



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2023 – 10:15 PM EDT

PDB ID : 6MCP
Title : L. pneumophila effector kinase LegK7 (AMP-PNP bound) in complex with human MOB1A
Authors : Beyrakhova, K.A.; Xu, C.; Boniecki, M.T.; Cygler, M.
Deposited on : 2018-09-01
Resolution : 2.50 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 2.50 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 9 unique types of molecules in this entry. The entry contains 11356 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 LegK7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	520	Total	C	N	O	S	0	1	0
			4142	2672	691	764	15			
1	C	507	Total	C	N	O	S	0	1	0
			3953	2556	662	721	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	SER	-	expression tag	UNP Q5ZU83
A	9	ASN	-	expression tag	UNP Q5ZU83
A	10	ALA	-	expression tag	UNP Q5ZU83
C	8	SER	-	expression tag	UNP Q5ZU83
C	9	ASN	-	expression tag	UNP Q5ZU83
C	10	ALA	-	expression tag	UNP Q5ZU83

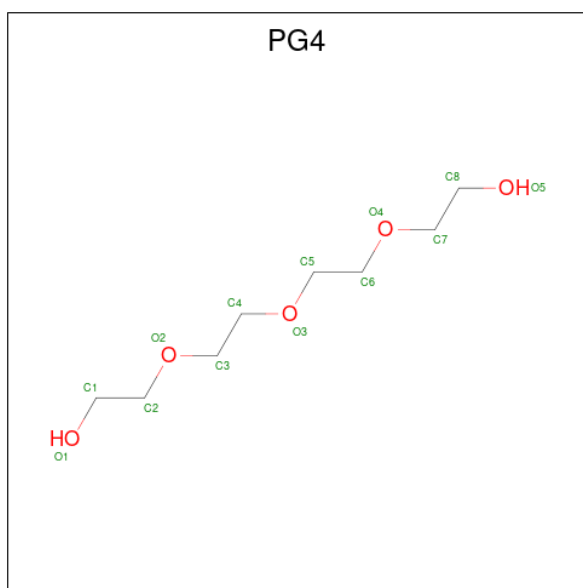
- Molecule 2 is a protein called MOB kinase activator 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	183	Total	C	N	O	S	0	2	0
			1473	953	240	271	9			
2	D	181	Total	C	N	O	S	0	0	0
			1404	908	223	264	9			

There are 6 discrepancies between the modelled and reference sequences:

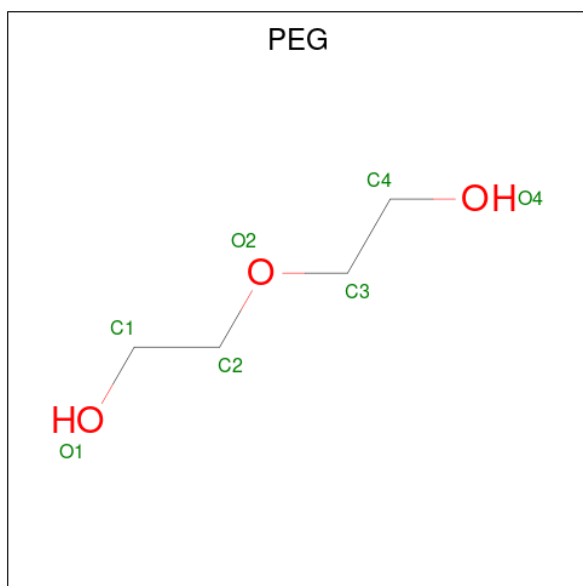
Chain	Residue	Modelled	Actual	Comment	Reference
B	30	SER	-	expression tag	UNP Q9H8S9
B	31	ASN	-	expression tag	UNP Q9H8S9
B	32	ALA	-	expression tag	UNP Q9H8S9
D	30	SER	-	expression tag	UNP Q9H8S9
D	31	ASN	-	expression tag	UNP Q9H8S9
D	32	ALA	-	expression tag	UNP Q9H8S9

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 19 12 7	0	0
5	A	1	Total C O 19 12 7	0	0
5	B	1	Total C O 19 12 7	0	0
5	C	1	Total C O 19 12 7	0	0

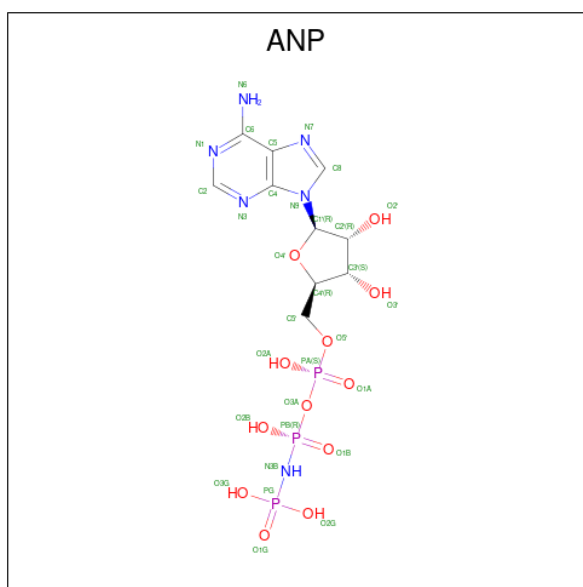
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Zn 1 1	0	0
6	D	1	Total Zn 1 1	0	0

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total Mn 1 1	0	0

- Molecule 8 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
8	C	1	31	10	6	12	3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	68	Total	O	0	0
			68	68		
9	B	23	Total	O	0	0
			23	23		
9	C	14	Total	O	0	0
			14	14		
9	D	4	Total	O	0	0
			4	4		

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

3 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.86Å 112.43Å 155.22Å 90.00° 105.58° 90.00°	Depositor
Resolution (Å)	48.67 – 2.50	Depositor
% Data completeness (in resolution range)	99.8 (48.67-2.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.194 , 0.233	Depositor
Wilson B-factor (Å ²)	57.1	Xtrriage
Anisotropy	0.338	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	11356	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5048e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

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](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 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	PEG	A	602	-	6,6,6	0.48	0	5,5,5	0.26	0
4	PEG	C	603	-	6,6,6	0.48	0	5,5,5	0.24	0
4	PEG	A	605	-	6,6,6	0.48	0	5,5,5	0.31	0
4	PEG	A	604	-	6,6,6	0.49	0	5,5,5	0.31	0
4	PEG	D	304	-	6,6,6	0.49	0	5,5,5	0.28	0
4	PEG	A	608	-	6,6,6	0.49	0	5,5,5	0.23	0
3	PG4	A	611	-	12,12,12	0.52	0	11,11,11	0.35	0
4	PEG	A	609	-	6,6,6	0.48	0	5,5,5	0.24	0
4	PEG	C	607	-	6,6,6	0.49	0	5,5,5	0.32	0
4	PEG	C	604	-	6,6,6	0.48	0	5,5,5	0.32	0
4	PEG	C	606	-	6,6,6	0.49	0	5,5,5	0.24	0
5	P6G	B	303	-	18,18,18	0.54	0	17,17,17	0.25	0
4	PEG	A	603	-	6,6,6	0.49	0	5,5,5	0.25	0
4	PEG	B	302	-	6,6,6	0.49	0	5,5,5	0.23	0
5	P6G	A	606	-	18,18,18	0.54	0	17,17,17	0.28	0
8	ANP	C	610	7	29,33,33	3.61	16 (55%)	31,52,52	1.99	7 (22%)
4	PEG	D	303	-	6,6,6	0.47	0	5,5,5	0.36	0
4	PEG	C	608	-	6,6,6	0.48	0	5,5,5	0.30	0
4	PEG	A	610	-	6,6,6	0.49	0	5,5,5	0.22	0
5	P6G	C	602	-	18,18,18	0.54	0	17,17,17	0.20	0
4	PEG	C	605	-	6,6,6	0.48	0	5,5,5	0.28	0
5	P6G	A	607	-	18,18,18	0.55	0	17,17,17	0.24	0
4	PEG	C	609	-	6,6,6	0.48	0	5,5,5	0.24	0
4	PEG	B	304	-	6,6,6	0.49	0	5,5,5	0.28	0
3	PG4	D	302	-	12,12,12	0.54	0	11,11,11	0.32	0
3	PG4	A	601	-	12,12,12	0.53	0	11,11,11	0.22	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
4	PEG	A	602	-	-	1/4/4/4	-
4	PEG	C	603	-	-	2/4/4/4	-
4	PEG	A	605	-	-	3/4/4/4	-
4	PEG	A	604	-	-	2/4/4/4	-
4	PEG	D	304	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	A	608	-	-	1/4/4/4	-
3	PG4	A	611	-	-	4/10/10/10	-
4	PEG	A	609	-	-	2/4/4/4	-
4	PEG	C	607	-	-	1/4/4/4	-
4	PEG	C	604	-	-	1/4/4/4	-
4	PEG	C	606	-	-	2/4/4/4	-
5	P6G	B	303	-	-	11/16/16/16	-
4	PEG	A	603	-	-	1/4/4/4	-
4	PEG	B	302	-	-	1/4/4/4	-
5	P6G	A	606	-	-	9/16/16/16	-
8	ANP	C	610	7	-	5/14/38/38	0/3/3/3
4	PEG	D	303	-	-	2/4/4/4	-
4	PEG	C	608	-	-	3/4/4/4	-
4	PEG	A	610	-	-	2/4/4/4	-
5	P6G	C	602	-	-	8/16/16/16	-
4	PEG	C	605	-	-	2/4/4/4	-
5	P6G	A	607	-	-	7/16/16/16	-
4	PEG	C	609	-	-	2/4/4/4	-
4	PEG	B	304	-	-	2/4/4/4	-
3	PG4	D	302	-	-	8/10/10/10	-
3	PG4	A	601	-	-	7/10/10/10	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	610	ANP	PG-N3B	-9.33	1.39	1.63
8	C	610	ANP	PG-O1G	9.21	1.60	1.46
8	C	610	ANP	PB-O1B	8.02	1.58	1.46
8	C	610	ANP	C2'-C1'	-3.94	1.47	1.53
8	C	610	ANP	PG-O2G	-3.66	1.46	1.56
8	C	610	ANP	C5-C4	-3.65	1.31	1.40
8	C	610	ANP	C6-C5	-3.23	1.31	1.43
8	C	610	ANP	PB-O2B	-3.22	1.48	1.56
8	C	610	ANP	C2-N3	3.11	1.37	1.32
8	C	610	ANP	C4-N3	-3.00	1.31	1.35
8	C	610	ANP	PB-N3B	-2.81	1.56	1.63
8	C	610	ANP	C3'-C4'	-2.73	1.46	1.53
8	C	610	ANP	PA-O1A	2.51	1.59	1.50
8	C	610	ANP	O4'-C4'	-2.39	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	610	ANP	C5-N7	-2.34	1.31	1.39
8	C	610	ANP	PA-O2A	-2.05	1.45	1.55

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	610	ANP	N3-C2-N1	-6.17	119.04	128.68
8	C	610	ANP	PB-O3A-PA	-5.03	114.92	132.62
8	C	610	ANP	O2B-PB-O3A	3.37	115.88	104.64
8	C	610	ANP	O1B-PB-N3B	-2.69	107.81	111.77
8	C	610	ANP	C5-C6-N6	-2.48	116.59	120.35
8	C	610	ANP	C5'-C4'-C3'	-2.35	106.39	115.18
8	C	610	ANP	O2G-PG-O1G	-2.07	108.25	113.45

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	610	ANP	PB-N3B-PG-O1G
8	C	610	ANP	PA-O3A-PB-O2B
8	C	610	ANP	O4'-C4'-C5'-O5'
8	C	610	ANP	C3'-C4'-C5'-O5'
3	D	302	PG4	O2-C3-C4-O3
4	A	604	PEG	O1-C1-C2-O2
5	A	606	P6G	C5-C6-O7-C8
5	A	607	P6G	O13-C14-C15-O16
5	A	606	P6G	O13-C14-C15-O16
5	A	607	P6G	O10-C11-C12-O13
4	C	604	PEG	O2-C3-C4-O4
4	C	606	PEG	O1-C1-C2-O2
5	A	606	P6G	C8-C9-O10-C11
5	A	607	P6G	O7-C8-C9-O10
5	C	602	P6G	O10-C11-C12-O13
5	B	303	P6G	O10-C11-C12-O13
4	A	605	PEG	O1-C1-C2-O2
5	A	606	P6G	O1-C2-C3-O4
5	A	607	P6G	O16-C17-C18-O19
4	C	608	PEG	O1-C1-C2-O2
5	A	607	P6G	O1-C2-C3-O4
4	A	602	PEG	O1-C1-C2-O2
4	B	304	PEG	O2-C3-C4-O4
4	C	609	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	A	601	PG4	C8-C7-O4-C6
5	C	602	P6G	O4-C5-C6-O7
3	A	601	PG4	O1-C1-C2-O2
3	D	302	PG4	O4-C7-C8-O5
4	A	609	PEG	O2-C3-C4-O4
4	A	610	PEG	O1-C1-C2-O2
4	C	607	PEG	O2-C3-C4-O4
3	D	302	PG4	C4-C3-O2-C2
5	C	602	P6G	O7-C8-C9-O10
3	D	302	PG4	O3-C5-C6-O4
5	A	606	P6G	O7-C8-C9-O10
4	C	603	PEG	O2-C3-C4-O4
4	C	608	PEG	O2-C3-C4-O4
4	D	303	PEG	C1-C2-O2-C3
3	D	302	PG4	C6-C5-O3-C4
5	A	606	P6G	O10-C11-C12-O13
5	B	303	P6G	C14-C15-O16-C17
4	C	603	PEG	C4-C3-O2-C2
4	A	609	PEG	C1-C2-O2-C3
3	A	611	PG4	C1-C2-O2-C3
3	A	611	PG4	C3-C4-O3-C5
3	A	601	PG4	C6-C5-O3-C4
5	B	303	P6G	O16-C17-C18-O19
5	A	607	P6G	C9-C8-O7-C6
4	B	302	PEG	C4-C3-O2-C2
4	C	606	PEG	C4-C3-O2-C2
5	C	602	P6G	C15-C14-O13-C12
5	A	607	P6G	C6-C5-O4-C3
4	C	608	PEG	C4-C3-O2-C2
4	A	608	PEG	C1-C2-O2-C3
5	C	602	P6G	C12-C11-O10-C9
5	A	606	P6G	C14-C15-O16-C17
4	A	605	PEG	C1-C2-O2-C3
5	B	303	P6G	C12-C11-O10-C9
3	D	302	PG4	C8-C7-O4-C6
3	A	601	PG4	O4-C7-C8-O5
5	A	606	P6G	C11-C12-O13-C14
5	B	303	P6G	C5-C6-O7-C8
5	A	606	P6G	O4-C5-C6-O7
5	B	303	P6G	C18-C17-O16-C15
4	C	605	PEG	C1-C2-O2-C3
4	A	605	PEG	O2-C3-C4-O4

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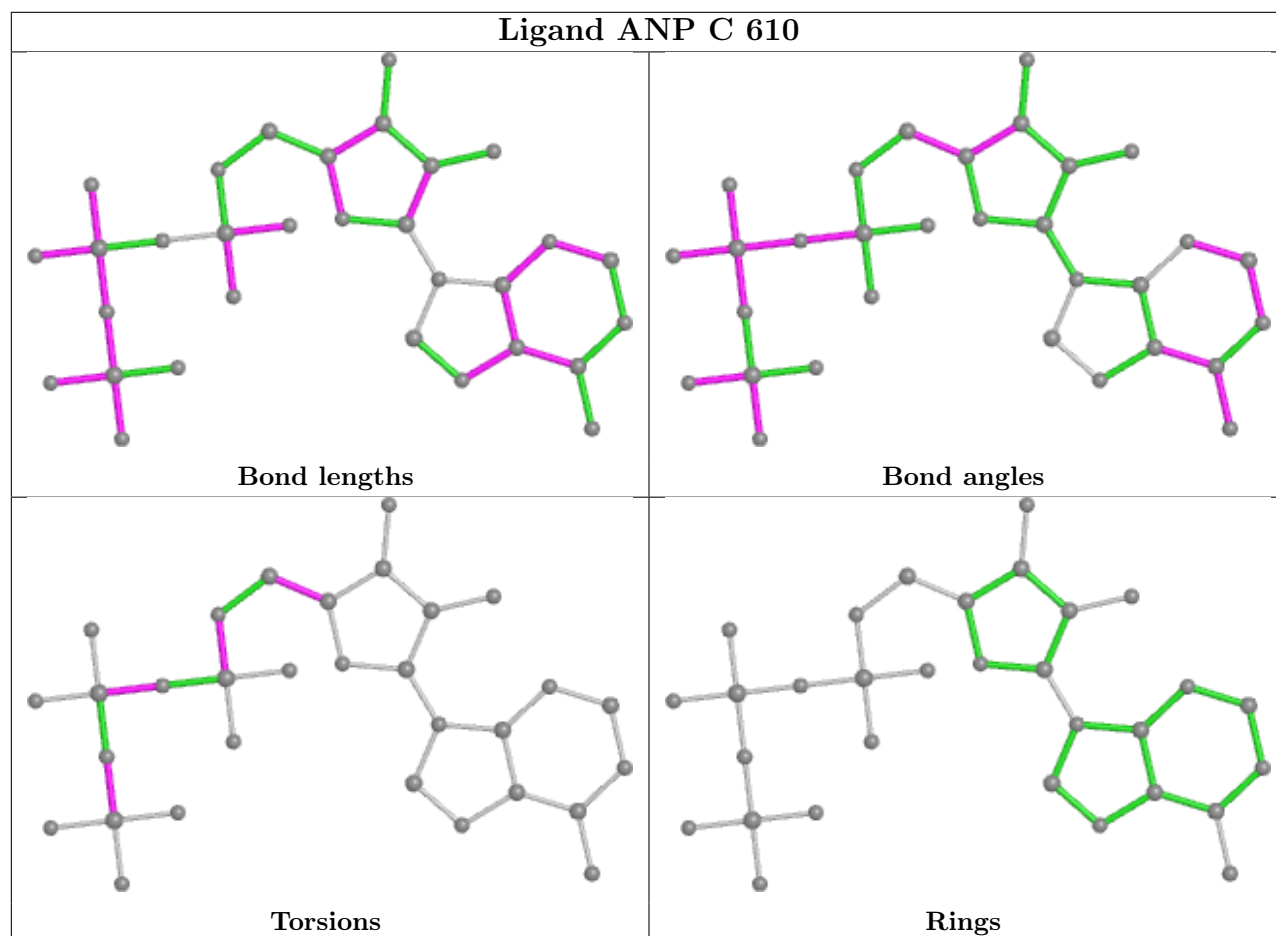
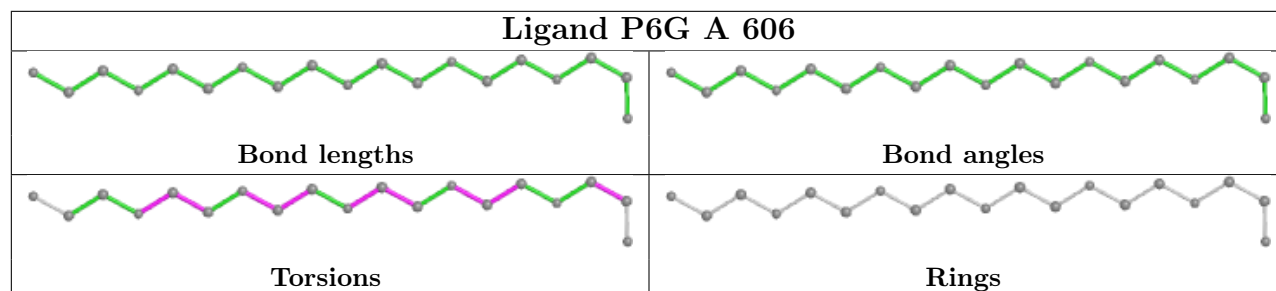
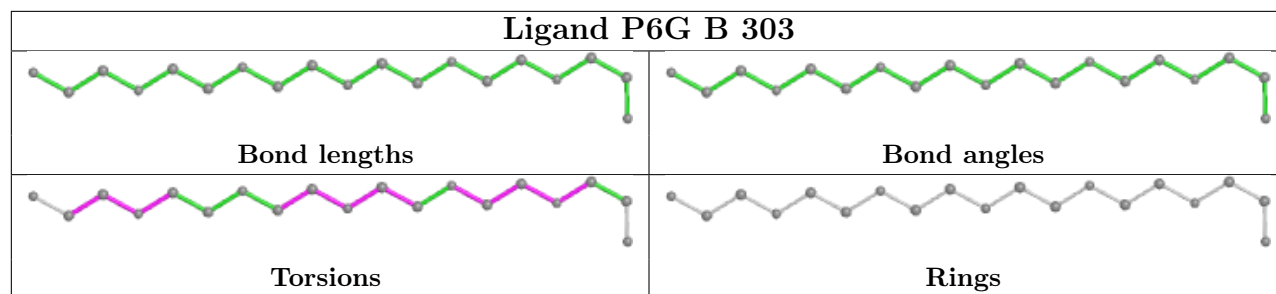
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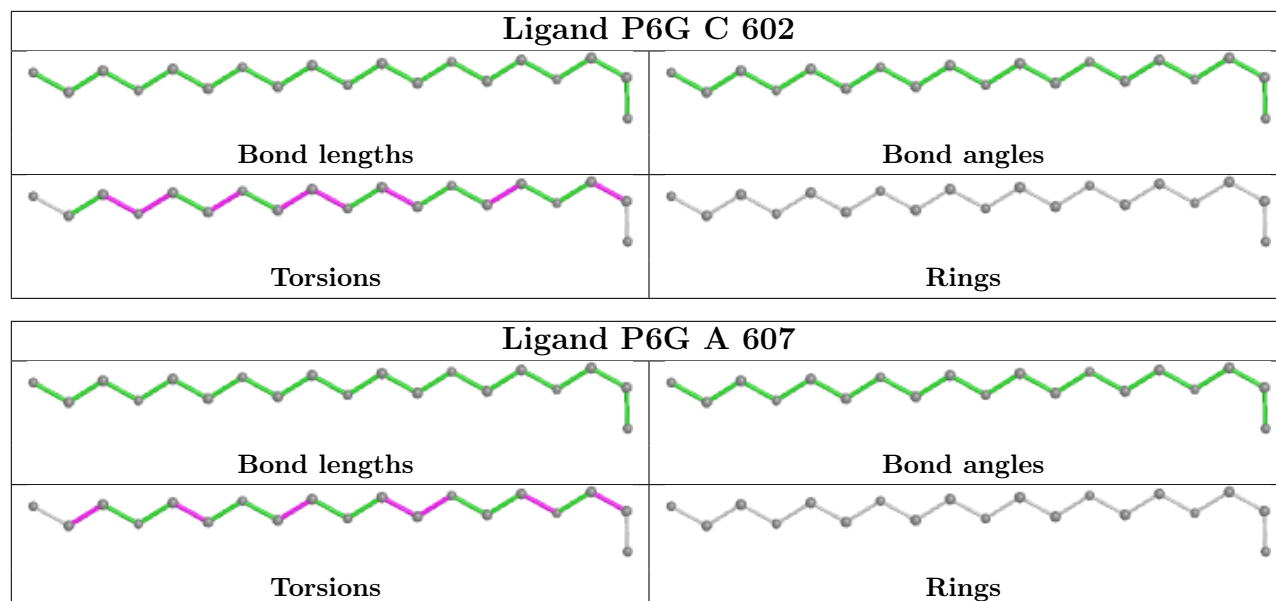
Mol	Chain	Res	Type	Atoms
3	D	302	PG4	O1-C1-C2-O2
4	D	303	PEG	O2-C3-C4-O4
3	D	302	PG4	C5-C6-O4-C7
5	C	602	P6G	C14-C15-O16-C17
5	C	602	P6G	O1-C2-C3-O4
4	C	609	PEG	C1-C2-O2-C3
5	B	303	P6G	C6-C5-O4-C3
3	A	601	PG4	C1-C2-O2-C3
4	C	605	PEG	O1-C1-C2-O2
4	A	603	PEG	C4-C3-O2-C2
5	B	303	P6G	O7-C8-C9-O10
3	A	601	PG4	C4-C3-O2-C2
3	A	601	PG4	O3-C5-C6-O4
3	A	611	PG4	C8-C7-O4-C6
4	A	604	PEG	C4-C3-O2-C2
4	A	610	PEG	C1-C2-O2-C3
5	B	303	P6G	C2-C3-O4-C5
5	C	602	P6G	C18-C17-O16-C15
4	D	304	PEG	O2-C3-C4-O4
5	B	303	P6G	O4-C5-C6-O7
4	B	304	PEG	C4-C3-O2-C2
8	C	610	ANP	C5'-O5'-PA-O3A
5	B	303	P6G	C8-C9-O10-C11
3	A	611	PG4	O2-C3-C4-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 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.