Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 04:23 AM EDT

PDB ID	:	6NES
Title	:	FAD-dependent monooxygenase TropB from T. stipitatus
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Deposited on	:	2018-12-18
Resolution	:	1.75 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 1.75 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

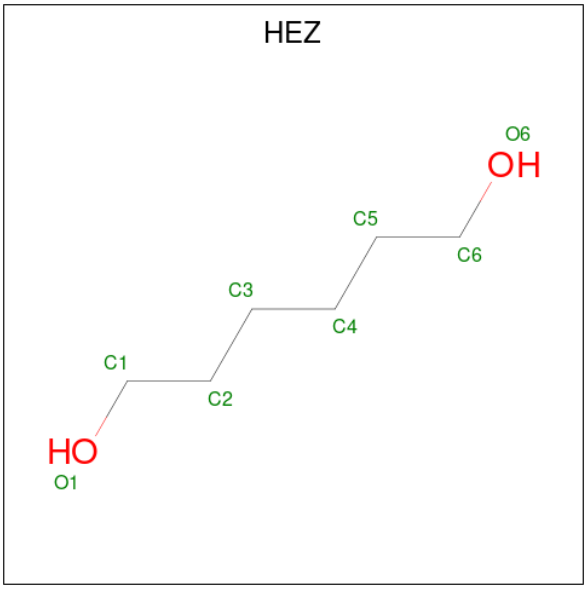
There are 6 unique types of molecules in this entry. The entry contains 14287 atoms, of which 6831 are hydrogens and 0 are deuteriums.

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 FAD-dependent monooxygenase tropB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	431	Total	C	H	N	O	S	0	5	0
			6750	2161	3341	615	610	23			
1	B	430	Total	C	H	N	O	S	0	7	0
			6762	2160	3350	618	612	22			

- Molecule 2 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			22	6	14	2		
2	A	1	Total	C	H	O	0	0
			22	6	14	2		
2	B	1	Total	C	H	O	0	0
			22	6	14	2		
2	B	1	Total	C	H	O	0	0
			22	6	14	2		

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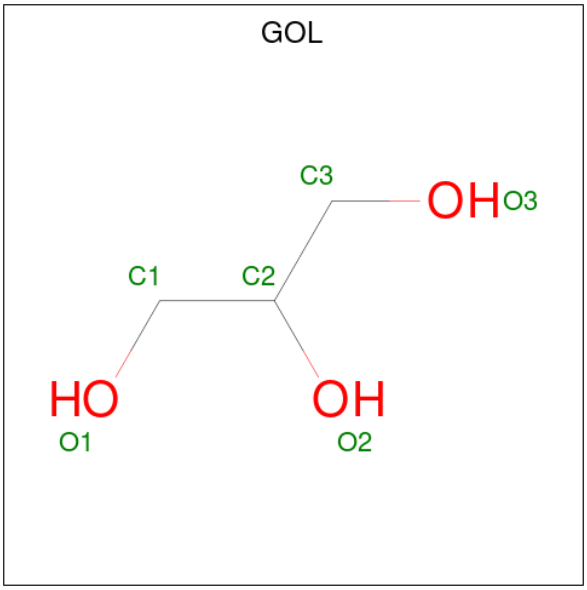
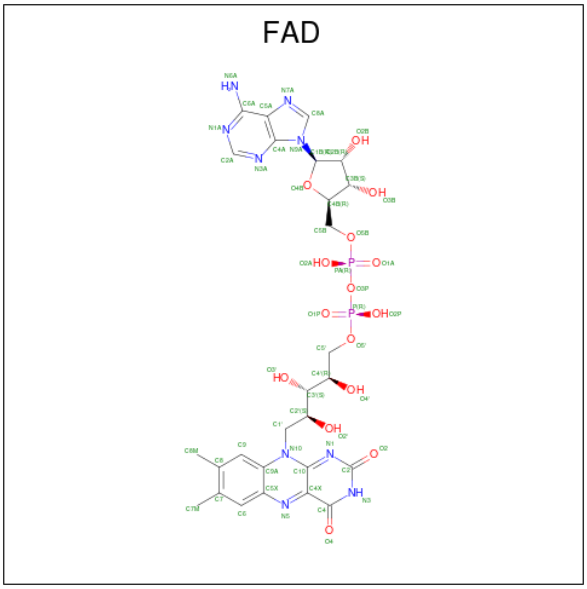
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
4	B	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	218	Total	O	0	0
			218	218		
6	B	263	Total	O	0	0
			263	263		

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	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	70.81Å 184.49Å 164.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.43 – 1.75	Depositor
% Data completeness (in resolution range)	99.6 (46.43-1.75)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.56 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.170 , 0.195	Depositor
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.316	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14287	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
2	HEZ	A	602	-	7,7,7	0.37	0	6,6,6	0.70	0
2	HEZ	B	502	-	7,7,7	0.34	0	6,6,6	0.70	0
3	GOL	A	603	-	5,5,5	1.34	1 (20%)	5,5,5	0.57	0
2	HEZ	A	601	-	7,7,7	0.34	0	6,6,6	1.12	1 (16%)
4	FAD	B	504	-	53,58,58	3.25	19 (35%)	68,89,89	2.04	15 (22%)
4	FAD	A	604	-	53,58,58	3.24	18 (33%)	68,89,89	1.81	16 (23%)
2	HEZ	B	501	-	7,7,7	0.41	0	6,6,6	0.72	0
2	HEZ	B	503	-	7,7,7	0.33	0	6,6,6	0.69	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	HEZ	A	602	-	-	3/5/5/5	-
2	HEZ	B	502	-	-	2/5/5/5	-
3	GOL	A	603	-	-	0/4/4/4	-
2	HEZ	A	601	-	-	0/5/5/5	-
4	FAD	B	504	-	-	1/30/50/50	0/6/6/6
4	FAD	A	604	-	-	1/30/50/50	0/6/6/6
2	HEZ	B	501	-	-	1/5/5/5	-
2	HEZ	B	503	-	-	2/5/5/5	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	504	FAD	C2B-C1B	-13.52	1.33	1.53
4	A	604	FAD	C2B-C1B	-13.32	1.33	1.53
4	B	504	FAD	O4B-C1B	12.35	1.58	1.41
4	A	604	FAD	O4B-C1B	11.89	1.57	1.41
4	B	504	FAD	C4X-N5	6.55	1.43	1.30
4	A	604	FAD	C4X-N5	5.66	1.41	1.30
4	A	604	FAD	C10-N1	4.54	1.42	1.33
4	B	504	FAD	O4B-C4B	-4.52	1.34	1.45
4	B	504	FAD	C10-N1	4.51	1.42	1.33
4	A	604	FAD	O4B-C4B	-4.31	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	FAD	C5X-N5	4.14	1.47	1.39
4	A	604	FAD	O2-C2	-3.99	1.16	1.24
4	B	504	FAD	C5X-N5	3.84	1.46	1.39
4	B	504	FAD	C9A-N10	3.69	1.47	1.41
4	A	604	FAD	C2-N1	3.56	1.45	1.36
4	A	604	FAD	C9A-N10	3.51	1.47	1.41
4	B	504	FAD	C4-N3	3.43	1.45	1.38
4	A	604	FAD	C2-N3	3.41	1.47	1.39
4	A	604	FAD	C4-N3	3.35	1.45	1.38
4	A	604	FAD	C6A-N6A	3.34	1.46	1.34
4	B	504	FAD	C6A-N6A	3.04	1.45	1.34
4	A	604	FAD	C2A-N3A	2.96	1.36	1.32
4	B	504	FAD	C2-N3	2.95	1.45	1.39
4	B	504	FAD	O4-C4	-2.91	1.18	1.23
4	A	604	FAD	C1'-C2'	2.70	1.56	1.52
4	B	504	FAD	C1'-C2'	2.68	1.56	1.52
4	B	504	FAD	O2B-C2B	2.64	1.49	1.43
4	A	604	FAD	O4-C4	-2.60	1.18	1.23
4	B	504	FAD	C2-N1	2.59	1.42	1.36
4	A	604	FAD	O3B-C3B	-2.57	1.36	1.43
4	B	504	FAD	C5A-C4A	-2.56	1.34	1.40
4	B	504	FAD	C10-N10	2.33	1.42	1.37
4	A	604	FAD	C5A-C4A	-2.32	1.34	1.40
4	B	504	FAD	O3B-C3B	-2.27	1.37	1.43
4	A	604	FAD	O2B-C2B	2.23	1.48	1.43
4	B	504	FAD	C2A-N3A	2.22	1.35	1.32
4	B	504	FAD	C5'-C4'	2.14	1.54	1.51
3	A	603	GOL	O1-C1	2.01	1.50	1.42

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	504	FAD	C5A-C6A-N6A	7.32	131.47	120.35
4	B	504	FAD	N3A-C2A-N1A	-5.58	119.96	128.68
4	A	604	FAD	N3A-C2A-N1A	-5.17	120.61	128.68
4	B	504	FAD	N6A-C6A-N1A	-4.83	108.54	118.57
4	B	504	FAD	C3B-C2B-C1B	4.69	108.04	100.98
4	A	604	FAD	C5A-C6A-N6A	4.57	127.30	120.35
4	B	504	FAD	O4B-C1B-C2B	-4.10	100.94	106.93
4	B	504	FAD	C4X-C10-N10	4.07	122.43	116.48
4	A	604	FAD	C4X-C10-N10	3.99	122.32	116.48
4	A	604	FAD	O2'-C2'-C1'	3.42	118.06	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	504	FAD	C7M-C7-C6	-3.40	113.20	119.49
4	A	604	FAD	C7M-C7-C6	-3.09	113.78	119.49
4	A	604	FAD	C3B-C2B-C1B	3.05	105.56	100.98
4	A	604	FAD	O4B-C1B-C2B	-2.79	102.86	106.93
4	A	604	FAD	O2'-C2'-C3'	-2.73	102.46	109.10
4	A	604	FAD	C4-N3-C2	-2.58	120.88	125.64
4	A	604	FAD	N6A-C6A-N1A	-2.55	113.29	118.57
4	B	504	FAD	C10-C4X-N5	-2.54	119.47	124.86
4	A	604	FAD	C7M-C7-C8	2.52	125.91	120.74
4	B	504	FAD	C8M-C8-C9	2.51	124.13	119.49
4	A	604	FAD	C10-C4X-N5	-2.49	119.58	124.86
4	B	504	FAD	C7M-C7-C8	2.48	125.83	120.74
4	B	504	FAD	O2-C2-N1	-2.42	117.81	121.83
4	B	504	FAD	C4-N3-C2	-2.29	121.42	125.64
4	A	604	FAD	O3'-C3'-C4'	2.27	114.30	108.81
4	B	504	FAD	O3B-C3B-C2B	2.27	119.16	111.82
4	A	604	FAD	O2-C2-N1	-2.27	118.07	121.83
2	A	601	HEZ	C4-C3-C2	-2.26	102.97	114.42
4	A	604	FAD	C5X-C9A-N10	2.24	120.27	117.95
4	B	504	FAD	C1B-N9A-C4A	-2.14	122.88	126.64
4	A	604	FAD	C4-C4X-C10	2.08	120.29	116.79
4	B	504	FAD	O2-C2-N3	2.08	122.70	118.65

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	HEZ	C1-C2-C3-C4
2	B	502	HEZ	C1-C2-C3-C4
2	B	501	HEZ	C4-C5-C6-O6
2	A	602	HEZ	O1-C1-C2-C3
2	B	503	HEZ	C4-C5-C6-O6
2	B	503	HEZ	O1-C1-C2-C3
2	B	502	HEZ	C2-C3-C4-C5
4	A	604	FAD	O4B-C4B-C5B-O5B
4	B	504	FAD	O4B-C4B-C5B-O5B
2	A	602	HEZ	C2-C3-C4-C5

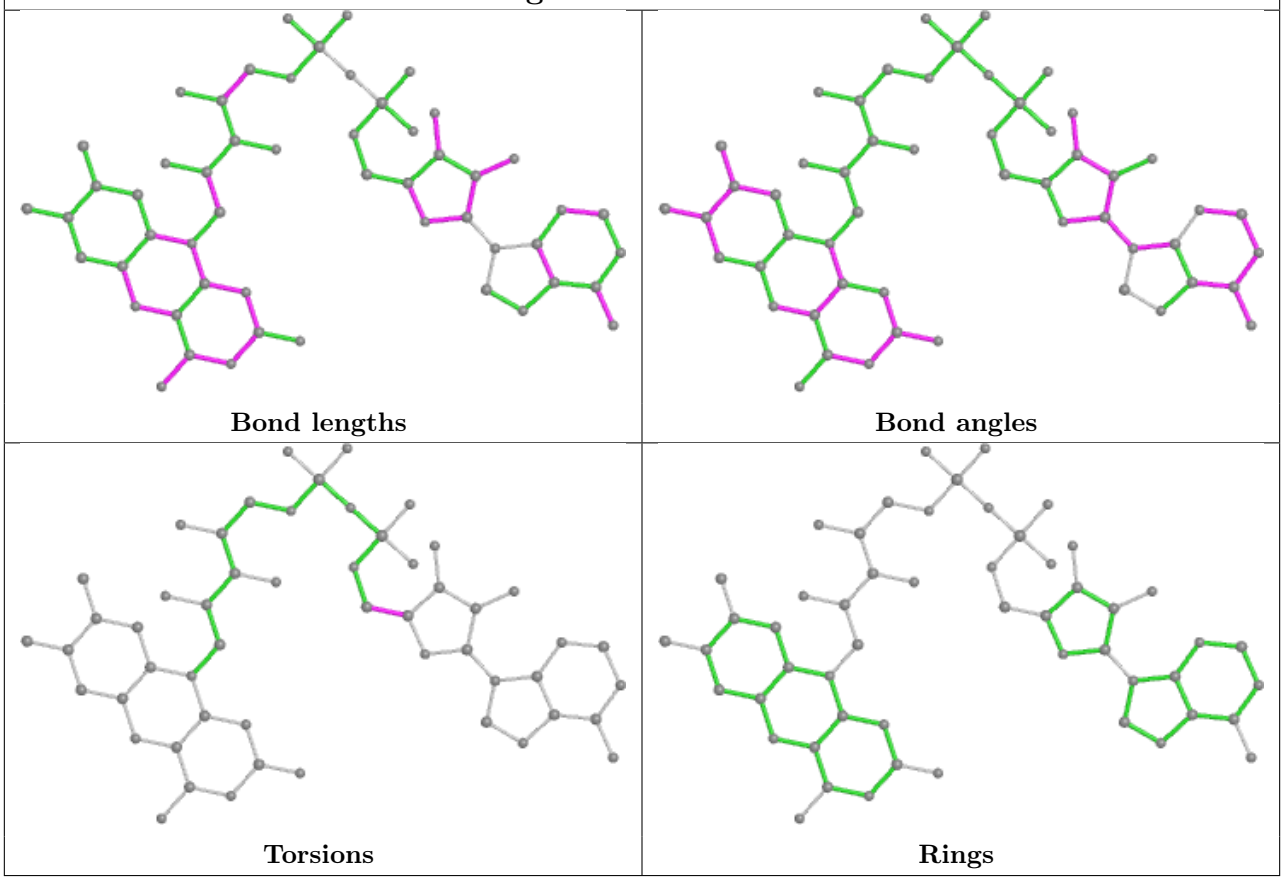
There are no ring outliers.

No monomer is involved in short contacts.

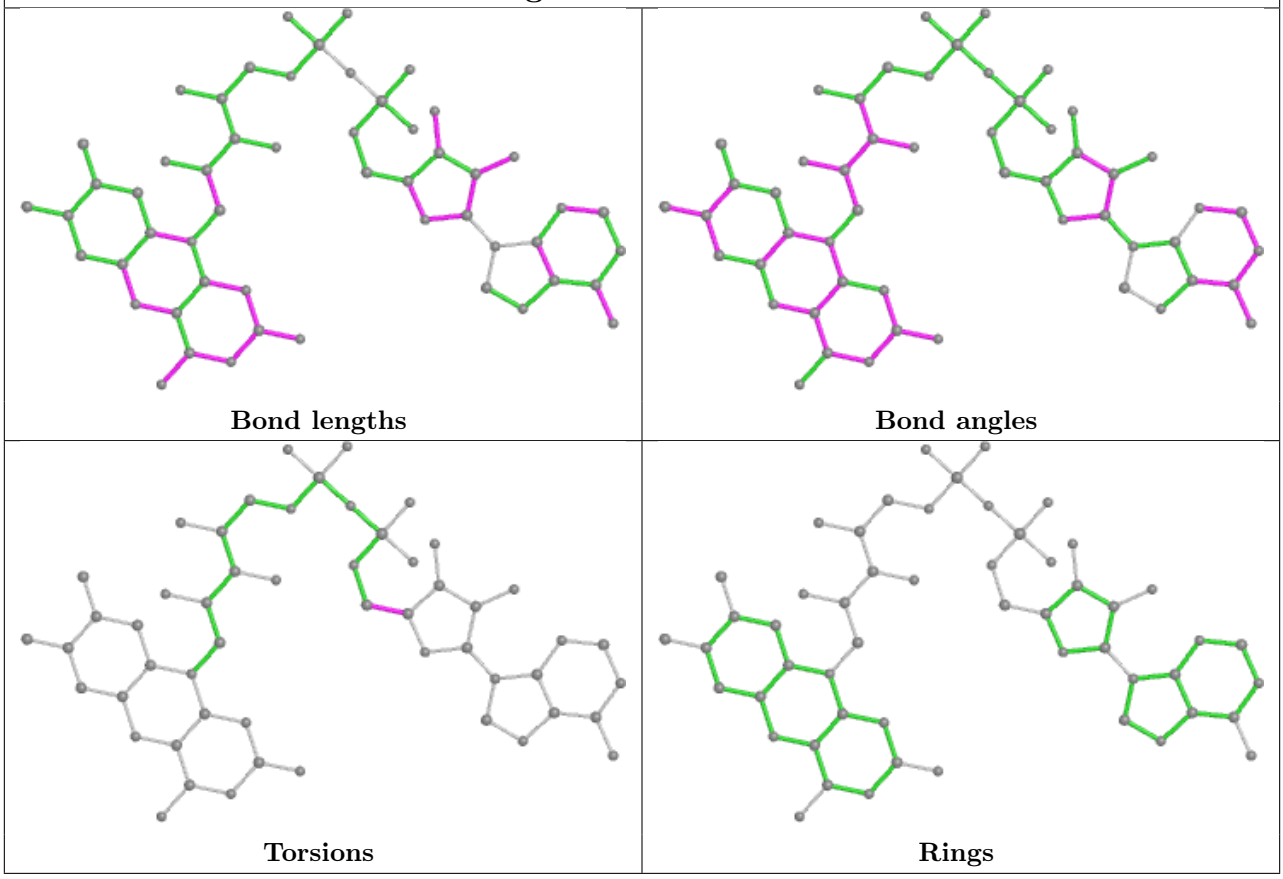
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 FAD B 504



Ligand FAD A 604



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.