WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB Geometry-Only Validation Report (i)

Oct 14, 2023 – 02:29 PM EDT

PDB ID	:	7T5D
Title	:	Neutron structure of Neurospora crassa Lytic Polysaccharide Monooxygenase 9D (NcLPMO9D) ascorbate soak
Authors	:	Schroder, G.C.; Meilleur, F.
Deposited on	:	2021-12-11
Resolution	:	2.40 Å(reported)

This is a Full wwPDB Geometry-Only 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 (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 (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
NEUTRON DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
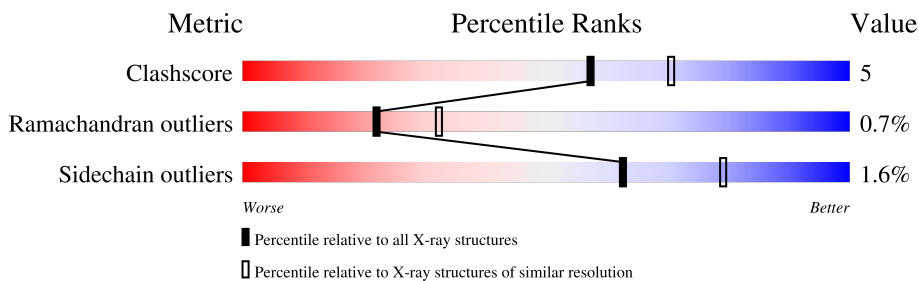
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	223	93% 7%
1	B	223	96% .
2	C	2	100%
2	D	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEO	A	302[A]	-	-	X	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 7807 atoms, of which 2640 are hydrogens and 1479 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 Lytic polysaccharide monooxygenase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	223	Total	C	D	H	N	O	S	0	145	0
			3234	1018	319	1302	279	310	6			
1	B	223	Total	C	D	H	N	O	S	0	155	0
			3213	1006	319	1295	277	310	6			

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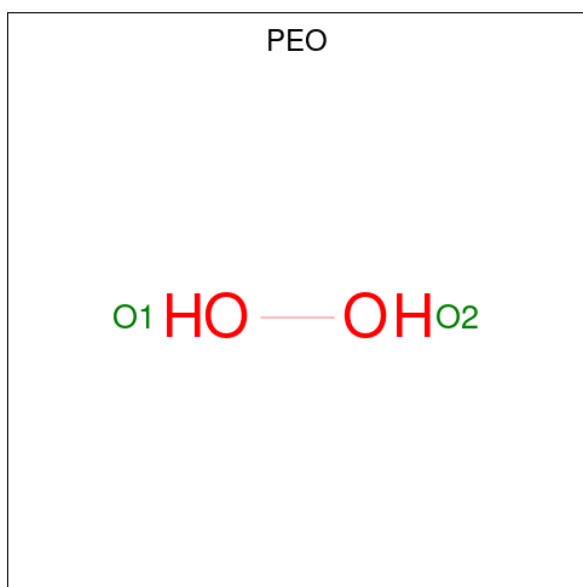

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	2	Total	C	D	H	N	O	0	1	0
			55	16	7	20	2	10			
2	D	2	Total	C	D	H	N	O	0	1	0
			56	16	5	23	2	10			

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cu	0	0
			1	1		
3	B	1	Total	Cu	0	0
			1	1		

- Molecule 4 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H_2O_2) (labeled as "Ligand of Interest" by depositor).

PEO

O1 HO —— OH O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 3	D 1	O 2	0	1

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2) (labeled as "Ligand of Interest" by depositor).

OXY

O1 O ═══ O O2
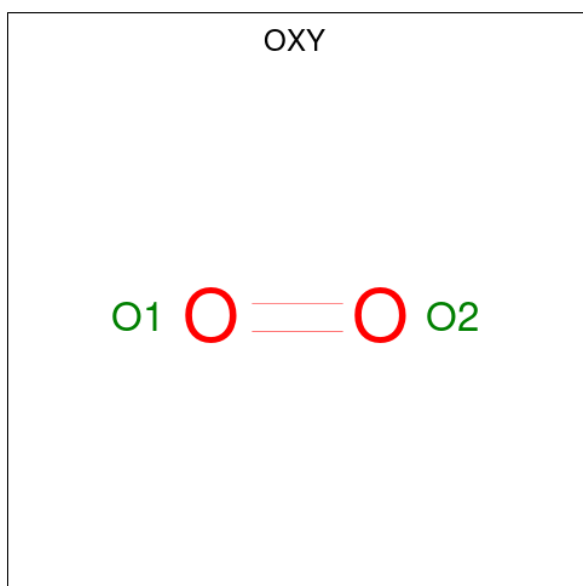
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 2	O 2	0	1

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	221	Total 663	D 442	O 221	0	0
6	B	192	Total 579	D 386	O 193	0	1

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: Lytic polysaccharide monooxygenase

Chain A:
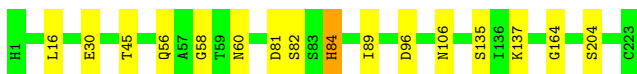
• Molecule 1: Lytic polysaccharide monooxygenase

Chain B:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

4 Model quality ⓘ

4.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CU, NAG, PEO, OXY

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.31	0/2495	0.50	0/3409
1	B	0.35	0/2505	0.58	6/3422 (0.2%)
All	All	0.33	0/5000	0.55	6/6831 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	21[A]	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	21[B]	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	21[A]	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	B	21[B]	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	B	59[A]	THR	O-C-N	-5.53	113.85	122.70
1	B	59[B]	THR	O-C-N	-5.53	113.85	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58[A]	GLY	Mainchain
1	A	58[B]	GLY	Mainchain
1	B	60[B]	ASN	Mainchain

4.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1932	1302	489	10	0
1	B	1918	1295	388	7	0
2	C	35	20	13	0	0
2	D	33	23	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	3	0	0	2	0
5	A	2	0	0	1	0
6	A	663	0	0	5	1
6	B	579	0	0	7	1
All	All	5167	2640	902	26	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (26) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:SER:O	6:A:401:HOH:O	2.02	0.76
1:A:16:LEU:HD21	6:A:461:HOH:O	1.82	0.74
5:A:303[B]:OXY:O2	1:B:30:GLU:OE1	2.06	0.73
4:A:302[A]:PEO:O2	1:B:30:GLU:OE1	2.08	0.71
1:A:30:GLU:OE1	6:A:402:HOH:O	2.12	0.67
1:A:84:HIS:CE1	4:A:302[A]:PEO:O1	2.62	0.51
1:A:81:ASP:OD1	1:A:82:SER:N	2.48	0.46
1:A:60:ASN:ND2	1:A:135:SER:OG	2.49	0.45
1:B:61:VAL:O	1:B:61:VAL:HG23	2.15	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:582:HOH:O	6:B:537:HOH:O[2_559]	2.16	0.04

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	328/223 (147%)	306 (93%)	20 (6%)	2 (1%)	25	36
1	B	329/223 (148%)	305 (93%)	22 (7%)	2 (1%)	25	36
All	All	657/446 (147%)	611 (93%)	42 (6%)	4 (1%)	22	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	164[B]	GLY
1	A	164[A]	GLY
1	A	164[B]	GLY
1	B	209	PRO

4.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	243/178 (136%)	237 (98%)	6 (2%)	47	67
1	B	244/178 (137%)	241 (99%)	3 (1%)	71	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	487/356 (137%)	478 (98%)	9 (2%)	62 76

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56[A]	GLN
1	A	56[B]	GLN
1	A	56[C]	GLN
1	A	56[D]	GLN
1	A	84	HIS
1	A	89[A]	ILE
1	B	124[A]	THR
1	B	124[B]	THR
1	B	140[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

5 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	2	2	14,14,15	0.21	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	D	1	1,2	14,14,15	0.27	0	17,19,21	0.43	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	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	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 C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D
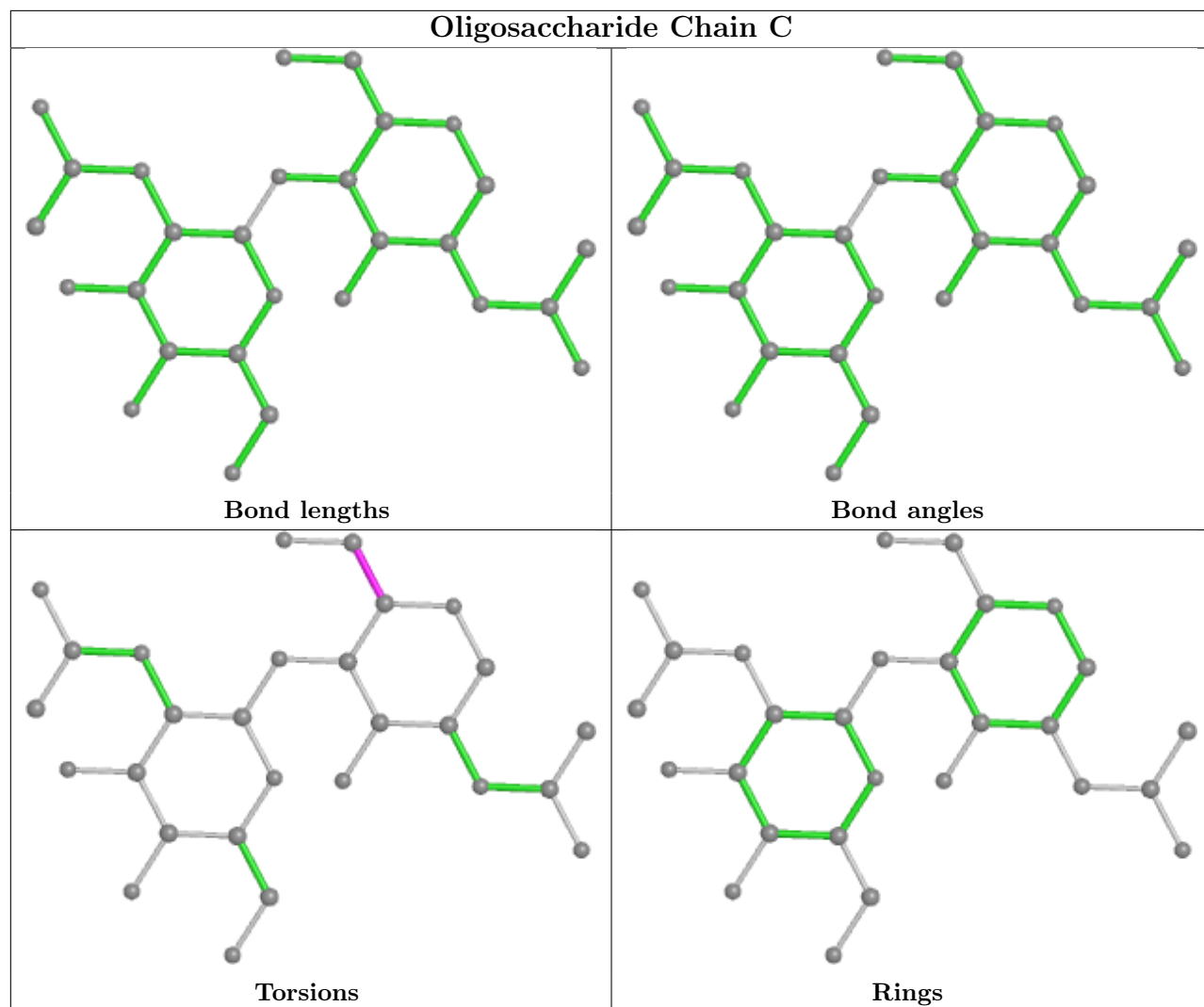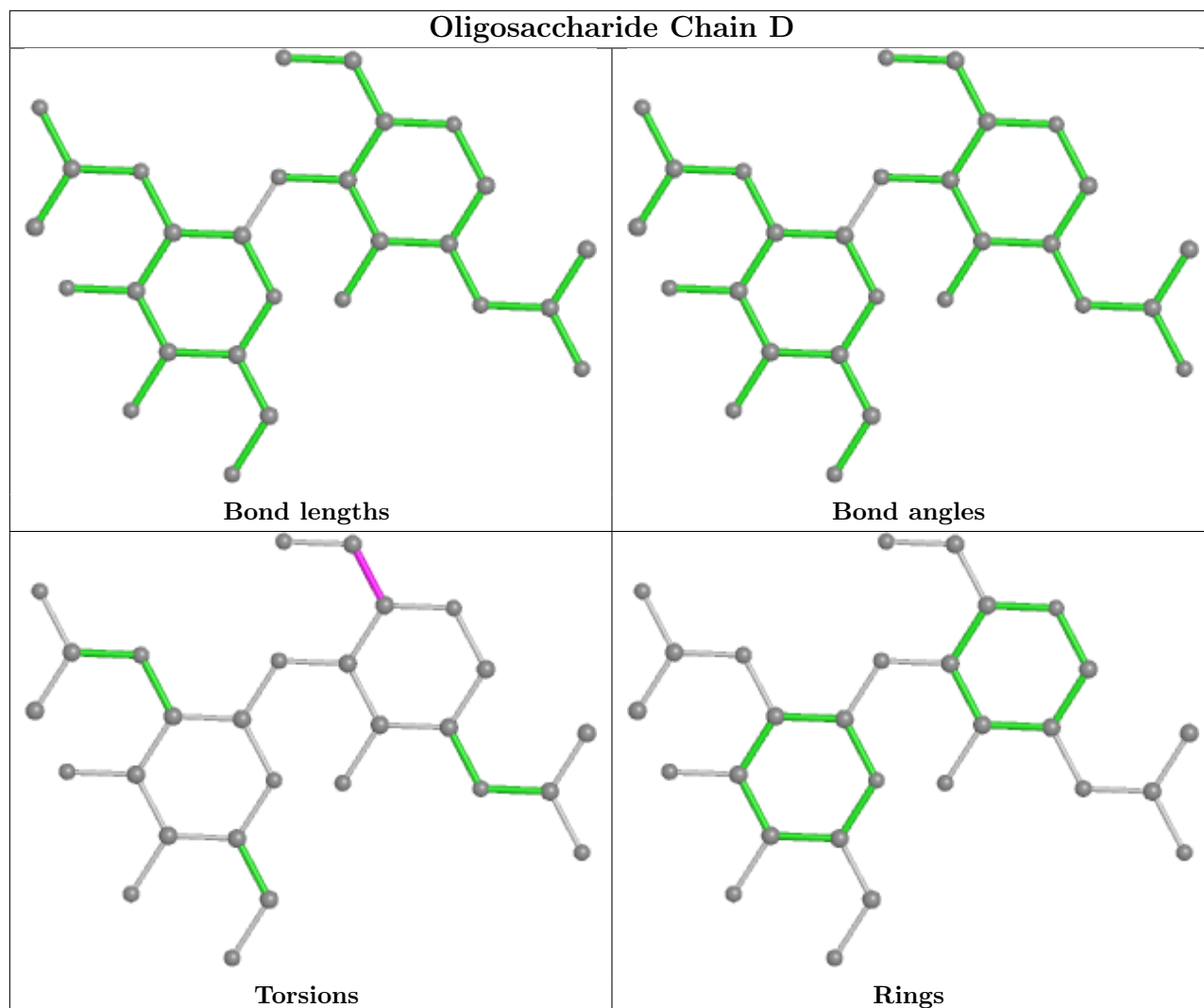
4.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#|Z| > 2$
4	PEO	A	302[A]	3	1,1,1	0.40	0	-		
5	OXY	A	303[B]	3	1,1,1	0.26	0	-		

There are no bond length outliers.

There are no bond angle outliers.
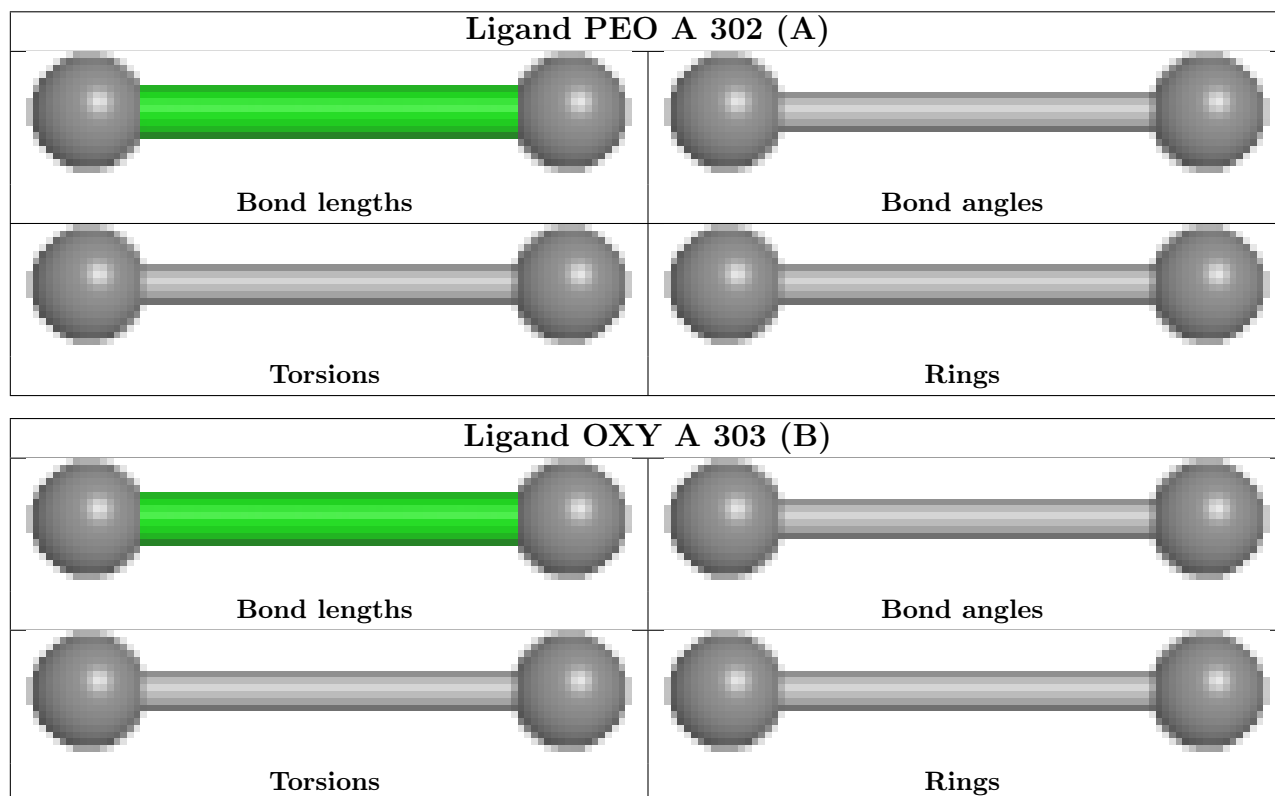
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	302[A]	PEO	2	0
5	A	303[B]	OXY	1	0

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 PEO A 302 (A)

Bond lengths   Bond angles

Torsions   Rings

Ligand OXY A 303 (B)

Bond lengths   Bond angles

Torsions   Rings

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.