Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 02:57 PM EDT

PDB ID	:	6NTG
Title	:	Crystal Structure of Recombinant Human Acetylcholinesterase Inhibited by A-234 in Complex with Reactivator, HI-6
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Deposited on	:	2019-01-29
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 6 unique types of molecules in this entry. The entry contains 9035 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.

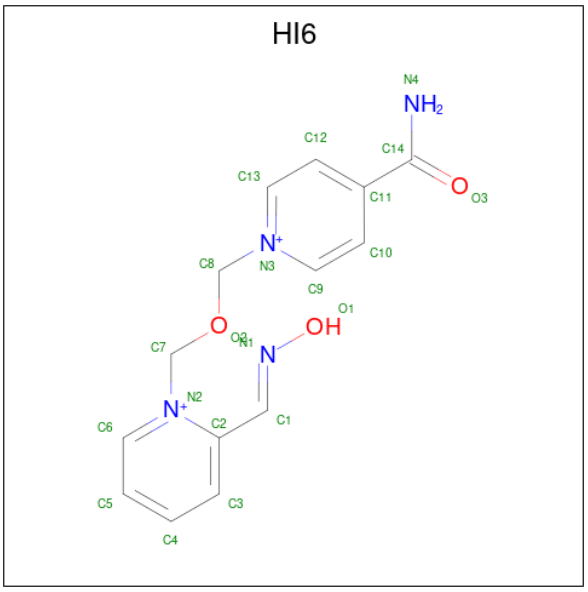
- Molecule 1 is a protein called Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	530	Total	C	N	O	S	0	3	0
			4152	2668	726	745	13			
1	B	532	Total	C	N	O	S	0	3	0
			4158	2669	727	749	13			

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

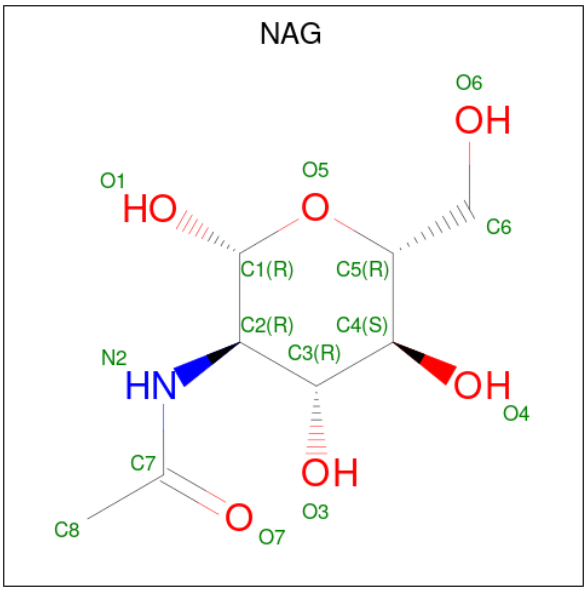
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	D	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is 4-(AMINOCARBONYL)-1-[({2-[(E)-(HYDROXYIMINO)METHYL]PYRIDINIUM-1-YL}METHOXY)METHYL]PYRIDINIUM (three-letter code: HI6) (formula: $C_{14}H_{16}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			42	28	8	6		
3	B	1	Total	C	N	O	0	0
			21	14	4	3		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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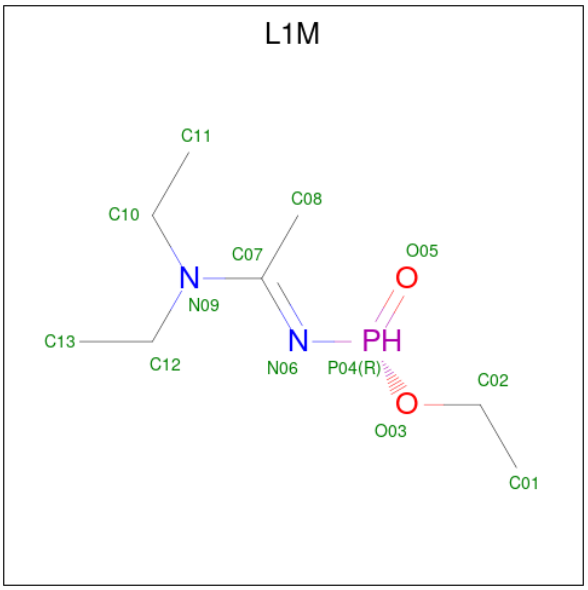
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is ethyl (R)-N-[(1E)-1-(diethylamino)ethylidene]phosphonamidate (three-letter code: L1M) (formula: $C_8H_{19}N_2O_2P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			13	8	2	2	1		
5	B	1	Total	C	N	O	P	0	0
			13	8	2	2	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	265	Total	O	0	0
			265	265		
6	B	229	Total	O	0	0
			229	229		

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	104.67Å 104.67Å 325.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.66 – 2.65	Depositor
% Data completeness (in resolution range)	99.6 (43.66-2.65)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.190 , 0.232	Depositor
Wilson B-factor (Å^2)	49.2	Xtriage
Anisotropy	0.521	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
Total number of atoms	9035	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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

9 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	0.41	0	17,19,21	0.62	0
2	NAG	C	2	2	14,14,15	0.61	1 (7%)	17,19,21	0.54	0
2	FUC	C	3	2	10,10,11	0.69	0	14,14,16	0.77	0
2	NAG	D	1	2,1	14,14,15	0.30	0	17,19,21	0.64	0
2	NAG	D	2	2	14,14,15	0.43	0	17,19,21	0.36	0
2	FUC	D	3	2	10,10,11	0.77	0	14,14,16	0.83	0
2	NAG	E	1	2,1	14,14,15	0.53	0	17,19,21	0.60	0
2	NAG	E	2	2	14,14,15	0.29	0	17,19,21	0.56	0
2	FUC	E	3	2	10,10,11	1.25	1 (10%)	14,14,16	1.23	1 (7%)

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	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1
2	NAG	D	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
2	FUC	D	3	2	-	-	0/1/1/1
2	NAG	E	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3	FUC	C2-C3	2.53	1.56	1.52
2	C	2	NAG	C1-C2	2.02	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	3	FUC	C1-C2-C3	2.69	112.97	109.67

There are no chirality outliers.

All (14) torsion outliers are listed below:

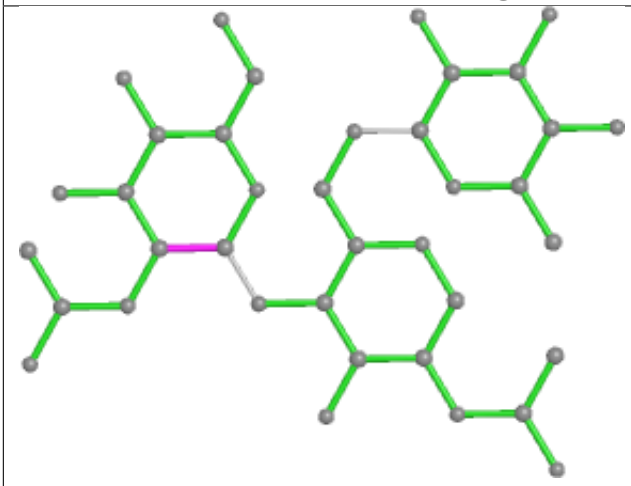
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

There are no ring outliers.

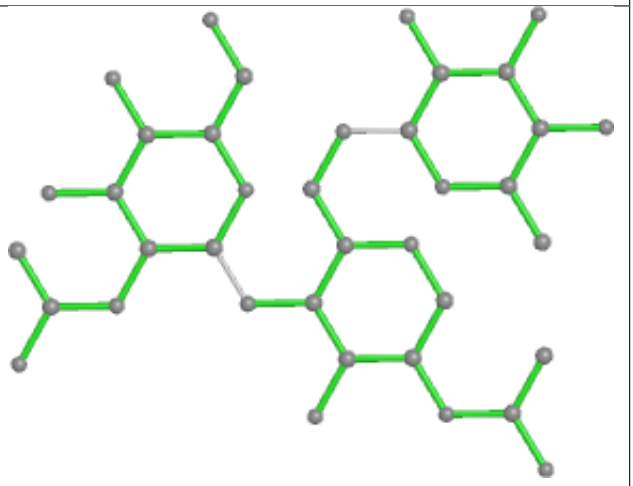
No monomer is involved in short contacts.

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

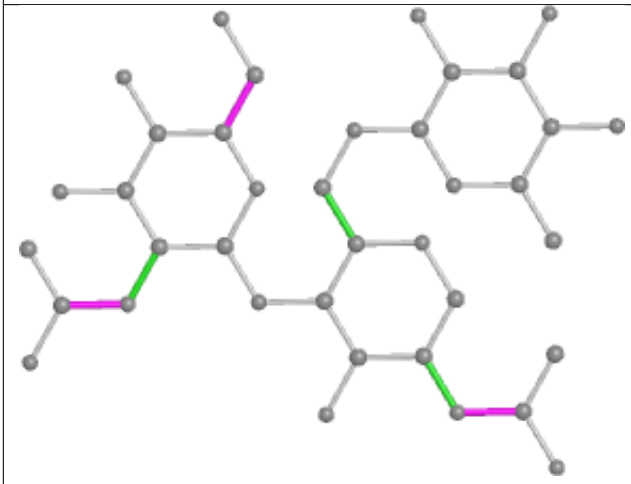
Oligosaccharide Chain C



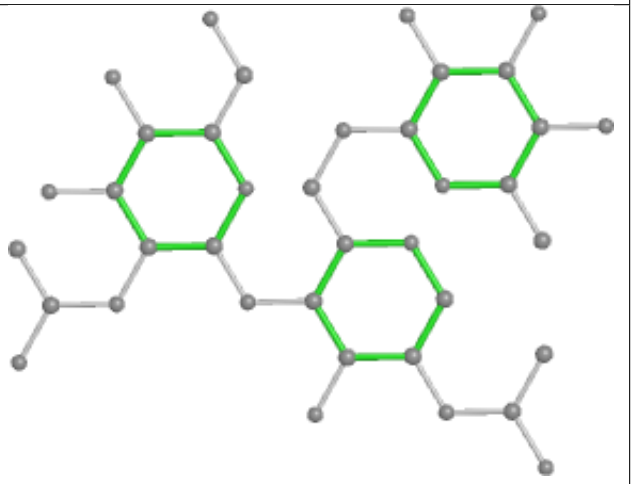
Bond lengths



Bond angles

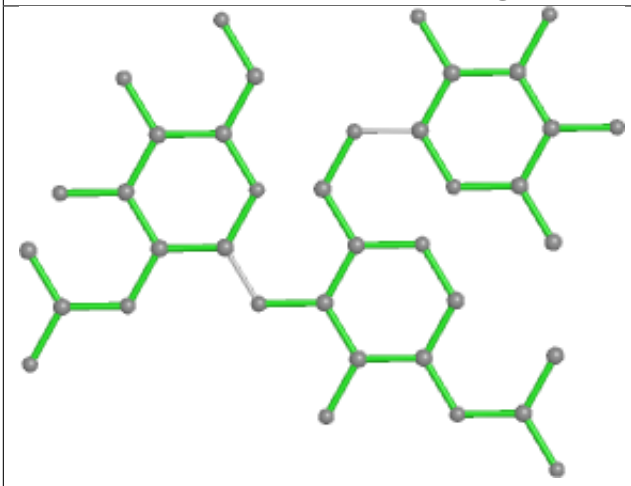


Torsions

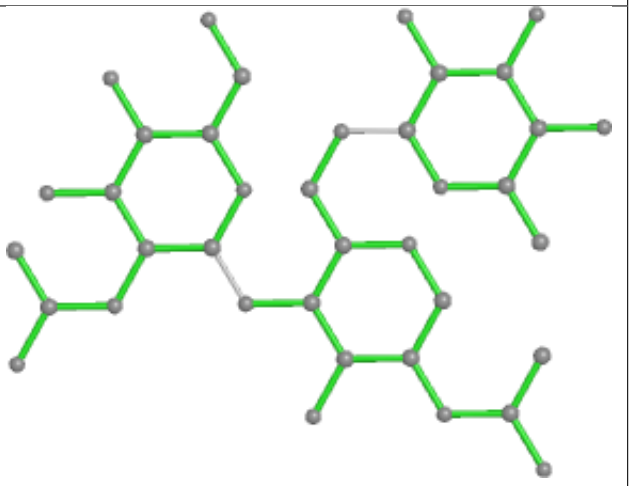


Rings

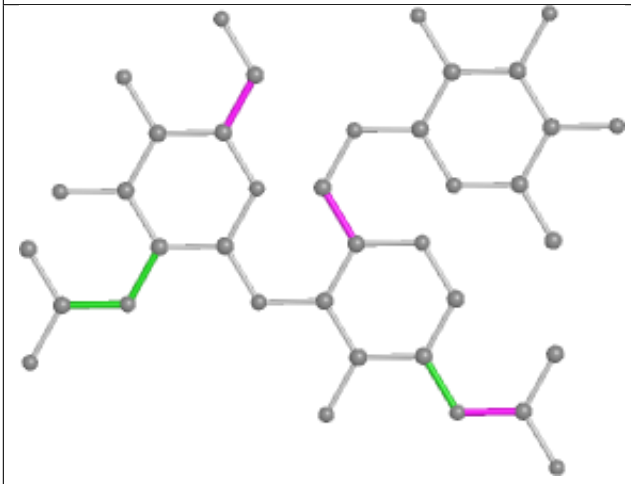
Oligosaccharide Chain D



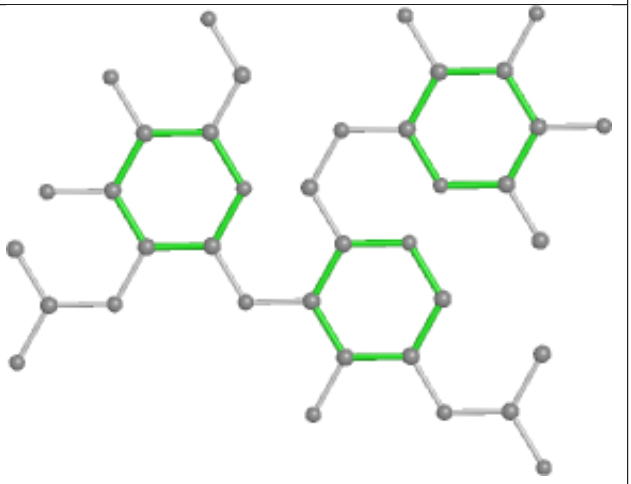
Bond lengths



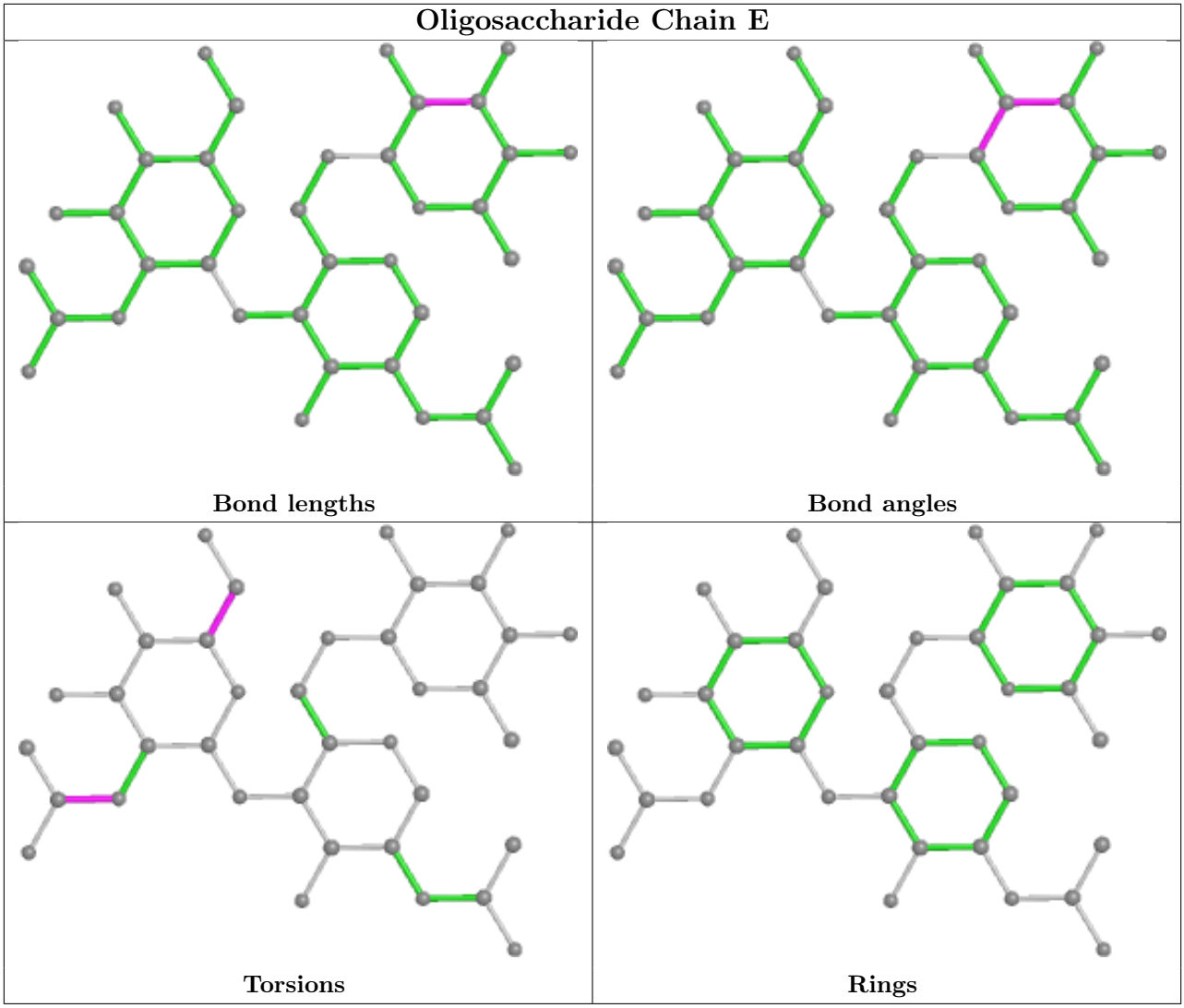
Bond angles



Torsions



Rings



4.6 Ligand geometry (i)

7 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	$\#\|Z\| > 2$
3	HI6	A	601[A]	-	18,22,22	5.32	7 (38%)	19,28,28	1.93	6 (31%)
3	HI6	B	601	-	18,22,22	4.27	6 (33%)	19,28,28	1.40	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	L1M	A	606	-	9,12,12	2.24	4 (44%)	6,14,14	0.96	0
5	L1M	B	609	1	9,12,12	2.21	4 (44%)	6,14,14	0.87	0
4	NAG	B	602	1	14,14,15	0.17	0	17,19,21	0.56	0
3	HI6	A	601[B]	-	18,22,22	4.38	6 (33%)	19,28,28	1.43	1 (5%)
4	NAG	A	605	1	14,14,15	0.31	0	17,19,21	0.51	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
3	HI6	A	601[A]	-	-	8/12/13/13	0/2/2/2
3	HI6	B	601	-	-	1/12/13/13	0/2/2/2
5	L1M	A	606	-	-	1/9/15/15	-
5	L1M	B	609	1	-	1/9/15/15	-
4	NAG	B	602	1	-	4/6/23/26	0/1/1/1
3	HI6	A	601[B]	-	-	3/12/13/13	0/2/2/2
4	NAG	A	605	1	-	3/6/23/26	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601[A]	HI6	C11-C14	-15.90	1.26	1.50
3	A	601[B]	HI6	C11-C14	-12.62	1.31	1.50
3	B	601	HI6	C11-C14	-12.06	1.32	1.50
3	A	601[B]	HI6	C1-N1	9.35	1.45	1.27
3	B	601	HI6	C1-N1	9.25	1.45	1.27
3	A	601[A]	HI6	C1-N1	9.02	1.45	1.27
3	A	601[A]	HI6	C2-N2	-8.05	1.29	1.37
3	B	601	HI6	C14-N4	6.59	1.45	1.33
3	A	601[B]	HI6	C14-N4	6.31	1.45	1.33
3	A	601[A]	HI6	O3-C14	-5.63	1.13	1.24
3	A	601[A]	HI6	C2-C1	-5.54	1.32	1.46
3	B	601	HI6	C2-C1	-5.40	1.32	1.46
3	A	601[B]	HI6	C2-C1	-5.39	1.32	1.46
3	A	601[A]	HI6	C14-N4	4.69	1.41	1.33
5	A	606	L1M	C07-N09	4.34	1.45	1.34
5	B	609	L1M	C07-N09	4.20	1.45	1.34
3	A	601[B]	HI6	C2-N2	-4.07	1.33	1.37
5	B	609	L1M	C07-N06	-3.67	1.25	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	606	L1M	C07-N06	-3.58	1.26	1.31
3	A	601[A]	HI6	C6-N2	-3.46	1.30	1.35
3	B	601	HI6	C2-N2	-3.36	1.33	1.37
3	A	601[B]	HI6	O3-C14	-2.73	1.18	1.24
3	B	601	HI6	O3-C14	-2.63	1.19	1.24
5	B	609	L1M	C08-C07	2.50	1.53	1.49
5	A	606	L1M	C08-C07	2.47	1.53	1.49
5	A	606	L1M	O03-C02	-2.22	1.39	1.44
5	B	609	L1M	O03-C02	-2.04	1.39	1.44

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601[B]	HI6	O1-N1-C1	4.39	119.62	111.86
3	A	601[A]	HI6	O1-N1-C1	4.39	119.61	111.86
3	B	601	HI6	O1-N1-C1	3.85	118.67	111.86
3	A	601[A]	HI6	C11-C14-N4	3.52	121.98	117.75
3	A	601[A]	HI6	C2-C1-N1	2.81	123.19	117.75
3	A	601[A]	HI6	C13-C12-C11	-2.67	115.63	119.44
3	A	601[A]	HI6	C12-C11-C10	2.55	122.22	118.59
3	B	601	HI6	C2-C1-N1	2.32	122.24	117.75
3	A	601[A]	HI6	C13-N3-C9	2.06	123.68	120.30

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601[A]	HI6	O2-C7-N2-C6
3	A	601[A]	HI6	N1-C1-C2-N2
3	A	601[A]	HI6	N1-C1-C2-C3
3	A	601[B]	HI6	O2-C8-N3-C9
3	A	601[B]	HI6	O2-C8-N3-C13
3	A	601[A]	HI6	C10-C11-C14-O3
3	A	601[A]	HI6	C12-C11-C14-O3
3	A	601[A]	HI6	C10-C11-C14-N4
3	A	601[A]	HI6	C12-C11-C14-N4
4	B	602	NAG	C4-C5-C6-O6
4	B	602	NAG	O5-C5-C6-O6
4	A	605	NAG	C8-C7-N2-C2
4	A	605	NAG	O7-C7-N2-C2
4	B	602	NAG	C8-C7-N2-C2
4	B	602	NAG	O7-C7-N2-C2

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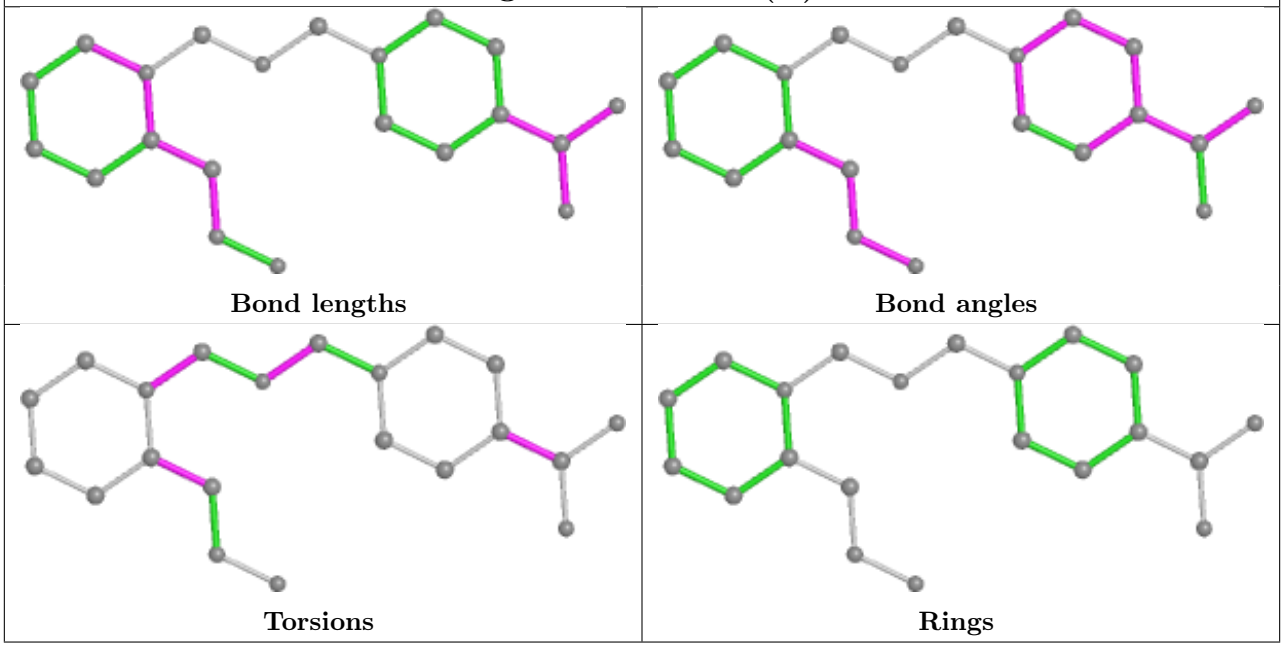
Mol	Chain	Res	Type	Atoms
5	B	609	L1M	C01-C02-O03-P04
4	A	605	NAG	O5-C5-C6-O6
3	A	601[A]	HI6	N3-C8-O2-C7
3	A	601[B]	HI6	N3-C8-O2-C7
3	B	601	HI6	N3-C8-O2-C7
5	A	606	L1M	C01-C02-O03-P04

There are no ring outliers.

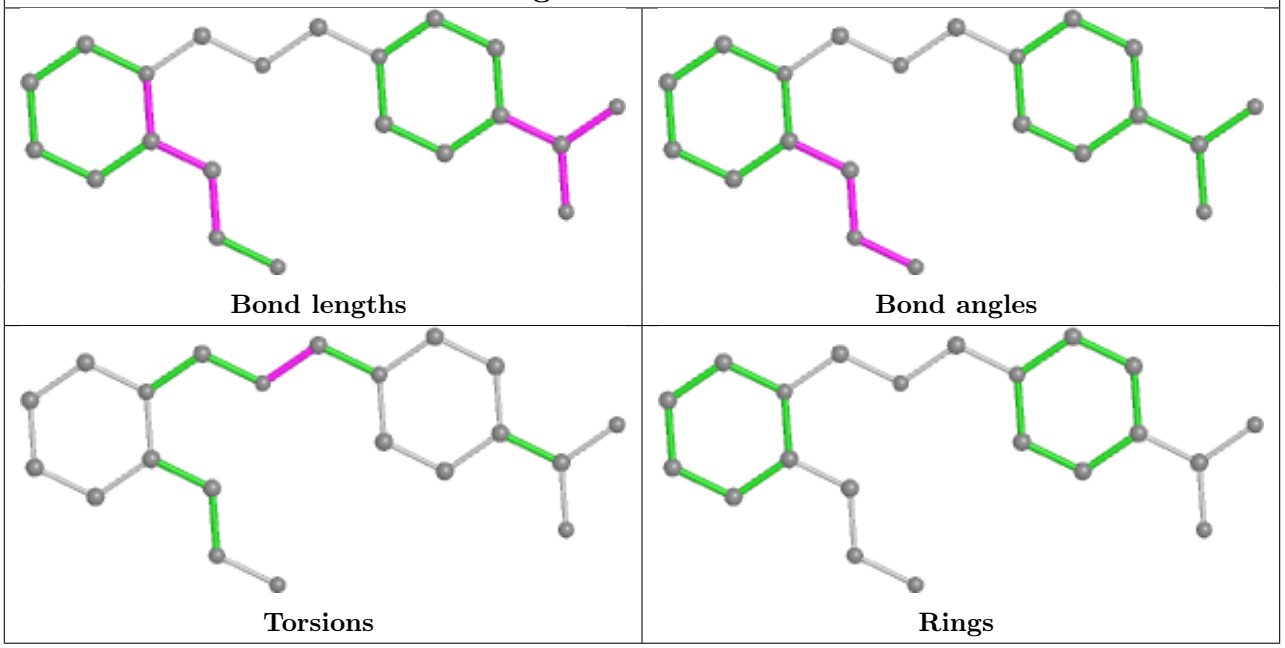
No monomer is involved in short contacts.

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.

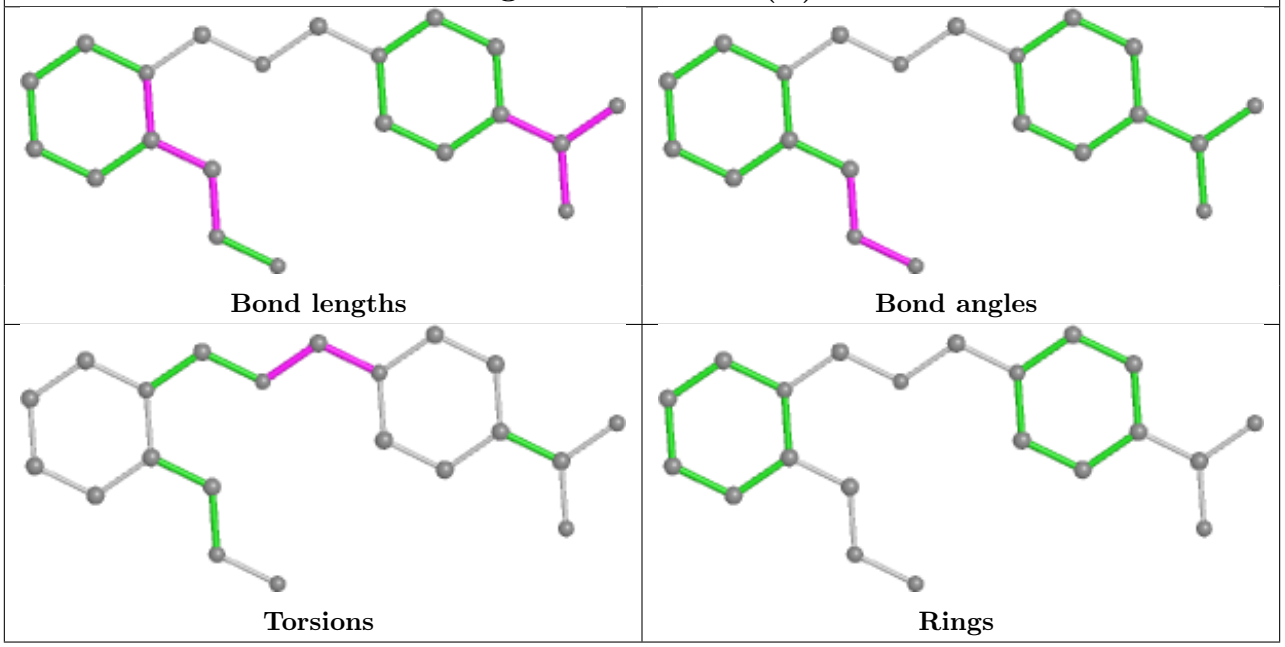
Ligand HI6 A 601 (A)



Ligand HI6 B 601



Ligand HI6 A 601 (B)



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.