



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 02:31 PM EDT

PDB ID : 6NTN
Title : Crystal Structure of Recombinant Human Acetylcholinesterase Inhibited by A-230 in Complex with the Reactivator, HI-6
Authors : Bester, S.M.; Guelta, M.A.; Height, J.J.; Pegan, S.D.
Deposited on : 2019-01-29
Resolution : 2.70 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)
Xtrriage (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

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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 8899 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.

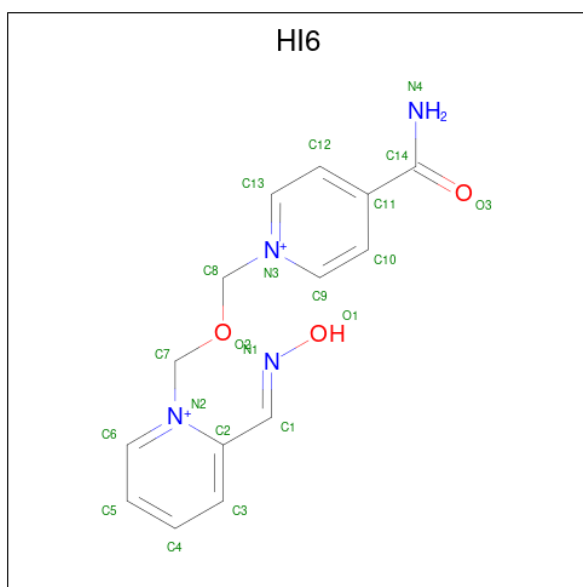
- Molecule 1 is a protein called Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	533	4138	2657	721	747	13	0	0	0
1	B	528	4111	2641	716	741	13	0	0	0

- 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.

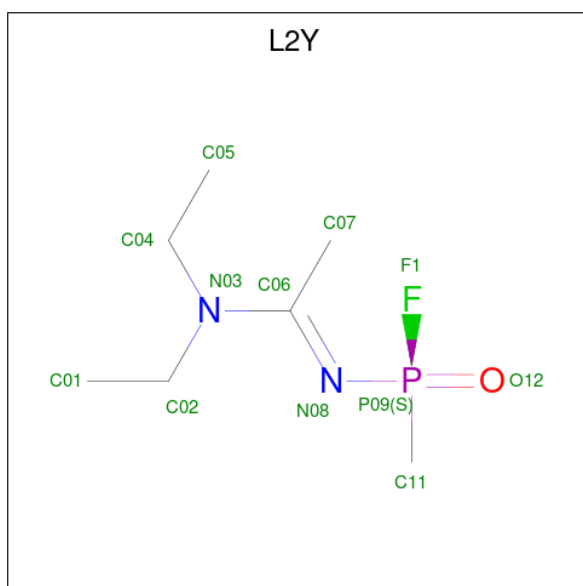
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	3	38	22	2	14	0	0	0
2	D	3	38	22	2	14	0	0	0
2	E	3	38	22	2	14	0	0	0

- Molecule 3 is 4-(AMINOCARBONYL)-1-[(2-[(E)-(HYDROXYIMINO)METHYL]PYRIDINIUM-1-YL}METHOXY)METHYL]PYRIDINIUM (three-letter code: HI6) (formula: C₁₄H₁₆N₄O₃).



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

- Molecule 4 is (S)-N-[(1E)-1-(diethylamino)ethylidene]-P-methylphosphonamidic fluoride (three-letter code: L2Y) (formula: C₇H₁₆FN₂OP).



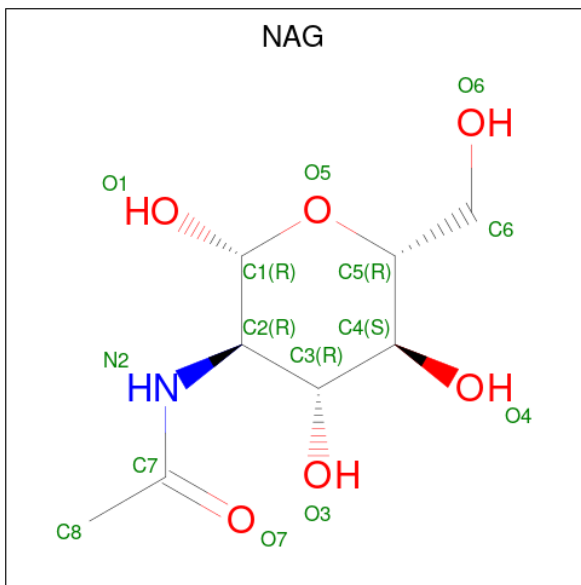
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			11	7	2	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	B	1	11	7	2	1	1	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	211	Total O 211 211	0	0
6	B	247	Total O 247 247	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	104.40Å 104.40Å 323.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.33 – 2.70	Depositor
% Data completeness (in resolution range)	99.3 (46.33-2.70)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (dev_3311: ???)	Depositor
R, R_{free}	0.171 , 0.215	Depositor
Wilson B-factor (Å ²)	52.5	Xtrriage
Anisotropy	0.758	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtrriage
Total number of atoms	8899	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

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	1,2	14,14,15	0.28	0	17,19,21	0.60	0
2	NAG	C	2	2	14,14,15	0.28	0	17,19,21	0.58	0
2	FUC	C	3	2	10,10,11	0.25	0	14,14,16	0.63	0
2	NAG	D	1	1,2	14,14,15	0.28	0	17,19,21	0.60	0
2	NAG	D	2	2	14,14,15	0.28	0	17,19,21	0.58	0
2	FUC	D	3	2	10,10,11	0.27	0	14,14,16	0.62	0
2	NAG	E	1	1,2	14,14,15	0.28	0	17,19,21	0.59	0
2	NAG	E	2	2	14,14,15	0.28	0	17,19,21	0.56	0
2	FUC	E	3	2	10,10,11	0.26	0	14,14,16	0.62	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	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	FUC	C	3	2	-	-	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	FUC	D	3	2	-	-	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	FUC	E	3	2	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C3-C2-N2-C7
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	E	1	NAG	C8-C7-N2-C2

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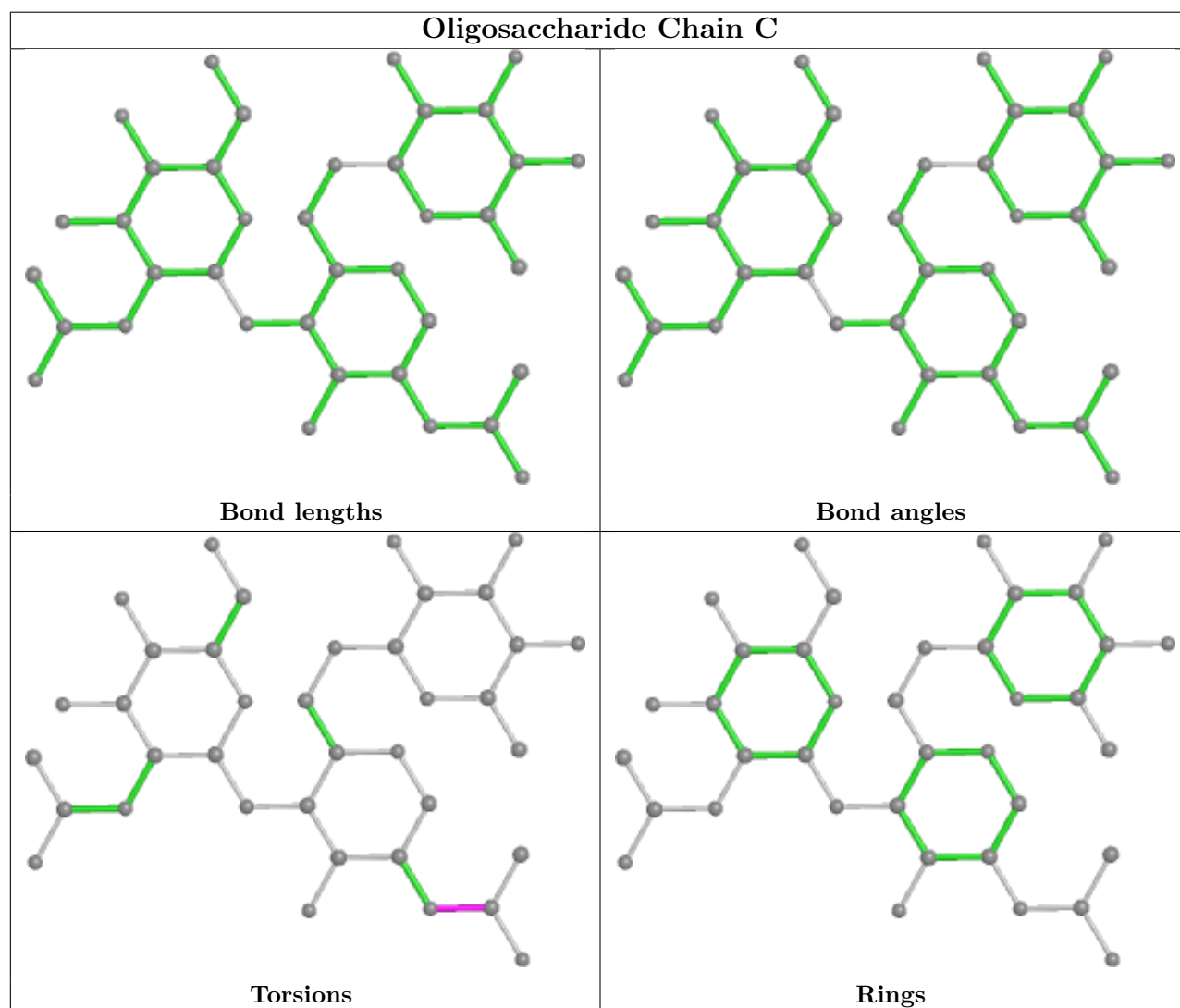
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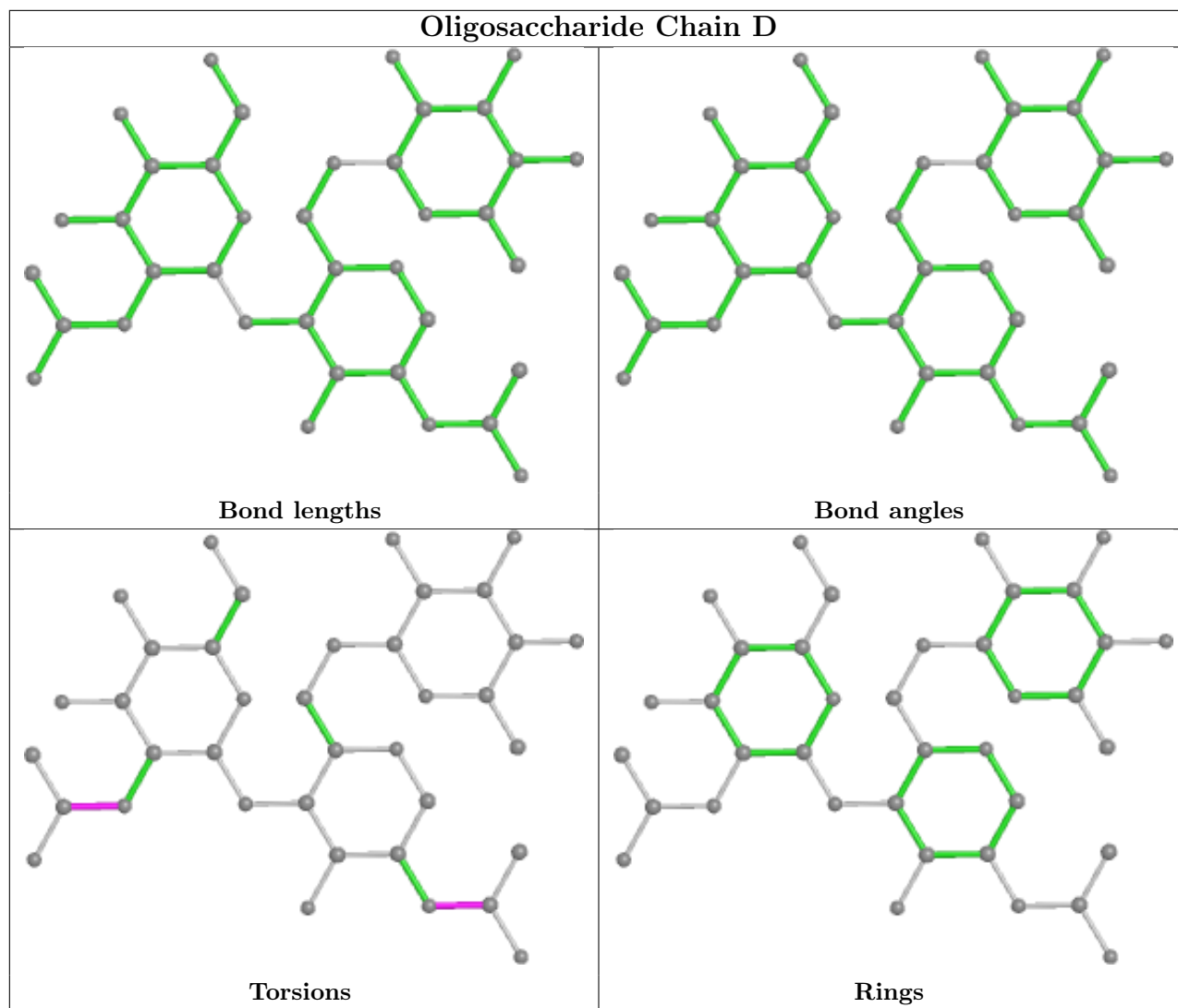
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2

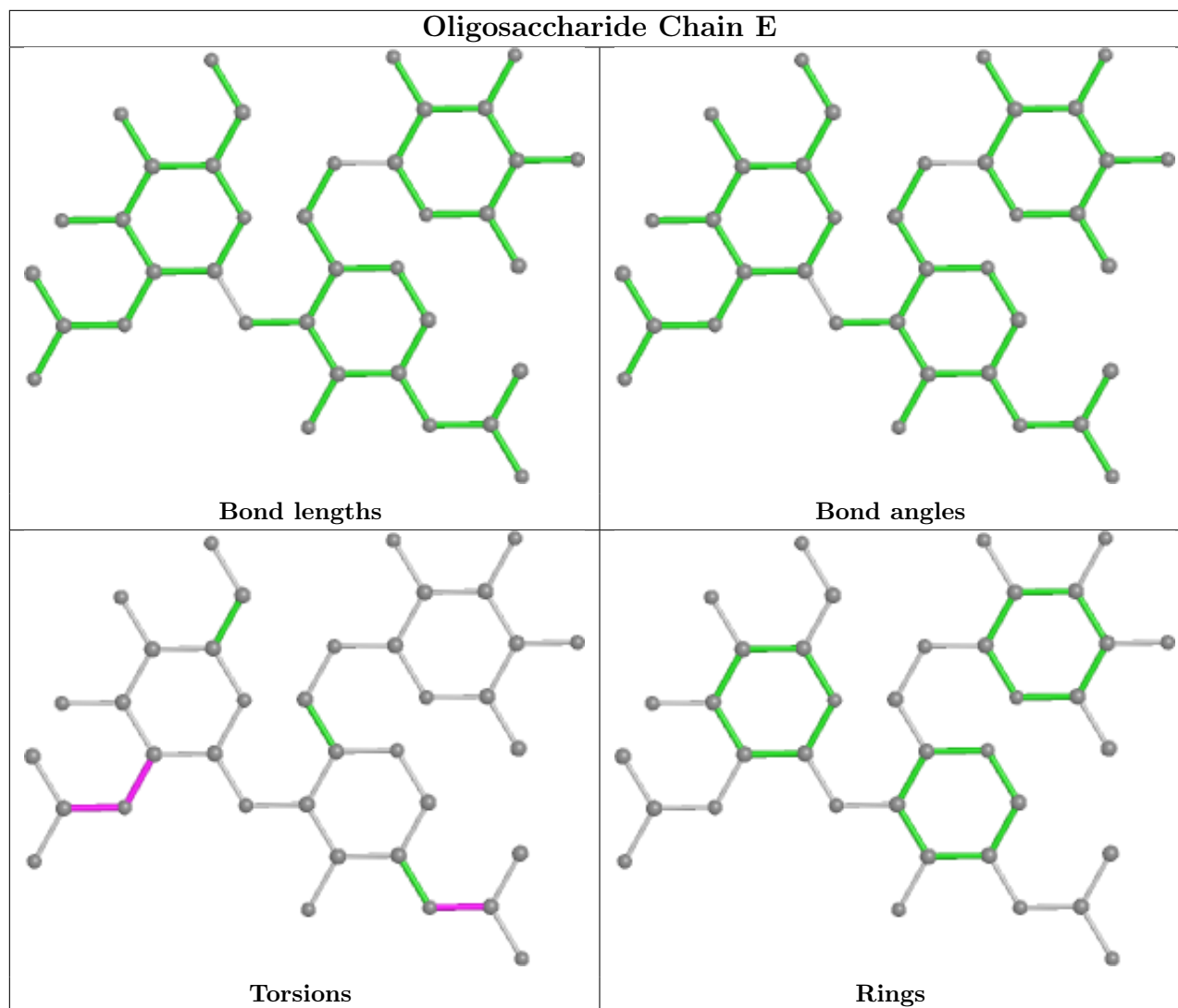
There are no ring outliers.

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.







4.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	L2Y	B	606	1	7,10,11	2.49	3 (42%)	5,12,15	0.87	0
5	NAG	B	605	1	14,14,15	0.29	0	17,19,21	0.57	0
3	HI6	B	601	-	18,22,22	2.52	7 (38%)	19,28,28	1.97	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	L2Y	A	608	1	7,10,11	2.44	3 (42%)	5,12,15	1.06	0
3	HI6	A	601	-	18,22,22	2.03	3 (16%)	19,28,28	1.61	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
4	L2Y	B	606	1	-	0/8/12/13	-
5	NAG	B	605	1	-	4/6/23/26	0/1/1/1
3	HI6	B	601	-	-	3/12/13/13	0/2/2/2
4	L2Y	A	608	1	-	1/8/12/13	-
3	HI6	A	601	-	-	4/12/13/13	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	HI6	C14-N4	6.64	1.45	1.33
3	B	601	HI6	O3-C14	-5.56	1.13	1.24
3	B	601	HI6	C14-N4	4.78	1.42	1.33
3	B	601	HI6	C2-N2	-4.39	1.32	1.37
4	A	608	L2Y	C06-N08	-4.30	1.25	1.31
4	B	606	L2Y	C06-N03	4.27	1.45	1.34
4	B	606	L2Y	C06-N08	-3.98	1.25	1.31
4	A	608	L2Y	C06-N03	3.89	1.44	1.34
3	B	601	HI6	C10-C11	-3.45	1.33	1.39
4	B	606	L2Y	C07-C06	2.69	1.53	1.49
3	B	601	HI6	C12-C11	-2.67	1.34	1.39
3	A	601	HI6	O3-C14	-2.62	1.19	1.24
3	A	601	HI6	C2-C1	2.62	1.54	1.46
3	B	601	HI6	C2-C1	2.50	1.53	1.46
4	A	608	L2Y	C07-C06	2.45	1.53	1.49
3	B	601	HI6	C4-C3	-2.17	1.34	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	HI6	O1-N1-C1	5.80	122.10	111.86
3	B	601	HI6	C11-C14-N4	4.58	123.25	117.75
3	B	601	HI6	O1-N1-C1	4.36	119.57	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	HI6	O3-C14-N4	-4.04	116.83	122.58
3	B	601	HI6	C2-C1-N1	3.02	123.59	117.75

There are no chirality outliers.

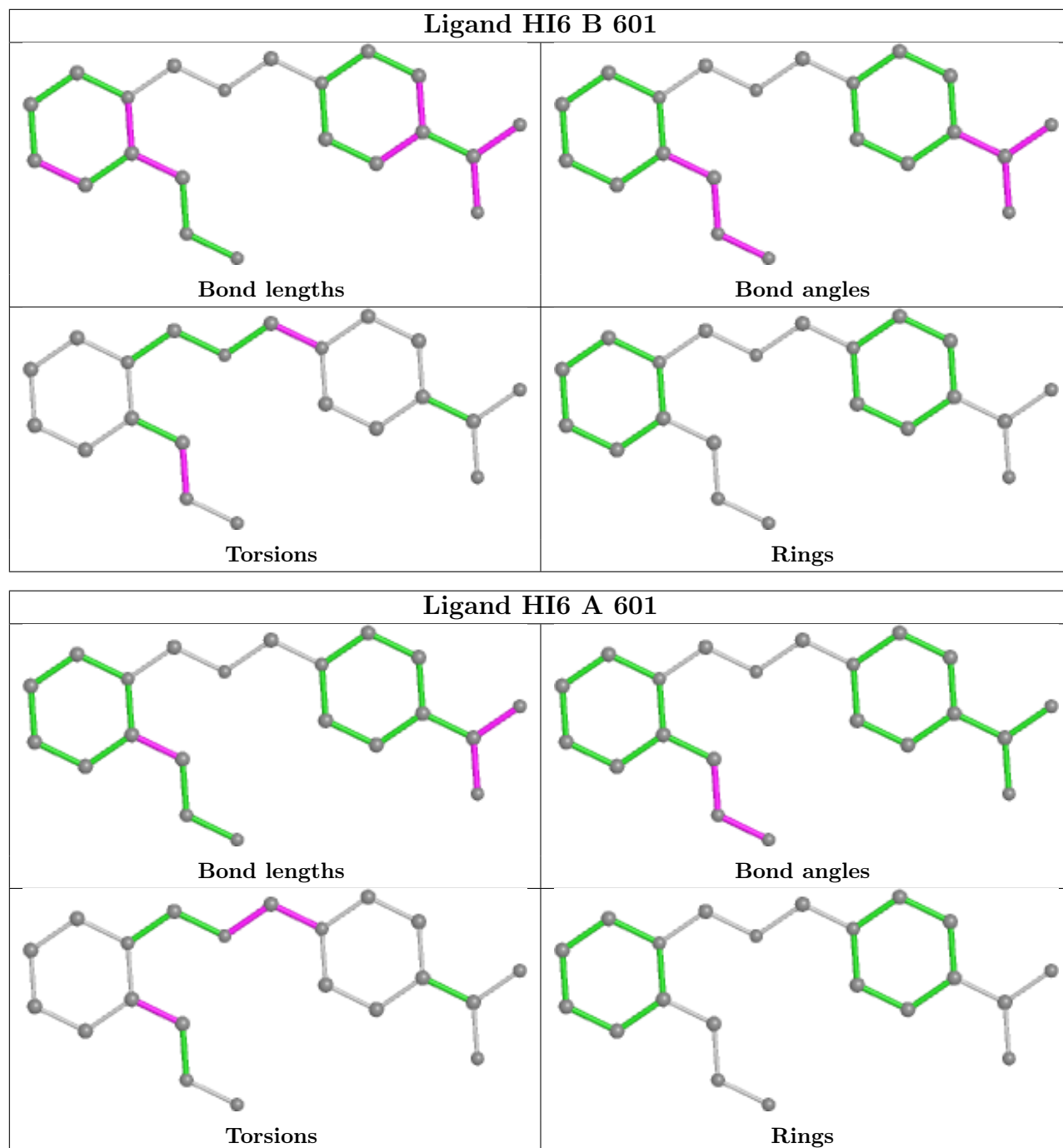
All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	HI6	O2-C8-N3-C13
3	A	601	HI6	N1-C1-C2-N2
3	B	601	HI6	O2-C8-N3-C9
3	B	601	HI6	O2-C8-N3-C13
5	B	605	NAG	C3-C2-N2-C7
5	B	605	NAG	C8-C7-N2-C2
3	A	601	HI6	N1-C1-C2-C3
3	A	601	HI6	N3-C8-O2-C7
5	B	605	NAG	O7-C7-N2-C2
3	B	601	HI6	C2-C1-N1-O1
4	A	608	L2Y	C01-C02-N03-C04
5	B	605	NAG	C1-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 than 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.



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.