Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 08:32 AM EDT

PDB ID	:	6MYW
Title	:	Gluconobacter Ene-Reductase (GluER) mutant - T36A
Authors	:	Garfinkle, S.E.; Jeffrey, P.; Hyster, T.K.
Deposited on	:	2018-11-02
Resolution	:	1.16 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 1.16 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 13184 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 N-ethylmaleimide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	2	0
			2752	1737	488	519	8			
1	B	356	Total	C	N	O	S	0	2	0
			2754	1738	491	517	8			
1	C	356	Total	C	N	O	S	0	2	0
			2754	1738	491	517	8			
1	D	356	Total	C	N	O	S	0	1	0
			2743	1732	487	516	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	ALA	THR	engineered mutation	UNP A1E8I9
A	362	LEU	-	expression tag	UNP A1E8I9
A	363	GLU	-	expression tag	UNP A1E8I9
A	364	HIS	-	expression tag	UNP A1E8I9
A	365	HIS	-	expression tag	UNP A1E8I9
A	366	HIS	-	expression tag	UNP A1E8I9
A	367	HIS	-	expression tag	UNP A1E8I9
A	368	HIS	-	expression tag	UNP A1E8I9
A	369	HIS	-	expression tag	UNP A1E8I9
B	36	ALA	THR	engineered mutation	UNP A1E8I9
B	362	LEU	-	expression tag	UNP A1E8I9
B	363	GLU	-	expression tag	UNP A1E8I9
B	364	HIS	-	expression tag	UNP A1E8I9
B	365	HIS	-	expression tag	UNP A1E8I9
B	366	HIS	-	expression tag	UNP A1E8I9
B	367	HIS	-	expression tag	UNP A1E8I9
B	368	HIS	-	expression tag	UNP A1E8I9
B	369	HIS	-	expression tag	UNP A1E8I9
C	36	ALA	THR	engineered mutation	UNP A1E8I9
C	362	LEU	-	expression tag	UNP A1E8I9
C	363	GLU	-	expression tag	UNP A1E8I9

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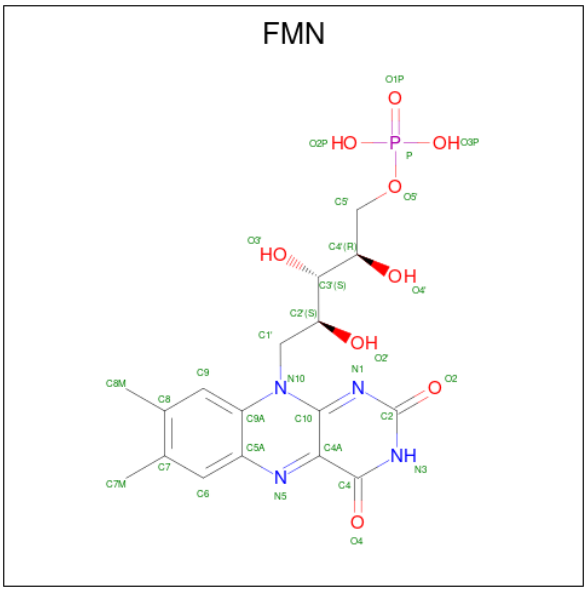
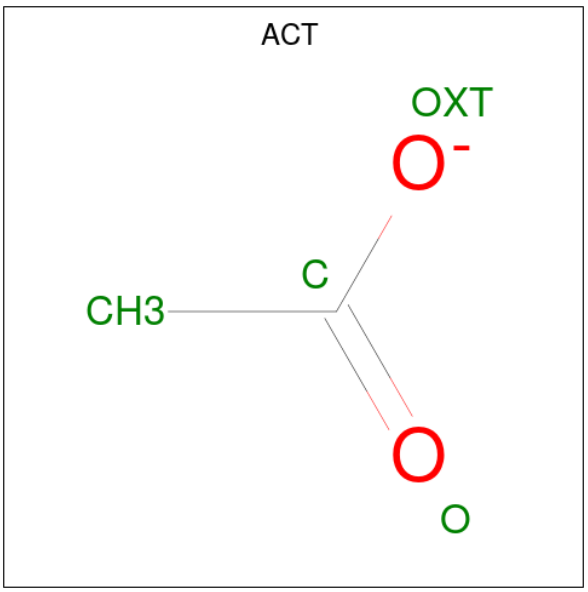
Chain	Residue	Modelled	Actual	Comment	Reference
C	364	HIS	-	expression tag	UNP A1E8I9
C	365	HIS	-	expression tag	UNP A1E8I9
C	366	HIS	-	expression tag	UNP A1E8I9
C	367	HIS	-	expression tag	UNP A1E8I9
C	368	HIS	-	expression tag	UNP A1E8I9
C	369	HIS	-	expression tag	UNP A1E8I9
D	36	ALA	THR	engineered mutation	UNP A1E8I9
D	362	LEU	-	expression tag	UNP A1E8I9
D	363	GLU	-	expression tag	UNP A1E8I9
D	364	HIS	-	expression tag	UNP A1E8I9
D	365	HIS	-	expression tag	UNP A1E8I9
D	366	HIS	-	expression tag	UNP A1E8I9
D	367	HIS	-	expression tag	UNP A1E8I9
D	368	HIS	-	expression tag	UNP A1E8I9
D	369	HIS	-	expression tag	UNP A1E8I9

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



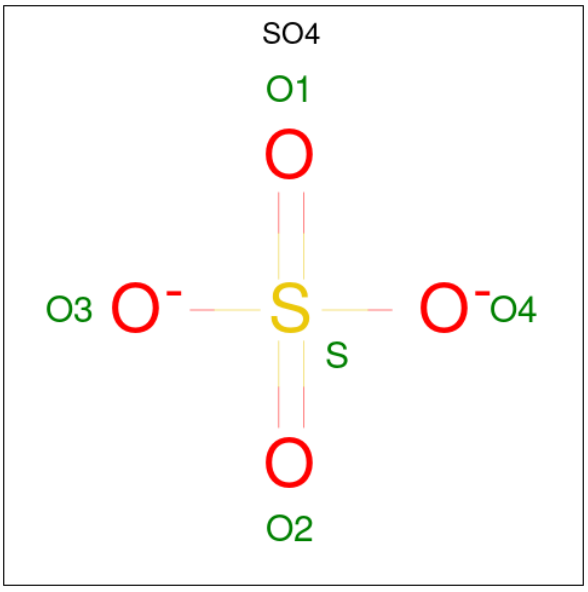
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

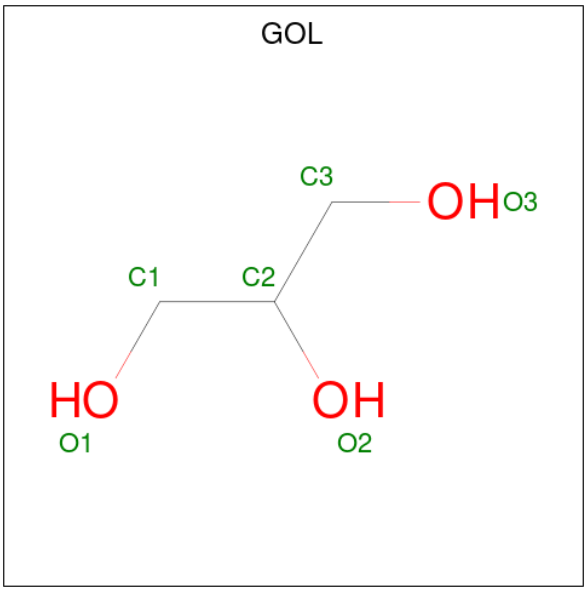


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Na 2 2	0	0
5	C	5	Total Na 5 5	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	491	Total O 491 491	0	0
7	B	520	Total O 520 520	0	0
7	C	477	Total O 477 477	0	0
7	D	490	Total O 490 490	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	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	99.47Å 45.15Å 163.74Å 90.00° 107.67° 90.00°	Depositor
Resolution (Å)	29.28 – 1.16	Depositor
% Data completeness (in resolution range)	95.0 (29.28-1.16)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 1.16Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.123 , 0.145	Depositor
Wilson B-factor (Å^2)	10.4	Xtriage
Anisotropy	0.534	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.534 for H, K, L 0.466 for -H, -K, H+L	Depositor
Outliers	13 of 458754 reflections (0.003%)	Xtriage
Total number of atoms	13184	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.31 % 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 1.8825e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 26 ligands modelled in this entry, 7 are monoatomic - leaving 19 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	$\#\|Z\| > 2$
3	ACT	A	402	-	3,3,3	1.03	0	3,3,3	0.81	0
4	SO4	C	403	-	4,4,4	0.40	0	6,6,6	0.36	0
4	SO4	B	403	-	4,4,4	0.41	0	6,6,6	0.29	0
2	FMN	B	401	-	33,33,33	1.05	1 (3%)	48,50,50	1.11	3 (6%)
4	SO4	D	405	-	4,4,4	0.66	0	6,6,6	0.18	0
4	SO4	C	405	-	4,4,4	0.35	0	6,6,6	0.05	0
3	ACT	D	402	-	3,3,3	0.94	0	3,3,3	1.45	1 (33%)
4	SO4	A	404	-	4,4,4	0.61	0	6,6,6	0.15	0
4	SO4	D	403	-	4,4,4	0.30	0	6,6,6	0.31	0
2	FMN	A	401	-	33,33,33	0.93	1 (3%)	48,50,50	1.21	6 (12%)
2	FMN	D	401	-	33,33,33	1.14	2 (6%)	48,50,50	1.18	4 (8%)
4	SO4	C	404	5	4,4,4	0.22	0	6,6,6	0.28	0
4	SO4	B	404	-	4,4,4	0.24	0	6,6,6	0.24	0
3	ACT	B	402	-	3,3,3	1.48	1 (33%)	3,3,3	0.86	0
4	SO4	A	403	-	4,4,4	0.44	0	6,6,6	0.31	0
2	FMN	C	401	-	33,33,33	1.15	1 (3%)	48,50,50	1.15	4 (8%)
3	ACT	C	402	-	3,3,3	0.71	0	3,3,3	0.26	0
4	SO4	D	404	-	4,4,4	0.47	0	6,6,6	0.29	0
6	GOL	C	411	-	5,5,5	0.11	0	5,5,5	0.65	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	FMN	D	401	-	-	1/18/18/18	0/3/3/3
2	FMN	B	401	-	-	1/18/18/18	0/3/3/3
2	FMN	C	401	-	-	1/18/18/18	0/3/3/3
6	GOL	C	411	-	-	4/4/4/4	-
2	FMN	A	401	-	-	1/18/18/18	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	FMN	C5'-C4'	3.35	1.56	1.51
2	C	401	FMN	C6-C7	-2.96	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	FMN	C4A-N5	2.45	1.35	1.30
3	B	402	ACT	OXT-C	-2.41	1.19	1.30
2	B	401	FMN	C5A-N5	-2.39	1.34	1.39
2	A	401	FMN	C1'-N10	-2.14	1.42	1.48

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	FMN	C6-C7-C8	-3.00	115.36	119.67
2	B	401	FMN	C4-C4A-N5	2.69	122.06	118.23
2	D	401	FMN	C9A-C5A-N5	-2.68	119.51	122.43
2	C	401	FMN	C9A-C9-C8	2.38	124.09	119.30
2	D	401	FMN	C8M-C8-C9	2.36	123.85	119.49
2	A	401	FMN	C9A-C9-C8	2.35	124.03	119.30
2	D	401	FMN	O3'-C3'-C2'	-2.33	103.17	108.81
2	B	401	FMN	C5A-C6-C7	2.31	124.95	120.71
2	C	401	FMN	C6-C5A-N5	2.29	122.52	118.51
2	A	401	FMN	C4A-C10-N10	2.27	119.80	116.48
2	C	401	FMN	C9A-C5A-N5	-2.23	120.01	122.43
2	C	401	FMN	C9-C8-C7	-2.20	116.52	119.67
2	A	401	FMN	O2'-C2'-C1'	2.19	115.09	109.80
2	D	401	FMN	C9A-C9-C8	2.13	123.59	119.30
2	A	401	FMN	C9A-N10-C10	-2.03	117.60	120.77
2	B	401	FMN	C7M-C7-C6	2.02	123.22	119.49
3	D	402	ACT	O-C-CH3	-2.01	114.52	122.33
2	A	401	FMN	C5A-C9A-N10	2.00	120.02	117.95

There are no chirality outliers.

All (8) torsion outliers are listed below:

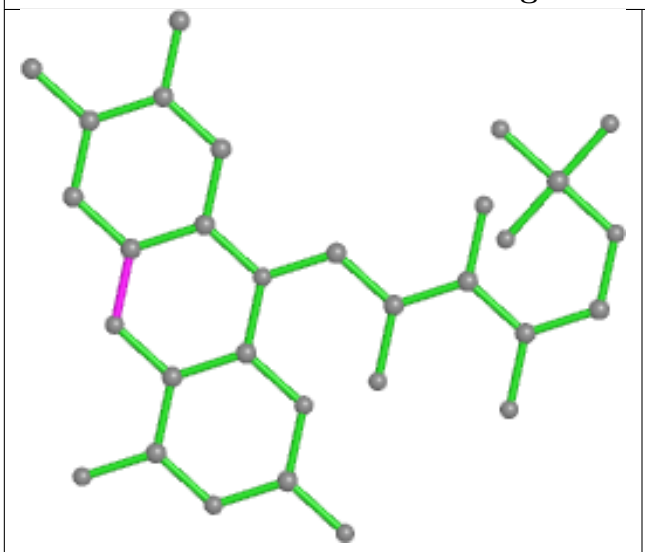
Mol	Chain	Res	Type	Atoms
6	C	411	GOL	O1-C1-C2-C3
6	C	411	GOL	O1-C1-C2-O2
6	C	411	GOL	O2-C2-C3-O3
2	A	401	FMN	C4'-C5'-O5'-P
2	C	401	FMN	C4'-C5'-O5'-P
2	D	401	FMN	C4'-C5'-O5'-P
2	B	401	FMN	C4'-C5'-O5'-P
6	C	411	GOL	C1-C2-C3-O3

There are no ring outliers.

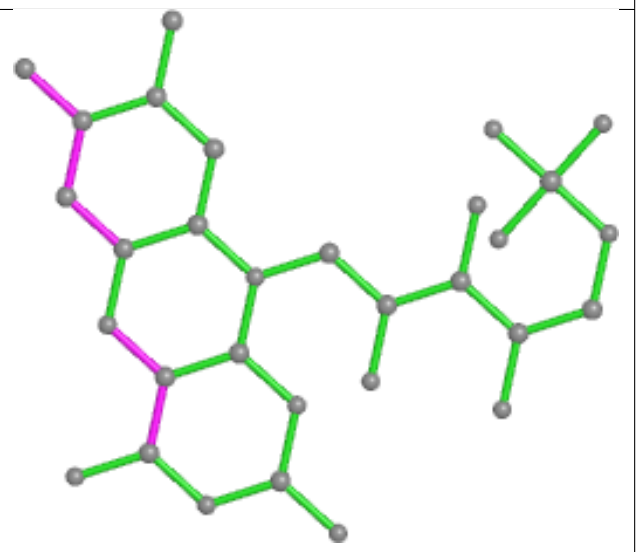
No monomer is involved in short contacts.

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 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.

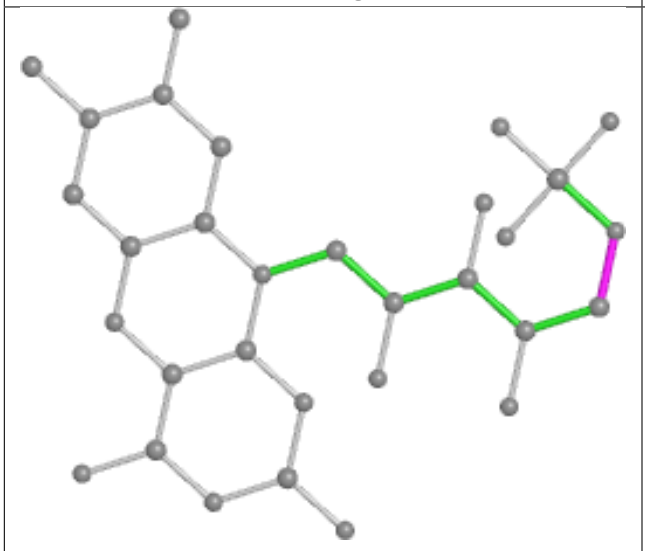
Ligand FMN B 401



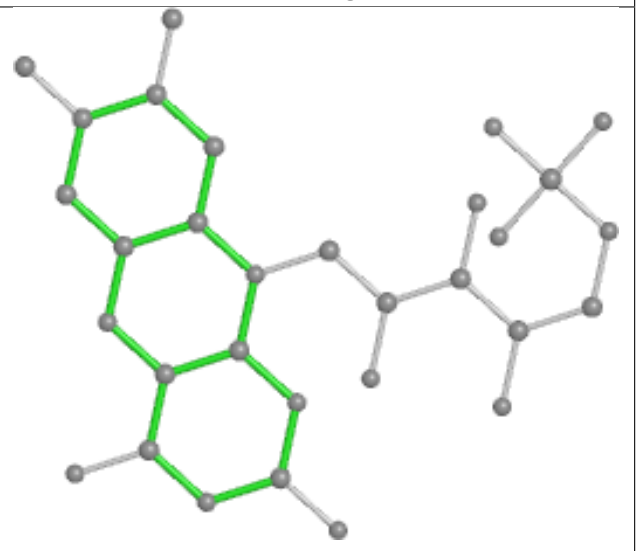
Bond lengths



Bond angles

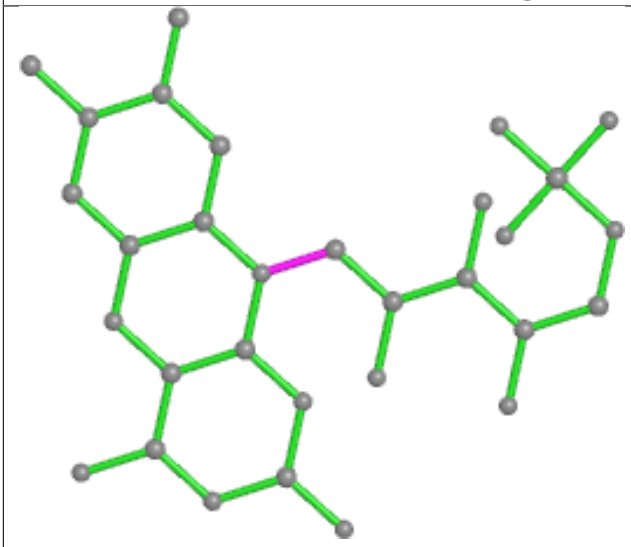


Torsions

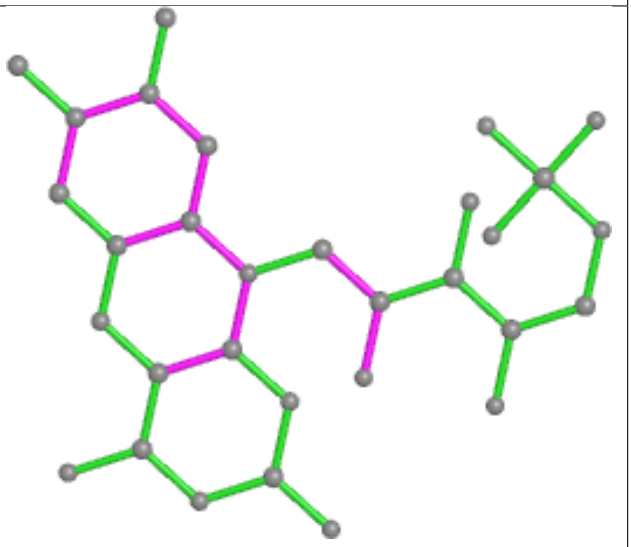


Rings

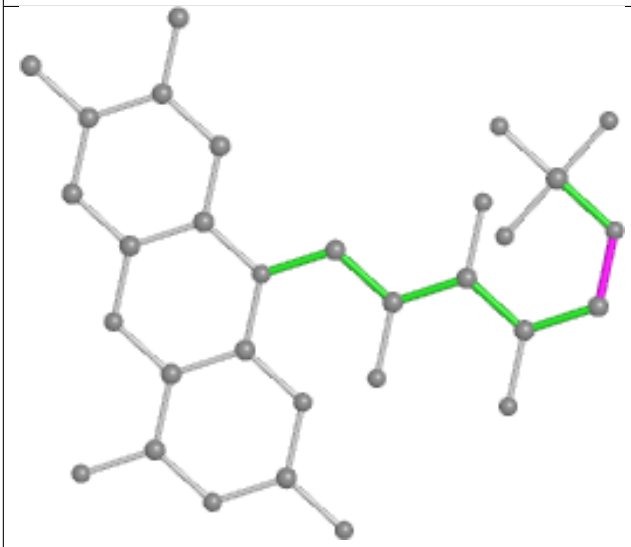
Ligand FMN A 401



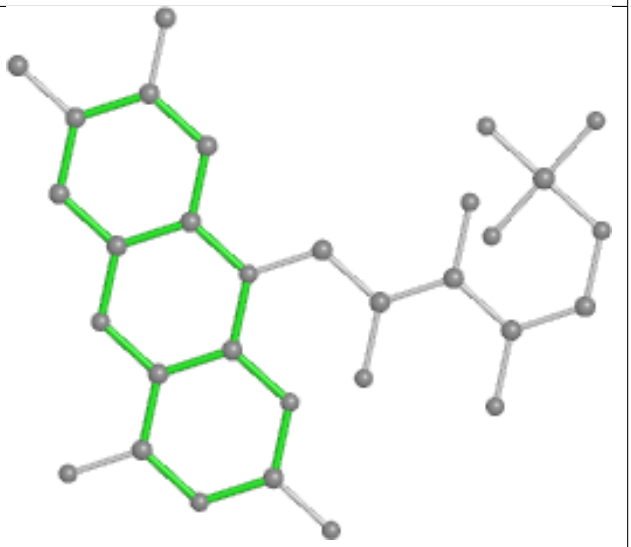
Bond lengths



Bond angles

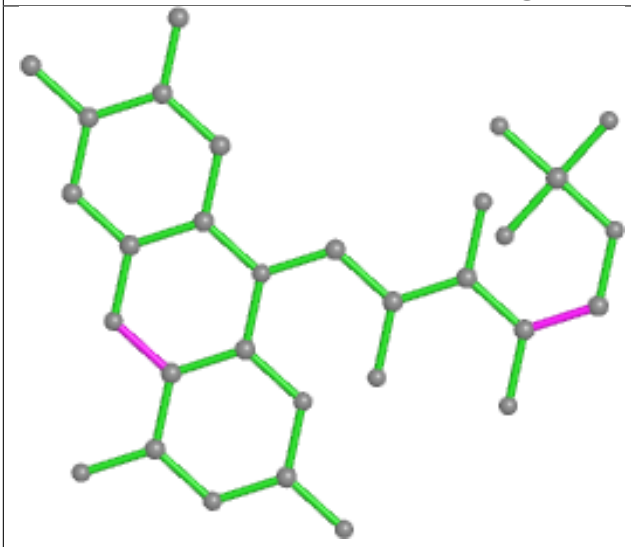


Torsions

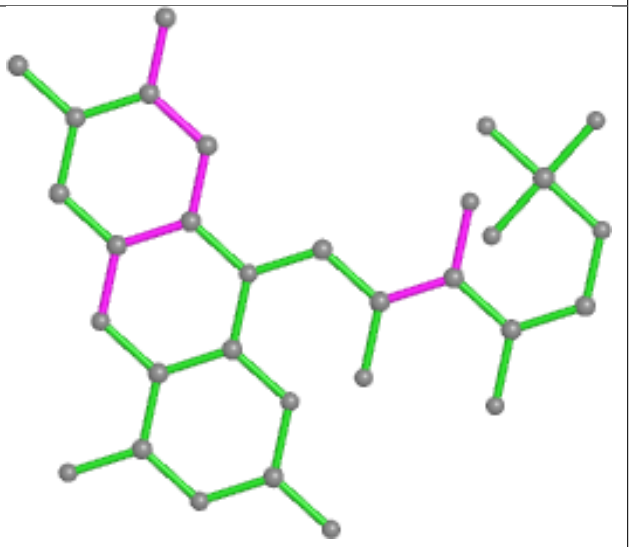


Rings

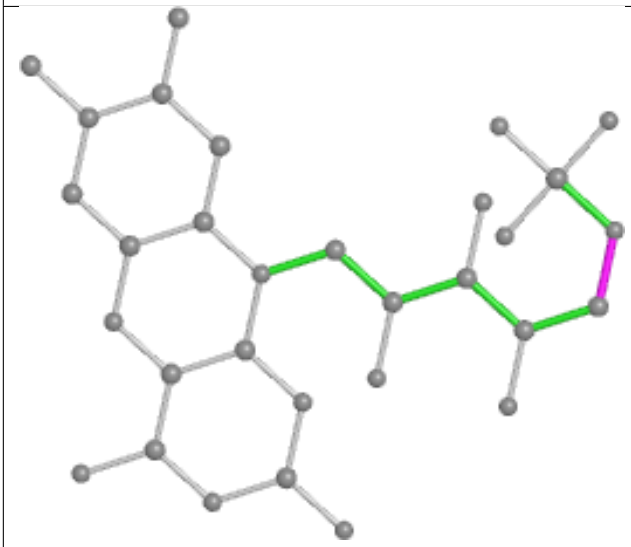
Ligand FMN D 401



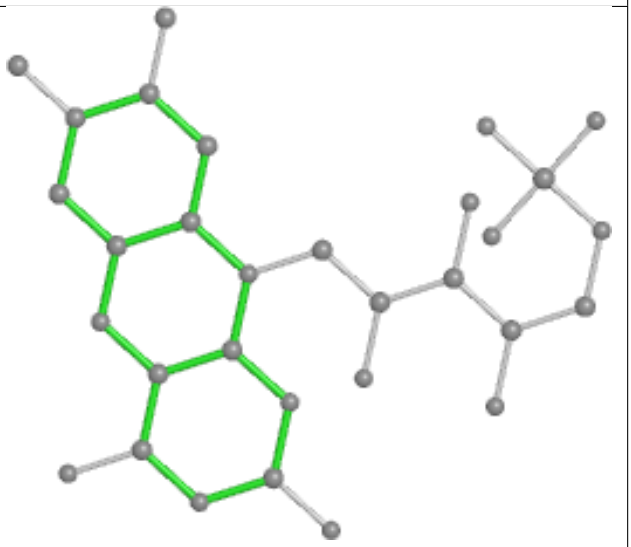
Bond lengths



Bond angles

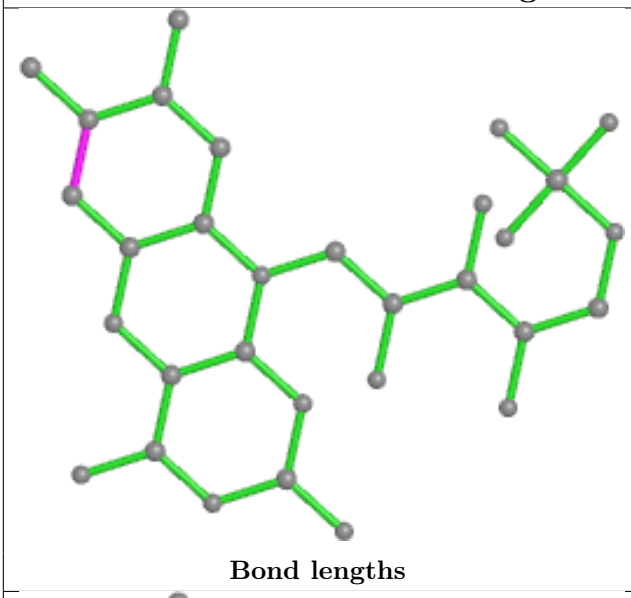


Torsions

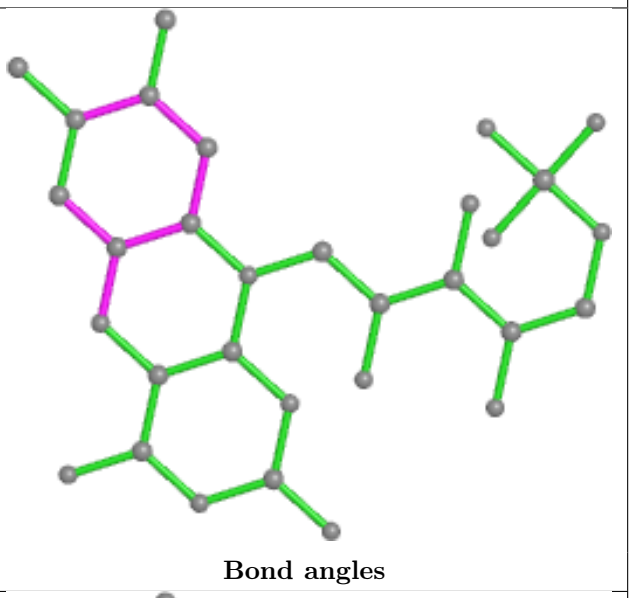


Rings

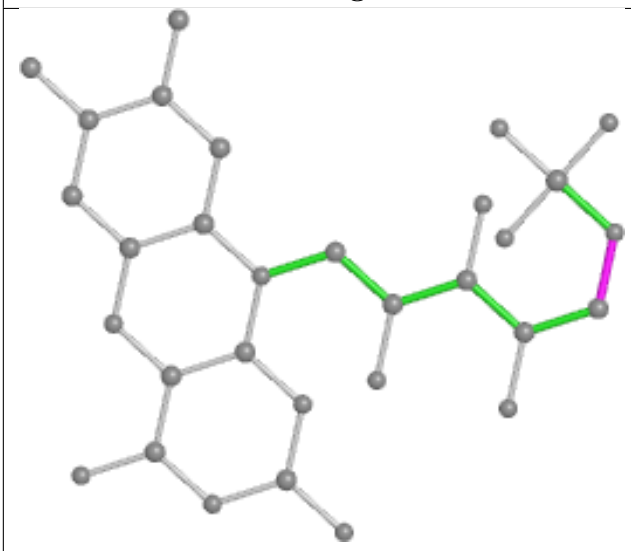
Ligand FMN C 401



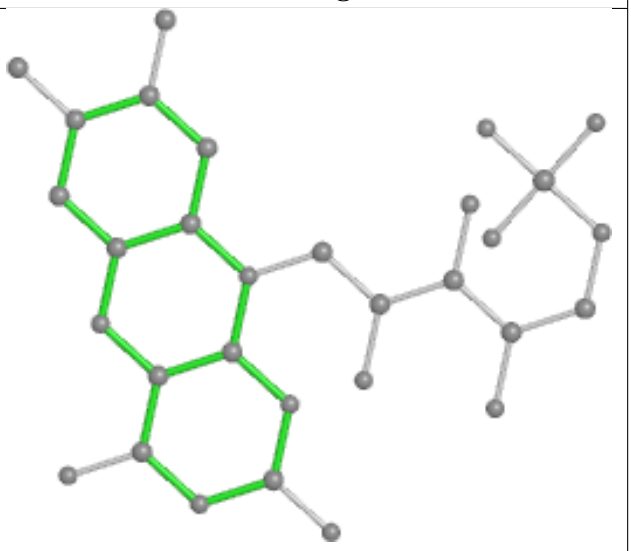
Bond lengths



Bond angles



Torsions



Rings

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

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.