B	1	Total Zn 1 1	0	0
6	C	1	Total Zn 1 1	0	0

- Molecule 7 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total X 1 1	0	0
7	B	1	Total X 1 1	0	0
7	C	1	Total X 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	14	Total O 14 14	0	0
8	B	14	Total O 14 14	0	0
8	C	8	Total O 8 8	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	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.14Å 234.70Å 132.28Å 90.00° 93.12° 90.00°	Depositor
Resolution (Å)	56.06 – 2.92	Depositor
% Data completeness (in resolution range)	81.7 (56.06-2.92)	Depositor
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.14_3211	Depositor
R, R_{free}	0.198 , 0.256	Depositor
Wilson B-factor (Å^2)	50.4	Xtriage
Anisotropy	0.061	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20671	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 2.96% 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

16 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	G	1	1,3	14,14,15	0.29	0	17,19,21	0.60	0
3	NAG	G	2	3	14,14,15	0.17	0	17,19,21	0.52	0
3	BMA	G	3	3	11,11,12	0.66	0	15,15,17	0.83	0
3	MAN	G	4	3	11,11,12	1.43	2 (18%)	15,15,17	1.24	1 (6%)
4	NAG	H	1	1,4	14,14,15	0.26	0	17,19,21	0.50	0
4	NAG	H	2	4	14,14,15	0.37	0	17,19,21	0.46	0
5	NAG	I	1	1,5	14,14,15	0.37	0	17,19,21	1.14	1 (5%)
5	NAG	I	2	5	14,14,15	0.31	0	17,19,21	0.87	1 (5%)
5	BMA	I	3	5	11,11,12	0.29	0	15,15,17	0.81	0
5	NAG	J	1	1,5	14,14,15	0.38	0	17,19,21	0.59	0
5	NAG	J	2	5	14,14,15	0.30	0	17,19,21	0.77	1 (5%)
5	BMA	J	3	5	11,11,12	1.14	2 (18%)	15,15,17	1.73	4 (26%)
4	NAG	K	1	1,4	14,14,15	0.18	0	17,19,21	0.51	0
4	NAG	K	2	4	14,14,15	0.57	0	17,19,21	0.64	0
4	NAG	L	1	1,4	14,14,15	0.32	0	17,19,21	0.50	0
4	NAG	L	2	4	14,14,15	0.27	0	17,19,21	0.77	1 (5%)

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	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	1/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	NAG	J	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	4	MAN	C4-C3	2.82	1.59	1.52
3	G	4	MAN	C1-C2	2.42	1.57	1.52
5	J	3	BMA	C4-C3	2.39	1.58	1.52
5	J	3	BMA	C4-C5	2.02	1.57	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	3	BMA	C1-C2-C3	-4.29	104.39	109.67
5	J	3	BMA	O5-C1-C2	-3.16	105.90	110.77
5	I	1	NAG	C2-N2-C7	-3.10	118.49	122.90
3	G	4	MAN	C1-O5-C5	2.55	115.65	112.19
5	J	2	NAG	O4-C4-C5	-2.51	103.06	109.30
5	J	3	BMA	C3-C4-C5	2.30	114.34	110.24
5	I	2	NAG	C2-N2-C7	-2.25	119.70	122.90
4	L	2	NAG	C2-N2-C7	2.18	126.01	122.90
5	J	3	BMA	O2-C2-C3	-2.07	106.00	110.14

There are no chirality outliers.

All (13) torsion outliers are listed below:

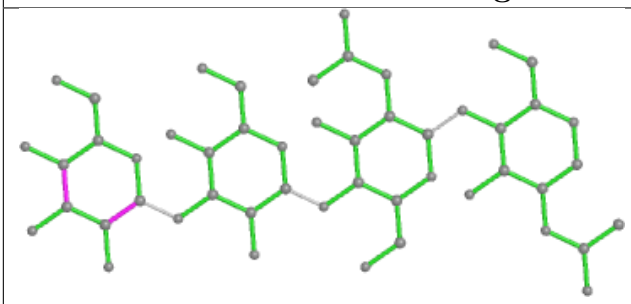
Mol	Chain	Res	Type	Atoms
4	L	2	NAG	C3-C2-N2-C7
5	I	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
4	H	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
5	J	1	NAG	C1-C2-N2-C7
5	J	2	NAG	C1-C2-N2-C7
5	J	1	NAG	C3-C2-N2-C7
5	I	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C3-C2-N2-C7
5	I	1	NAG	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
3	G	4	MAN	O5-C5-C6-O6

There are no ring outliers.

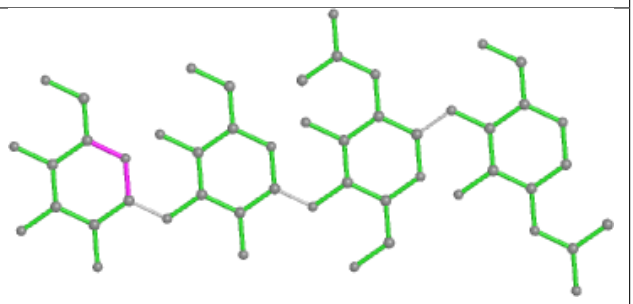
No monomer is involved in short contacts.

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

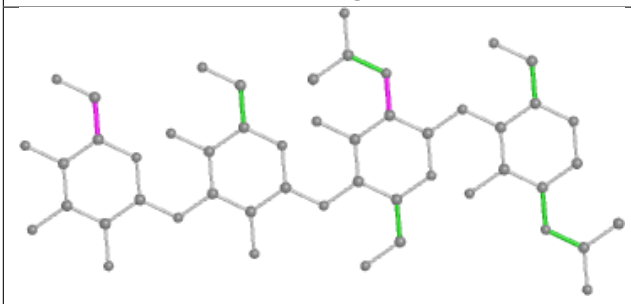
Oligosaccharide Chain G



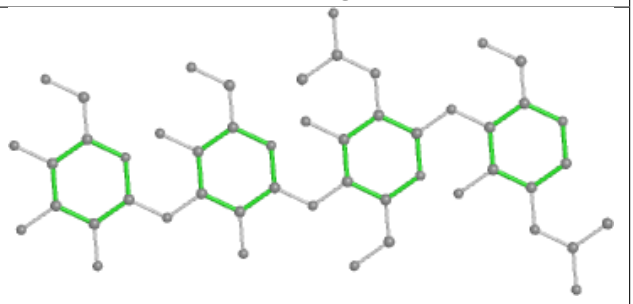
Bond lengths



Bond angles

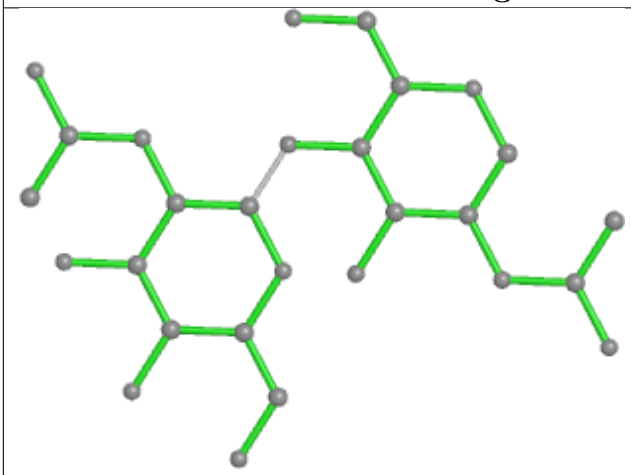


Torsions

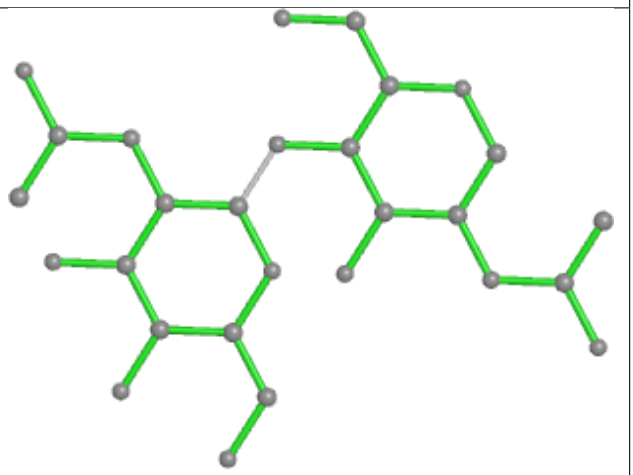


Rings

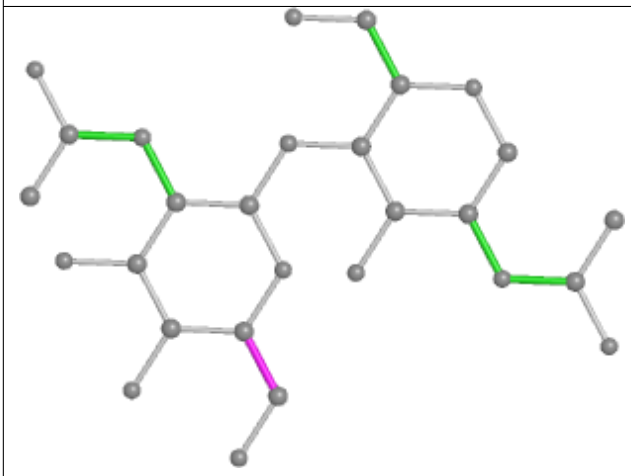
Oligosaccharide Chain H



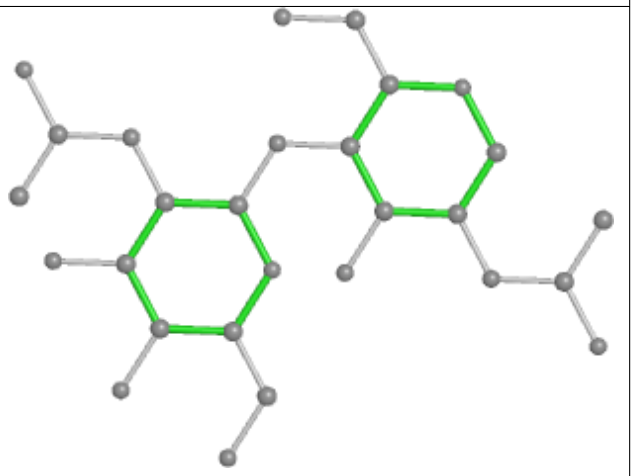
Bond lengths



Bond angles

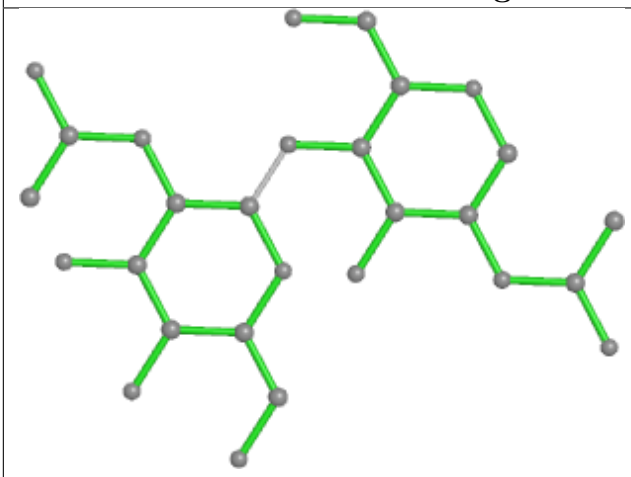


Torsions

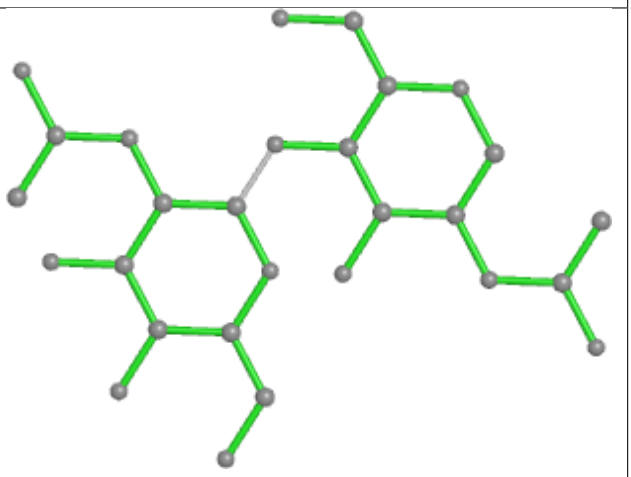


Rings

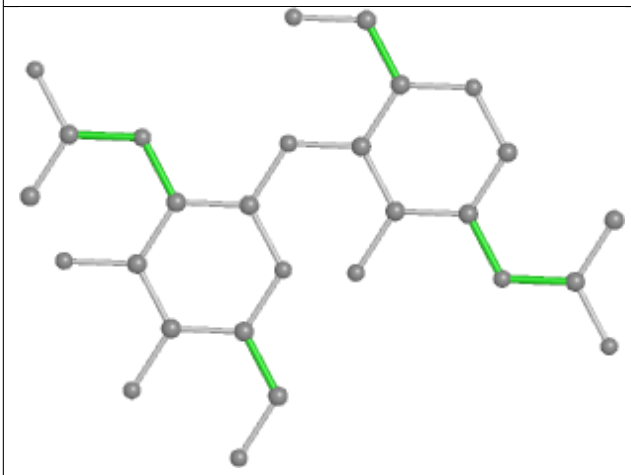
Oligosaccharide Chain K



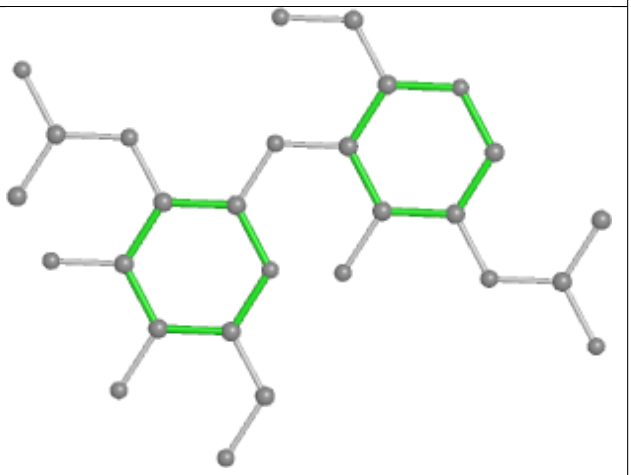
Bond lengths



Bond angles

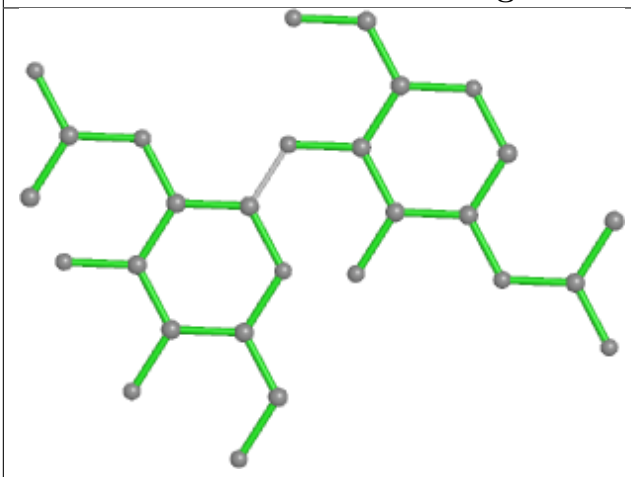


Torsions

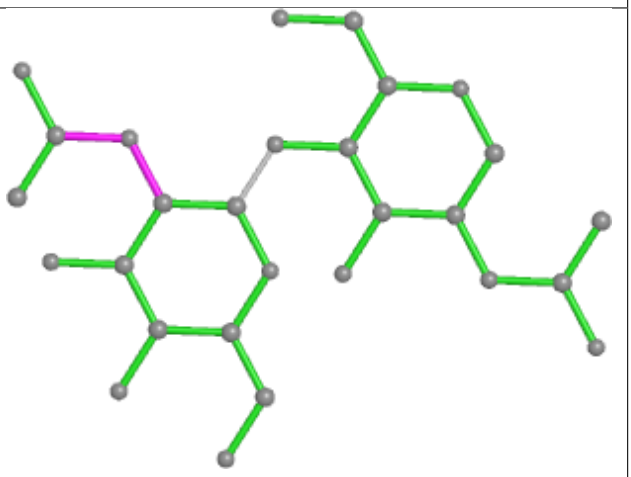


Rings

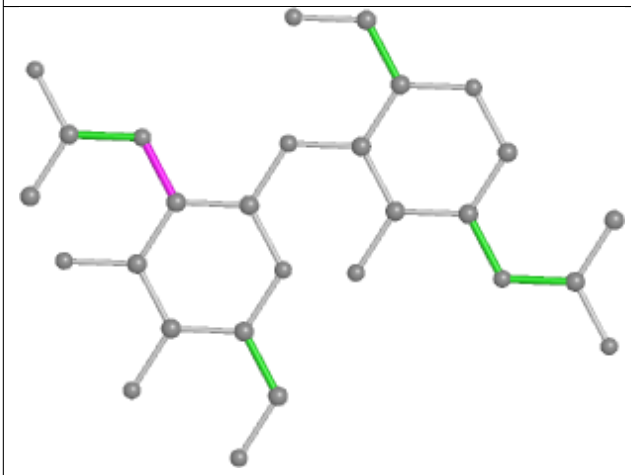
Oligosaccharide Chain L



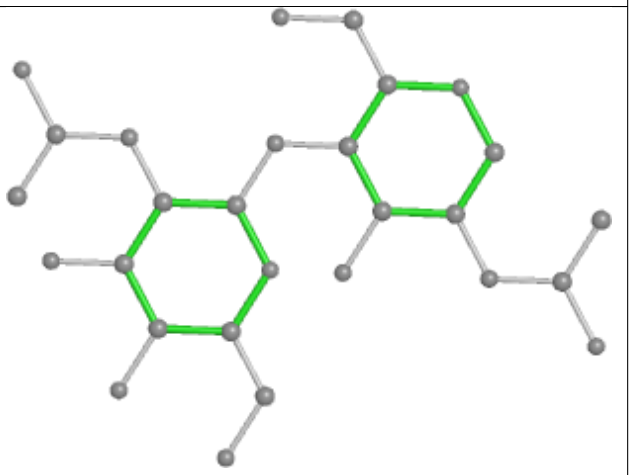
Bond lengths



Bond angles

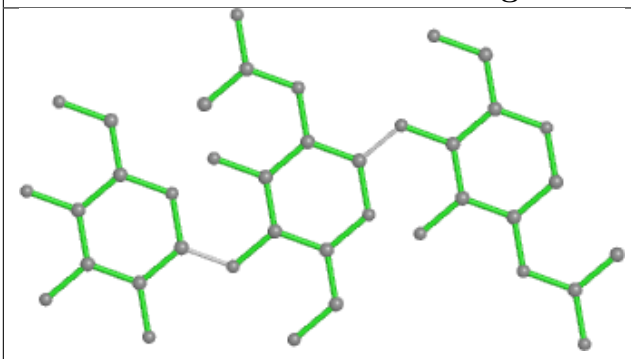


Torsions

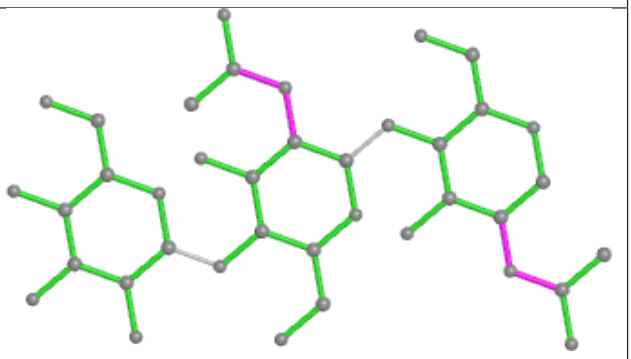


Rings

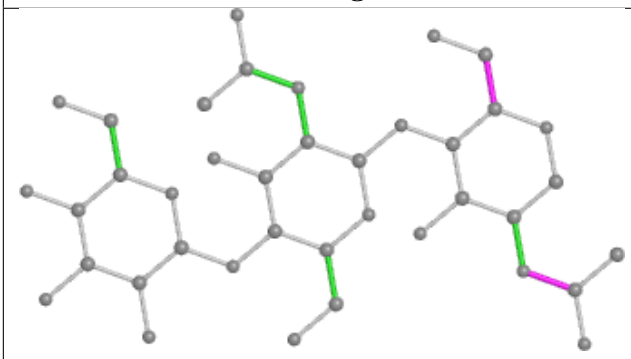
Oligosaccharide Chain I



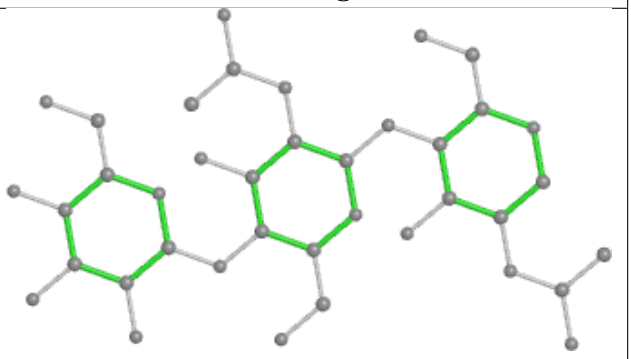
Bond lengths



Bond angles

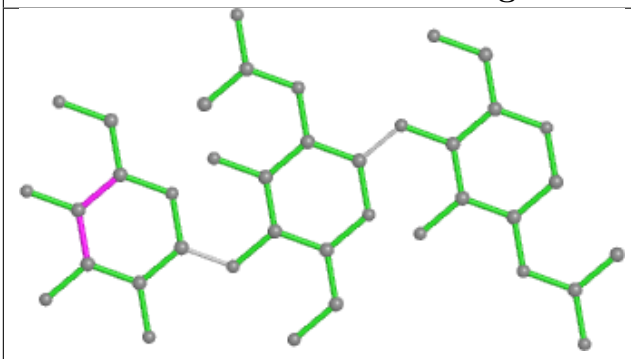


Torsions

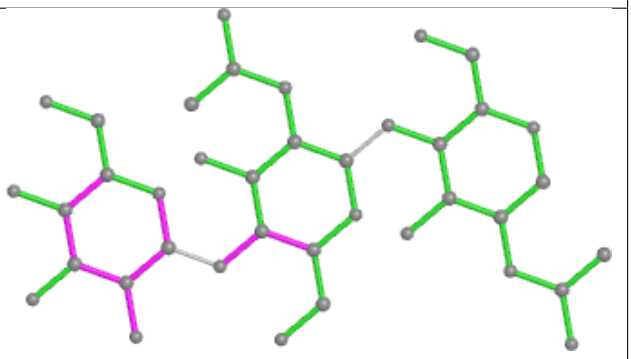


Rings

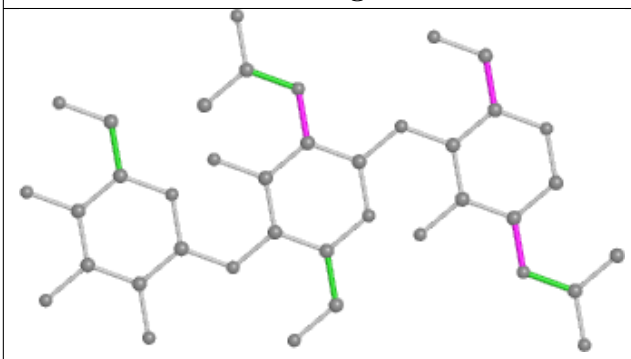
Oligosaccharide Chain J



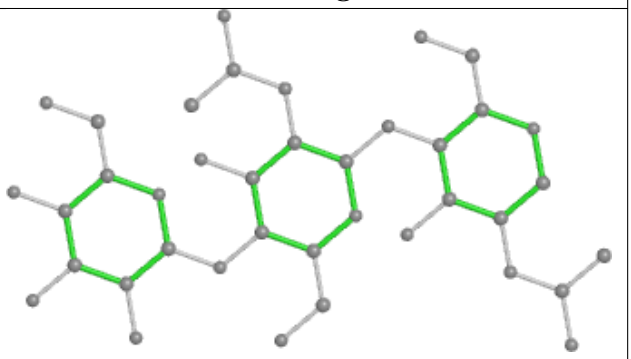
Bond lengths



Bond angles



Torsions



Rings

4.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 3 are monoatomic and 3 are unknown - 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.

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.