Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 04:38 PM EDT

PDB ID	:	6N7F
Title	:	1.90 Angstrom Resolution Crystal Structure of Glutathione Reductase from Streptococcus pyogenes in Complex with FAD.
Authors	:	Minasov, G.; Shuvalova, L.; Shabalin, I.G.; Grabowski, M.; Olphie, A.; Cardona-Correa, A.; Anderson, W.F.; Satchell, K.J.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2018-11-27
Resolution	:	1.90 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 1.90 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 8 unique types of molecules in this entry. The entry contains 16456 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.

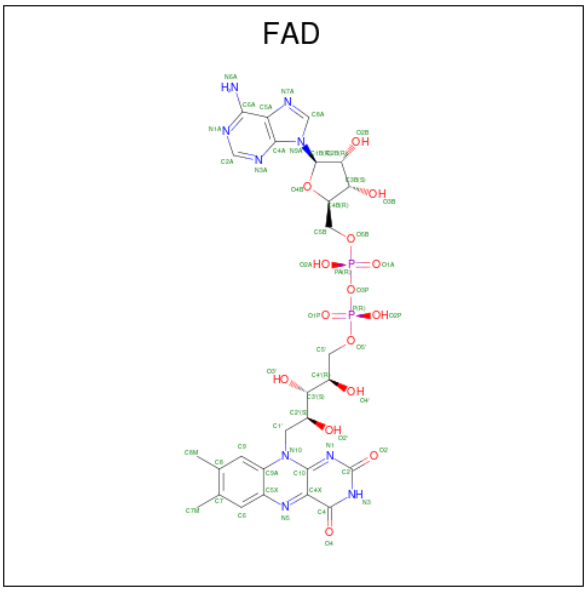
- Molecule 1 is a protein called Putative glutathione reductase (GR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	14	0
			3576	2271	613	680	12			
1	B	450	Total	C	N	O	S	0	13	0
			3565	2268	611	674	12			
1	C	450	Total	C	N	O	S	0	15	0
			3576	2275	611	676	14			
1	D	451	Total	C	N	O	S	0	17	0
			3589	2281	613	682	13			

There are 12 discrepancies between the modelled and reference sequences:

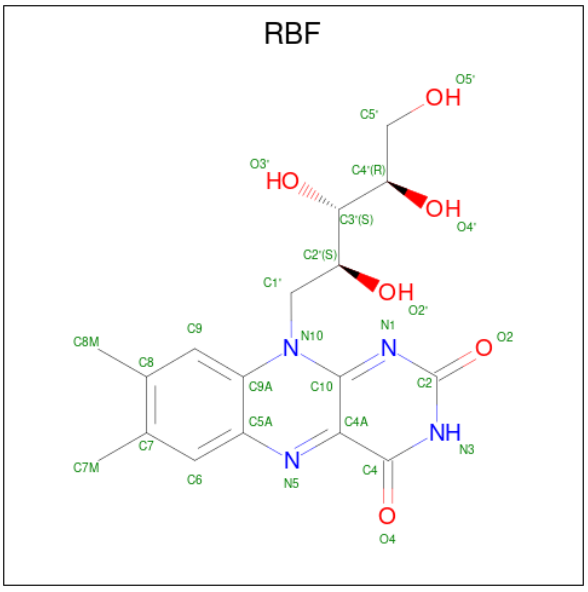
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9A0E2
A	-1	ASN	-	expression tag	UNP Q9A0E2
A	0	ALA	-	expression tag	UNP Q9A0E2
B	-2	SER	-	expression tag	UNP Q9A0E2
B	-1	ASN	-	expression tag	UNP Q9A0E2
B	0	ALA	-	expression tag	UNP Q9A0E2
C	-2	SER	-	expression tag	UNP Q9A0E2
C	-1	ASN	-	expression tag	UNP Q9A0E2
C	0	ALA	-	expression tag	UNP Q9A0E2
D	-2	SER	-	expression tag	UNP Q9A0E2
D	-1	ASN	-	expression tag	UNP Q9A0E2
D	0	ALA	-	expression tag	UNP Q9A0E2

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



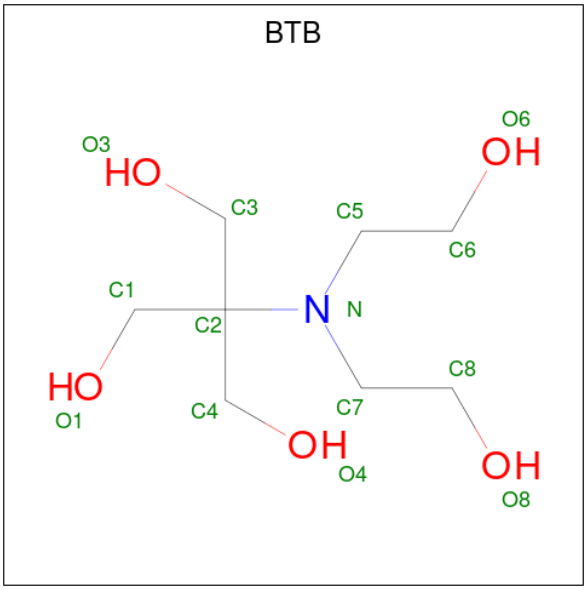
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is RIBOFLAVIN (three-letter code: RBF) (formula: $C_{17}H_{20}N_4O_6$).



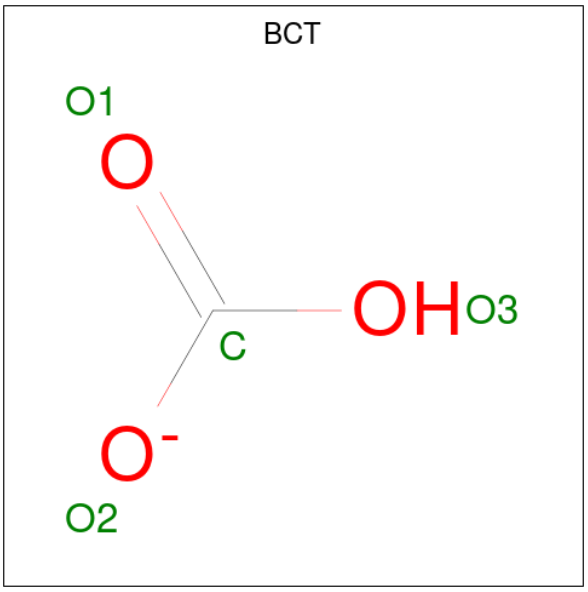
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			54	34	8	12		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

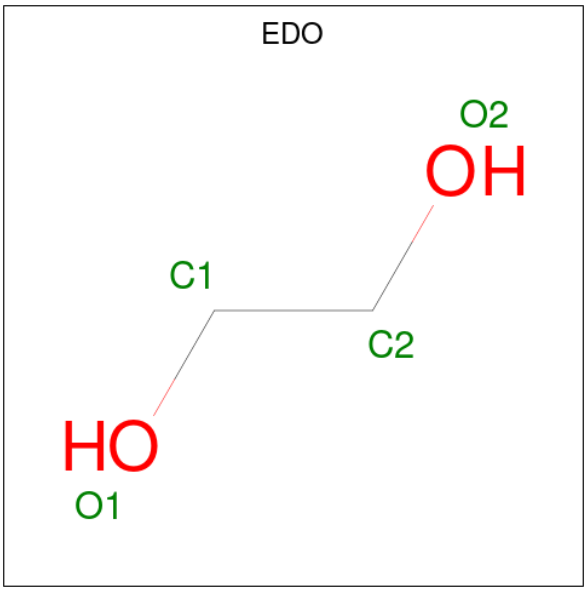


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 1 3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total Cl 4 4	0	0
6	B	4	Total Cl 4 4	0	0
6	C	5	Total Cl 5 5	0	0
6	D	4	Total Cl 4 4	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	471	Total O 495 495	0	39
8	B	405	Total O 436 436	0	40
8	C	382	Total O 406 406	0	27
8	D	450	Total O 466 466	0	26

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	Depositor
Cell constants a, b, c, α, β, γ	76.40Å 86.65Å 86.67Å 67.13° 74.15° 74.11°	Depositor
Resolution (Å)	29.47 – 1.90	Depositor
% Data completeness (in resolution range)	97.5 (29.47-1.90)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.169 , 0.210	Depositor
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.376	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.469 for -h,-l,-k	Xtriage
Total number of atoms	16456	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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 29 ligands modelled in this entry, 17 are monoatomic - leaving 12 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	FAD	C	501	-	53,58,58	0.58	0	68,89,89	0.72	1 (1%)
4	BTB	B	502	-	13,13,13	1.25	1 (7%)	7,16,16	0.42	0
4	BTB	D	502	-	13,13,13	1.11	2 (15%)	7,16,16	0.32	0
7	EDO	D	507	-	3,3,3	0.20	0	2,2,2	0.34	0
2	FAD	B	501	-	53,58,58	0.58	0	68,89,89	0.72	2 (2%)
5	BCT	A	504	-	2,3,3	0.92	0	2,3,3	1.66	1 (50%)
4	BTB	A	503	-	13,13,13	1.08	1 (7%)	7,16,16	0.25	0
2	FAD	D	501	-	53,58,58	0.62	0	68,89,89	0.71	1 (1%)
2	FAD	A	501	-	53,58,58	0.63	0	68,89,89	0.71	1 (1%)
4	BTB	C	502	-	13,13,13	1.18	1 (7%)	7,16,16	0.33	0
3	RBF	A	502[B]	-	29,29,29	0.53	0	41,43,43	0.64	0
3	RBF	A	502[A]	-	29,29,29	0.49	0	41,43,43	0.65	1 (2%)

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	C	501	-	-	3/30/50/50	0/6/6/6
4	BTB	B	502	-	-	0/21/21/21	-
4	BTB	D	502	-	-	3/21/21/21	-
7	EDO	D	507	-	-	1/1/1/1	-
2	FAD	B	501	-	-	3/30/50/50	0/6/6/6
4	BTB	A	503	-	-	5/21/21/21	-
2	FAD	D	501	-	-	3/30/50/50	0/6/6/6
2	FAD	A	501	-	-	3/30/50/50	0/6/6/6
4	BTB	C	502	-	-	1/21/21/21	-
3	RBF	A	502[B]	-	-	6/14/14/14	0/3/3/3
3	RBF	A	502[A]	-	-	11/14/14/14	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	BTB	C2-N	3.53	1.55	1.48
4	C	502	BTB	C2-N	3.14	1.54	1.48
4	D	502	BTB	C2-N	2.74	1.54	1.48
4	A	503	BTB	C2-N	2.72	1.54	1.48
4	D	502	BTB	C5-N	2.01	1.50	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	FAD	C5A-C6A-N6A	2.59	124.29	120.35
2	A	501	FAD	C5A-C6A-N6A	2.58	124.27	120.35
2	B	501	FAD	C5A-C6A-N6A	2.40	123.99	120.35
2	C	501	FAD	C5A-C6A-N6A	2.39	123.99	120.35
5	A	504	BCT	O2-C-O1	2.20	125.24	119.55
2	B	501	FAD	C4-N3-C2	-2.07	121.83	125.64
3	A	502[A]	RBF	C4-N3-C2	-2.05	121.85	125.64

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	FAD	PA-O3P-P-O5'
3	A	502[A]	RBF	N10-C1'-C2'-O2'
3	A	502[A]	RBF	C1'-C2'-C3'-O3'
3	A	502[A]	RBF	C1'-C2'-C3'-C4'
3	A	502[A]	RBF	O2'-C2'-C3'-O3'
3	A	502[A]	RBF	O2'-C2'-C3'-C4'
3	A	502[B]	RBF	C1'-C2'-C3'-O3'
3	A	502[B]	RBF	C1'-C2'-C3'-C4'
3	A	502[B]	RBF	O2'-C2'-C3'-O3'
3	A	502[B]	RBF	O2'-C2'-C3'-C4'
3	A	502[B]	RBF	O4'-C4'-C5'-O5'
3	A	502[B]	RBF	C3'-C4'-C5'-O5'
2	A	501	FAD	O4B-C4B-C5B-O5B
2	B	501	FAD	O4B-C4B-C5B-O5B
3	A	502[A]	RBF	C2'-C3'-C4'-C5'
3	A	502[A]	RBF	O4'-C4'-C5'-O5'
3	A	502[A]	RBF	C3'-C4'-C5'-O5'
3	A	502[A]	RBF	O3'-C3'-C4'-C5'
3	A	502[A]	RBF	O3'-C3'-C4'-O4'
2	A	501	FAD	C3B-C4B-C5B-O5B
7	D	507	EDO	O1-C1-C2-O2

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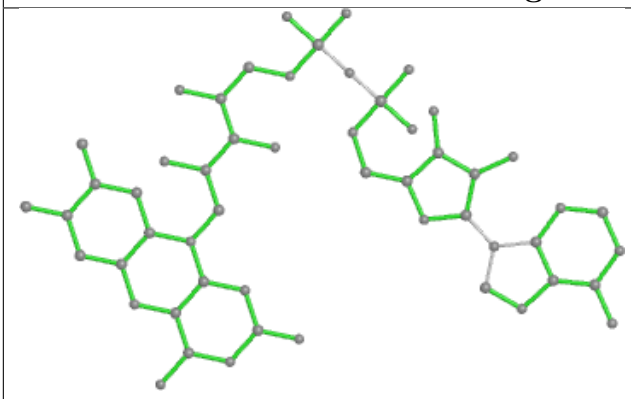
Mol	Chain	Res	Type	Atoms
3	A	502[A]	RBF	C2'-C3'-C4'-O4'
4	A	503	BTB	N-C5-C6-O6
2	B	501	FAD	C3B-C4B-C5B-O5B
4	D	502	BTB	N-C7-C8-O8
2	A	501	FAD	PA-O3P-P-O5'
2	B	501	FAD	PA-O3P-P-O5'
2	C	501	FAD	PA-O3P-P-O5'
2	C	501	FAD	O4B-C4B-C5B-O5B
2	D	501	FAD	O4B-C4B-C5B-O5B
4	A	503	BTB	O1-C1-C2-C4
4	A	503	BTB	C3-C2-C4-O4
4	A	503	BTB	N-C7-C8-O8
4	C	502	BTB	N-C7-C8-O8
4	D	502	BTB	N-C5-C6-O6
2	D	501	FAD	C3B-C4B-C5B-O5B
2	C	501	FAD	C3B-C4B-C5B-O5B
4	A	503	BTB	O1-C1-C2-C3
4	D	502	BTB	C1-C2-C3-O3

There are no ring outliers.

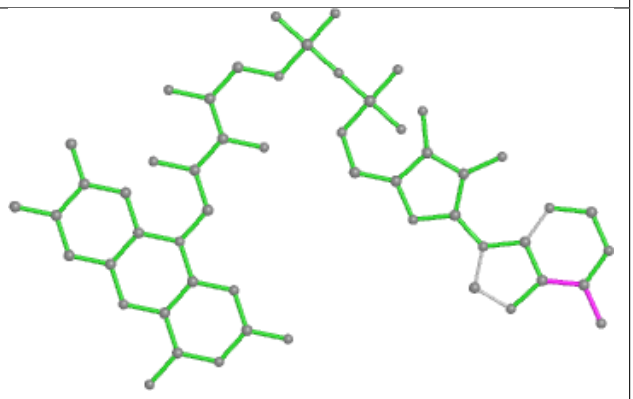
No monomer is involved in short contacts.

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.

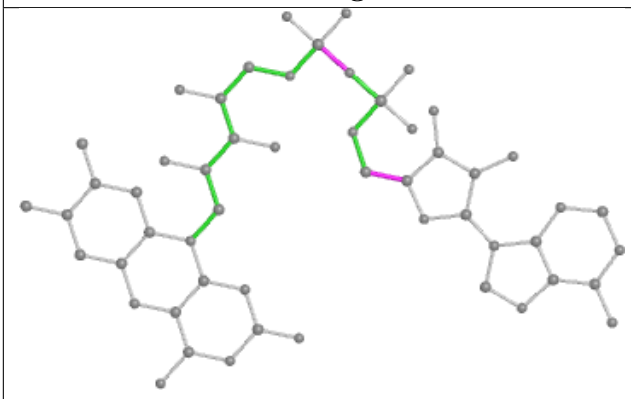
Ligand FAD C 501



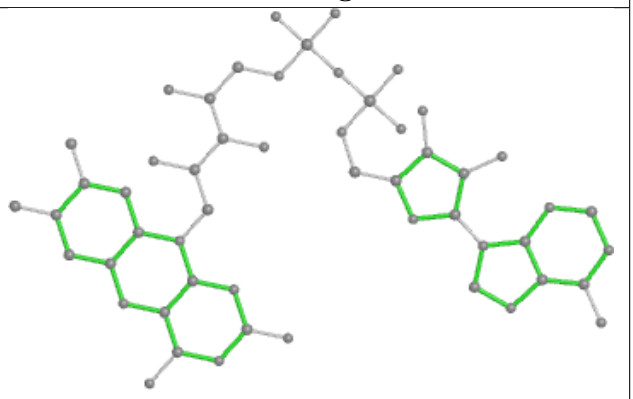
Bond lengths



Bond angles

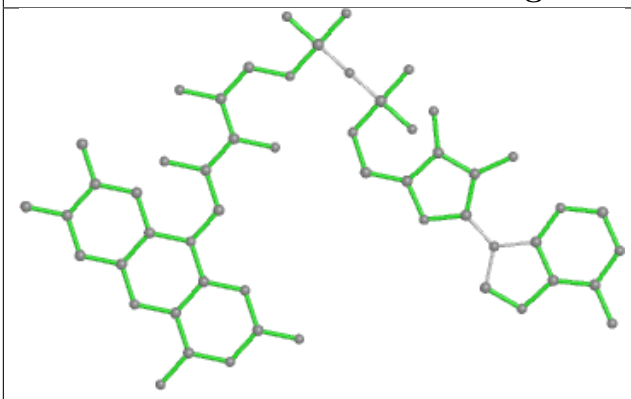


Torsions

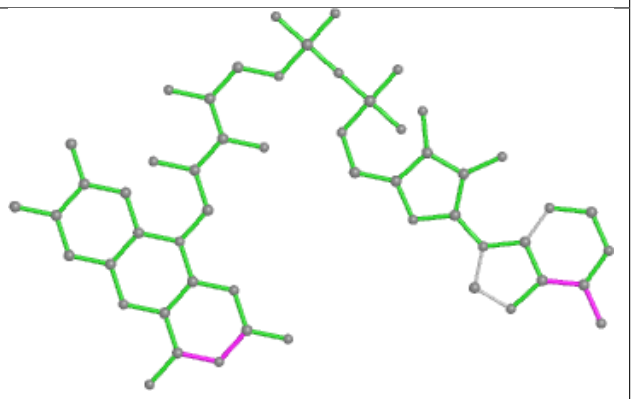


Rings

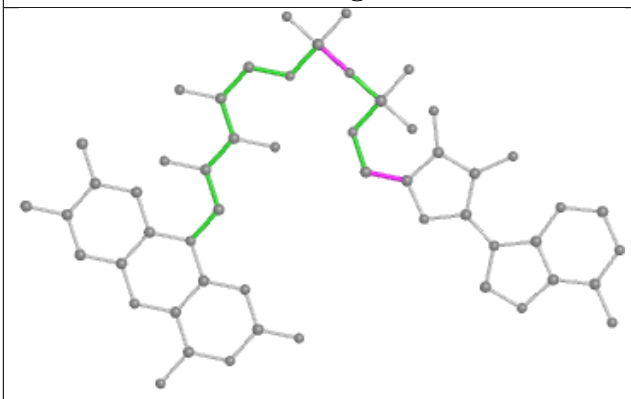
Ligand FAD B 501



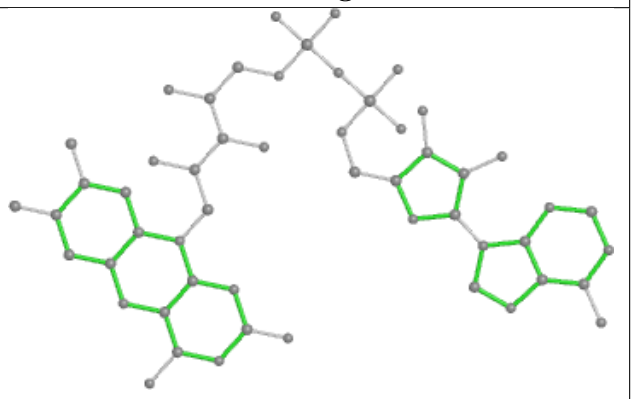
Bond lengths



Bond angles

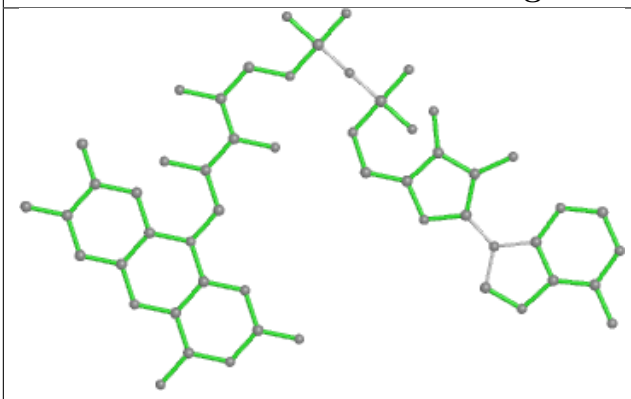


Torsions

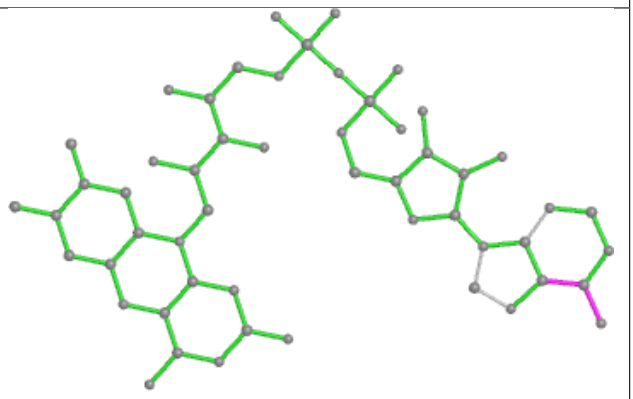


Rings

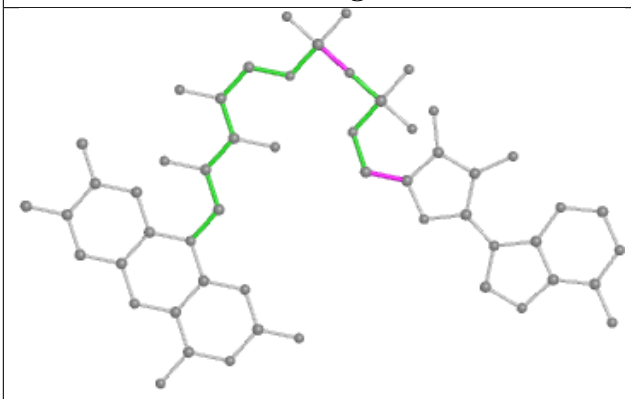
Ligand FAD D 501



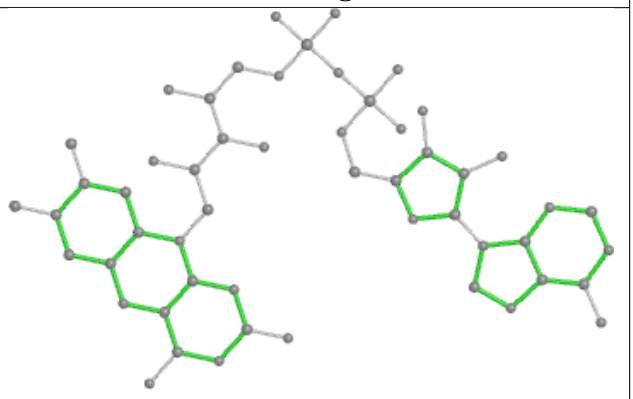
Bond lengths



Bond angles

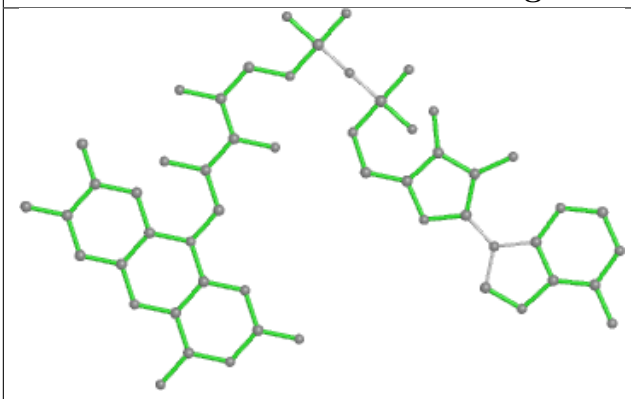


Torsions

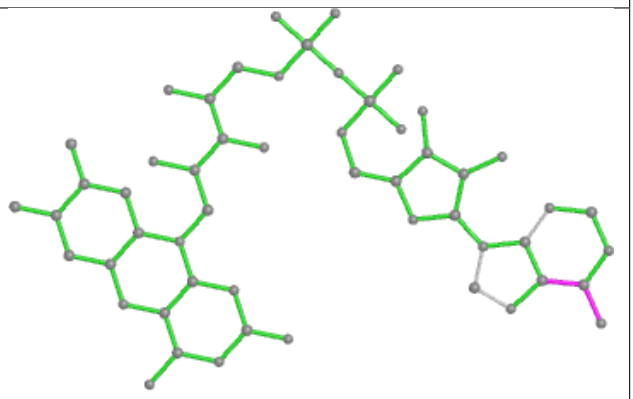


Rings

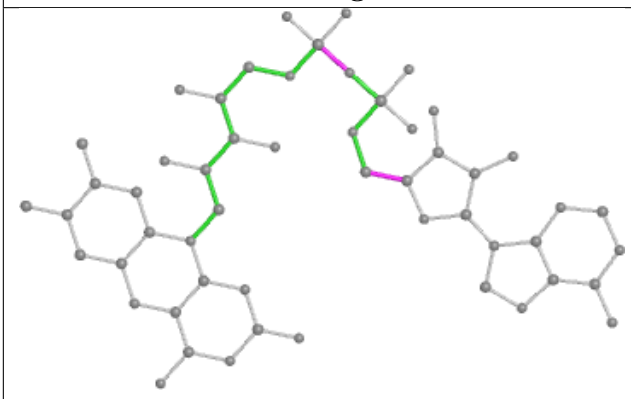
Ligand FAD A 501



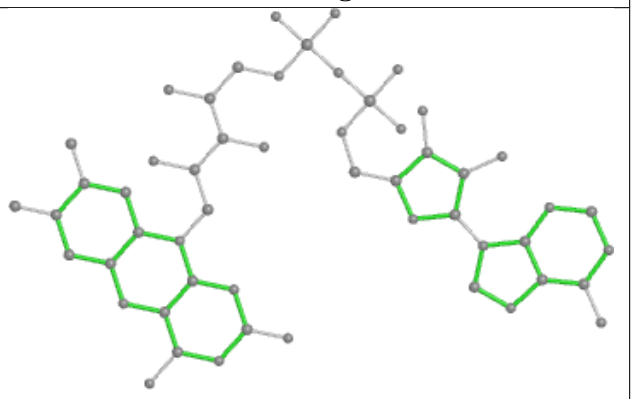
Bond lengths



Bond angles

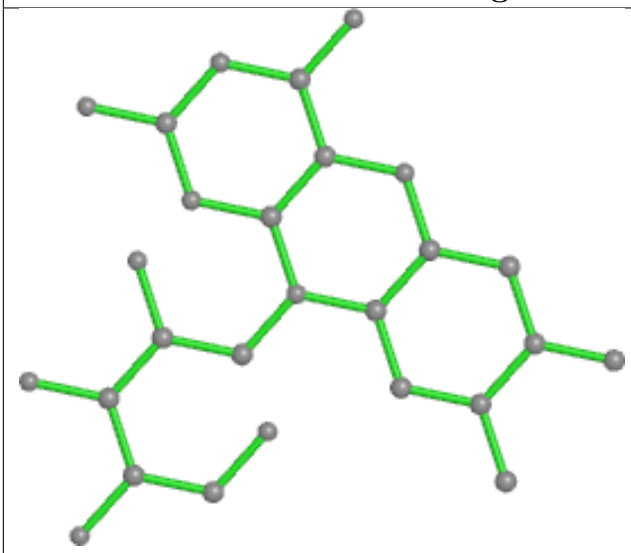


Torsions

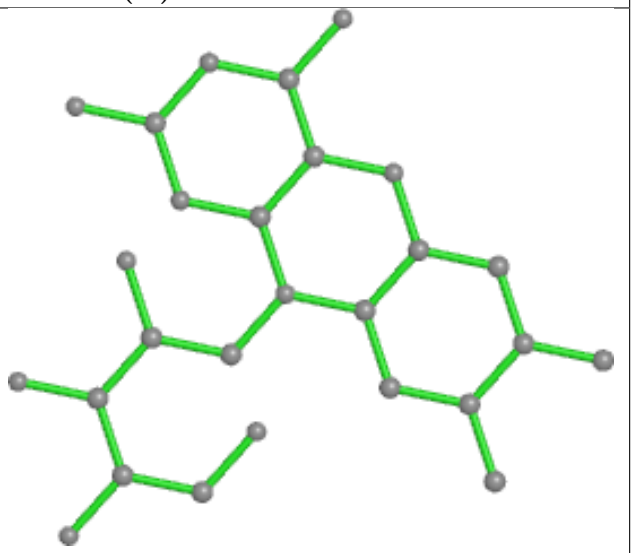


Rings

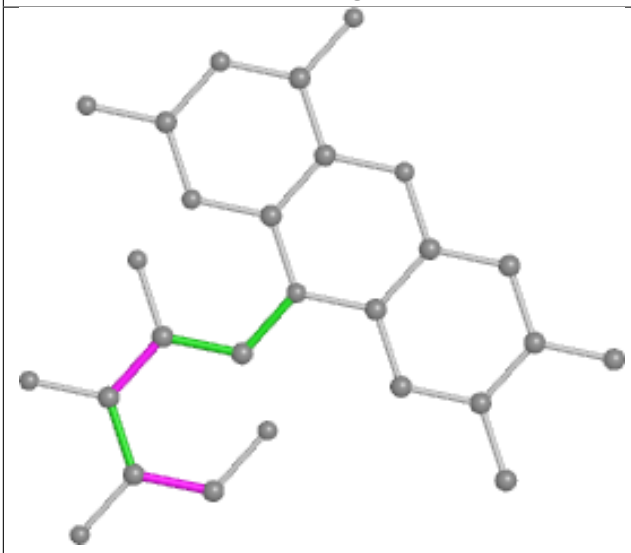
Ligand RBF A 502 (B)



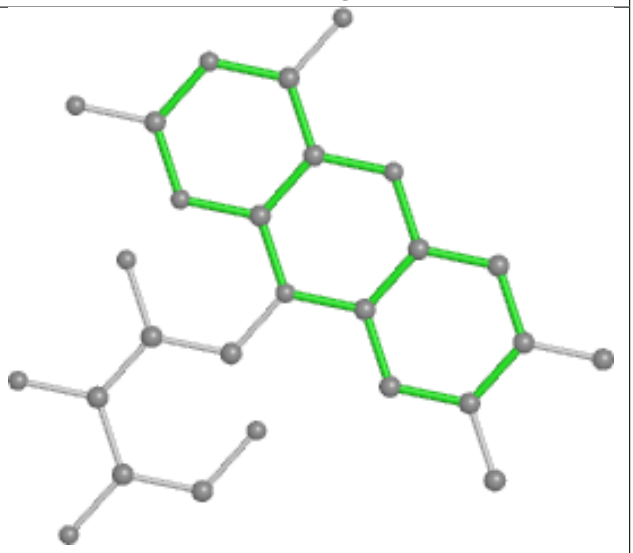
Bond lengths



Bond angles

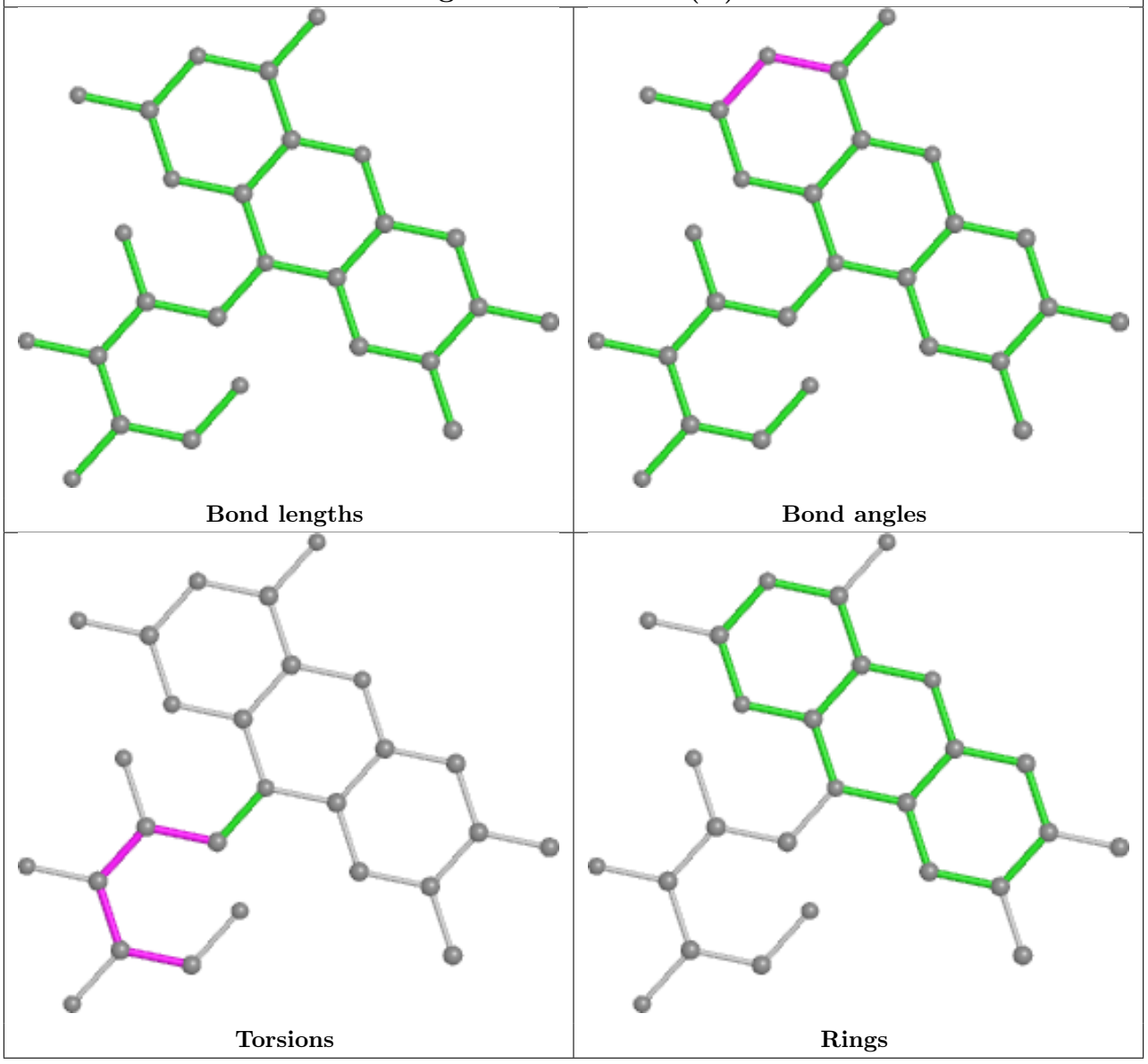


Torsions



Rings

Ligand RBF A 502 (A)



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.