Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 01:06 PM EDT

PDB ID	:	6NWE
Title	:	Crystal structure of bovine opsin with beta octyl glucoside bound
Authors	:	Eger, B.T.; Morizumi, T.; Ernst, O.P.
Deposited on	:	2019-02-06
Resolution	:	2.71 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 (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 2.71 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 7 unique types of molecules in this entry. The entry contains 2886 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 Rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	326	2606	1736	402	442	26	0	1	0

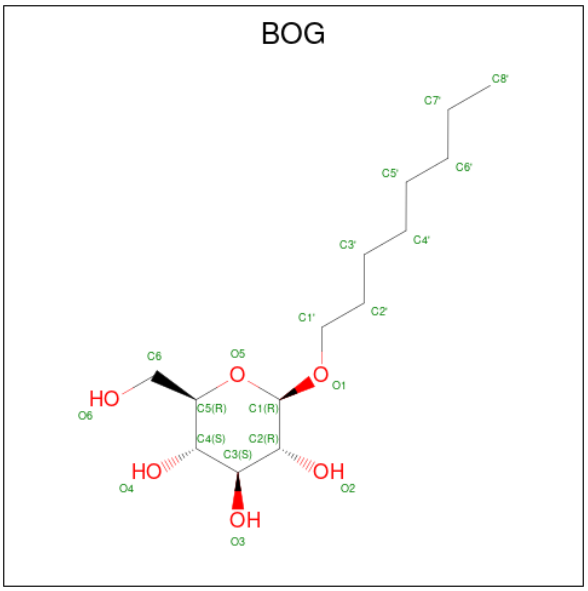
- Molecule 2 is a protein called ILENLKDVGLF peptide CT2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	11	89	59	13	17	0	0	0

- Molecule 3 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-glucopyranose.

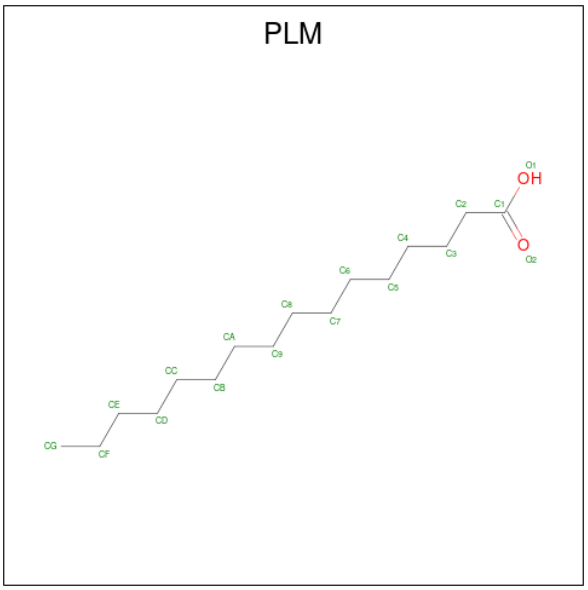
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	4	50	28	2	20	0	0	0

- Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$) (labeled as "Ligand of Interest" by depositor).



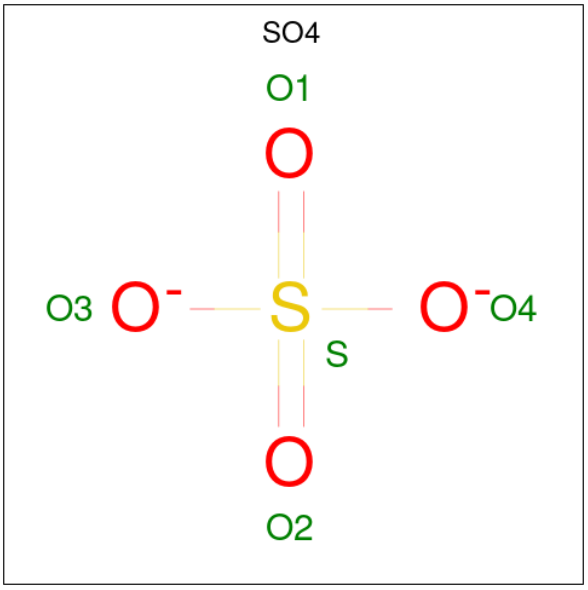
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	20	14	6	0	0
			Total	C	O		
4	A	1	20	14	6	0	0
			Total	C	O		
4	A	1	20	14	6	0	0
			Total	C	O		
4	A	1	20	14	6	0	0
			Total	C	O		
4	A	1	20	14	6	0	0

- Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	17	16	1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	9	9	9	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	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	242.17Å 242.17Å 110.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.10 – 2.71	Depositor
% Data completeness (in resolution range)	99.3 (40.10-2.71)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.10_2155)	Depositor
R, R_{free}	0.196 , 0.223	Depositor
Wilson B-factor (Å^2)	65.6	Xtriage
Anisotropy	0.585	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2886	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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 (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

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)

4 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	C	1	3,1	14,14,15	0.70	0	17,19,21	0.78	0
3	NAG	C	2	3	14,14,15	0.85	1 (7%)	17,19,21	1.37	2 (11%)
3	BMA	C	3	3	11,11,12	0.60	0	15,15,17	0.83	0
3	BMA	C	4	3	11,11,12	0.51	0	15,15,17	0.74	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	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	BMA	C	4	3	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	NAG	O5-C1	2.05	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2	NAG	O5-C5-C6	3.85	113.23	107.20
3	C	2	NAG	C6-C5-C4	-2.28	107.67	113.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

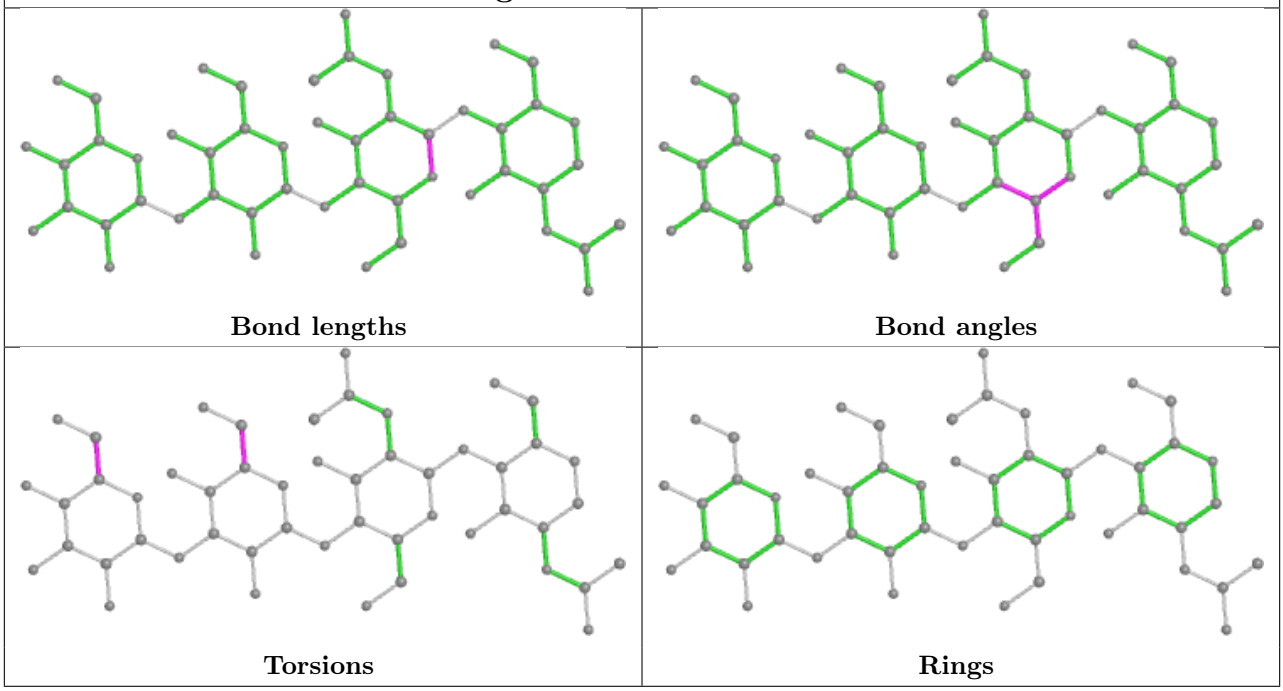
Mol	Chain	Res	Type	Atoms
3	C	3	BMA	C4-C5-C6-O6
3	C	3	BMA	O5-C5-C6-O6
3	C	4	BMA	O5-C5-C6-O6

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



4.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
5	PLM	A	409	1	16,16,17	0.30	0	15,15,17	0.76	0
6	SO4	A	411	-	4,4,4	0.16	0	6,6,6	0.12	0
6	SO4	B	401	-	4,4,4	0.14	0	6,6,6	0.10	0
4	BOG	A	408	-	20,20,20	0.92	2 (10%)	25,25,25	1.37	3 (12%)
6	SO4	A	410	-	4,4,4	0.13	0	6,6,6	0.07	0
4	BOG	A	412	-	20,20,20	0.96	1 (5%)	25,25,25	1.34	4 (16%)
4	BOG	A	405	-	20,20,20	0.84	0	25,25,25	1.62	4 (16%)
4	BOG	A	407	-	20,20,20	0.99	1 (5%)	25,25,25	1.62	3 (12%)
4	BOG	A	406	-	20,20,20	1.01	2 (10%)	25,25,25	1.31	2 (8%)

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
5	PLM	A	409	1	-	6/13/14/15	-
4	BOG	A	408	-	-	7/11/31/31	0/1/1/1
4	BOG	A	412	-	-	8/11/31/31	0/1/1/1
4	BOG	A	405	-	-	5/11/31/31	0/1/1/1
4	BOG	A	407	-	-	8/11/31/31	0/1/1/1
4	BOG	A	406	-	-	5/11/31/31	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	412	BOG	O5-C1	2.63	1.48	1.41
4	A	406	BOG	O5-C1	2.34	1.47	1.41
4	A	406	BOG	C4-C3	-2.33	1.46	1.52
4	A	407	BOG	C3-C2	-2.28	1.46	1.52
4	A	408	BOG	C4-C3	-2.06	1.47	1.52
4	A	408	BOG	O5-C1	2.01	1.47	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	407	BOG	C3-C4-C5	4.78	118.77	110.24
4	A	405	BOG	C4-C3-C2	4.52	118.72	110.82
4	A	407	BOG	O5-C5-C4	4.40	117.69	109.69
4	A	405	BOG	C3-C4-C5	3.76	116.94	110.24
4	A	408	BOG	C1-C2-C3	3.73	117.76	110.00
4	A	412	BOG	O5-C1-C2	3.72	118.22	110.35
4	A	406	BOG	C1-C2-C3	3.48	117.23	110.00
4	A	406	BOG	O5-C1-C2	3.34	117.41	110.35
4	A	408	BOG	C4-C3-C2	3.33	116.63	110.82
4	A	405	BOG	C1-C2-C3	3.07	116.40	110.00
4	A	412	BOG	C3-C4-C5	-2.87	105.12	110.24
4	A	407	BOG	C4-C3-C2	2.75	115.62	110.82
4	A	412	BOG	C1-C2-C3	2.71	115.64	110.00
4	A	412	BOG	O5-C5-C6	2.60	112.89	106.44
4	A	408	BOG	O5-C1-C2	2.29	115.20	110.35
4	A	405	BOG	C1-O5-C5	-2.05	109.66	113.69

There are no chirality outliers.

All (39) torsion outliers are listed below:

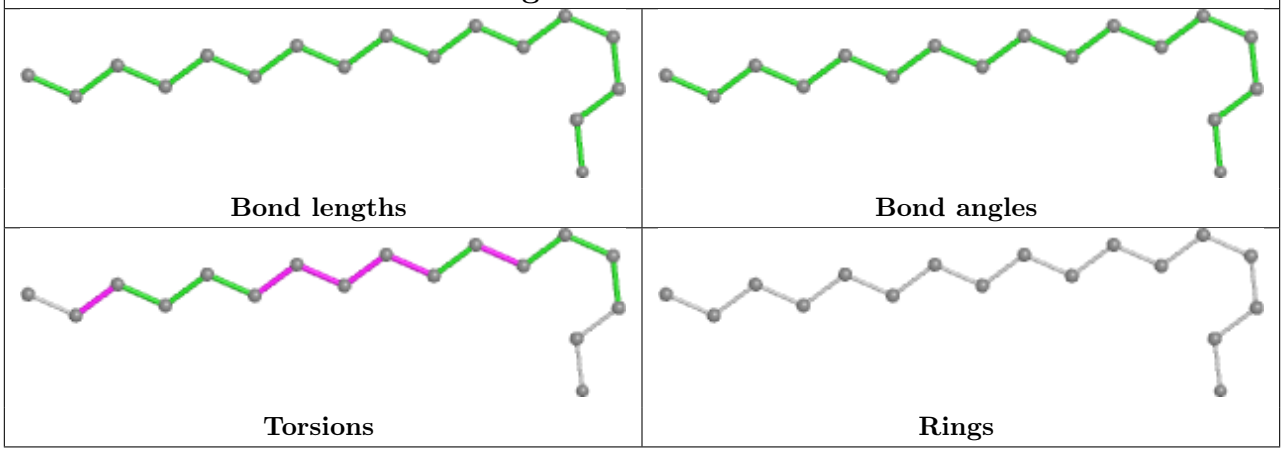
Mol	Chain	Res	Type	Atoms
4	A	406	BOG	O5-C1-O1-C1'
4	A	407	BOG	C2-C1-O1-C1'
4	A	407	BOG	O5-C1-O1-C1'
4	A	408	BOG	C2'-C1'-O1-C1
4	A	412	BOG	O5-C1-O1-C1'
4	A	407	BOG	C4-C5-C6-O6
4	A	408	BOG	O5-C5-C6-O6
4	A	407	BOG	O5-C5-C6-O6
4	A	408	BOG	C4-C5-C6-O6
4	A	406	BOG	C2-C1-O1-C1'
4	A	407	BOG	O1-C1'-C2'-C3'
4	A	412	BOG	C4-C5-C6-O6
4	A	412	BOG	O1-C1'-C2'-C3'
4	A	405	BOG	C4-C5-C6-O6
4	A	405	BOG	O5-C5-C6-O6
4	A	408	BOG	C4'-C5'-C6'-C7'
4	A	406	BOG	C2'-C3'-C4'-C5'
5	A	409	PLM	C6-C7-C8-C9
4	A	405	BOG	C4'-C5'-C6'-C7'
4	A	412	BOG	C2'-C1'-O1-C1
4	A	412	BOG	C1'-C2'-C3'-C4'
4	A	412	BOG	O5-C5-C6-O6
4	A	408	BOG	C5'-C6'-C7'-C8'
4	A	406	BOG	O5-C5-C6-O6
4	A	408	BOG	C2'-C3'-C4'-C5'
4	A	405	BOG	C2-C1-O1-C1'
5	A	409	PLM	C8-C9-CA-CB
4	A	406	BOG	C2'-C1'-O1-C1
4	A	407	BOG	C2'-C1'-O1-C1
5	A	409	PLM	C7-C8-C9-CA
4	A	408	BOG	C3'-C4'-C5'-C6'
5	A	409	PLM	C9-CA-CB-CC
4	A	407	BOG	C3'-C4'-C5'-C6'
4	A	405	BOG	O1-C1'-C2'-C3'
4	A	412	BOG	C5'-C6'-C7'-C8'
4	A	407	BOG	C4'-C5'-C6'-C7'
4	A	412	BOG	C3'-C4'-C5'-C6'
5	A	409	PLM	C4-C5-C6-C7
5	A	409	PLM	CD-CE-CF-CG

There are no ring outliers.

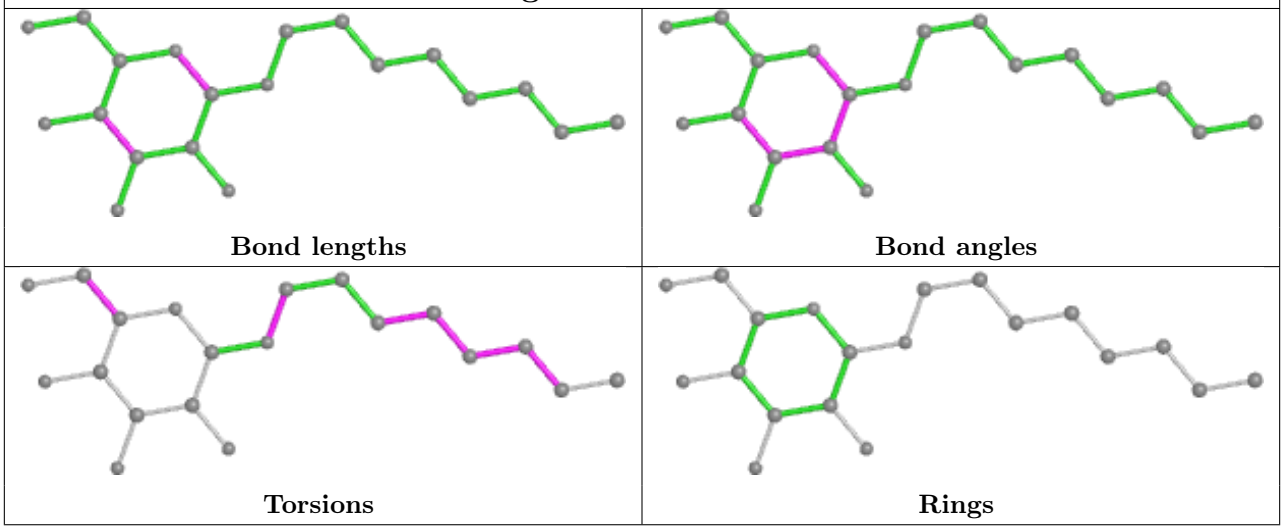
No monomer is involved in short contacts.

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.

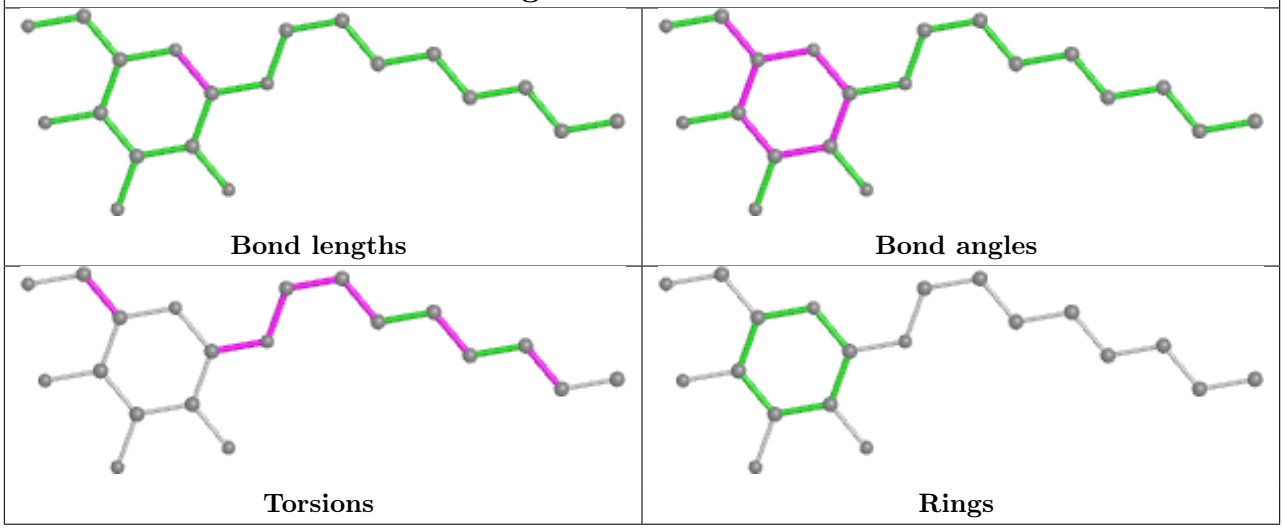
Ligand PLM A 409



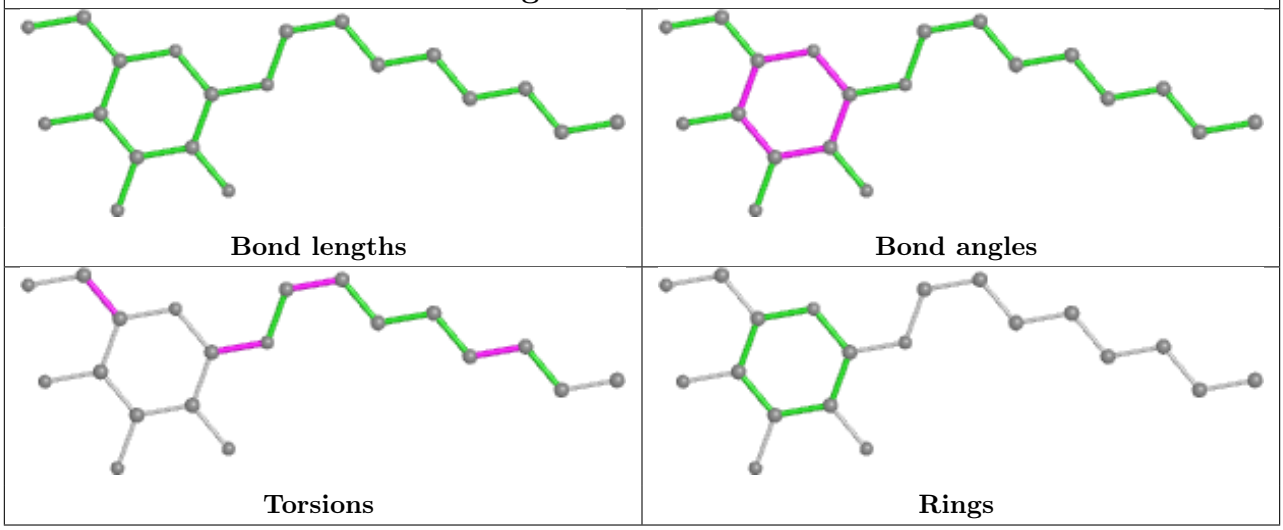
Ligand BOG A 408



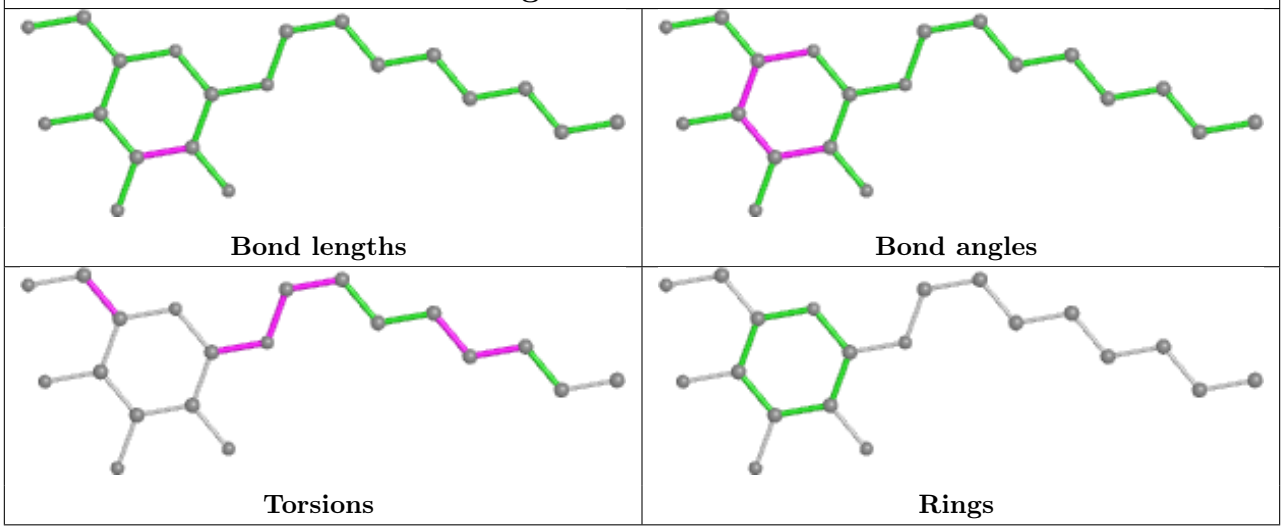
Ligand BOG A 412

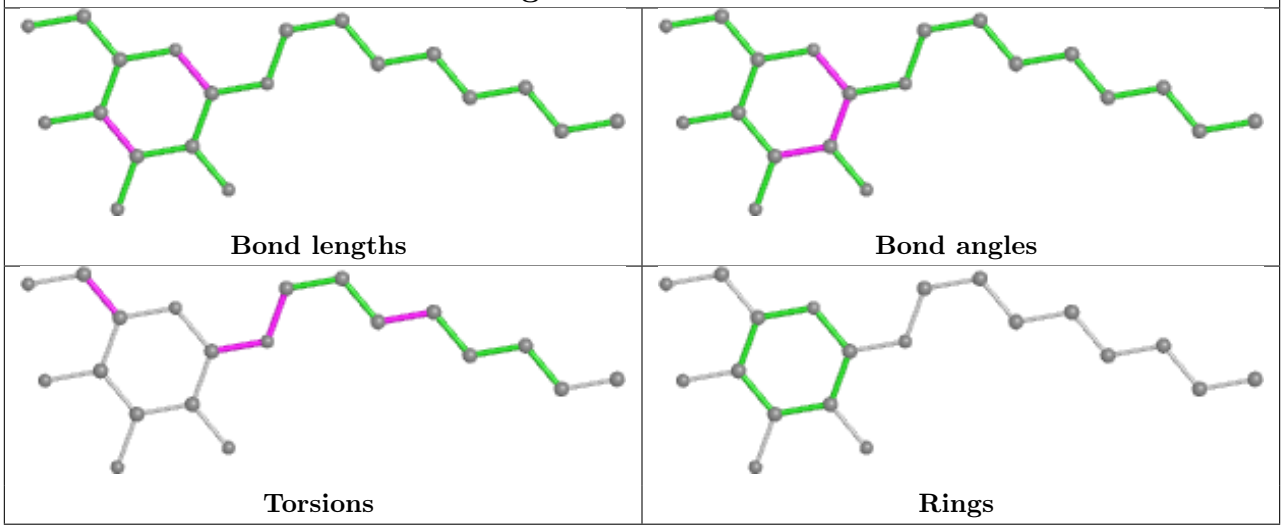


Ligand BOG A 405



Ligand BOG A 407



Ligand BOG A 406	
	
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 (i)

5.1 Protein, DNA and RNA chains (i)

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

5.2 Non-standard residues in protein, DNA, RNA chains (i)

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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