Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 03:04 AM EDT

PDB ID	:	6MYR
Title	:	Avian mitochondrial complex II with thiapronil bound
Authors	:	Huang, L.-S.; Luemmen, P.; Berry, E.A.
Deposited on	:	2018-11-02
Resolution	:	2.15 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 2.15 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 18 unique types of molecules in this entry. The entry contains 9126 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 Succinate dehydrogenase [ubiquinone] flavoprotein subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	611	4734	2962	847	896	29	0	2	0

- Molecule 2 is a protein called Succinate dehydrogenase [ubiquinone] iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	240	1928	1219	326	361	22	0	0	0

- Molecule 3 is a protein called Succinate dehydrogenase cytochrome b, large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	139	1075	706	178	186	5	0	0	0

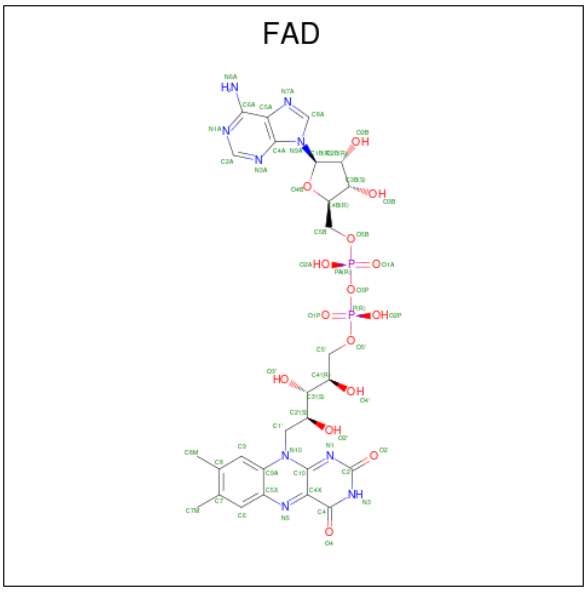
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	139	ALA	SER	conflict	UNP D0VWW3
C	140	MET	GLU	conflict	UNP D0VWW3

- Molecule 4 is a protein called Succinate dehydrogenase [ubiquinone] cytochrome b small subunit, mitochondrial.

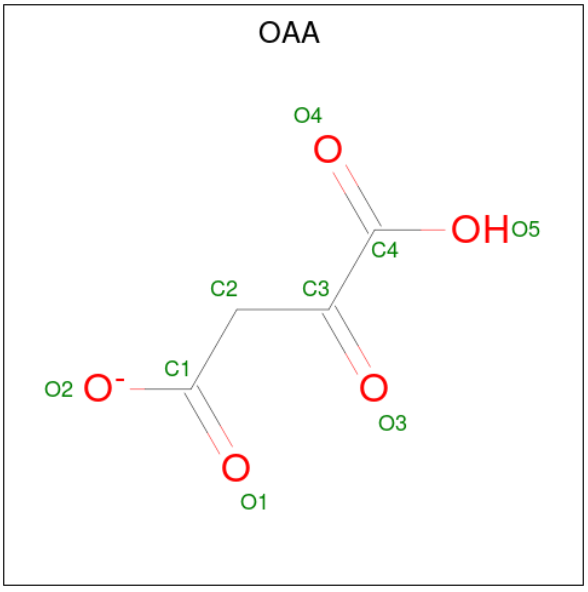
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	102	771	508	122	138	3	0	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 6 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).

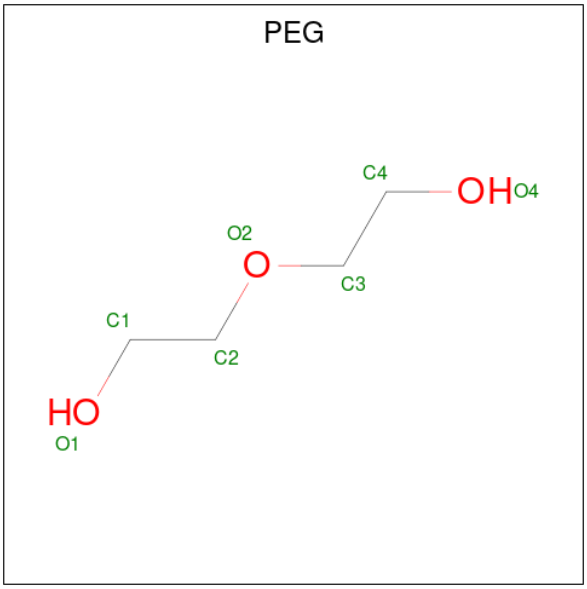


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O		0	0
			9	4	5			

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total K 1 1	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

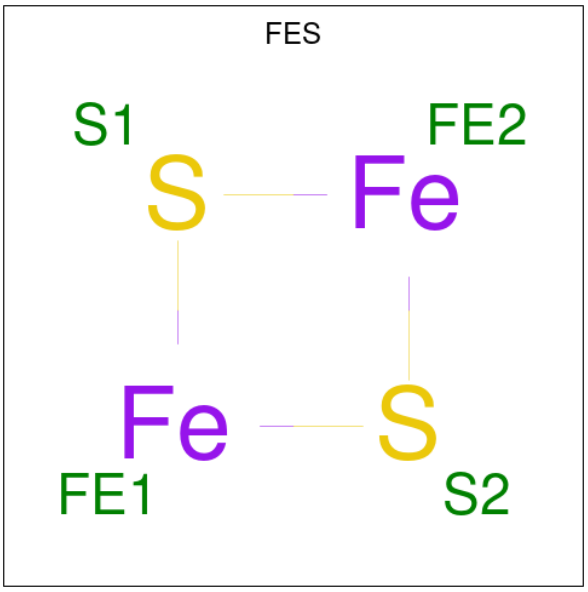


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 5 3 2	0	0

- Molecule 9 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

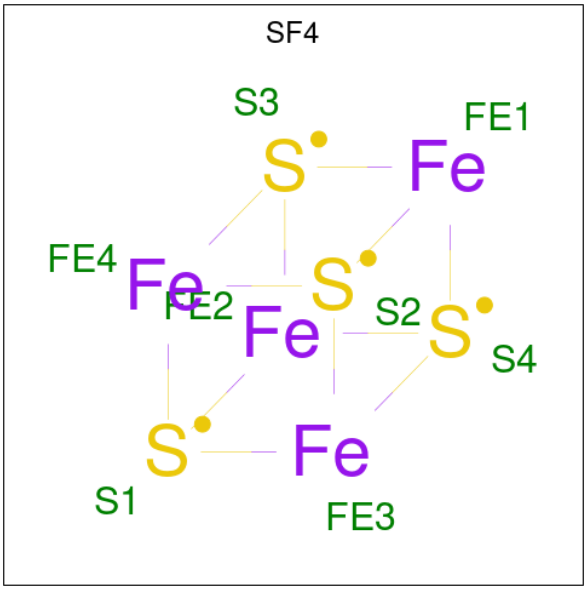
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	15	Total C N O P S 53 20 10 19 1 3	0	0
9	B	12	Total C N O S 53 21 11 19 2	0	0
9	C	5	Total C O 13 6 7	0	0
9	D	11	Total C N O 65 36 3 26	0	0

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



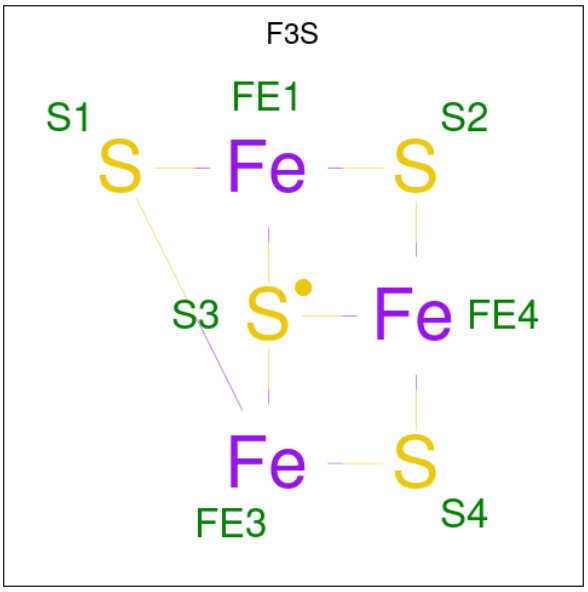
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
10	B	1	4	2	2	0	0

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



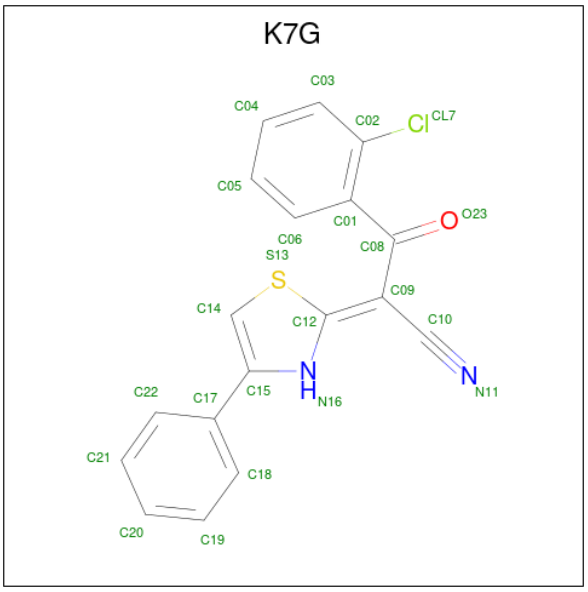
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
11	B	1	8	4	4	0	0

- Molecule 12 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



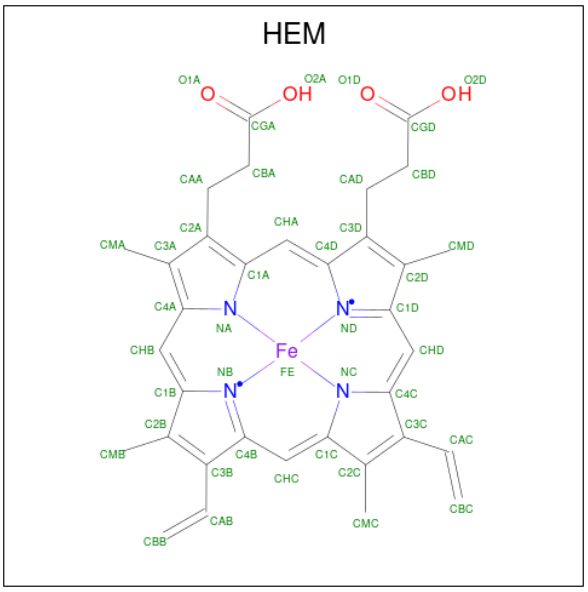
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Fe	S			
12	B	1	7	3	4		0	0

- Molecule 13 is thiapronil (three-letter code: K7G) (formula: $C_{18}H_{11}ClN_2OS$) (labeled as "Ligand of Interest" by depositor).



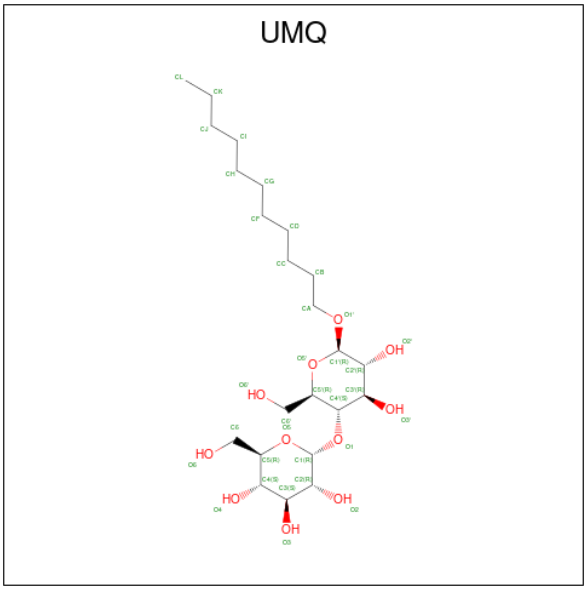
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
13	C	1	23	18	1	2	1	1	0	0

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



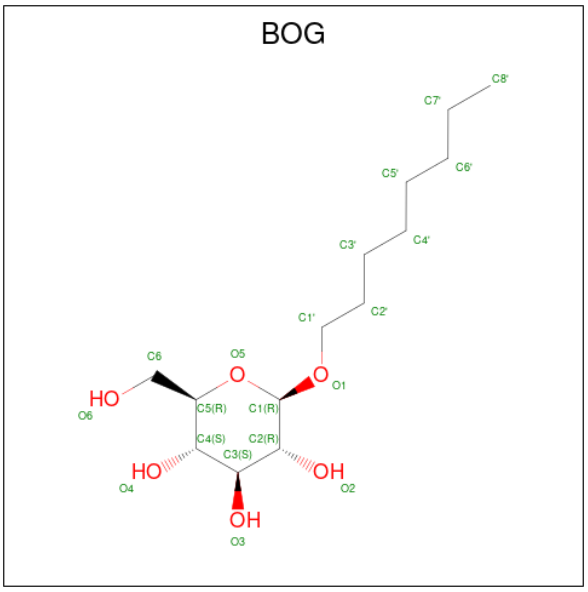
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	Fe	N	O	0	0
			41	32	1	4	4		

- Molecule 15 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



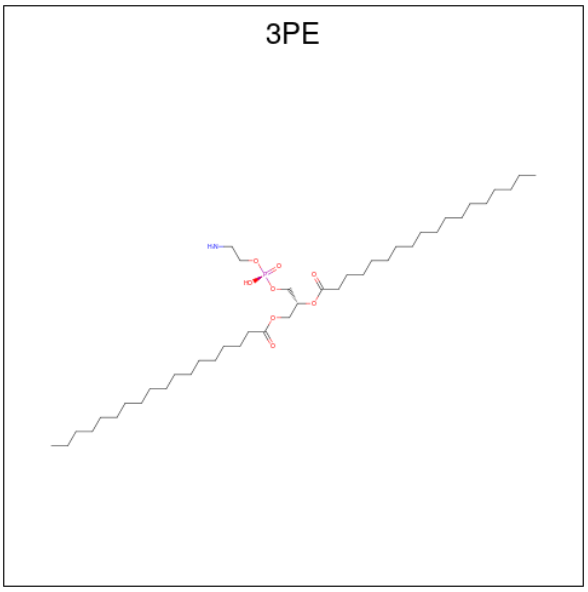
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			34	23	11		

- Molecule 16 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	D	1	Total	C	O		0	0
			20	14	6			

- Molecule 17 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	73	Total O 73 73	0	0
18	B	82	Total O 82 82	0	0
18	C	23	Total O 23 23	0	0
18	D	11	Total O 11 11	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 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.36Å 84.62Å 293.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.93 – 2.15	Depositor
% Data completeness (in resolution range)	89.7 (47.93-2.15)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 2.14Å)	Xtriage
Refinement program	PHENIX dev_3150	Depositor
R, R_{free}	0.218 , 0.238	Depositor
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.487	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9126	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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 55 ligands modelled in this entry, 1 is monoatomic and 43 are unknown - leaving 11 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	$\#\|Z\| > 2$
17	3PE	D	201	-	39,39,50	1.07	2 (5%)	42,44,55	1.06	3 (7%)
10	FES	B	1001	2	0,4,4	-	-	-		
14	HEM	C	201	3,4	40,48,50	1.31	3 (7%)	46,80,82	1.48	9 (19%)
8	PEG	A	1004	-	4,4,6	0.45	0	3,3,5	0.26	0
11	SF4	B	1002	2	0,12,12	-	-	-		
6	OAA	A	1002	-	8,8,8	2.58	4 (50%)	9,10,10	1.54	2 (22%)
13	K7G	C	202	-	24,25,25	2.18	8 (33%)	24,34,34	2.71	3 (12%)
16	BOG	D	1001	-	20,20,20	0.58	1 (5%)	25,25,25	0.82	1 (4%)
5	FAD	A	1001	1	53,58,58	0.82	1 (1%)	68,89,89	1.31	10 (14%)
15	UMQ	C	203	-	35,35,35	0.49	0	46,46,46	0.81	0
12	F3S	B	1003	2	0,9,9	-	-	-		

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
17	3PE	D	201	-	-	18/43/43/54	-
10	FES	B	1001	2	-	-	0/1/1/1
14	HEM	C	201	3,4	-	5/10/50/54	-
8	PEG	A	1004	-	-	2/2/2/4	-
6	OAA	A	1002	-	-	3/8/8/8	-
13	K7G	C	202	-	-	3/17/18/18	0/3/3/3
16	BOG	D	1001	-	-	3/11/31/31	0/1/1/1
11	SF4	B	1002	2	-	-	0/6/5/5
5	FAD	A	1001	1	-	6/30/50/50	0/6/6/6
15	UMQ	C	203	-	-	3/20/60/60	0/2/2/2
12	F3S	B	1003	2	-	-	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1002	OAA	O3-C3	5.30	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	202	K7G	C10-C09	4.94	1.53	1.43
17	D	201	3PE	O31-C31	4.42	1.46	1.33
13	C	202	K7G	C12-S13	-4.29	1.68	1.73
13	C	202	K7G	C09-C12	-4.26	1.32	1.39
17	D	201	3PE	O21-C21	4.10	1.45	1.34
13	C	202	K7G	C17-C15	4.04	1.53	1.47
13	C	202	K7G	C14-C15	3.90	1.42	1.35
6	A	1002	OAA	C2-C3	-3.39	1.37	1.51
13	C	202	K7G	C02-CL7	2.57	1.79	1.73
5	A	1001	FAD	C4-N3	-2.46	1.34	1.38
14	C	201	HEM	FE-ND	2.32	2.08	1.96
14	C	201	HEM	C2C-C3C	-2.26	1.34	1.41
13	C	202	K7G	O23-C08	-2.23	1.18	1.23
16	D	1001	BOG	O1-C1	2.19	1.43	1.40
14	C	201	HEM	CAB-C3B	2.16	1.55	1.50
13	C	202	K7G	C12-N16	-2.12	1.33	1.38
6	A	1002	OAA	O5-C4	-2.09	1.24	1.30
6	A	1002	OAA	C2-C1	2.08	1.54	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	202	K7G	C14-S13-C12	12.23	98.66	90.27
5	A	1001	FAD	C4-N3-C2	-4.17	117.94	125.64
17	D	201	3PE	O21-C21-C22	3.65	119.38	111.50
5	A	1001	FAD	C4X-C4-N3	3.52	122.13	113.19
14	C	201	HEM	C4D-ND-C1D	3.07	108.24	105.07
14	C	201	HEM	CAD-CBD-CGD	-3.00	107.15	113.60
6	A	1002	OAA	O3-C3-C2	2.96	124.87	120.58
14	C	201	HEM	C1B-NB-C4B	2.89	108.06	105.07
5	A	1001	FAD	O4-C4-C4X	-2.83	119.09	126.60
17	D	201	3PE	C2-O21-C21	-2.78	110.96	117.79
13	C	202	K7G	C02-C01-C08	-2.63	119.77	123.13
17	D	201	3PE	O31-C31-C32	2.57	119.98	111.91
5	A	1001	FAD	P-O3P-PA	-2.51	124.20	132.83
13	C	202	K7G	C09-C12-S13	2.48	127.89	122.96
14	C	201	HEM	C4C-CHD-C1D	2.48	125.83	122.56
5	A	1001	FAD	C4X-C10-N1	-2.47	118.99	124.73
5	A	1001	FAD	C10-N1-C2	2.45	121.81	116.90
14	C	201	HEM	C3D-C4D-ND	-2.41	107.48	110.17
5	A	1001	FAD	C4'-C3'-C2'	-2.37	108.44	113.36
14	C	201	HEM	C4B-CHC-C1C	2.33	125.63	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	D	1001	BOG	O1-C1-C2	2.18	111.70	108.30
14	C	201	HEM	CMA-C3A-C4A	-2.16	125.14	128.46
5	A	1001	FAD	O2-C2-N1	-2.14	118.29	121.83
5	A	1001	FAD	C4A-C5A-N7A	-2.11	107.20	109.40
5	A	1001	FAD	C4-C4X-N5	2.09	121.21	118.23
14	C	201	HEM	CAD-C3D-C2D	-2.08	124.00	127.88
6	A	1002	OAA	O2-C1-C2	2.07	121.16	114.54
14	C	201	HEM	C4C-C3C-C2C	2.05	108.26	106.85

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	FAD	N10-C1'-C2'-O2'
5	A	1001	FAD	N10-C1'-C2'-C3'
5	A	1001	FAD	PA-O3P-P-O5'
6	A	1002	OAA	O3-C3-C4-O4
6	A	1002	OAA	C2-C3-C4-O4
6	A	1002	OAA	C2-C3-C4-O5
13	C	202	K7G	C08-C09-C10-N11
17	D	201	3PE	C1-O11-P-O14
17	D	201	3PE	C11-O13-P-O12
17	D	201	3PE	O11-C1-C2-O21
17	D	201	3PE	C22-C21-O21-C2
17	D	201	3PE	O22-C21-O21-C2
15	C	203	UMQ	O5'-C1'-O1'-CA
16	D	1001	BOG	O5-C1-O1-C1'
17	D	201	3PE	C1-O11-P-O13
16	D	1001	BOG	C2'-C1'-O1-C1
15	C	203	UMQ	CG-CH-CI-CJ
17	D	201	3PE	O11-C1-C2-C3
16	D	1001	BOG	O1-C1'-C2'-C3'
14	C	201	HEM	C2A-CAA-CBA-CGA
14	C	201	HEM	C2D-C3D-CAD-CBD
14	C	201	HEM	C4D-C3D-CAD-CBD
17	D	201	3PE	C1-O11-P-O12
8	A	1004	PEG	O2-C3-C4-O4
17	D	201	3PE	C25-C26-C27-C28
13	C	202	K7G	N16-C15-C17-C18
13	C	202	K7G	N16-C15-C17-C22
5	A	1001	FAD	P-O3P-PA-O2A
17	D	201	3PE	C33-C34-C35-C36

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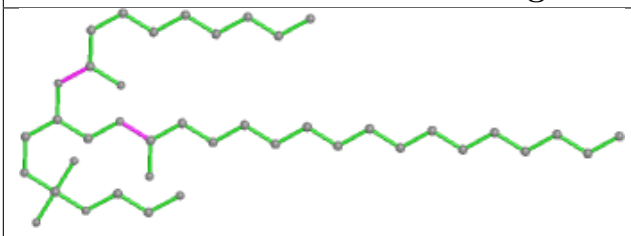
Mol	Chain	Res	Type	Atoms
15	C	203	UMQ	CC-CD-CF-CG
8	A	1004	PEG	C4-C3-O2-C2
17	D	201	3PE	C23-C24-C25-C26
17	D	201	3PE	O32-C31-O31-C3
17	D	201	3PE	C32-C31-O31-C3
17	D	201	3PE	O31-C31-C32-C33
5	A	1001	FAD	P-O3P-PA-O1A
17	D	201	3PE	C38-C39-C3A-C3B
14	C	201	HEM	CAA-CBA-CGA-O2A
17	D	201	3PE	C39-C3A-C3B-C3C
17	D	201	3PE	C11-O13-P-O14
5	A	1001	FAD	O4B-C4B-C5B-O5B
17	D	201	3PE	O32-C31-C32-C33
14	C	201	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

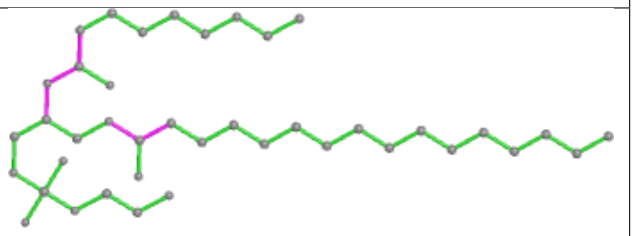
No monomer is involved in short contacts.

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.

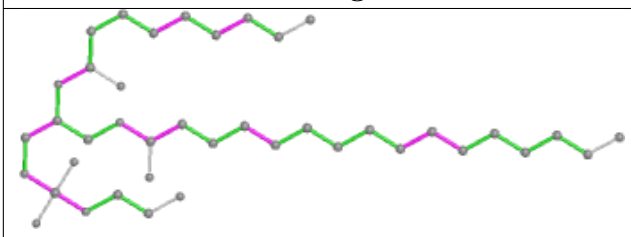
Ligand 3PE D 201



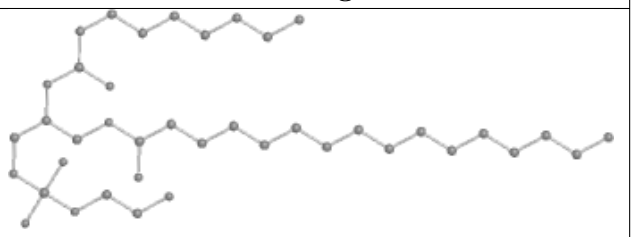
Bond lengths



Bond angles

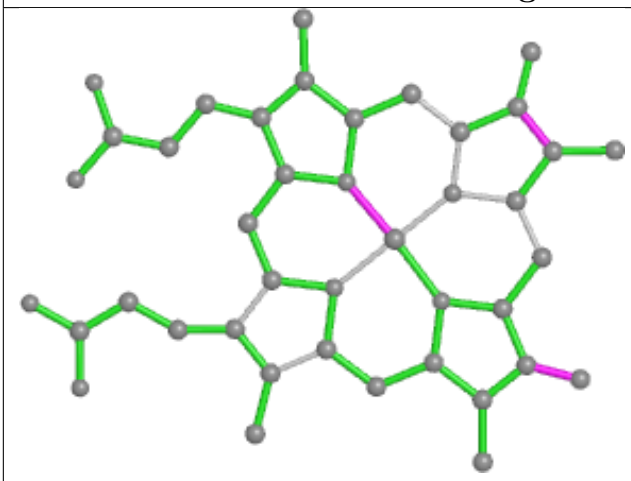


Torsions

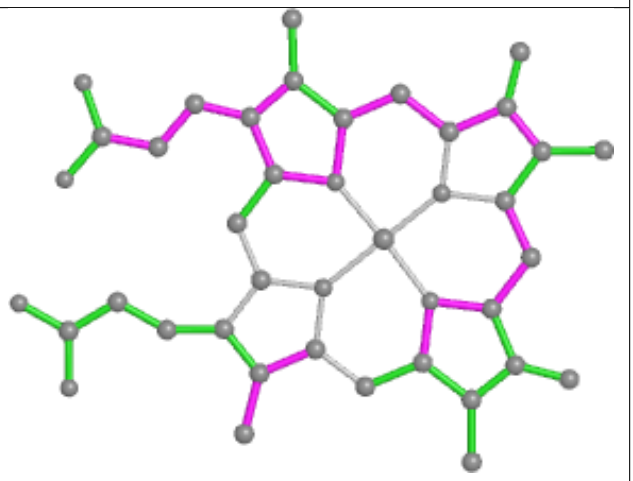


Rings

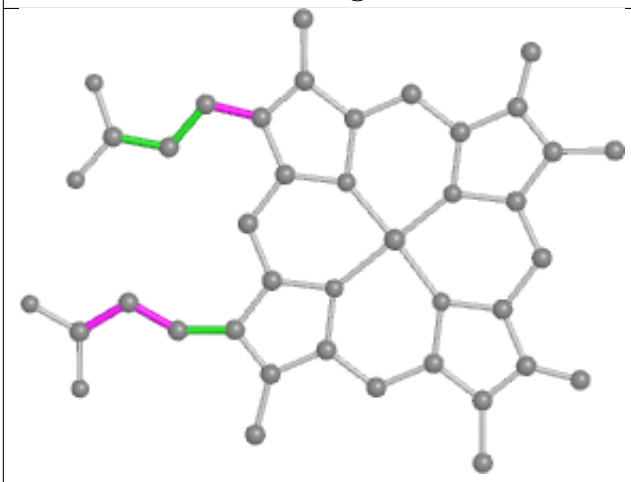
Ligand HEM C 201



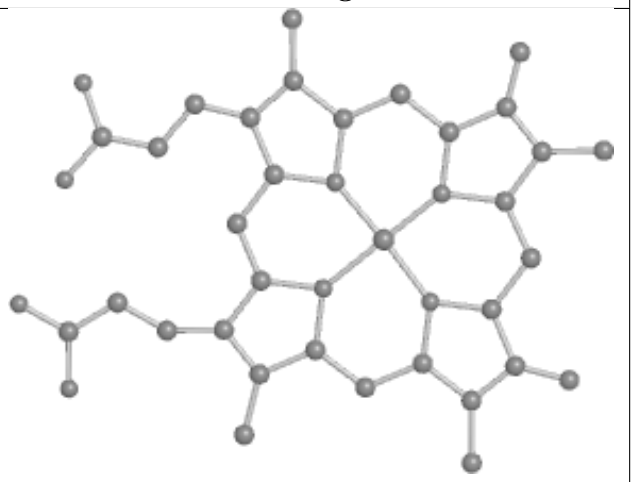
Bond lengths



Bond angles

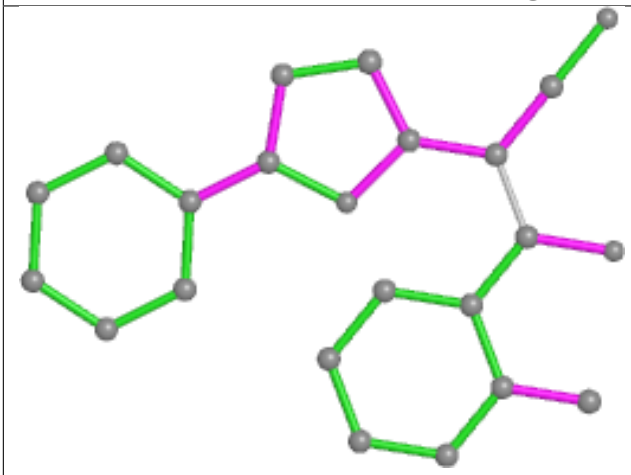


Torsions

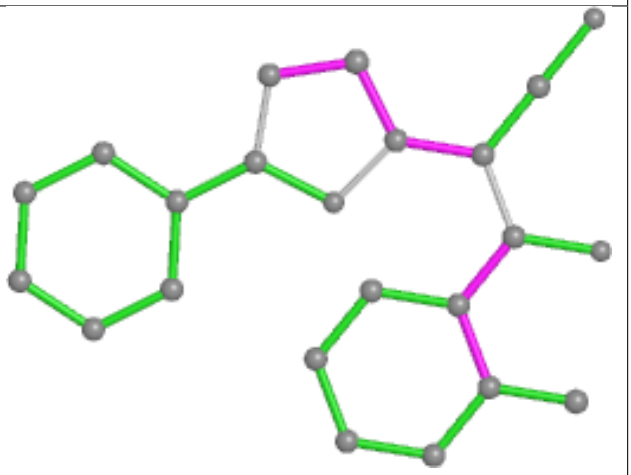


Rings

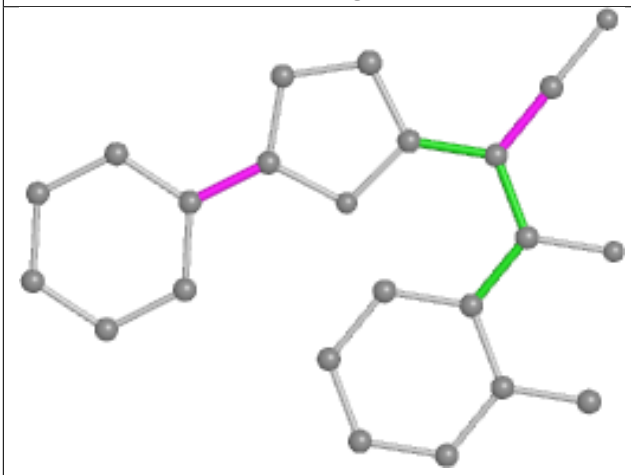
Ligand K7G C 202



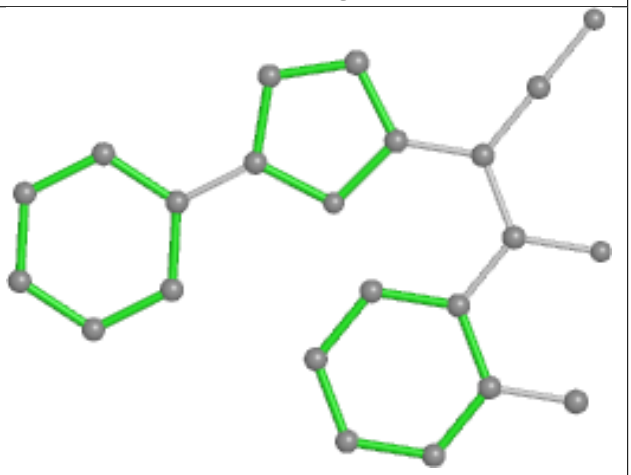
Bond lengths



Bond angles

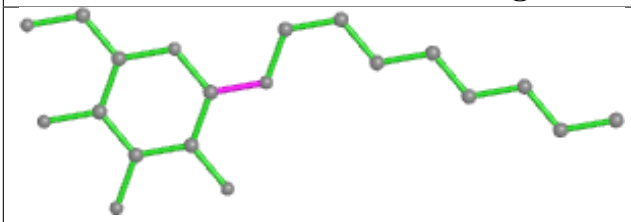


Torsions

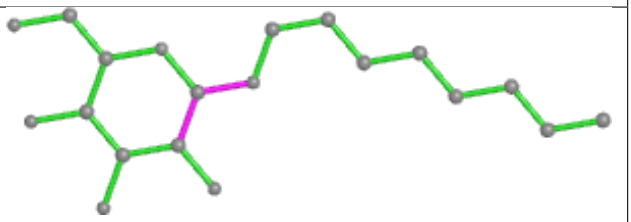


Rings

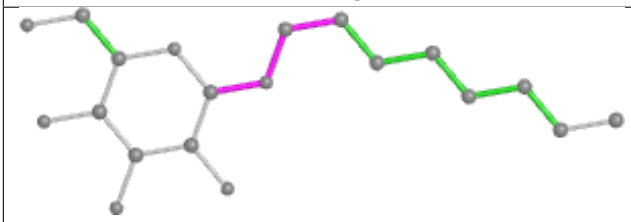
Ligand BOG D 1001



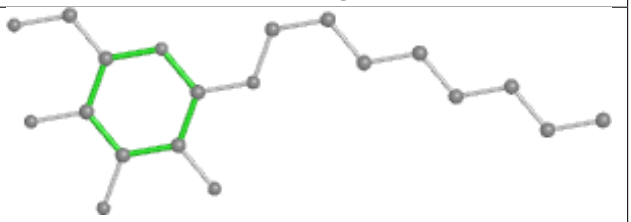
Bond lengths



Bond angles

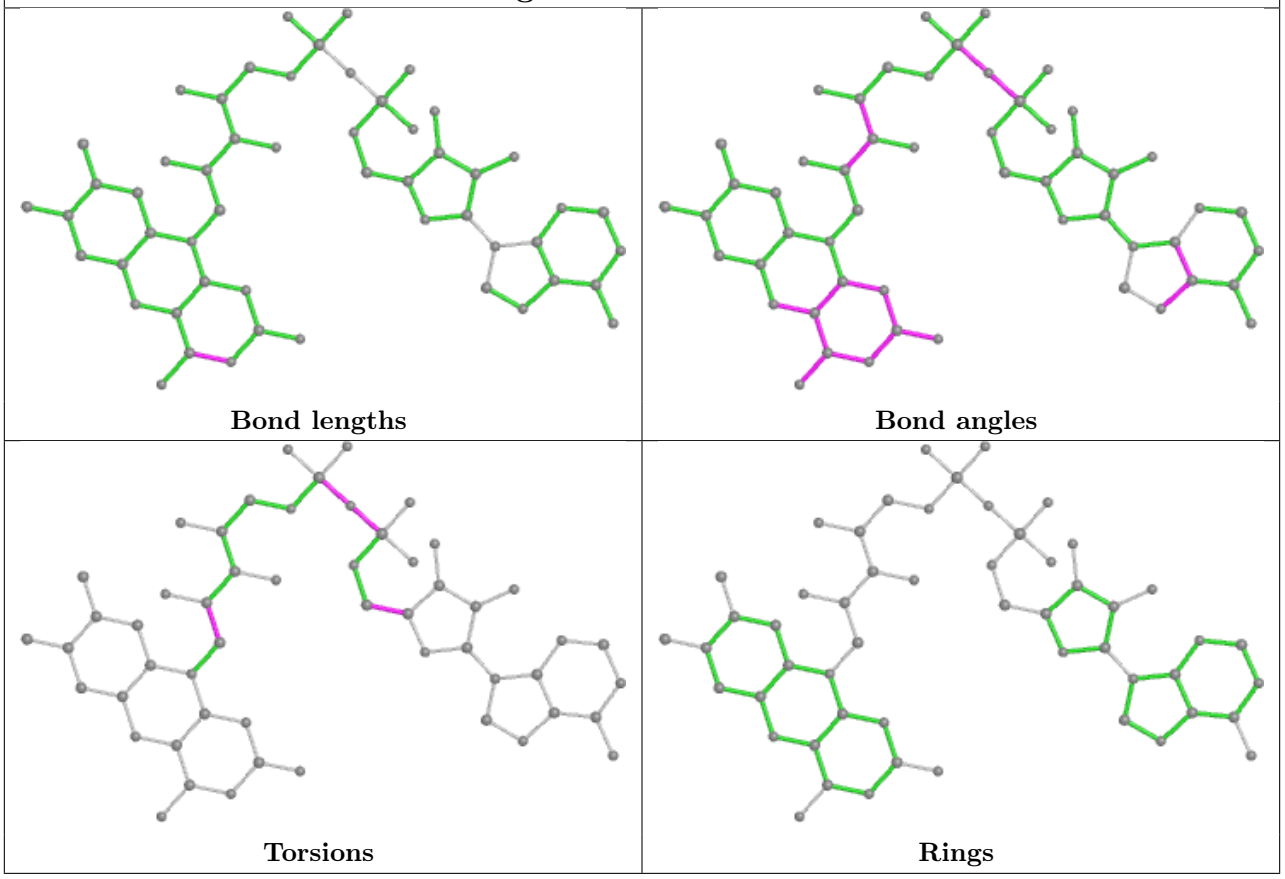


Torsions

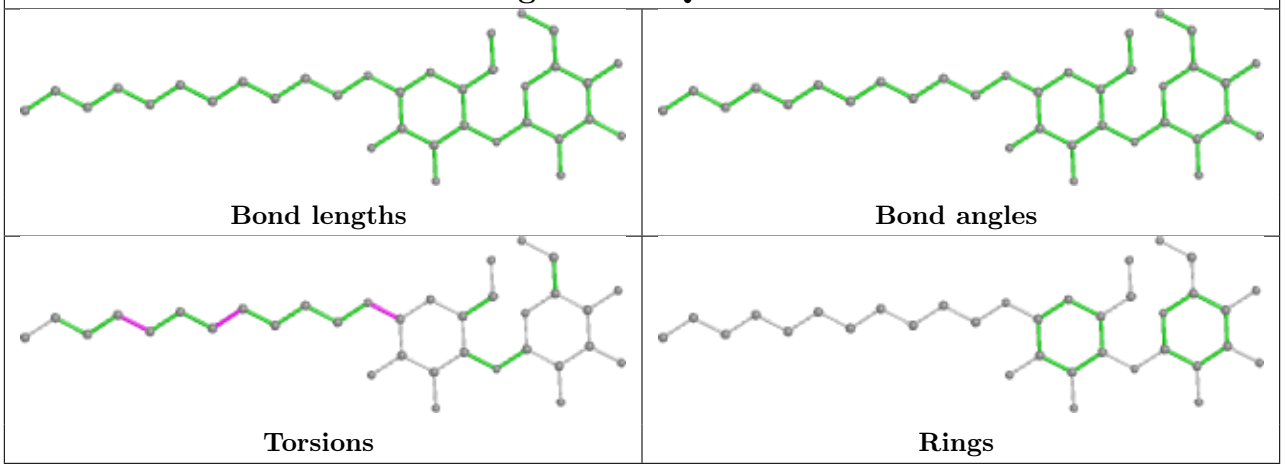


Rings

Ligand FAD A 1001



Ligand UMQ C 203



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.