Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 05:18 AM EDT

PDB ID	:	6P2V
Title	:	RebH Variant 10S, Tryptamine 5-halogenase
Authors	:	Andorfer, M.C.; Sukumar, N.; Lewis, J.C.
Deposited on	:	2019-05-22
Resolution	:	2.55 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 2.55 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 3 unique types of molecules in this entry. The entry contains 8885 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 Flavin-dependent tryptophan halogenase RebH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	523	Total	C	N	O	S	0	0	0
			4185	2655	730	780	20			
1	B	521	Total	C	N	O	S	0	0	0
			4162	2642	727	773	20			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8KHZ8
A	-18	GLY	-	expression tag	UNP Q8KHZ8
A	-17	SER	-	expression tag	UNP Q8KHZ8
A	-16	SER	-	expression tag	UNP Q8KHZ8
A	-15	HIS	-	expression tag	UNP Q8KHZ8
A	-14	HIS	-	expression tag	UNP Q8KHZ8
A	-13	HIS	-	expression tag	UNP Q8KHZ8
A	-12	HIS	-	expression tag	UNP Q8KHZ8
A	-11	HIS	-	expression tag	UNP Q8KHZ8
A	-10	HIS	-	expression tag	UNP Q8KHZ8
A	-9	SER	-	expression tag	UNP Q8KHZ8
A	-8	SER	-	expression tag	UNP Q8KHZ8
A	-7	GLY	-	expression tag	UNP Q8KHZ8
A	-6	LEU	-	expression tag	UNP Q8KHZ8
A	-5	VAL	-	expression tag	UNP Q8KHZ8
A	-4	PRO	-	expression tag	UNP Q8KHZ8
A	-3	ARG	-	expression tag	UNP Q8KHZ8
A	-2	GLY	-	expression tag	UNP Q8KHZ8
A	-1	SER	-	expression tag	UNP Q8KHZ8
A	0	HIS	-	expression tag	UNP Q8KHZ8
A	52	HIS	ILE	engineered mutation	UNP Q8KHZ8
A	380	PHE	LEU	engineered mutation	UNP Q8KHZ8
A	465	CYS	PHE	engineered mutation	UNP Q8KHZ8
A	470	SER	ASN	engineered mutation	UNP Q8KHZ8
A	494	ARG	GLN	engineered mutation	UNP Q8KHZ8

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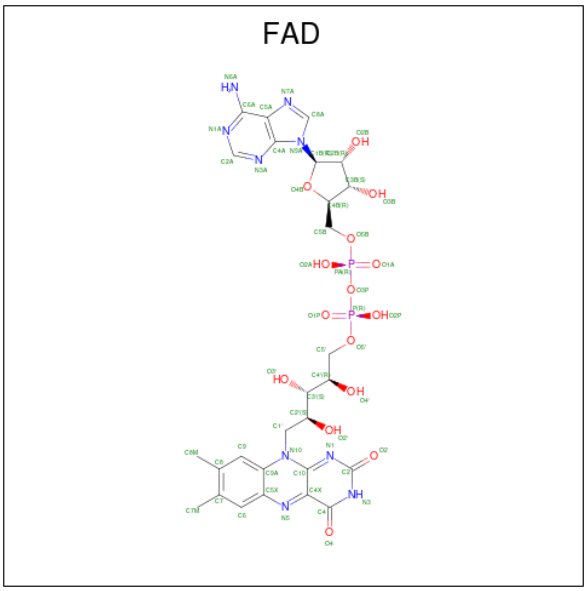
Chain	Residue	Modelled	Actual	Comment	Reference
A	509	GLN	ARG	engineered mutation	UNP Q8KHZ8
B	-19	MET	-	initiating methionine	UNP Q8KHZ8
B	-18	GLY	-	expression tag	UNP Q8KHZ8
B	-17	SER	-	expression tag	UNP Q8KHZ8
B	-16	SER	-	expression tag	UNP Q8KHZ8
B	-15	HIS	-	expression tag	UNP Q8KHZ8
B	-14	HIS	-	expression tag	UNP Q8KHZ8
B	-13	HIS	-	expression tag	UNP Q8KHZ8
B	-12	HIS	-	expression tag	UNP Q8KHZ8
B	-11	HIS	-	expression tag	UNP Q8KHZ8
B	-10	HIS	-	expression tag	UNP Q8KHZ8
B	-9	SER	-	expression tag	UNP Q8KHZ8
B	-8	SER	-	expression tag	UNP Q8KHZ8
B	-7	GLY	-	expression tag	UNP Q8KHZ8
B	-6	LEU	-	expression tag	UNP Q8KHZ8
B	-5	VAL	-	expression tag	UNP Q8KHZ8
B	-4	PRO	-	expression tag	UNP Q8KHZ8
B	-3	ARG	-	expression tag	UNP Q8KHZ8
B	-2	GLY	-	expression tag	UNP Q8KHZ8
B	-1	SER	-	expression tag	UNP Q8KHZ8
B	0	HIS	-	expression tag	UNP Q8KHZ8
B	52	HIS	ILE	engineered mutation	UNP Q8KHZ8
B	380	PHE	LEU	engineered mutation	UNP Q8KHZ8
B	465	CYS	PHE	engineered mutation	UNP Q8KHZ8
B	470	SER	ASN	engineered mutation	UNP Q8KHZ8
B	494	ARG	GLN	engineered mutation	UNP Q8KHZ8
B	509	GLN	ARG	engineered mutation	UNP Q8KHZ8

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	224	Total	O	0	0
			224	224		
3	B	208	Total	O	0	0
			208	208		

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 62	Depositor
Cell constants a, b, c, α, β, γ	115.16Å 115.16Å 230.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.73 – 2.55	Depositor
% Data completeness (in resolution range)	99.8 (48.73-2.55)	Depositor
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.171 , 0.210	Depositor
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.339	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.052 for h,-h-k,-l	Xtriage
Total number of atoms	8885	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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

2 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	$\#\|Z\| > 2$
2	FAD	A	601	-	53,58,58	3.95	18 (33%)	68,89,89	2.23	13 (19%)
2	FAD	B	601	-	53,58,58	3.96	18 (33%)	68,89,89	2.21	14 (20%)

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	FAD	A	601	-	-	9/30/50/50	0/6/6/6
2	FAD	B	601	-	-	16/30/50/50	0/6/6/6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	O4B-C1B	15.50	1.62	1.41
2	B	601	FAD	C2B-C1B	-15.36	1.30	1.53
2	B	601	FAD	O4B-C1B	15.29	1.62	1.41
2	A	601	FAD	C2B-C1B	-14.88	1.31	1.53
2	B	601	FAD	C4X-N5	7.76	1.45	1.30
2	A	601	FAD	C4X-N5	7.76	1.45	1.30
2	A	601	FAD	C10-N1	6.61	1.46	1.33
2	B	601	FAD	C10-N1	6.59	1.46	1.33
2	A	601	FAD	O4B-C4B	-6.39	1.30	1.45
2	B	601	FAD	O4B-C4B	-6.18	1.31	1.45
2	A	601	FAD	C5X-N5	5.16	1.49	1.39
2	B	601	FAD	C5X-N5	5.16	1.49	1.39
2	B	601	FAD	C9A-N10	5.03	1.50	1.41
2	A	601	FAD	C9A-N10	5.02	1.50	1.41
2	B	601	FAD	C2-N1	4.99	1.48	1.36
2	A	601	FAD	C2-N1	4.99	1.48	1.36
2	A	601	FAD	C2-N3	4.48	1.49	1.39
2	B	601	FAD	C2-N3	4.46	1.49	1.39
2	B	601	FAD	C4-N3	3.99	1.46	1.38
2	A	601	FAD	C4-N3	3.97	1.46	1.38
2	B	601	FAD	C10-N10	3.75	1.45	1.37
2	A	601	FAD	C10-N10	3.68	1.45	1.37
2	A	601	FAD	O2B-C2B	3.11	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	O2B-C2B	3.04	1.50	1.43
2	B	601	FAD	C6A-N6A	3.00	1.45	1.34
2	A	601	FAD	C6A-N6A	3.00	1.45	1.34
2	A	601	FAD	O2-C2	-2.99	1.18	1.24
2	B	601	FAD	O2-C2	-2.97	1.18	1.24
2	B	601	FAD	O3B-C3B	-2.93	1.36	1.43
2	A	601	FAD	O3B-C3B	-2.92	1.36	1.43
2	A	601	FAD	C5A-C4A	-2.71	1.33	1.40
2	B	601	FAD	C5A-C4A	-2.69	1.33	1.40
2	A	601	FAD	O4-C4	-2.55	1.18	1.23
2	B	601	FAD	O4-C4	-2.52	1.18	1.23
2	A	601	FAD	C2A-N3A	2.26	1.35	1.32
2	B	601	FAD	C2A-N3A	2.25	1.35	1.32

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	FAD	C5A-C6A-N6A	9.86	135.33	120.35
2	A	601	FAD	C5A-C6A-N6A	9.82	135.28	120.35
2	B	601	FAD	N6A-C6A-N1A	-6.71	104.64	118.57
2	A	601	FAD	N6A-C6A-N1A	-6.71	104.65	118.57
2	B	601	FAD	C7M-C7-C6	-6.29	107.87	119.49
2	A	601	FAD	C7M-C7-C6	-6.27	107.90	119.49
2	B	601	FAD	C7M-C7-C8	5.56	132.13	120.74
2	B	601	FAD	N3A-C2A-N1A	-5.53	120.03	128.68
2	A	601	FAD	N3A-C2A-N1A	-5.52	120.06	128.68
2	A	601	FAD	C7M-C7-C8	5.50	132.01	120.74
2	A	601	FAD	C3B-C2B-C1B	3.54	106.30	100.98
2	B	601	FAD	C4-N3-C2	-3.19	119.75	125.64
2	A	601	FAD	C4-N3-C2	-3.16	119.81	125.64
2	A	601	FAD	P-O3P-PA	-2.68	123.62	132.83
2	B	601	FAD	P-O3P-PA	-2.68	123.63	132.83
2	A	601	FAD	C4X-C4-N3	2.58	119.74	113.19
2	B	601	FAD	C4X-C4-N3	2.57	119.72	113.19
2	A	601	FAD	O4-C4-C4X	-2.43	120.15	126.60
2	B	601	FAD	O4-C4-C4X	-2.43	120.16	126.60
2	A	601	FAD	C4X-C10-N10	2.38	119.96	116.48
2	A	601	FAD	C10-C4X-N5	-2.37	119.82	124.86
2	B	601	FAD	C4X-C10-N10	2.34	119.90	116.48
2	B	601	FAD	C10-C4X-N5	-2.33	119.91	124.86
2	B	601	FAD	C9A-C5X-N5	-2.15	120.10	122.43
2	A	601	FAD	C9A-C5X-N5	-2.15	120.10	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	FAD	C3B-C2B-C1B	2.10	104.14	100.98
2	B	601	FAD	C5X-C9A-N10	2.06	120.08	117.95

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	C5B-O5B-PA-O2A
2	A	601	FAD	O4B-C4B-C5B-O5B
2	A	601	FAD	C3B-C4B-C5B-O5B
2	A	601	FAD	N10-C1'-C2'-O2'
2	A	601	FAD	N10-C1'-C2'-C3'
2	A	601	FAD	C5'-O5'-P-O1P
2	A	601	FAD	C5'-O5'-P-O3P
2	B	601	FAD	C5B-O5B-PA-O1A
2	B	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	C3B-C4B-C5B-O5B
2	B	601	FAD	N10-C1'-C2'-O2'
2	B	601	FAD	N10-C1'-C2'-C3'
2	B	601	FAD	C1'-C2'-C3'-O3'
2	B	601	FAD	C1'-C2'-C3'-C4'
2	B	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	O3'-C3'-C4'-O4'
2	B	601	FAD	O2'-C2'-C3'-O3'
2	B	601	FAD	O2'-C2'-C3'-C4'
2	B	601	FAD	O3'-C3'-C4'-C5'
2	B	601	FAD	C2'-C3'-C4'-C5'
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	PA-O3P-P-O2P
2	A	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	PA-O3P-P-O1P

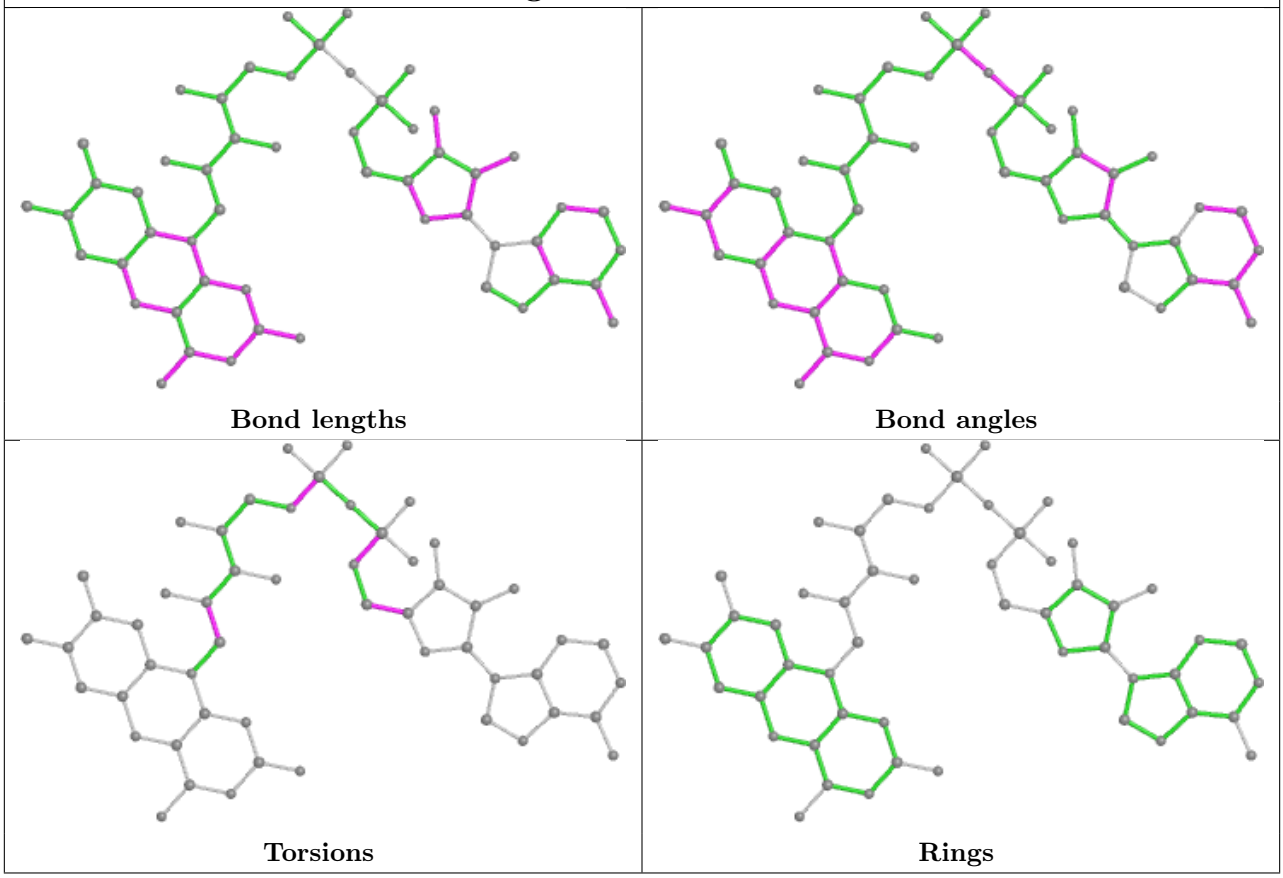
There are no ring outliers.

No monomer is involved in short contacts.

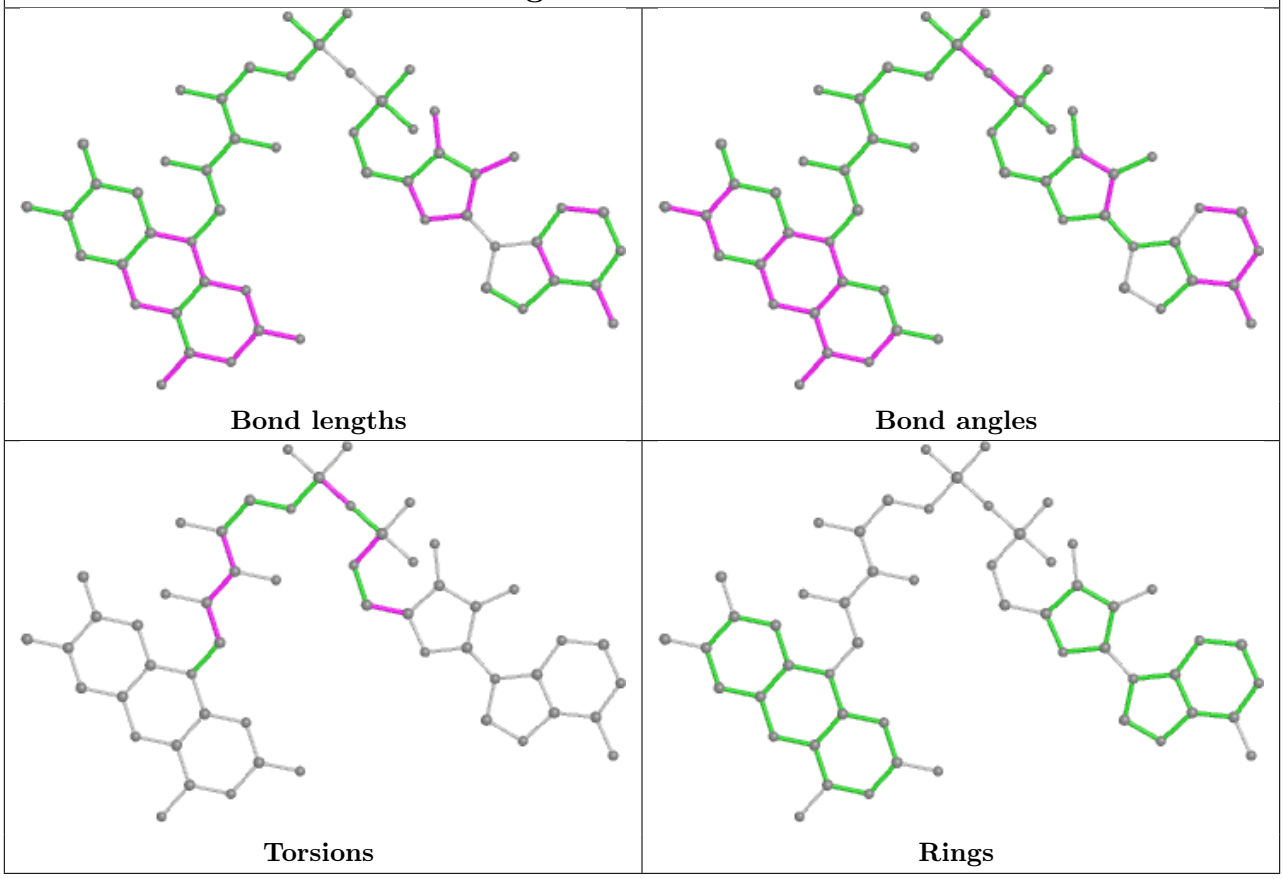
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A 601



Ligand FAD B 601



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.