wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 10:56 PM EDT

PDB ID	:	6VJ7
Title	:	Crystal structure of red kidney bean purple acid phosphatase in complex with adenosine 5'-(beta,gamma imido)triphosphate
Authors	:	Feder, D.; Schenk, G.; Guddat, L.W.; McGeary, R.P.; Mitic, N.; Furtado, A.; Schulz, B.L.; Henry, R.J.; Schmidt, S.
Deposited on	:	2020-01-15
Resolution	:	2.60 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 (1)) 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 2.60 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 18 unique types of molecules in this entry. The entry contains 15691 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 Fe(3+)-Zn(2+) purple acid phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	2	0
			3506	2250	608	638	10			
1	B	425	Total	C	N	O	S	0	3	0
			3521	2260	611	640	10			
1	C	423	Total	C	N	O	S	0	0	0
			3482	2237	603	632	10			
1	D	426	Total	C	N	O	S	0	5	0
			3546	2275	618	642	11			

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose -(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucop yranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	G	4	Total C N O 50 28 2 20	0	0	0

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[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 38 22 2 14	0	0	0
5	J	3	Total C N O 38 22 2 14	0	0	0

- Molecule 6 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
6	K	2	Total C N O 28 16 2 10	0	0	0
6	L	2	Total C N O 28 16 2 10	0	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Fe 1 1	0	0
8	B	1	Total Fe 1 1	0	0
8	C	1	Total Fe 1 1	0	0

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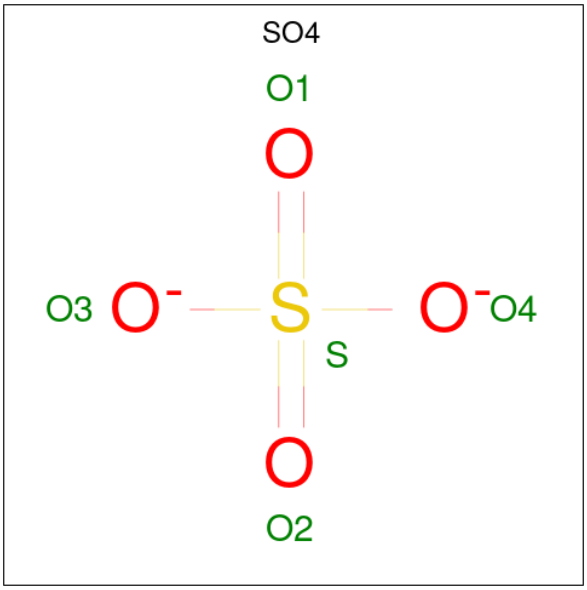
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Fe 1 1	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O S 5 4 1	0	0
9	A	1	Total O S 5 4 1	0	0
9	A	1	Total O S 5 4 1	0	0
9	B	1	Total O S 5 4 1	0	0
9	B	1	Total O S 5 4 1	0	0
9	B	1	Total O S 5 4 1	0	0
9	B	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0

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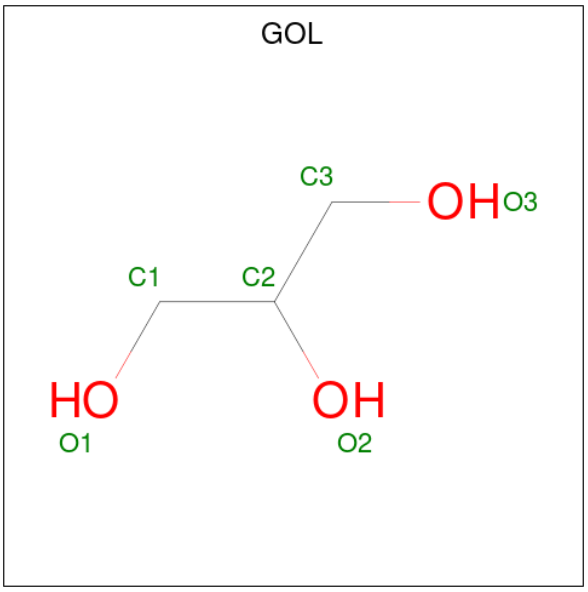
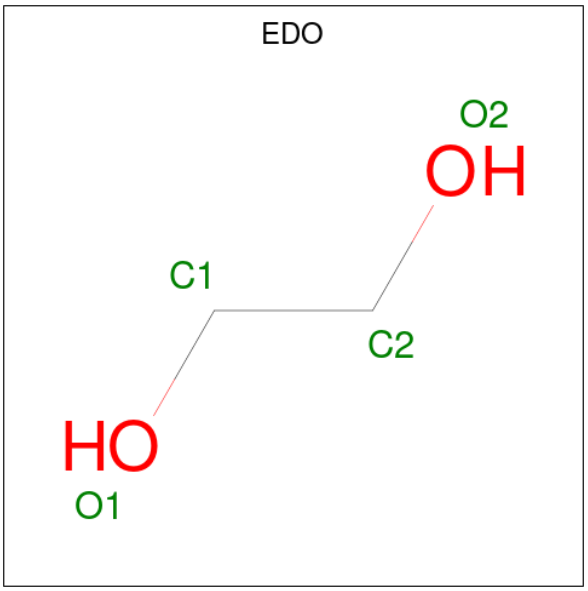
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	1
			12	6	6		
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			4	2	2		
11	A	1	Total	C	O	0	0
			4	2	2		
11	A	1	Total	C	O	0	0
			4	2	2		
11	A	1	Total	C	O	0	0
			4	2	2		
11	A	1	Total	C	O	0	0
			4	2	2		
11	B	1	Total	C	O	0	0
			4	2	2		
11	B	1	Total	C	O	0	0
			4	2	2		
11	B	1	Total	C	O	0	0
			4	2	2		
11	B	1	Total	C	O	0	0
			4	2	2		
11	B	1	Total	C	O	0	0
			4	2	2		
11	B	1	Total	C	O	0	0
			4	2	2		
11	C	1	Total	C	O	0	0
			4	2	2		
11	C	1	Total	C	O	0	0
			4	2	2		
11	C	1	Total	C	O	0	0
			4	2	2		

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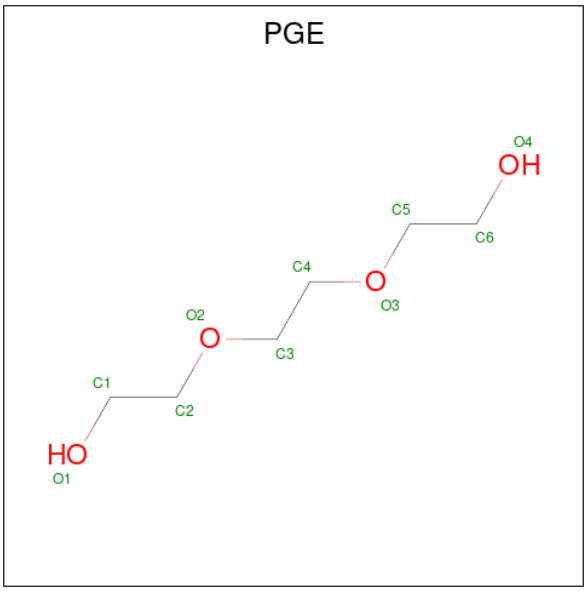
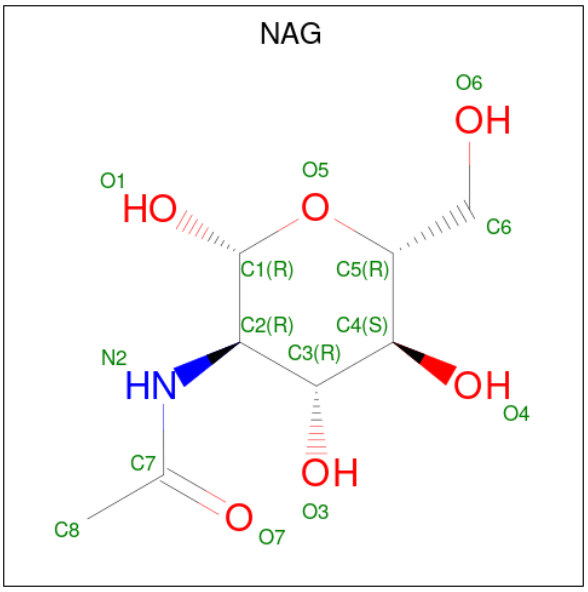
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	C	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0
11	D	1	Total C O 4 2 2	0	0

- Molecule 12 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



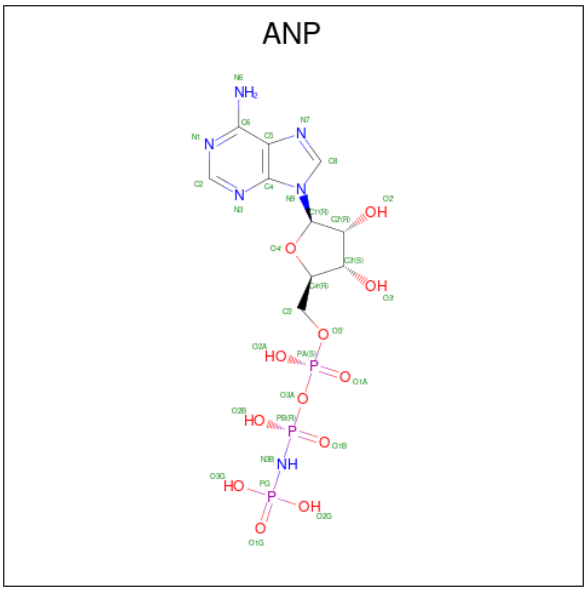
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 7 4 3	0	0
12	B	1	Total C O 7 4 3	0	0
12	B	1	Total C O 7 4 3	0	0
12	C	1	Total C O 10 6 4	0	0
12	C	1	Total C O 7 4 3	0	0
12	D	1	Total C O 7 4 3	0	0
12	D	1	Total C O 7 4 3	0	0

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



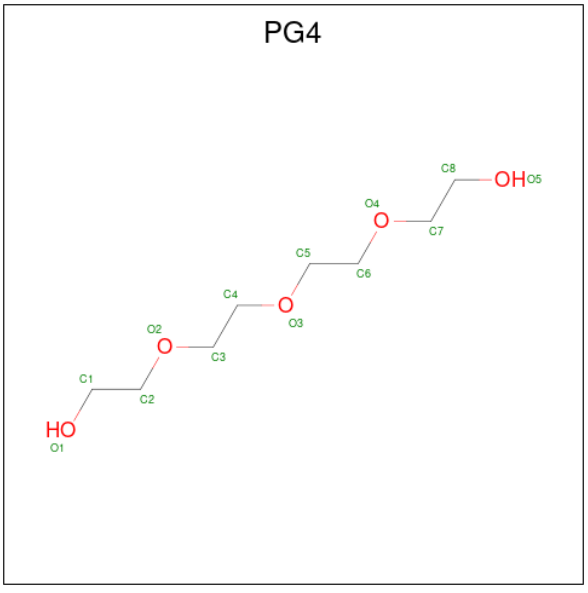
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C N O 14 8 1 5	0	0
13	A	1	Total C N O 14 8 1 5	0	0
13	B	1	Total C N O 14 8 1 5	0	0
13	C	1	Total C N O 14 8 1 5	0	0
13	C	1	Total C N O 14 8 1 5	0	0
13	D	1	Total C N O 14 8 1 5	0	0
13	D	1	Total C N O 14 8 1 5	0	0

- Molecule 14 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total C N O P 31 10 6 12 3	0	0
14	C	1	Total C N O P 15 2 1 9 3	0	0
14	D	1	Total C N O P 14 1 1 9 3	0	0

- Molecule 15 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C O 13 8 5	0	0

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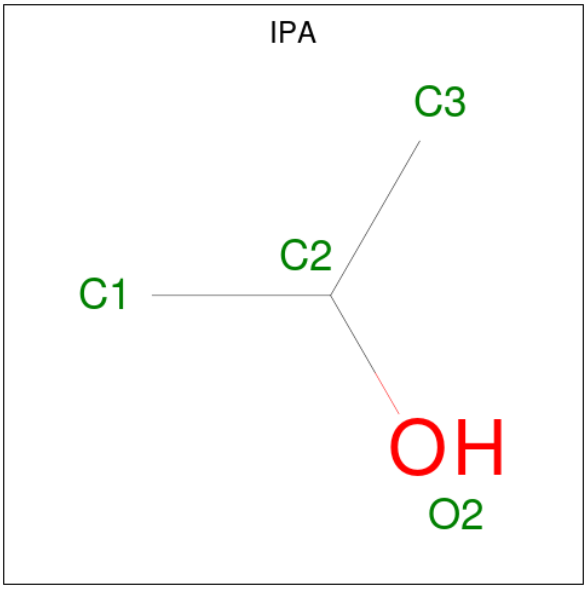
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	D	1	Total C O 13 8 5	0	0

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	B	1	Total Na 1 1	0	0
16	C	1	Total Na 1 1	0	0

- Molecule 17 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	C	1	Total C O 4 3 1	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	208	Total O 208 208	0	0
18	B	179	Total O 179 179	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	C	192	Total O 192 192	0	0
18	D	192	Total O 192 192	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 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	125.70Å 125.70Å 298.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.76 – 2.60	Depositor
% Data completeness (in resolution range)	74.9 (40.76-2.60)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.213 , 0.274	Depositor
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.108	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
Total number of atoms	15691	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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

24 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	E	1	2,1	14,14,15	0.39	0	17,19,21	0.69	0
2	NAG	E	2	2	14,14,15	0.48	0	17,19,21	0.51	0
2	BMA	E	3	2	11,11,12	1.07	1 (9%)	15,15,17	2.50	2 (13%)
2	BMA	E	4	2	11,11,12	0.60	0	15,15,17	0.86	1 (6%)
3	NAG	F	1	3,1	14,14,15	0.44	0	17,19,21	1.14	1 (5%)
3	NAG	F	2	3	14,14,15	1.50	1 (7%)	17,19,21	1.68	1 (5%)
3	BMA	F	3	3	11,11,12	1.59	3 (27%)	15,15,17	1.49	3 (20%)
4	NAG	G	1	4,1	14,14,15	0.42	0	17,19,21	0.85	0
4	NAG	G	2	4	14,14,15	0.30	0	17,19,21	0.72	1 (5%)
4	BMA	G	3	4	11,11,12	1.11	1 (9%)	15,15,17	1.08	1 (6%)
4	BMA	G	4	4	11,11,12	1.40	2 (18%)	15,15,17	2.49	6 (40%)
3	NAG	H	1	3,1	14,14,15	0.60	1 (7%)	17,19,21	0.53	0
3	NAG	H	2	3	14,14,15	0.37	0	17,19,21	0.73	0
3	BMA	H	3	3	11,11,12	1.62	3 (27%)	15,15,17	1.88	4 (26%)
5	NAG	I	1	5,1	14,14,15	0.47	0	17,19,21	1.56	2 (11%)
5	FUC	I	2	5	10,10,11	1.02	1 (10%)	14,14,16	1.64	3 (21%)
5	NAG	I	3	5	14,14,15	0.46	0	17,19,21	0.44	0
5	NAG	J	1	5,1	14,14,15	0.55	0	17,19,21	1.29	4 (23%)
5	FUC	J	2	5	10,10,11	1.17	1 (10%)	14,14,16	2.12	4 (28%)
5	NAG	J	3	5	14,14,15	0.28	0	17,19,21	1.23	2 (11%)
6	NAG	K	1	6,1	14,14,15	0.90	1 (7%)	17,19,21	0.92	1 (5%)
6	NAG	K	2	6	14,14,15	0.56	0	17,19,21	1.45	2 (11%)
6	NAG	L	1	6,1	14,14,15	0.49	0	17,19,21	0.54	0
6	NAG	L	2	6	14,14,15	0.40	0	17,19,21	0.36	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	NAG	E	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
2	BMA	E	4	2	-	0/2/19/22	1/1/1/1
3	NAG	F	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	1/1/1/1
4	BMA	G	4	4	-	1/2/19/22	1/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	0/1/1/1
5	NAG	I	1	5,1	-	0/6/23/26	0/1/1/1
5	FUC	I	2	5	-	-	0/1/1/1
5	NAG	I	3	5	-	0/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	2/6/23/26	0/1/1/1
5	FUC	J	2	5	-	-	0/1/1/1
5	NAG	J	3	5	-	5/6/23/26	0/1/1/1
6	NAG	K	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	5/6/23/26	0/1/1/1
6	NAG	L	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	O5-C1	5.48	1.52	1.43
3	H	3	BMA	C1-C2	3.62	1.60	1.52
3	F	3	BMA	C2-C3	3.37	1.57	1.52
5	J	2	FUC	C1-C2	3.00	1.59	1.52
3	H	3	BMA	C2-C3	2.83	1.56	1.52

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	3	BMA	C1-O5-C5	8.28	123.41	112.19
4	G	4	BMA	C1-O5-C5	6.65	121.20	112.19
3	F	2	NAG	C1-O5-C5	6.45	120.93	112.19
6	K	2	NAG	C2-N2-C7	4.64	129.51	122.90
5	I	1	NAG	C1-O5-C5	4.59	118.41	112.19

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

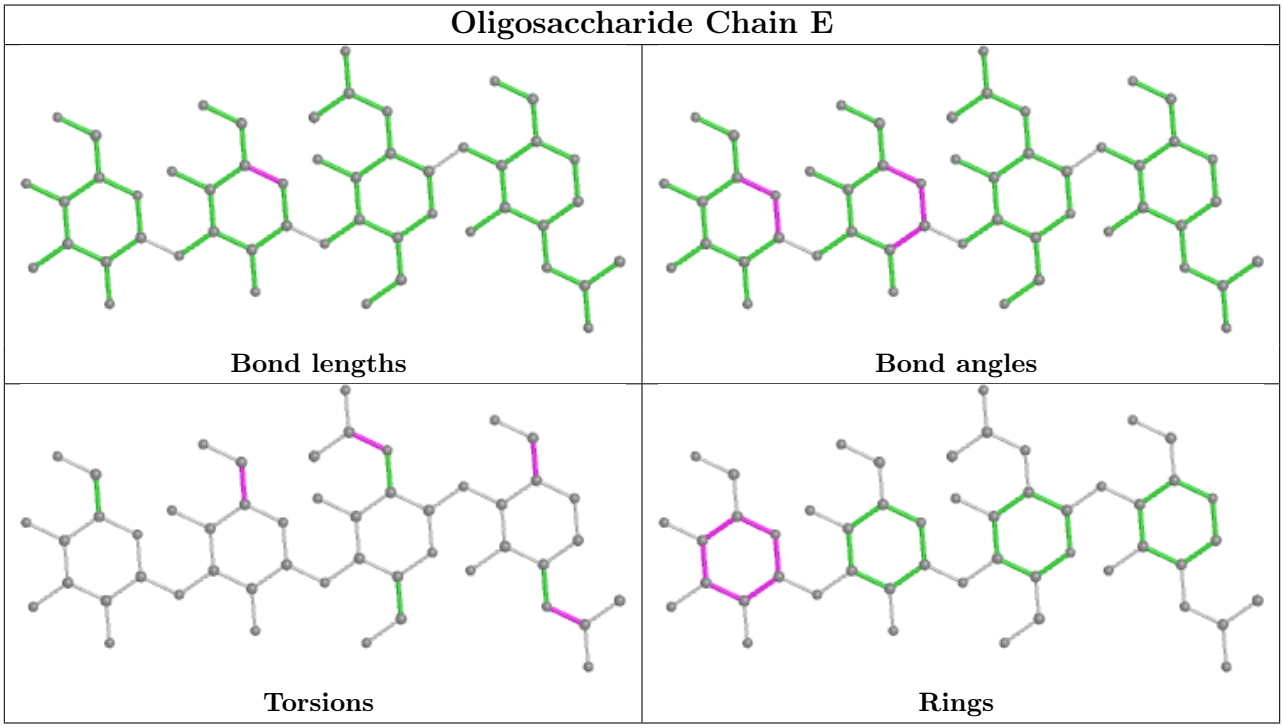
Mol	Chain	Res	Type	Atoms
3	F	1	NAG	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6

All (3) ring outliers are listed below:

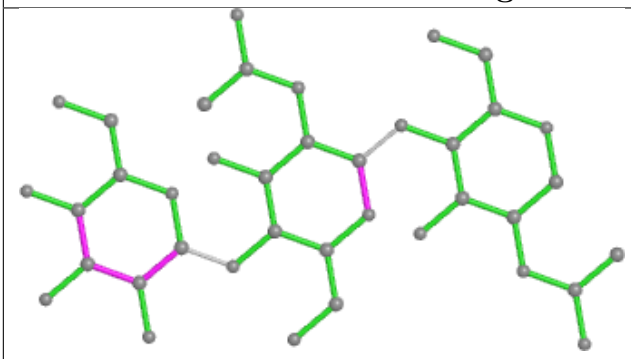
Mol	Chain	Res	Type	Atoms
4	G	4	BMA	C1-C2-C3-C4-C5-O5
4	G	3	BMA	C1-C2-C3-C4-C5-O5
2	E	4	BMA	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

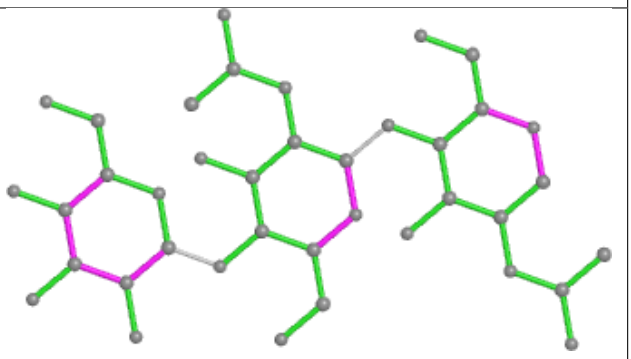
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



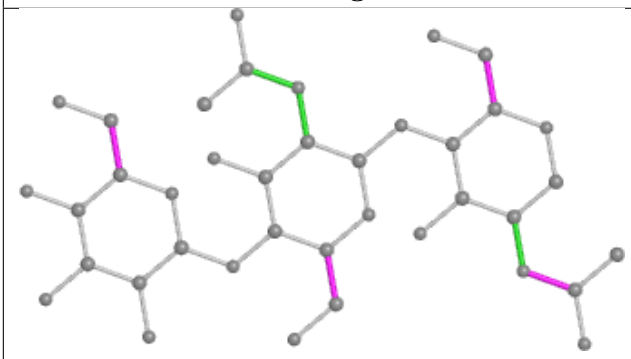
Oligosaccharide Chain F



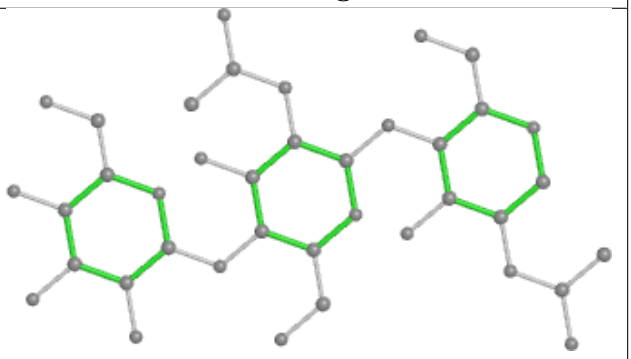
Bond lengths



Bond angles

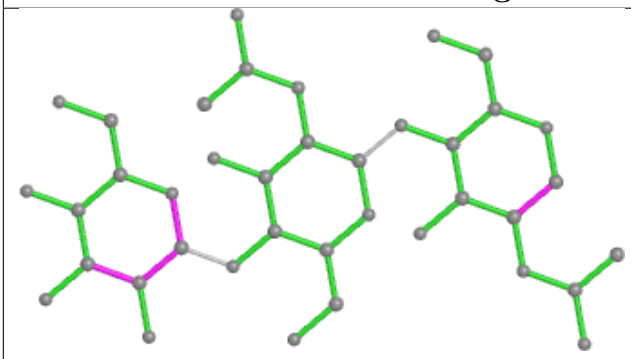


Torsions

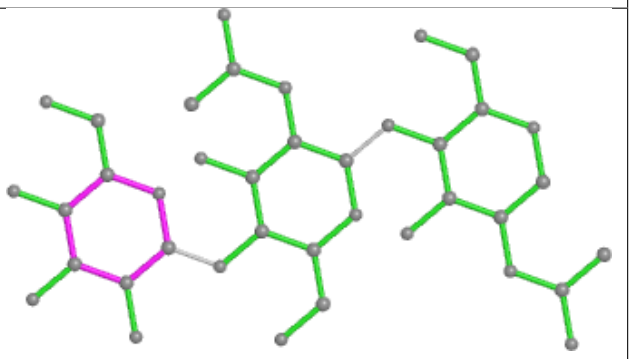


Rings

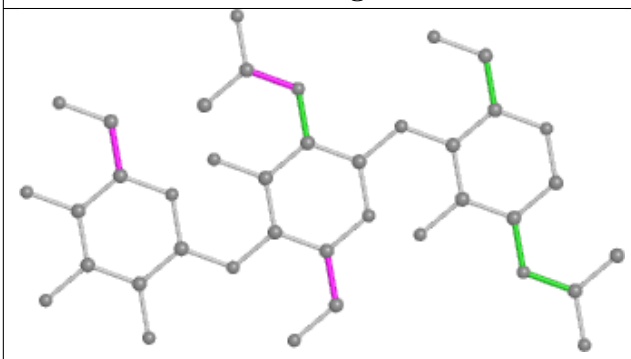
Oligosaccharide Chain H



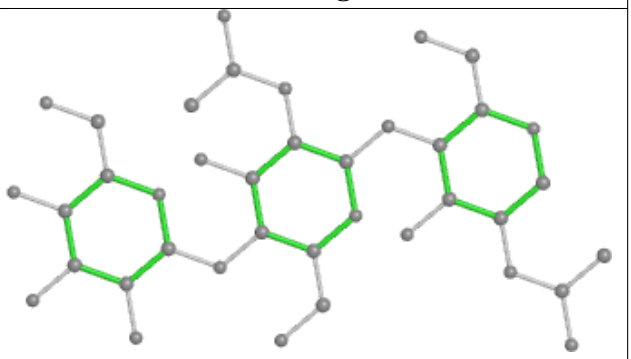
Bond lengths



Bond angles

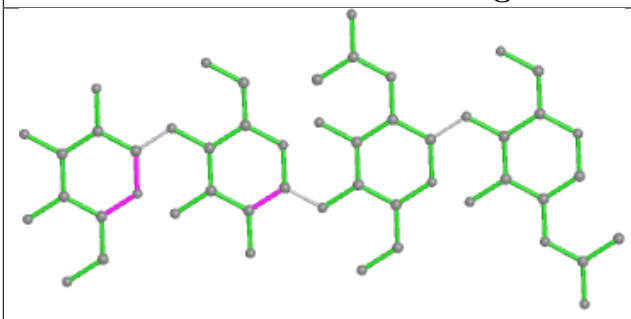


Torsions

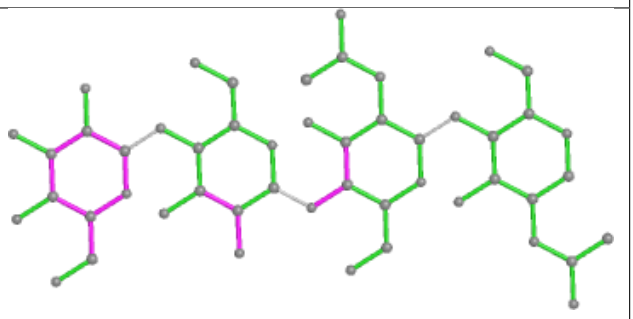


Rings

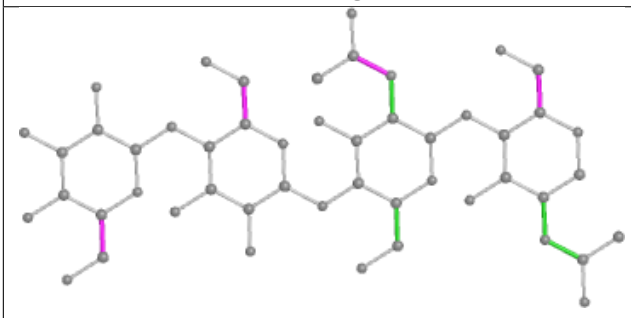
Oligosaccharide Chain G



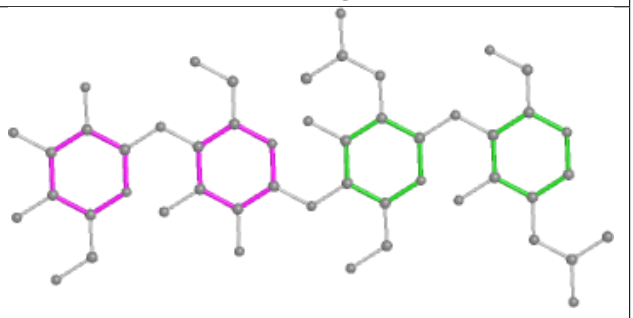
Bond lengths



Bond angles

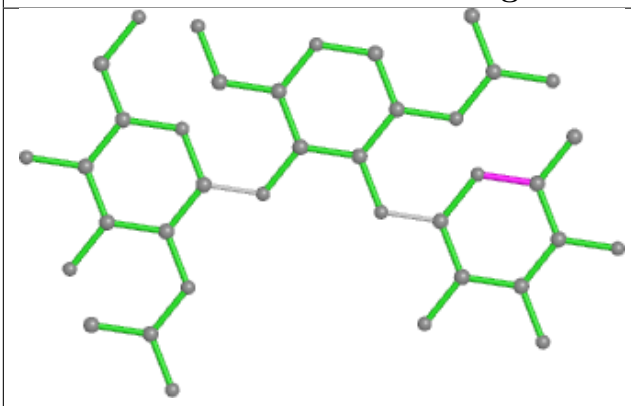


Torsions

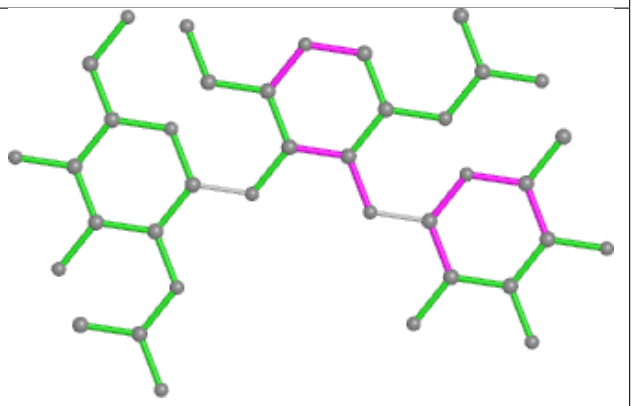


Rings

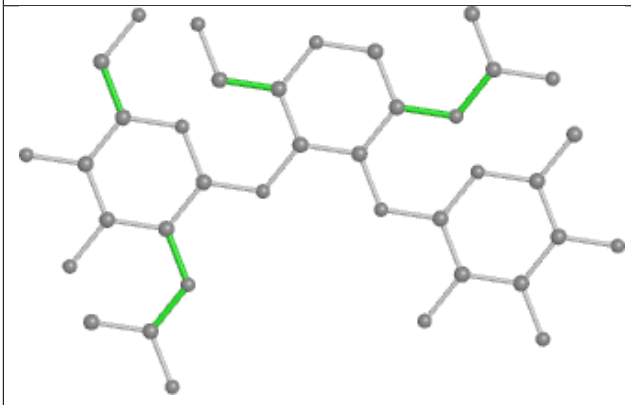
Oligosaccharide Chain I



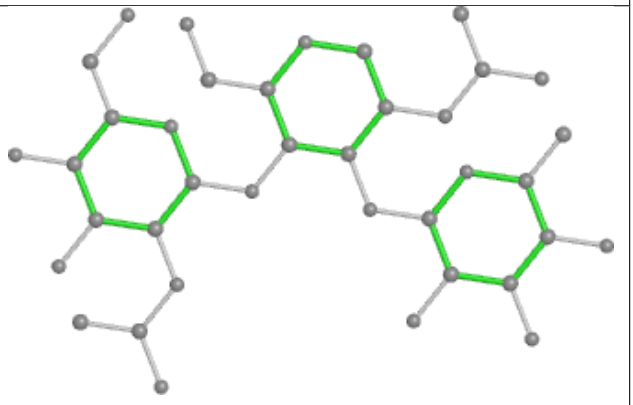
Bond lengths



Bond angles

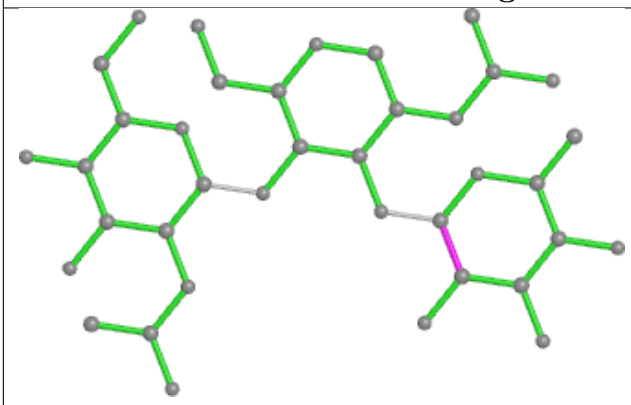


Torsions

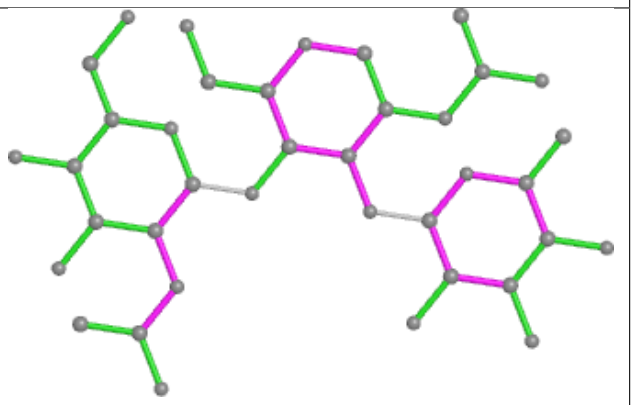


Rings

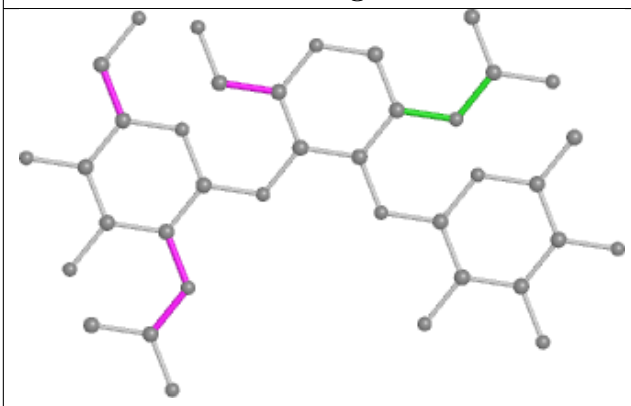
Oligosaccharide Chain J



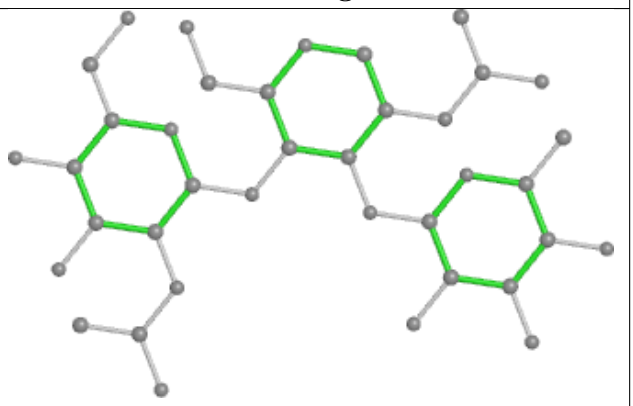
Bond lengths



Bond angles

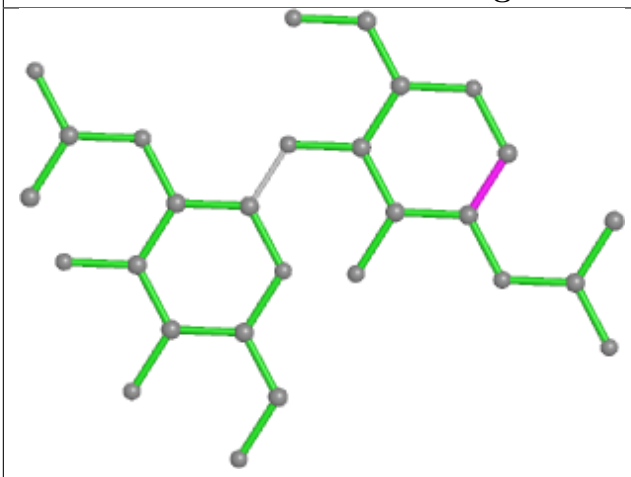


Torsions

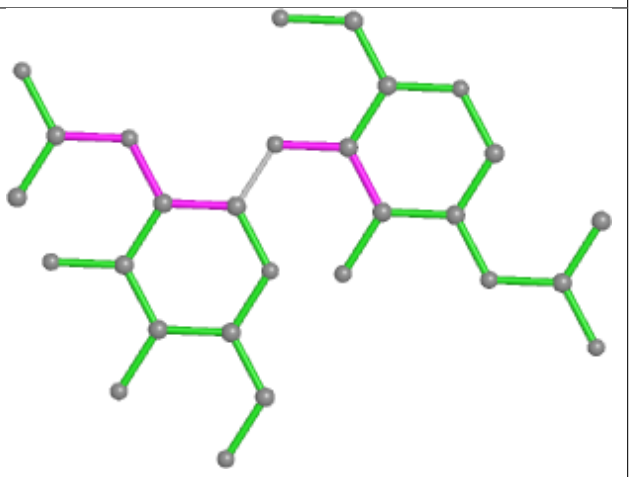


Rings

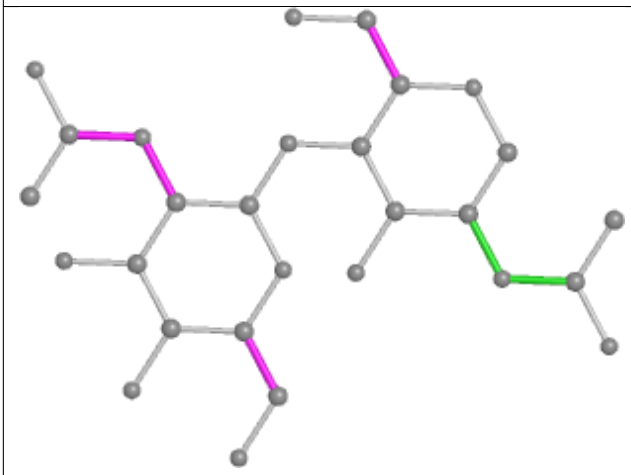
Oligosaccharide Chain K



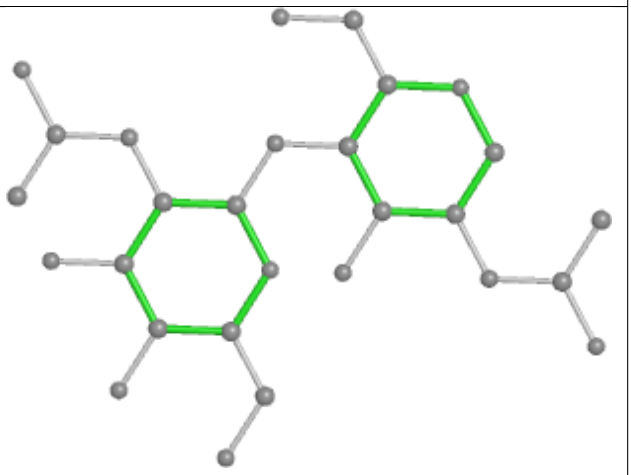
Bond lengths



Bond angles

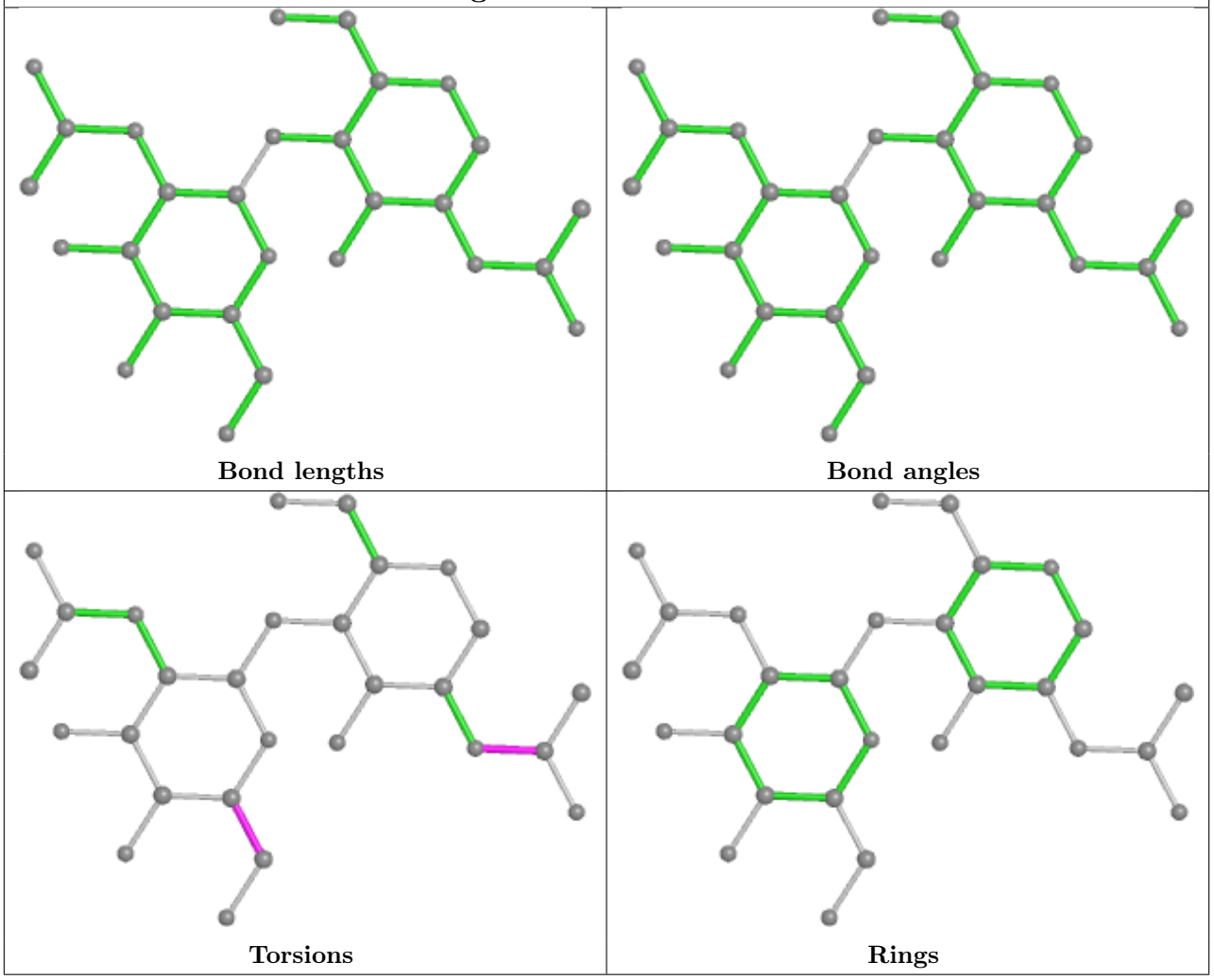


Torsions



Rings

Oligosaccharide Chain L



4.6 Ligand geometry (i)

Of 96 ligands modelled in this entry, 11 are monoatomic - leaving 85 for Mogul analysis.

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	$\#\|Z\| > 2$
11	EDO	C	514	-	3,3,3	0.48	0	2,2,2	0.43	0
9	SO4	C	511	-	4,4,4	0.13	0	6,6,6	0.12	0
10	GOL	A	506	-	5,5,5	1.01	0	5,5,5	0.89	0
11	EDO	C	513	-	3,3,3	0.54	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	EDO	D	721	-	3,3,3	0.54	0	2,2,2	0.53	0
9	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.15	0
9	SO4	D	707	-	4,4,4	0.15	0	6,6,6	0.24	0
11	EDO	C	520	-	3,3,3	0.71	0	2,2,2	0.04	0
9	SO4	D	709	-	4,4,4	0.16	0	6,6,6	0.08	0
9	SO4	D	711	-	4,4,4	0.14	0	6,6,6	0.07	0
12	PGE	B	513	-	6,6,9	0.30	0	5,5,8	0.43	0
9	SO4	C	507	-	4,4,4	0.16	0	6,6,6	0.12	0
9	SO4	D	704	-	4,4,4	0.15	0	6,6,6	0.07	0
11	EDO	D	717	-	3,3,3	0.51	0	2,2,2	0.29	0
11	EDO	C	518	-	3,3,3	0.68	0	2,2,2	0.56	0
11	EDO	A	510	-	3,3,3	0.53	0	2,2,2	0.22	0
11	EDO	C	515	-	3,3,3	0.53	0	2,2,2	0.29	0
15	PG4	A	526	-	12,12,12	0.44	0	11,11,11	0.38	0
9	SO4	B	504	-	4,4,4	0.13	0	6,6,6	0.16	0
9	SO4	C	508	-	4,4,4	0.15	0	6,6,6	0.10	0
9	SO4	D	706	-	4,4,4	0.12	0	6,6,6	0.19	0
14	ANP	C	530	8,7	13,14,33	2.68	4 (30%)	14,22,52	2.06	3 (21%)
11	EDO	D	727	-	3,3,3	0.54	0	2,2,2	0.81	0
10	GOL	C	512	-	5,5,5	0.86	0	5,5,5	1.02	0
9	SO4	C	510	-	4,4,4	0.12	0	6,6,6	0.10	0
10	GOL	D	715	-	5,5,5	0.92	0	5,5,5	1.03	0
9	SO4	A	505	-	4,4,4	0.47	0	6,6,6	0.42	0
9	SO4	B	503	-	4,4,4	0.14	0	6,6,6	0.17	0
11	EDO	B	509	-	3,3,3	0.51	0	2,2,2	0.16	0
11	EDO	C	517	-	3,3,3	0.66	0	2,2,2	0.33	0
13	NAG	C	502	1	14,14,15	2.18	2 (14%)	17,19,21	2.31	1 (5%)
11	EDO	D	728	-	3,3,3	0.58	0	2,2,2	0.37	0
9	SO4	D	708	-	4,4,4	0.10	0	6,6,6	0.12	0
11	EDO	D	726	-	3,3,3	0.69	0	2,2,2	0.40	0
13	NAG	D	733	1	14,14,15	0.96	1 (7%)	17,19,21	1.91	5 (29%)
9	SO4	C	509	-	4,4,4	0.15	0	6,6,6	0.12	0
11	EDO	A	514	-	3,3,3	0.70	0	2,2,2	0.33	0
10	GOL	D	713	-	5,5,5	0.92	0	5,5,5	0.78	0
12	PGE	D	729	-	6,6,9	0.26	0	5,5,8	0.70	0
10	GOL	A	508	-	5,5,5	1.31	1 (20%)	5,5,5	0.88	0
11	EDO	A	513	-	3,3,3	0.63	0	2,2,2	0.47	0
9	SO4	D	712	-	4,4,4	0.15	0	6,6,6	0.09	0
13	NAG	B	522	1	14,14,15	0.25	0	17,19,21	0.36	0
11	EDO	D	723	-	3,3,3	0.72	0	2,2,2	0.53	0
9	SO4	C	506	-	4,4,4	0.16	0	6,6,6	0.10	0
11	EDO	A	512	-	3,3,3	0.70	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	EDO	D	725	-	3,3,3	0.68	0	2,2,2	0.28	0
15	PG4	D	701	-	12,12,12	0.47	0	11,11,11	0.38	0
9	SO4	D	710	-	4,4,4	0.12	0	6,6,6	0.20	0
11	EDO	D	724	-	3,3,3	0.72	0	2,2,2	0.20	0
9	SO4	B	506	-	4,4,4	0.13	0	6,6,6	0.08	0
11	EDO	B	512	-	3,3,3	0.53	0	2,2,2	0.34	0
11	EDO	D	718	-	3,3,3	0.50	0	2,2,2	0.18	0
11	EDO	D	720	-	3,3,3	0.53	0	2,2,2	0.26	0
12	PGE	A	515	-	6,6,9	0.29	0	5,5,8	0.30	0
12	PGE	C	521	-	9,9,9	0.34	0	8,8,8	0.23	0
9	SO4	B	505	-	4,4,4	0.14	0	6,6,6	0.16	0
11	EDO	B	507	-	3,3,3	0.48	0	2,2,2	0.42	0
12	PGE	B	514	-	6,6,9	0.44	0	5,5,8	0.44	0
11	EDO	B	511	-	3,3,3	0.53	0	2,2,2	0.17	0
10	GOL	A	507[A]	-	5,5,5	0.97	0	5,5,5	0.98	0
11	EDO	D	722	-	3,3,3	0.42	0	2,2,2	0.32	0
12	PGE	C	522	-	6,6,9	0.31	0	5,5,8	0.26	0
11	EDO	D	719	-	3,3,3	0.45	0	2,2,2	0.53	0
11	EDO	A	511	-	3,3,3	0.54	0	2,2,2	0.27	0
14	ANP	A	525	8,7	29,33,33	2.03	6 (20%)	31,52,52	1.70	5 (16%)
10	GOL	D	714	-	5,5,5	0.82	0	5,5,5	1.02	0
14	ANP	D	735	8,7	12,13,33	2.94	4 (33%)	14,21,52	1.83	4 (28%)
13	NAG	D	734	1	14,14,15	0.45	0	17,19,21	0.74	1 (5%)
9	SO4	C	505	-	4,4,4	0.15	0	6,6,6	0.07	0
13	NAG	A	520	1	14,14,15	0.38	0	17,19,21	0.56	0
11	EDO	B	508	-	3,3,3	0.59	0	2,2,2	0.15	0
13	NAG	A	521	-	14,14,15	1.69	3 (21%)	17,19,21	1.36	3 (17%)
17	IPA	C	529	-	3,3,3	0.56	0	3,3,3	0.23	0
9	SO4	D	705	-	4,4,4	0.16	0	6,6,6	0.16	0
10	GOL	D	716	-	5,5,5	0.89	0	5,5,5	1.00	0
10	GOL	A	507[B]	-	5,5,5	0.85	0	5,5,5	1.05	0
11	EDO	B	510	-	3,3,3	0.49	0	2,2,2	0.28	0
12	PGE	D	730	-	6,6,9	0.56	0	5,5,8	0.56	0
10	GOL	A	509	-	5,5,5	1.13	0	5,5,5	0.94	0
13	NAG	C	526	1	14,14,15	0.30	0	17,19,21	0.65	1 (5%)
9	SO4	A	504	-	4,4,4	0.16	0	6,6,6	0.12	0
9	SO4	C	501	16	4,4,4	0.22	0	6,6,6	0.34	0
11	EDO	C	516	-	3,3,3	0.45	0	2,2,2	0.35	0
11	EDO	C	519	-	3,3,3	0.66	0	2,2,2	0.28	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
11	EDO	C	514	-	-	0/1/1/1	-
13	NAG	D	733	1	-	3/6/23/26	0/1/1/1
14	ANP	A	525	8,7	-	3/14/38/38	0/3/3/3
10	GOL	D	714	-	-	2/4/4/4	-
10	GOL	A	506	-	-	0/4/4/4	-
14	ANP	D	735	8,7	-	1/11/15/38	-
13	NAG	D	734	1	-	2/6/23/26	0/1/1/1
11	EDO	C	513	-	-	0/1/1/1	-
11	EDO	D	721	-	-	0/1/1/1	-
13	NAG	A	520	1	-	2/6/23/26	0/1/1/1
11	EDO	A	514	-	-	1/1/1/1	-
11	EDO	C	520	-	-	0/1/1/1	-
10	GOL	D	713	-	-	2/4/4/4	-
14	ANP	C	530	8,7	-	1/12/16/38	-
12	PGE	D	729	-	-	1/4/4/7	-
10	GOL	A	508	-	-	4/4/4/4	-
11	EDO	D	727	-	-	1/1/1/1	-
11	EDO	A	513	-	-	1/1/1/1	-
10	GOL	C	512	-	-	4/4/4/4	-
13	NAG	B	522	1	-	2/6/23/26	0/1/1/1
10	GOL	D	715	-	-	2/4/4/4	-
11	EDO	B	508	-	-	0/1/1/1	-
11	EDO	D	723	-	-	0/1/1/1	-
11	EDO	A	512	-	-	1/1/1/1	-
11	EDO	D	725	-	-	1/1/1/1	-
13	NAG	A	521	-	-	2/6/23/26	0/1/1/1
15	PG4	D	701	-	-	5/10/10/10	-
12	PGE	B	513	-	-	2/4/4/7	-
11	EDO	D	724	-	-	1/1/1/1	-
11	EDO	D	720	-	-	0/1/1/1	-
11	EDO	B	512	-	-	0/1/1/1	-
11	EDO	D	718	-	-	0/1/1/1	-
10	GOL	D	716	-	-	1/4/4/4	-
11	EDO	D	717	-	-	0/1/1/1	-
12	PGE	A	515	-	-	3/4/4/7	-
10	GOL	A	507[B]	-	-	2/4/4/4	-
11	EDO	B	510	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PGE	D	730	-	-	1/4/4/7	-
11	EDO	B	509	-	-	0/1/1/1	-
11	EDO	C	517	-	-	1/1/1/1	-
10	GOL	A	509	-	-	1/4/4/4	-
12	PGE	C	521	-	-	4/7/7/7	-
11	EDO	C	518	-	-	0/1/1/1	-
13	NAG	C	526	1	-	2/6/23/26	0/1/1/1
11	EDO	A	510	-	-	0/1/1/1	-
11	EDO	C	516	-	-	0/1/1/1	-
11	EDO	B	507	-	-	1/1/1/1	-
11	EDO	C	515	-	-	1/1/1/1	-
12	PGE	B	514	-	-	2/4/4/7	-
11	EDO	B	511	-	-	1/1/1/1	-
10	GOL	A	507[A]	-	-	2/4/4/4	-
13	NAG	C	502	1	-	2/6/23/26	0/1/1/1
11	EDO	D	728	-	-	1/1/1/1	-
15	PG4	A	526	-	-	3/10/10/10	-
11	EDO	D	719	-	-	1/1/1/1	-
11	EDO	D	722	-	-	1/1/1/1	-
12	PGE	C	522	-	-	1/4/4/7	-
11	EDO	C	519	-	-	1/1/1/1	-
11	EDO	A	511	-	-	0/1/1/1	-
11	EDO	D	726	-	-	0/1/1/1	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	502	NAG	O5-C1	7.47	1.55	1.43
14	D	735	ANP	PG-O1G	6.98	1.57	1.46
14	A	525	ANP	PG-O1G	6.57	1.56	1.46
14	C	530	ANP	PG-O1G	6.18	1.56	1.46
14	C	530	ANP	PB-O1B	5.97	1.55	1.46

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	502	NAG	C1-O5-C5	8.73	124.02	112.19
14	C	530	ANP	PB-O3A-PA	-6.05	111.30	132.62
13	D	733	NAG	C1-O5-C5	5.25	119.30	112.19
14	D	735	ANP	PB-O3A-PA	-4.80	115.72	132.62
14	A	525	ANP	PB-O3A-PA	-4.63	116.29	132.62

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

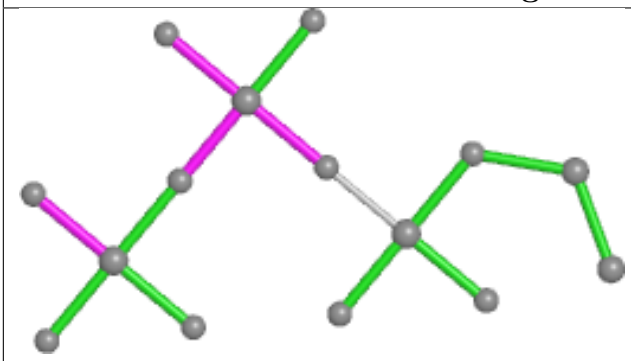
Mol	Chain	Res	Type	Atoms
10	A	507[A]	GOL	O1-C1-C2-O2
10	A	507[A]	GOL	O1-C1-C2-C3
10	A	507[B]	GOL	O1-C1-C2-C3
10	A	508	GOL	O1-C1-C2-C3
10	A	509	GOL	C1-C2-C3-O3

There are no ring outliers.

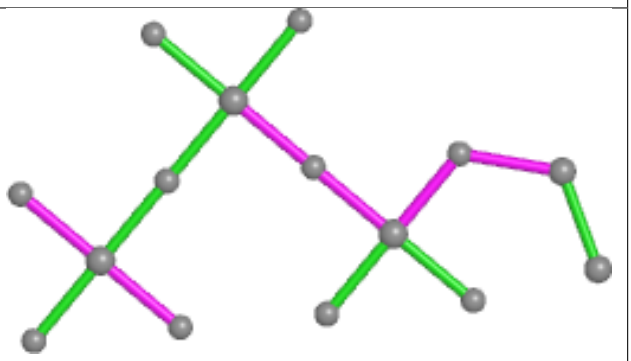
No monomer is involved in short contacts.

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.

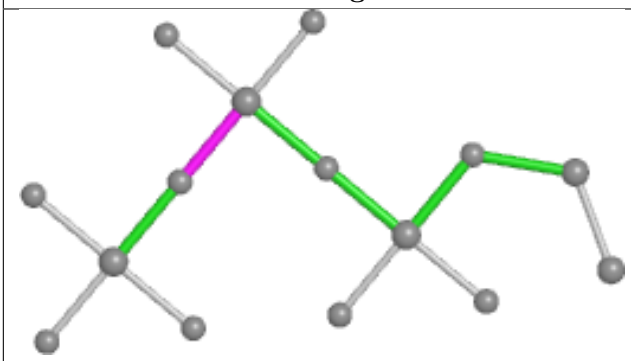
Ligand ANP C 530



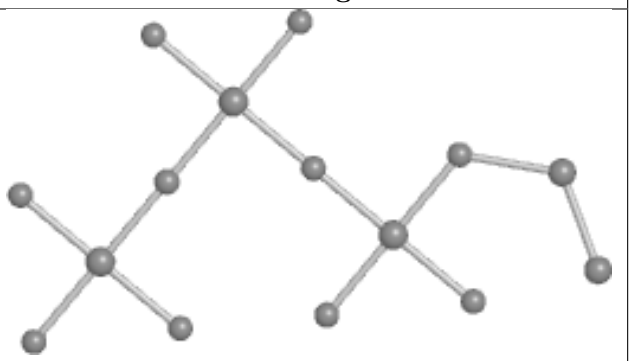
Bond lengths



Bond angles

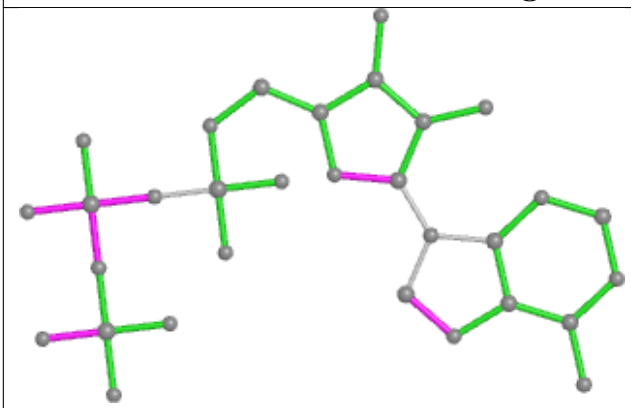


Torsions

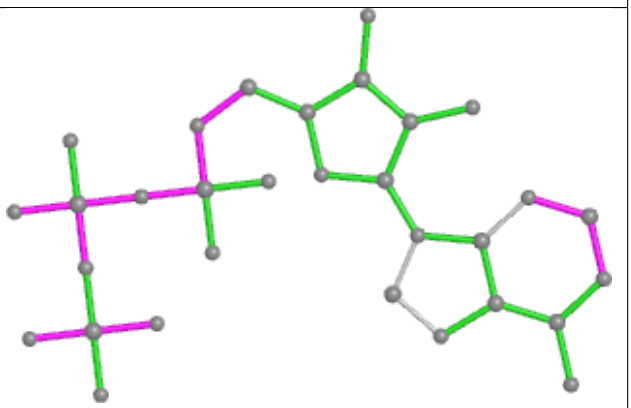


Rings

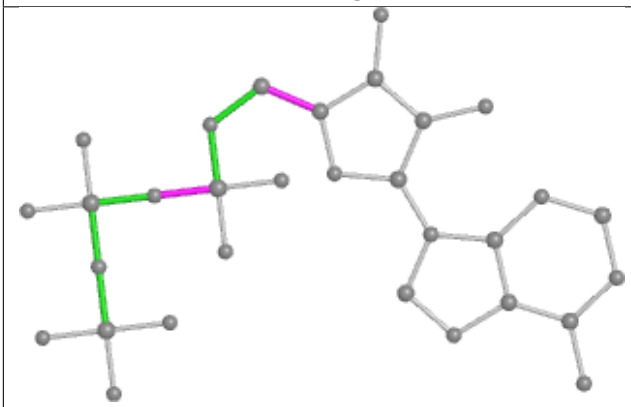
Ligand ANP A 525



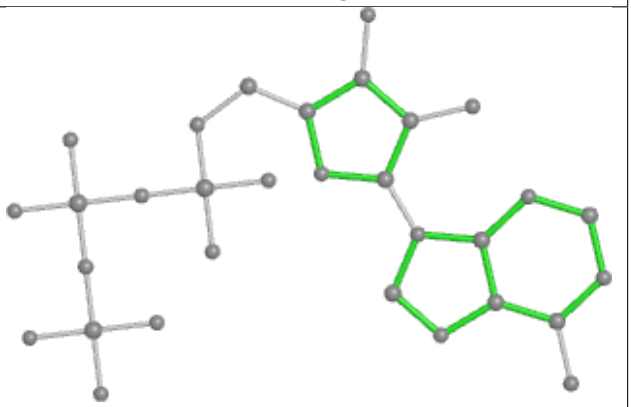
Bond lengths



Bond angles

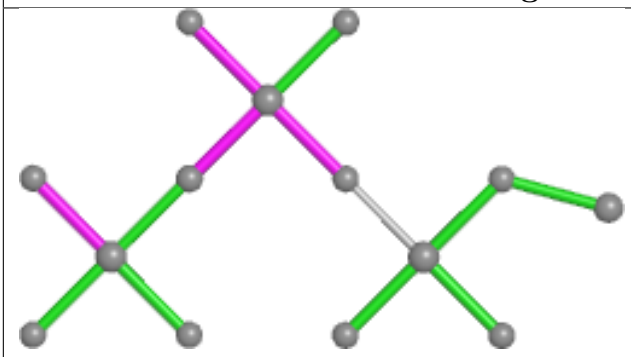


Torsions

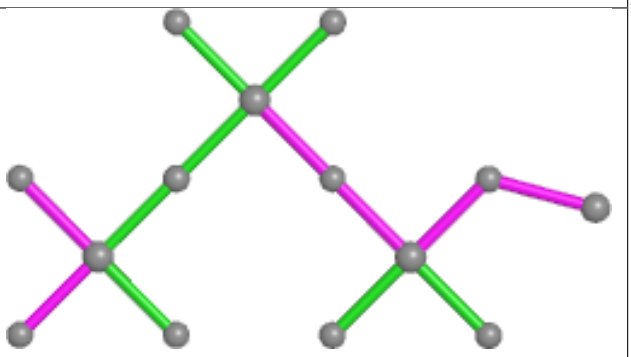


Rings

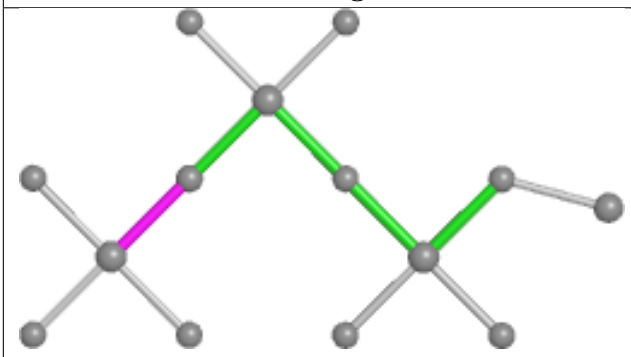
Ligand ANP D 735



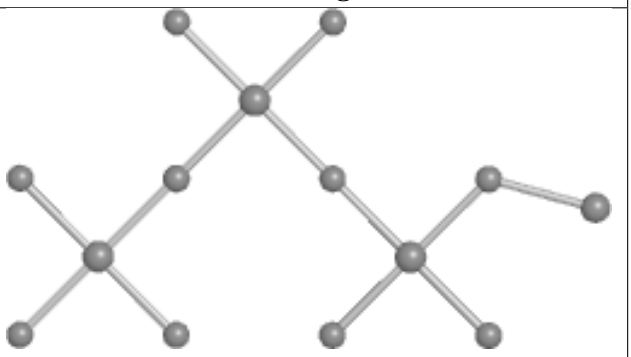
Bond lengths



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.