wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 08:31 AM EDT

PDB ID	:	6VTY
Title	:	Crystal structure of Plasmodium falciparum dihydroorotate dehydrogenase bound with Inhibitor DSM483
Authors	:	Deng, X.; Phillips, M.
Deposited on	:	2020-02-13
Resolution	:	1.78 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 1.78 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 5 unique types of molecules in this entry. The entry contains 25167 atoms, of which 12193 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 Dihydroorotate dehydrogenase (quinone), mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	377	Total	C	H	N	O	S	0	1	0
			6025	1916	3031	501	563	14			
1	B	372	Total	C	H	N	O	S	0	2	0
			5972	1894	3012	498	553	15			
1	C	366	Total	C	H	N	O	S	0	7	0
			5947	1880	3012	494	546	15			
1	D	368	Total	C	H	N	O	S	0	3	0
			5914	1875	2986	491	547	15			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	MET	-	initiating methionine	UNP Q08210
A	140	GLY	-	expression tag	UNP Q08210
A	141	HIS	-	expression tag	UNP Q08210
A	142	HIS	-	expression tag	UNP Q08210
A	143	HIS	-	expression tag	UNP Q08210
A	144	HIS	-	expression tag	UNP Q08210
A	145	HIS	-	expression tag	UNP Q08210
A	146	HIS	-	expression tag	UNP Q08210
A	147	ALA	-	expression tag	UNP Q08210
A	148	GLU	-	expression tag	UNP Q08210
A	149	ASN	-	expression tag	UNP Q08210
A	150	LEU	-	expression tag	UNP Q08210
A	151	TYR	-	expression tag	UNP Q08210
A	152	PHE	-	expression tag	UNP Q08210
A	153	GLN	-	expression tag	UNP Q08210
A	154	GLY	-	expression tag	UNP Q08210
A	155	ALA	-	expression tag	UNP Q08210
A	156	ASP	-	expression tag	UNP Q08210
A	157	PRO	-	expression tag	UNP Q08210
B	139	MET	-	initiating methionine	UNP Q08210
B	140	GLY	-	expression tag	UNP Q08210

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Chain	Residue	Modelled	Actual	Comment	Reference
B	141	HIS	-	expression tag	UNP Q08210
B	142	HIS	-	expression tag	UNP Q08210
B	143	HIS	-	expression tag	UNP Q08210
B	144	HIS	-	expression tag	UNP Q08210
B	145	HIS	-	expression tag	UNP Q08210
B	146	HIS	-	expression tag	UNP Q08210
B	147	ALA	-	expression tag	UNP Q08210
B	148	GLU	-	expression tag	UNP Q08210
B	149	ASN	-	expression tag	UNP Q08210
B	150	LEU	-	expression tag	UNP Q08210
B	151	TYR	-	expression tag	UNP Q08210
B	152	PHE	-	expression tag	UNP Q08210
B	153	GLN	-	expression tag	UNP Q08210
B	154	GLY	-	expression tag	UNP Q08210
B	155	ALA	-	expression tag	UNP Q08210
B	156	ASP	-	expression tag	UNP Q08210
B	157	PRO	-	expression tag	UNP Q08210
C	139	MET	-	initiating methionine	UNP Q08210
C	140	GLY	-	expression tag	UNP Q08210
C	141	HIS	-	expression tag	UNP Q08210
C	142	HIS	-	expression tag	UNP Q08210
C	143	HIS	-	expression tag	UNP Q08210
C	144	HIS	-	expression tag	UNP Q08210
C	145	HIS	-	expression tag	UNP Q08210
C	146	HIS	-	expression tag	UNP Q08210
C	147	ALA	-	expression tag	UNP Q08210
C	148	GLU	-	expression tag	UNP Q08210
C	149	ASN	-	expression tag	UNP Q08210
C	150	LEU	-	expression tag	UNP Q08210
C	151	TYR	-	expression tag	UNP Q08210
C	152	PHE	-	expression tag	UNP Q08210
C	153	GLN	-	expression tag	UNP Q08210
C	154	GLY	-	expression tag	UNP Q08210
C	155	ALA	-	expression tag	UNP Q08210
C	156	ASP	-	expression tag	UNP Q08210
C	157	PRO	-	expression tag	UNP Q08210
D	139	MET	-	initiating methionine	UNP Q08210
D	140	GLY	-	expression tag	UNP Q08210
D	141	HIS	-	expression tag	UNP Q08210
D	142	HIS	-	expression tag	UNP Q08210
D	143	HIS	-	expression tag	UNP Q08210
D	144	HIS	-	expression tag	UNP Q08210

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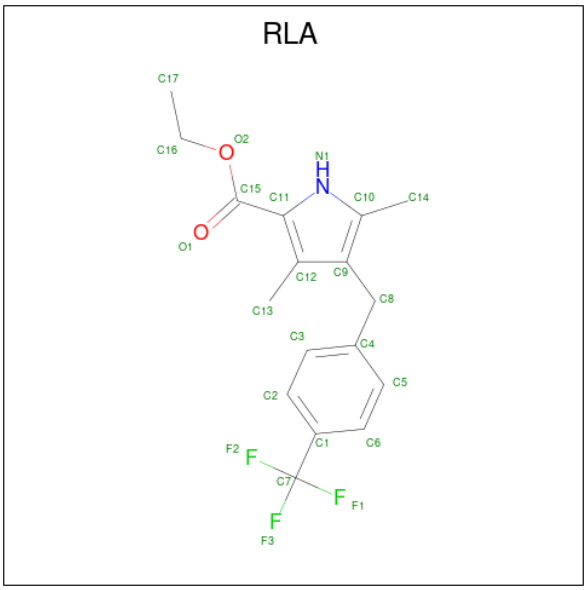
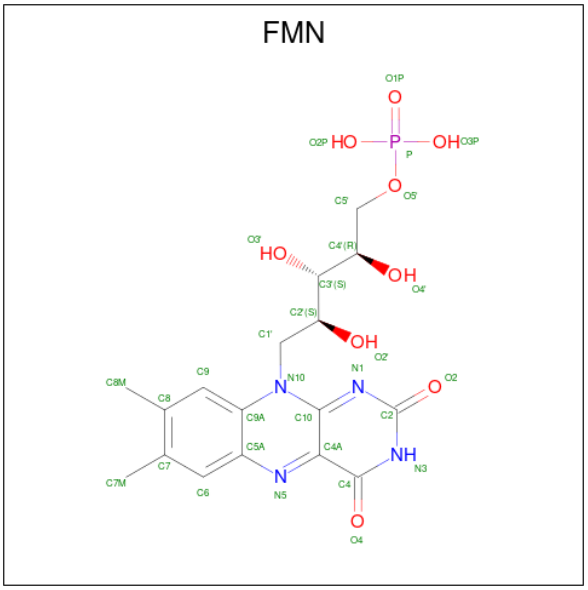
Chain	Residue	Modelled	Actual	Comment	Reference
D	145	HIS	-	expression tag	UNP Q08210
D	146	HIS	-	expression tag	UNP Q08210
D	147	ALA	-	expression tag	UNP Q08210
D	148	GLU	-	expression tag	UNP Q08210
D	149	ASN	-	expression tag	UNP Q08210
D	150	LEU	-	expression tag	UNP Q08210
D	151	TYR	-	expression tag	UNP Q08210
D	152	PHE	-	expression tag	UNP Q08210
D	153	GLN	-	expression tag	UNP Q08210
D	154	GLY	-	expression tag	UNP Q08210
D	155	ALA	-	expression tag	UNP Q08210
D	156	ASP	-	expression tag	UNP Q08210
D	157	PRO	-	expression tag	UNP Q08210

- Molecule 2 is ethyl 3,5-dimethyl-4-{[4-(trifluoromethyl)phenyl]methyl}-1H-pyrrole-2-carboxylate (three-letter code: RLA) (formula: $C_{17}H_{18}F_3NO_2$) (labeled as "Ligand of Interest" by depositor).



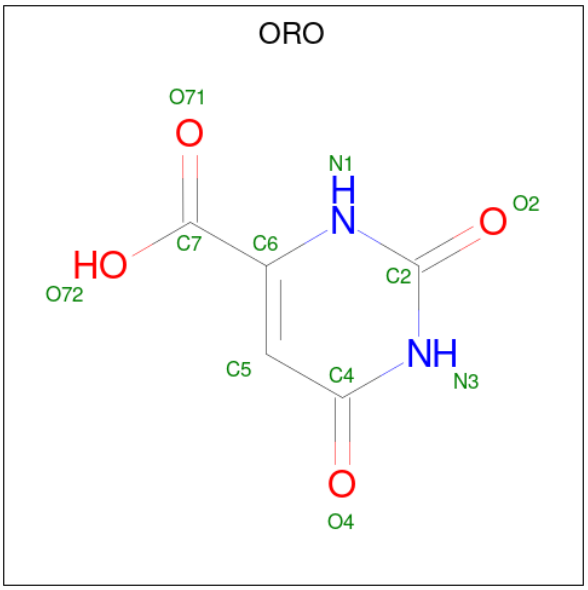
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	0	0
			40	17	3	17	1	2		
2	B	1	Total	C	F	H	N	O	0	0
			40	17	3	17	1	2		
2	C	1	Total	C	F	H	N	O	0	0
			40	17	3	17	1	2		
2	D	1	Total	C	F	H	N	O	0	0
			40	17	3	17	1	2		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			49	17	18	4	9	1		
3	B	1	Total	C	H	N	O	P	0	0
			49	17	18	4	9	1		
3	C	1	Total	C	H	N	O	P	0	0
			49	17	18	4	9	1		
3	D	1	Total	C	H	N	O	P	0	0
			49	17	18	4	9	1		

- Molecule 4 is OROTIC ACID (three-letter code: ORO) (formula: $C_5H_4N_2O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			14	5	3	2	4		
4	B	1	Total	C	H	N	O	0	0
			14	5	3	2	4		
4	C	1	Total	C	H	N	O	0	0
			14	5	3	2	4		
4	D	1	Total	C	H	N	O	0	0
			14	5	3	2	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	283	Total	O	0	0
			283	283		
5	B	196	Total	O	0	0
			196	196		
5	C	253	Total	O	0	0
			253	253		
5	D	165	Total	O	0	0
			165	165		

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 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.09Å 97.52Å 186.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.03 – 1.78	Depositor
% Data completeness (in resolution range)	92.2 (42.03-1.78)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 1.77Å)	Xtriage
Refinement program	PHENIX V1.16	Depositor
R, R_{free}	0.151 , 0.194	Depositor
Wilson B-factor (Å^2)	19.0	Xtriage
Anisotropy	0.109	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	25167	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.82% 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

12 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	RLA	D	1001	-	22,24,24	1.21	3 (13%)	28,35,35	1.27	3 (10%)
3	FMN	B	1002	-	33,33,33	1.59	6 (18%)	48,50,50	1.23	6 (12%)
4	ORO	A	1003	-	9,11,11	1.54	1 (11%)	8,15,15	2.35	2 (25%)
4	ORO	D	1003	-	9,11,11	1.36	1 (11%)	8,15,15	2.83	4 (50%)
3	FMN	D	1002	-	33,33,33	1.12	1 (3%)	48,50,50	1.48	8 (16%)
4	ORO	B	1003	-	9,11,11	1.53	1 (11%)	8,15,15	2.40	4 (50%)
2	RLA	C	1001	-	22,24,24	1.55	3 (13%)	28,35,35	2.10	8 (28%)
2	RLA	A	1001	-	22,24,24	1.55	5 (22%)	28,35,35	1.67	9 (32%)
2	RLA	B	1001	-	22,24,24	1.55	3 (13%)	28,35,35	1.50	7 (25%)
4	ORO	C	1003	-	9,11,11	1.30	1 (11%)	8,15,15	2.35	2 (25%)
3	FMN	A	1002	-	33,33,33	1.26	4 (12%)	48,50,50	1.23	5 (10%)
3	FMN	C	1002	-	33,33,33	1.23	2 (6%)	48,50,50	1.30	6 (12%)

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	RLA	D	1001	-	-	3/17/17/17	0/2/2/2
3	FMN	B	1002	-	-	1/18/18/18	0/3/3/3
4	ORO	A	1003	-	-	3/4/4/4	0/1/1/1
4	ORO	D	1003	-	-	4/4/4/4	0/1/1/1
3	FMN	D	1002	-	-	1/18/18/18	0/3/3/3
4	ORO	B	1003	-	-	4/4/4/4	0/1/1/1
2	RLA	C	1001	-	-	2/17/17/17	0/2/2/2
2	RLA	A	1001	-	-	2/17/17/17	0/2/2/2
2	RLA	B	1001	-	-	2/17/17/17	0/2/2/2
4	ORO	C	1003	-	-	3/4/4/4	0/1/1/1
3	FMN	A	1002	-	-	1/18/18/18	0/3/3/3
3	FMN	C	1002	-	-	1/18/18/18	0/3/3/3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	FMN	C4A-N5	4.75	1.40	1.30
3	B	1002	FMN	C4A-N5	4.75	1.40	1.30
2	B	1001	RLA	O2-C15	4.72	1.45	1.33
2	A	1001	RLA	O2-C15	4.42	1.44	1.33
2	C	1001	RLA	O2-C15	4.33	1.44	1.33

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1003	ORO	C5-C4-N3	-5.88	117.22	124.08
4	C	1003	ORO	C5-C4-N3	-5.41	117.76	124.08
2	C	1001	RLA	C5-C4-C3	5.03	126.07	118.17
4	D	1003	ORO	O72-C7-C6	4.51	124.97	114.69
4	B	1003	ORO	C6-C5-C4	4.48	119.62	116.73

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

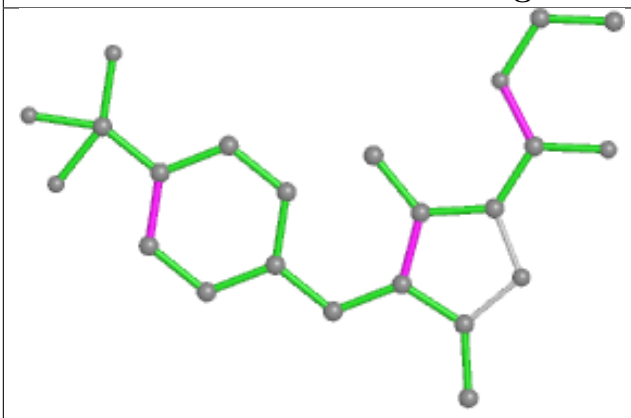
Mol	Chain	Res	Type	Atoms
4	A	1003	ORO	C5-C6-C7-O72
4	B	1003	ORO	C5-C6-C7-O72
4	C	1003	ORO	C5-C6-C7-O72
4	D	1003	ORO	N1-C6-C7-O71
4	D	1003	ORO	C5-C6-C7-O71

There are no ring outliers.

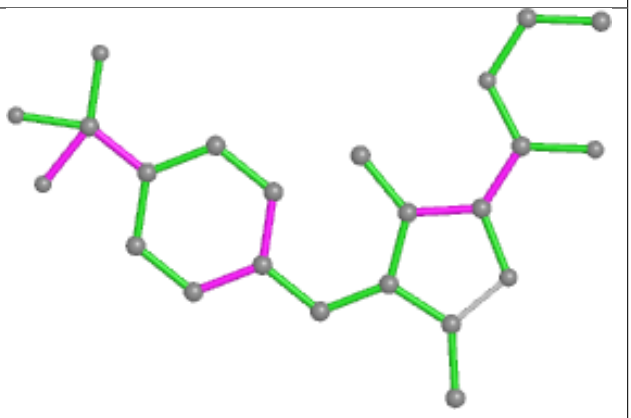
No monomer is involved in short contacts.

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.

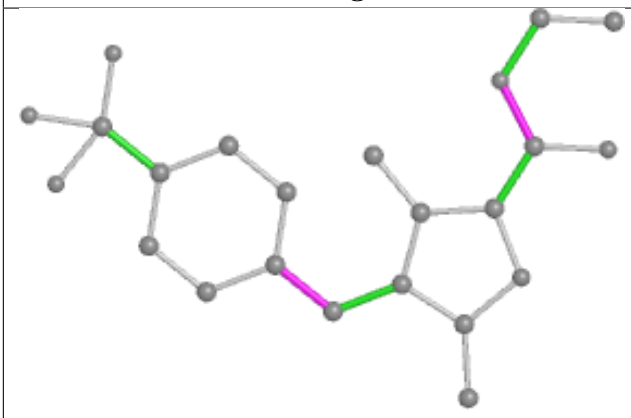
Ligand RLA D 1001



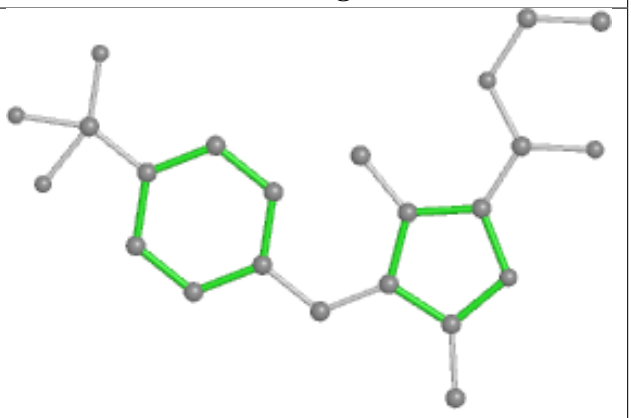
Bond lengths



Bond angles

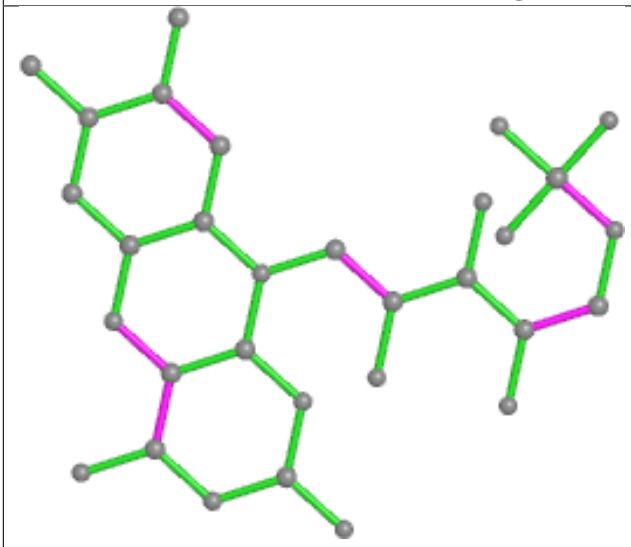


Torsions

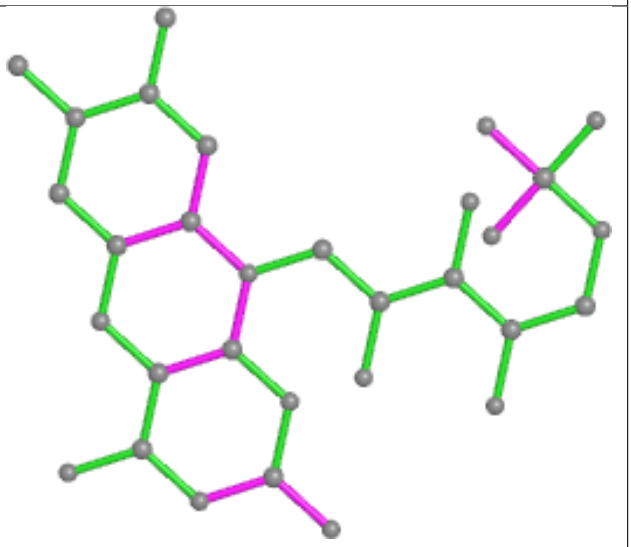


Rings

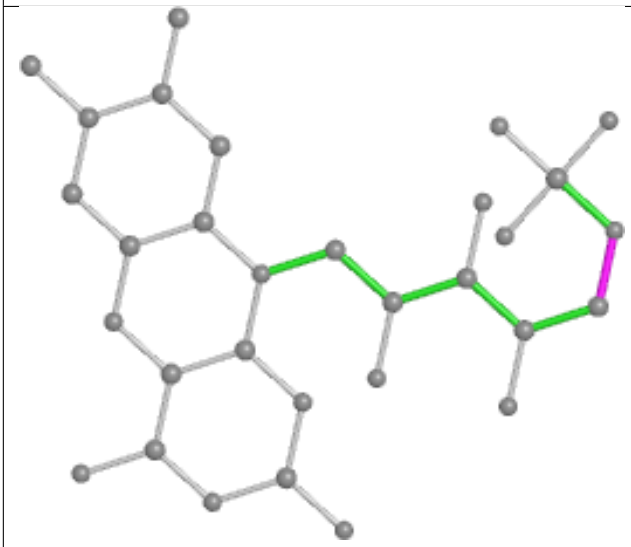
Ligand FMN B 1002



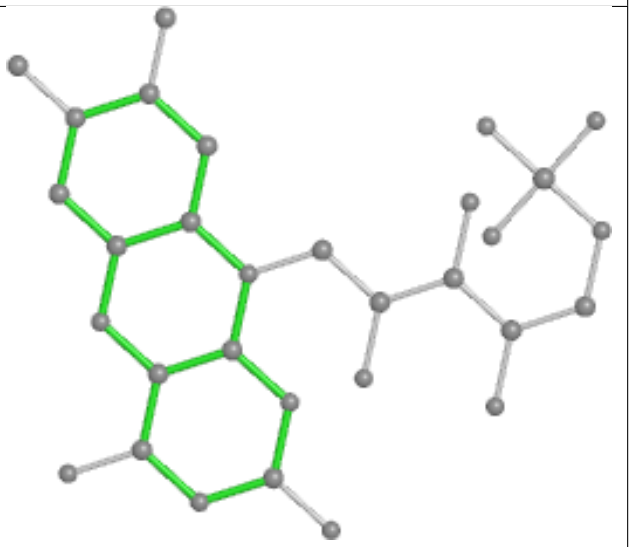
Bond lengths



Bond angles

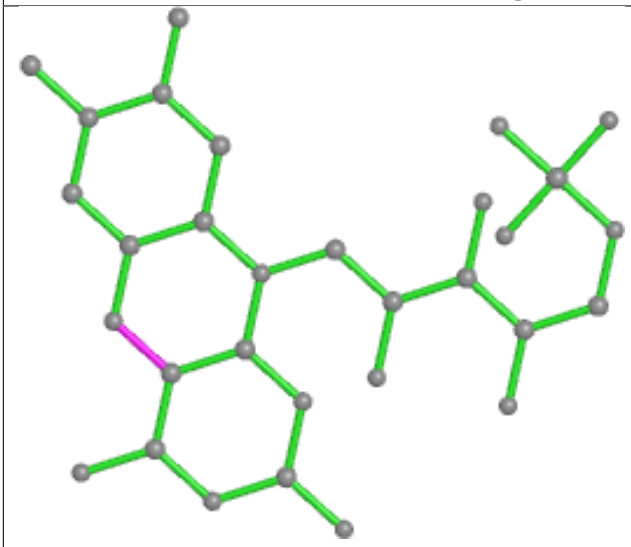


Torsions

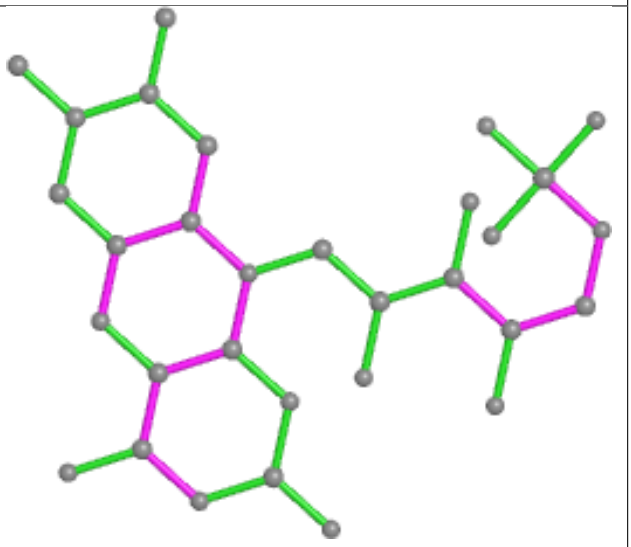


Rings

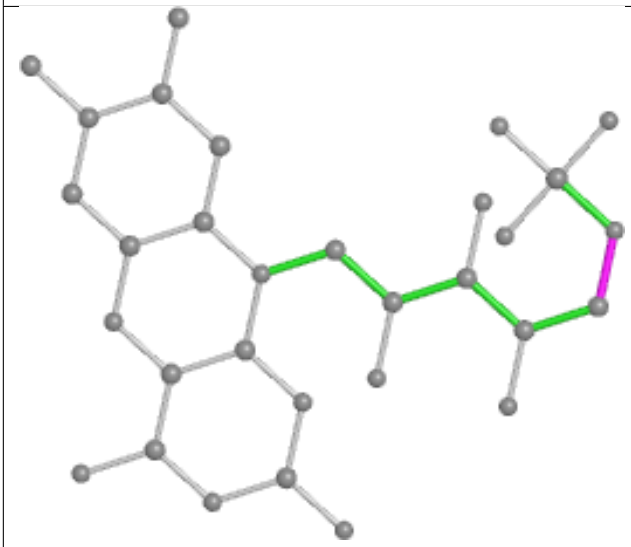
Ligand FMN D 1002



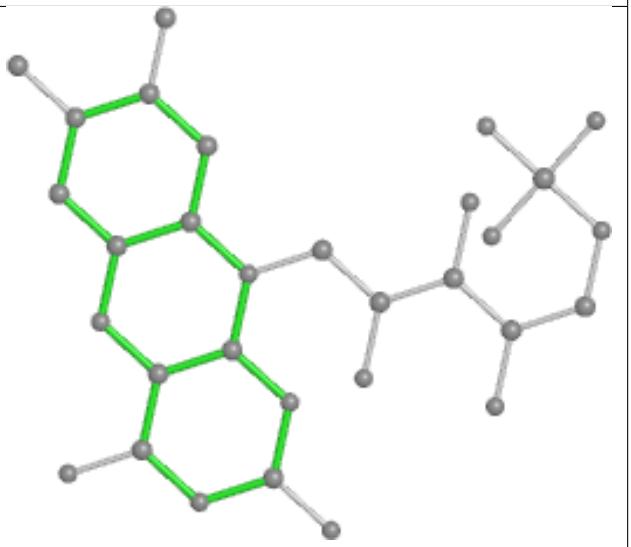
Bond lengths



Bond angles

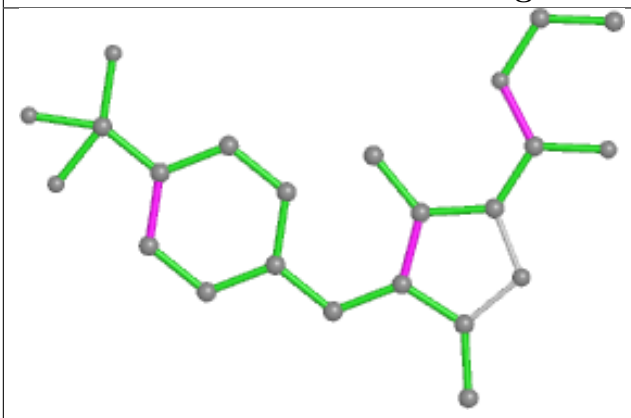


Torsions

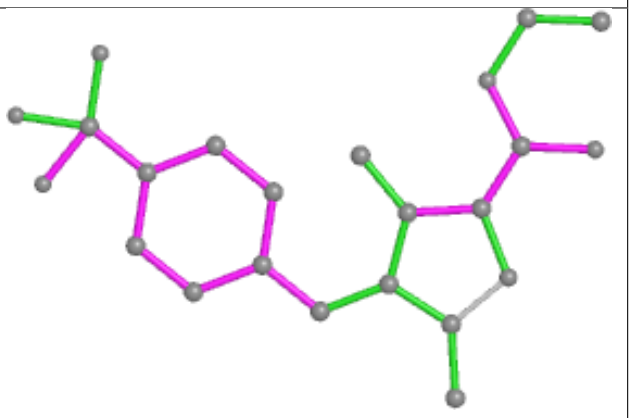


Rings

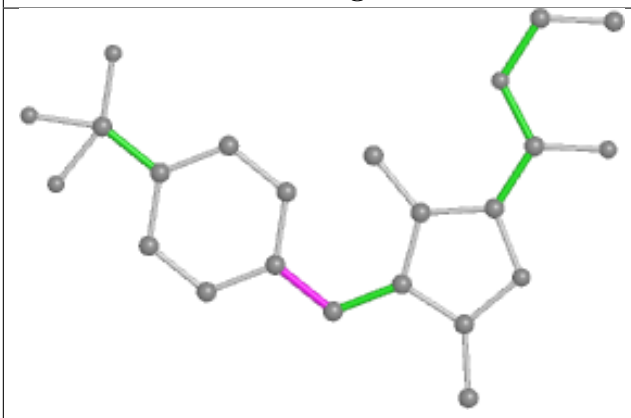
Ligand RLA C 1001



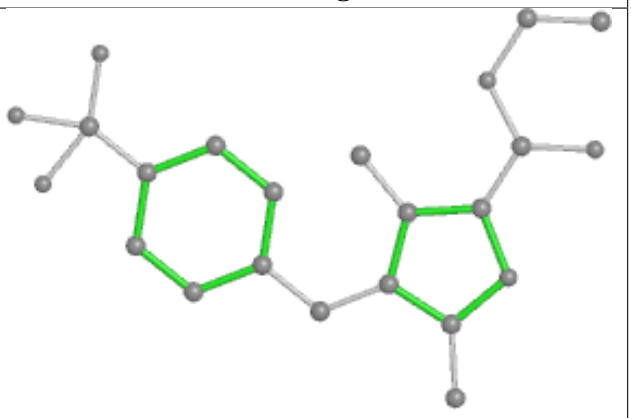
Bond lengths



Bond angles

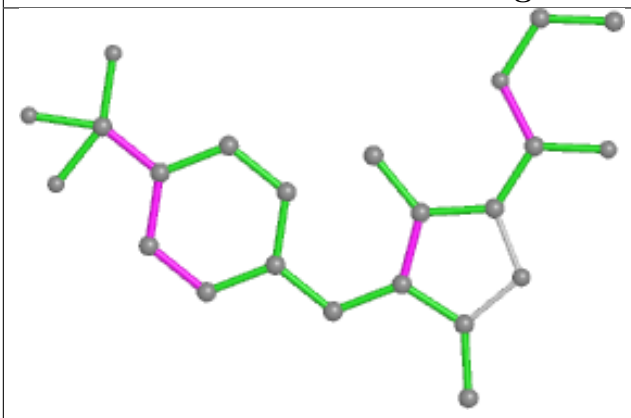


Torsions



Rings

Ligand RLA A 1001



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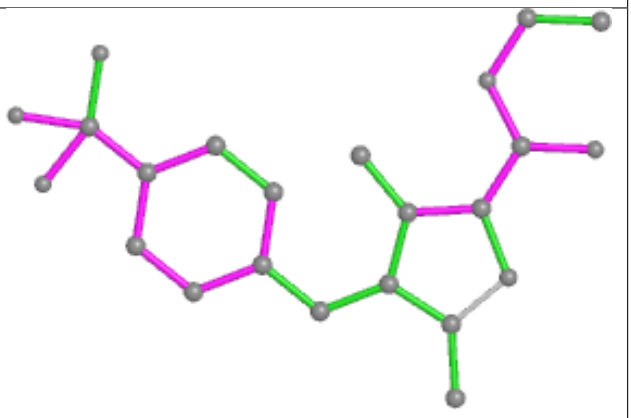
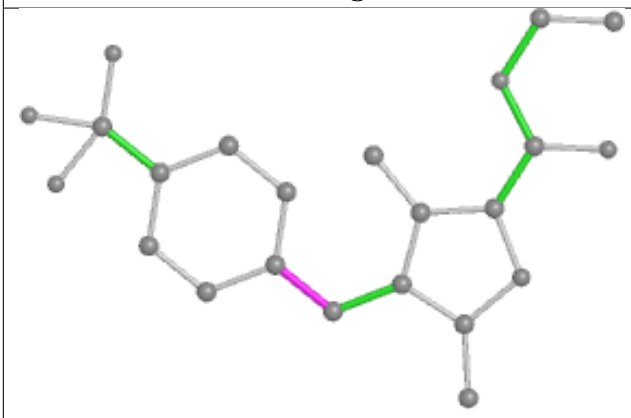
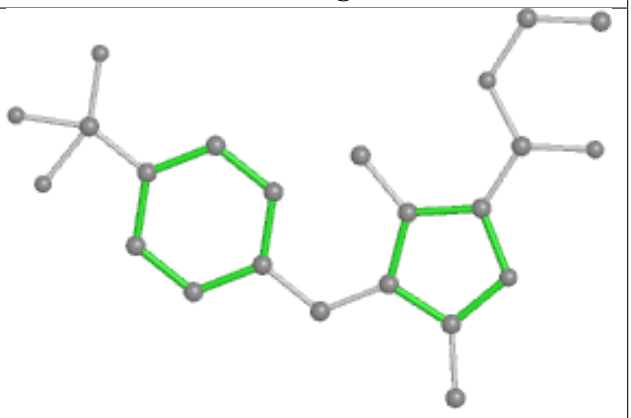


Bond angles

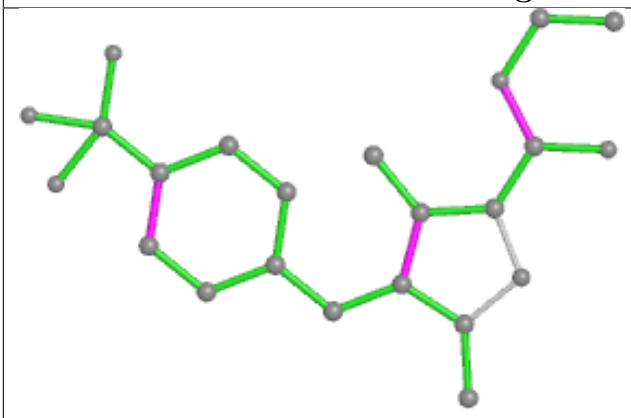


Torsions



Rings

Ligand RLA B 1001



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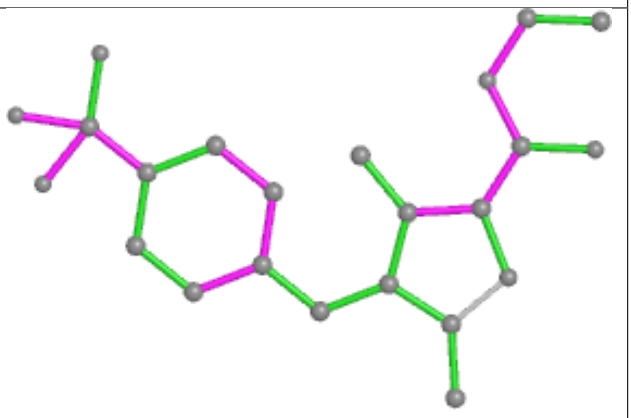
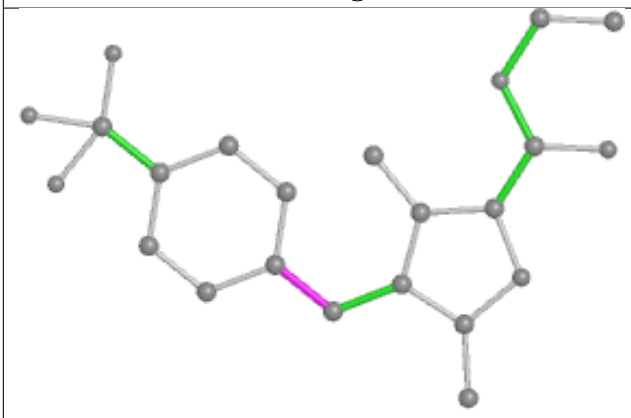
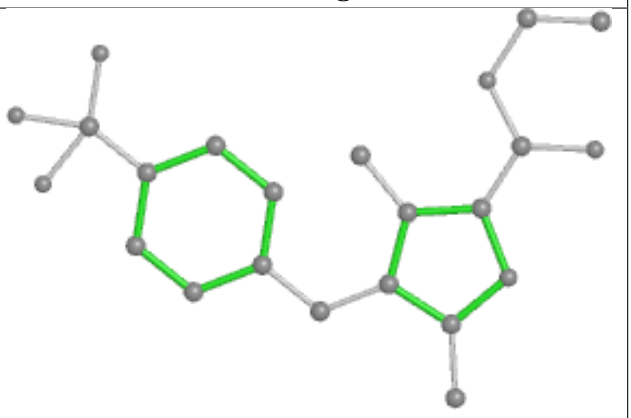


Bond angles

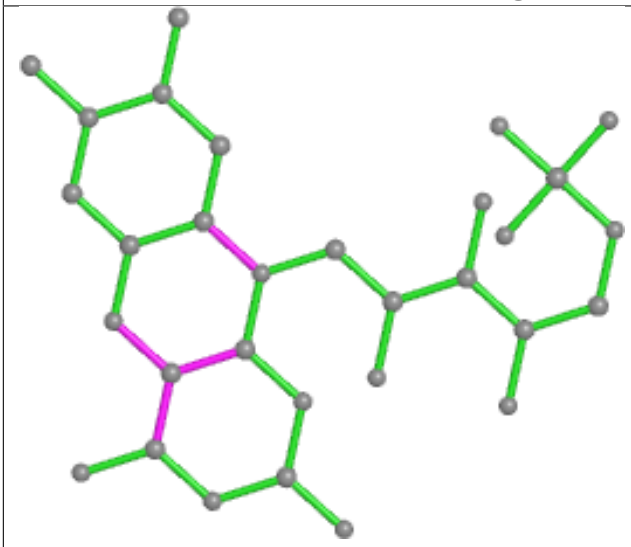


Torsions

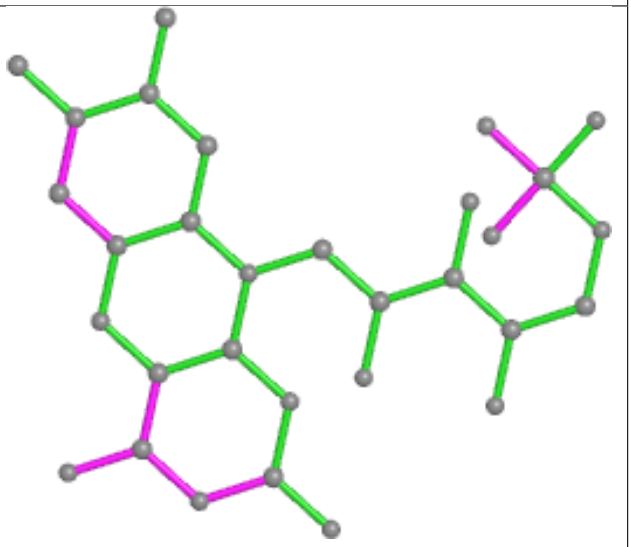


Rings

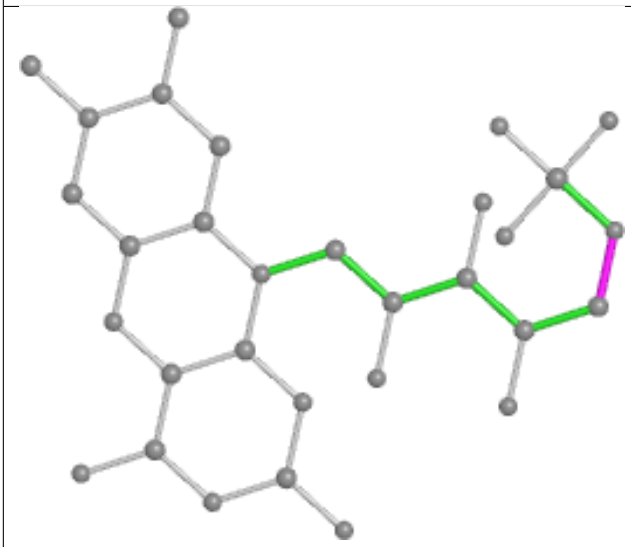
Ligand FMN A 1002



Bond lengths



Bond angles



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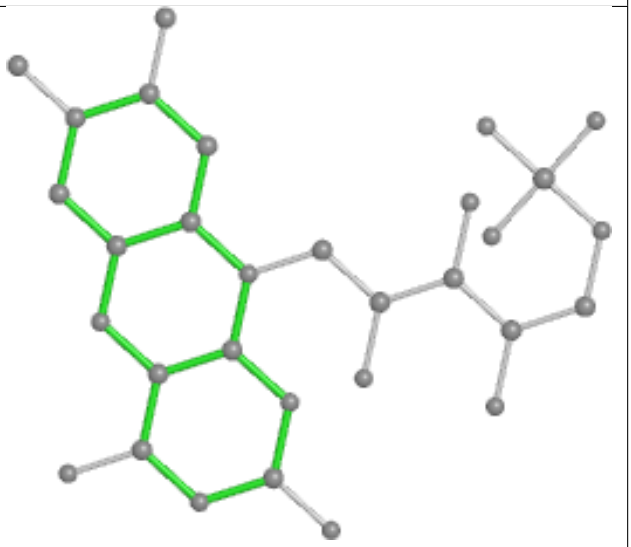
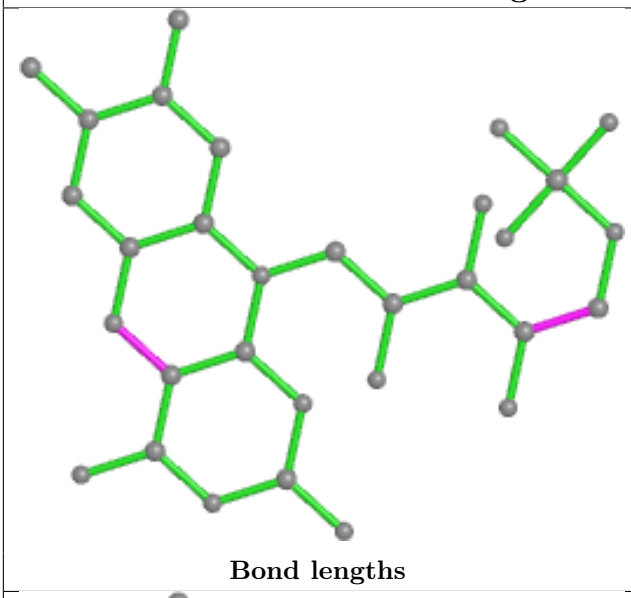


Rings

Ligand FMN C 1002



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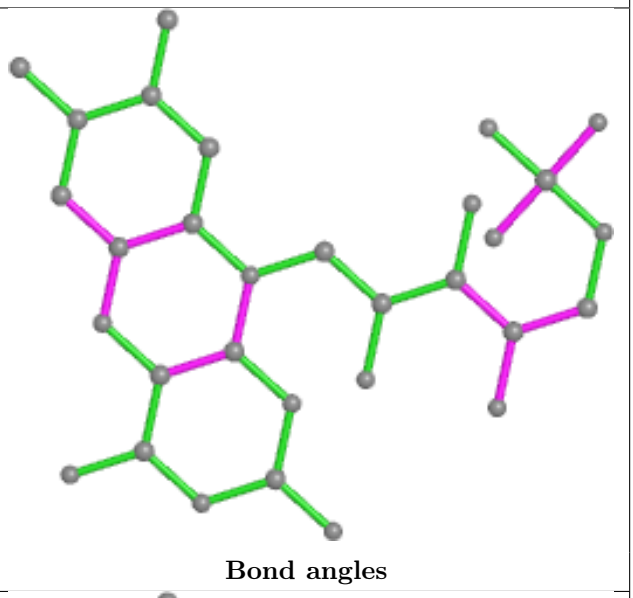
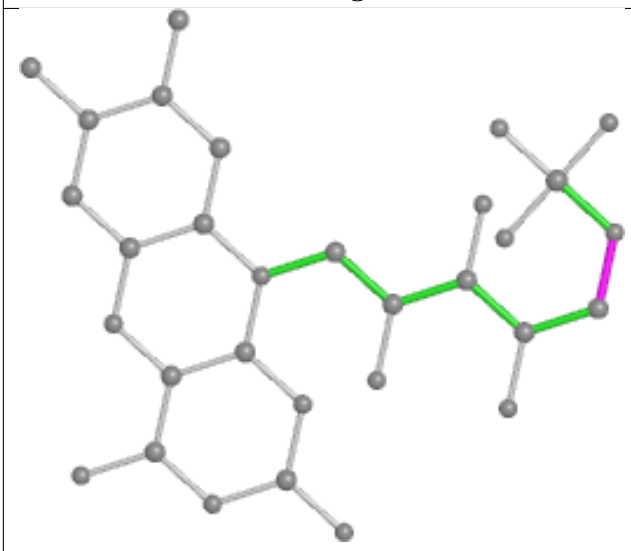


Bond angles



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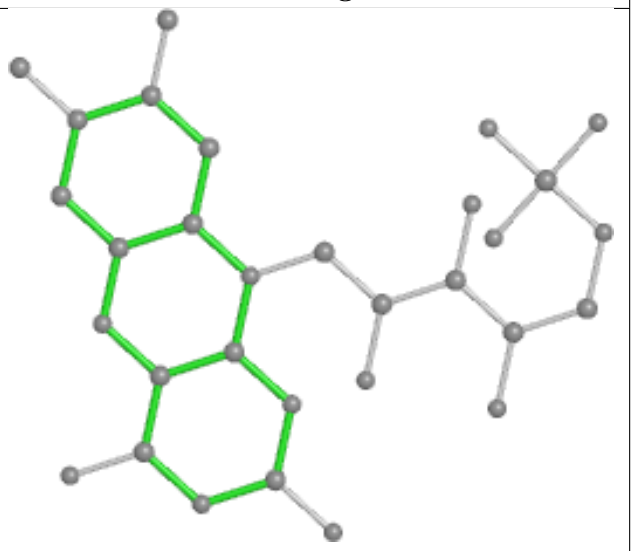

Rings

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

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.