Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 02:48 AM EDT

PDB ID	:	6U0S
Title	:	Crystal structure of the flavin-dependent monooxygenase PieE in complex with FAD and substrate
Authors	:	Shi, R.; Manenda, M.
Deposited on	:	2019-08-14
Resolution	:	2.52 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 2.52 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 27918 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 2,4-dichlorophenol 6-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	579	Total 4423	C 2764	N 828	O 821	S 10	0	0	0
1	B	579	Total 4423	C 2764	N 828	O 821	S 10	0	0	0
1	C	580	Total 4430	C 2768	N 829	O 823	S 10	0	0	0
1	D	579	Total 4423	C 2764	N 828	O 821	S 10	0	0	0
1	E	579	Total 4423	C 2764	N 828	O 821	S 10	0	0	0
1	F	580	Total 4427	C 2765	N 829	O 823	S 10	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP W0C4C9
A	-1	SER	-	expression tag	UNP W0C4C9
A	0	HIS	-	expression tag	UNP W0C4C9
B	-2	GLY	-	expression tag	UNP W0C4C9
B	-1	SER	-	expression tag	UNP W0C4C9
B	0	HIS	-	expression tag	UNP W0C4C9
C	-2	GLY	-	expression tag	UNP W0C4C9
C	-1	SER	-	expression tag	UNP W0C4C9
C	0	HIS	-	expression tag	UNP W0C4C9
D	-2	GLY	-	expression tag	UNP W0C4C9
D	-1	SER	-	expression tag	UNP W0C4C9
D	0	HIS	-	expression tag	UNP W0C4C9
E	-2	GLY	-	expression tag	UNP W0C4C9
E	-1	SER	-	expression tag	UNP W0C4C9
E	0	HIS	-	expression tag	UNP W0C4C9
F	-2	GLY	-	expression tag	UNP W0C4C9
F	-1	SER	-	expression tag	UNP W0C4C9

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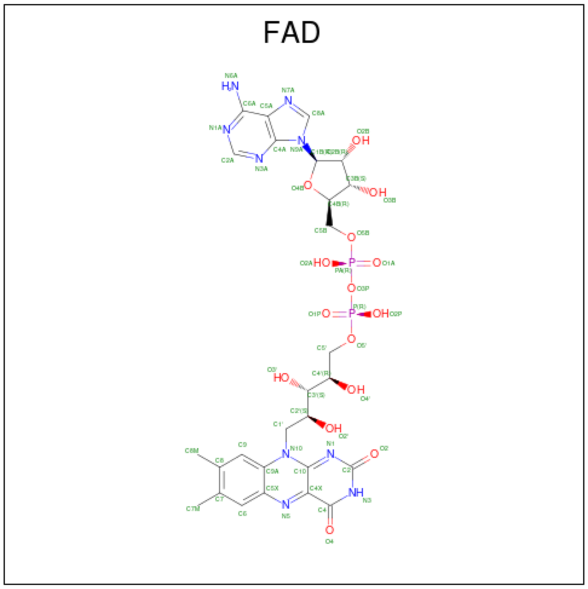
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP W0C4C9

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0
3	B	2	Total Cl 2 2	0	0

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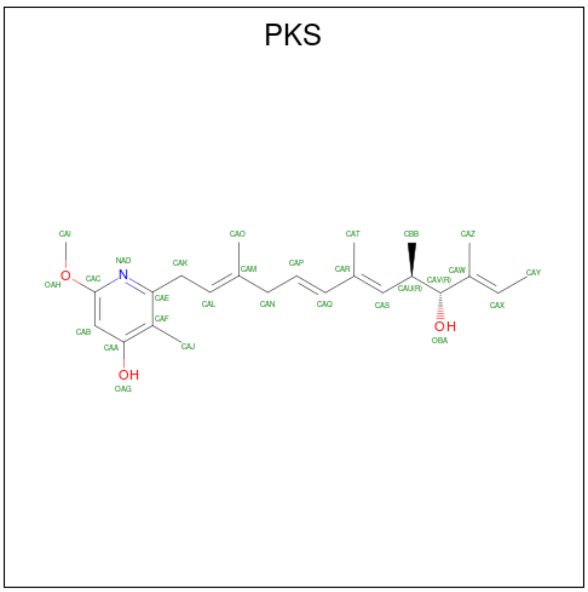
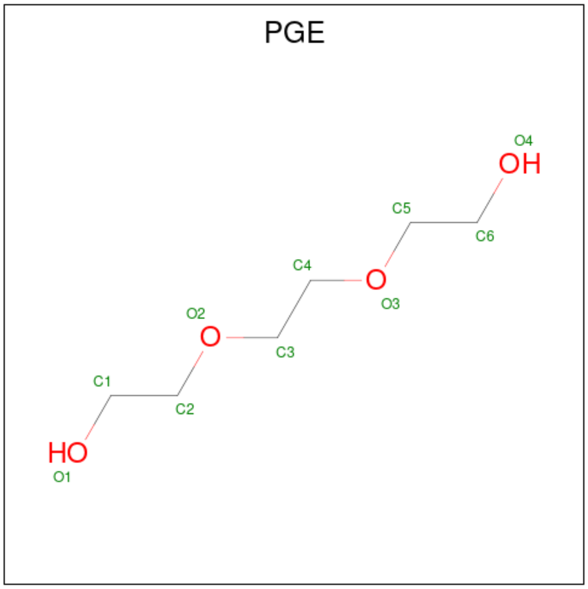
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Cl 1	0	0
3	D	2	Total 2	Cl 2	0	0
3	E	2	Total 2	Cl 2	0	0
3	F	2	Total 2	Cl 2	0	0

- Molecule 4 is 2-[(2E,5E,7E,9R,10R,11E)-10-hydroxy-3,7,9,11-tetramethyltrideca-2,5,7,11-tetraen-1-yl]-6-methoxy-3-methylpyridin-4-ol (three-letter code: PKS) (formula: $C_{24}H_{35}NO_3$) (labeled as "Ligand of Interest" by depositor).



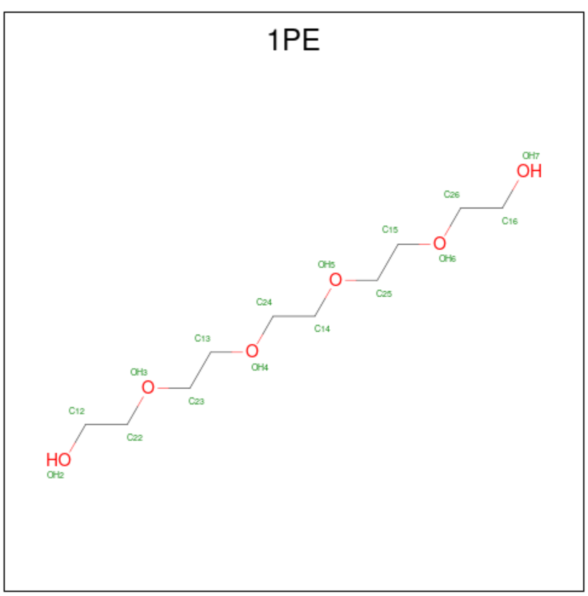
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 28	C 24	N 1	O 3	0	0
4	B	1	Total 28	C 24	N 1	O 3	0	0
4	C	1	Total 28	C 24	N 1	O 3	0	0
4	D	1	Total 28	C 24	N 1	O 3	0	0
4	E	1	Total 28	C 24	N 1	O 3	0	0
4	F	1	Total 28	C 24	N 1	O 3	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



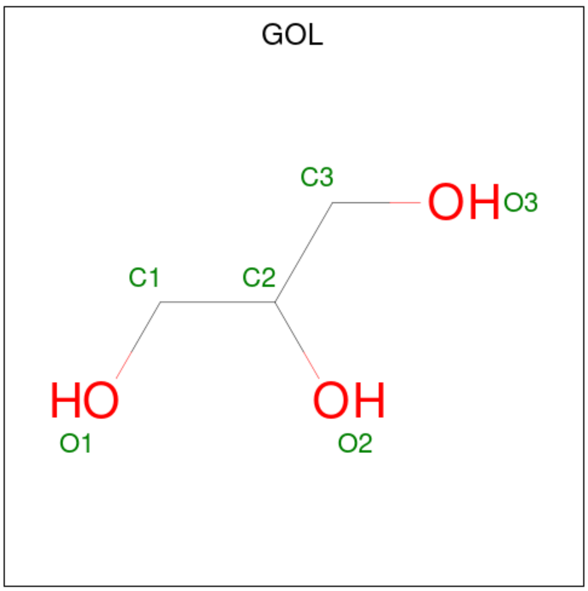
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 6 4	0	0
5	C	1	Total C O 10 6 4	0	0
5	C	1	Total C O 10 6 4	0	0
5	E	1	Total C O 10 6 4	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 16 10 6	0	0
6	B	1	Total C O 16 10 6	0	0
6	C	1	Total C O 16 10 6	0	0
6	D	1	Total C O 16 10 6	0	0
6	E	1	Total C O 16 10 6	0	0
6	F	1	Total C O 16 10 6	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0
7	E	1	Total C O 6 3 3	0	0
7	E	1	Total C O 6 3 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	177	Total O 177 177	0	0
8	B	113	Total O 113 113	0	0
8	C	205	Total O 205 205	0	0
8	D	88	Total O 88 88	0	0
8	E	56	Total O 56 56	0	0
8	F	61	Total O 61 61	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	91.34Å 187.13Å 239.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 2.52	Depositor
% Data completeness (in resolution range)	100.0 (49.12-2.52)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.187 , 0.239	Depositor
Wilson B-factor (Å^2)	47.4	Xtriage
Anisotropy	0.097	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	27918	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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 (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 11 are monoatomic - leaving 28 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	F	601	-	53,58,58	1.54	9 (16%)	68,89,89	1.58	11 (16%)
4	PKS	B	603	-	28,28,28	1.99	8 (28%)	35,37,37	2.23	10 (28%)
4	PKS	E	603	-	28,28,28	2.05	8 (28%)	35,37,37	2.17	8 (22%)
7	GOL	A	608	-	5,5,5	0.11	0	5,5,5	0.25	0
4	PKS	F	603	-	28,28,28	2.07	5 (17%)	35,37,37	2.29	8 (22%)
7	GOL	D	601	-	5,5,5	0.18	0	5,5,5	0.46	0
5	PGE	A	604	-	9,9,9	0.27	0	8,8,8	0.18	0
7	GOL	E	607	-	5,5,5	0.16	0	5,5,5	0.53	0
5	PGE	C	701	-	9,9,9	0.31	0	8,8,8	0.16	0
6	1PE	E	605	-	15,15,15	0.59	0	14,14,14	0.48	0
6	1PE	B	604	-	15,15,15	0.58	0	14,14,14	0.42	0
4	PKS	D	604	-	28,28,28	2.34	9 (32%)	35,37,37	1.80	7 (20%)
4	PKS	C	703	-	28,28,28	2.29	8 (28%)	35,37,37	2.23	13 (37%)
2	FAD	B	601	-	53,58,58	1.56	10 (18%)	68,89,89	1.54	13 (19%)
7	GOL	D	607	-	5,5,5	0.12	0	5,5,5	0.39	0
7	GOL	A	607	-	5,5,5	0.13	0	5,5,5	0.33	0
6	1PE	C	705	-	15,15,15	0.67	0	14,14,14	0.61	0
6	1PE	A	605	-	15,15,15	0.52	0	14,14,14	0.48	0
7	GOL	E	608	-	5,5,5	0.15	0	5,5,5	0.50	0
5	PGE	C	704	-	9,9,9	0.28	0	8,8,8	0.16	0
5	PGE	E	604	-	9,9,9	0.34	0	8,8,8	0.18	0
6	1PE	F	604	-	15,15,15	0.65	0	14,14,14	0.39	0
6	1PE	D	605	-	15,15,15	0.60	0	14,14,14	0.30	0
4	PKS	A	603	-	28,28,28	2.48	9 (32%)	35,37,37	2.65	16 (45%)
2	FAD	E	601	-	53,58,58	1.50	7 (13%)	68,89,89	1.58	16 (23%)
2	FAD	A	601	-	53,58,58	1.73	10 (18%)	68,89,89	1.68	17 (25%)
2	FAD	D	602	-	53,58,58	1.56	8 (15%)	68,89,89	1.48	18 (26%)
2	FAD	C	702	-	53,58,58	1.79	13 (24%)	68,89,89	1.55	11 (16%)

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	F	601	-	-	4/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PKS	B	603	-	-	4/27/27/27	0/1/1/1
4	PKS	E	603	-	-	10/27/27/27	0/1/1/1
7	GOL	A	608	-	-	4/4/4/4	-
4	PKS	F	603	-	-	9/27/27/27	0/1/1/1
7	GOL	D	601	-	-	4/4/4/4	-
5	PGE	A	604	-	-	5/7/7/7	-
7	GOL	E	607	-	-	0/4/4/4	-
5	PGE	C	701	-	-	4/7/7/7	-
6	1PE	E	605	-	-	12/13/13/13	-
6	1PE	B	604	-	-	10/13/13/13	-
4	PKS	D	604	-	-	10/27/27/27	0/1/1/1
4	PKS	C	703	-	-	11/27/27/27	0/1/1/1
2	FAD	B	601	-	-	13/30/50/50	0/6/6/6
7	GOL	D	607	-	-	4/4/4/4	-
7	GOL	A	607	-	-	4/4/4/4	-
6	1PE	C	705	-	-	7/13/13/13	-
6	1PE	A	605	-	-	7/13/13/13	-
7	GOL	E	608	-	-	4/4/4/4	-
5	PGE	C	704	-	-	3/7/7/7	-
5	PGE	E	604	-	-	3/7/7/7	-
6	1PE	F	604	-	-	10/13/13/13	-
6	1PE	D	605	-	-	9/13/13/13	-
4	PKS	A	603	-	-	9/27/27/27	0/1/1/1
2	FAD	E	601	-	-	4/30/50/50	0/6/6/6
2	FAD	A	601	-	-	7/30/50/50	0/6/6/6
2	FAD	D	602	-	-	10/30/50/50	0/6/6/6
2	FAD	C	702	-	-	8/30/50/50	0/6/6/6

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	PKS	CAK-CAE	9.19	1.58	1.51
4	C	703	PKS	CAK-CAE	7.73	1.57	1.51
4	D	604	PKS	CAK-CAE	7.45	1.57	1.51
2	C	702	FAD	C9A-C5X	6.69	1.52	1.41
4	F	603	PKS	CAK-CAE	6.48	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	603	PKS	CAK-CAE	6.26	1.56	1.51
2	D	602	FAD	C9A-C5X	5.83	1.50	1.41
2	E	601	FAD	C9A-C5X	5.71	1.50	1.41
2	B	601	FAD	C9A-C5X	5.55	1.50	1.41
2	A	601	FAD	C9A-C5X	5.51	1.50	1.41
2	F	601	FAD	C9A-C5X	5.49	1.50	1.41
2	A	601	FAD	C8-C7	4.85	1.53	1.40
4	B	603	PKS	OAH-CAC	4.82	1.43	1.35
4	F	603	PKS	OAH-CAC	4.58	1.42	1.35
4	D	604	PKS	CAQ-CAR	4.40	1.55	1.45
4	E	603	PKS	CAQ-CAR	4.31	1.55	1.45
2	E	601	FAD	C8-C7	4.25	1.51	1.40
4	D	604	PKS	OAH-CAC	4.16	1.42	1.35
4	C	703	PKS	OAH-CAC	4.05	1.41	1.35
4	C	703	PKS	CAQ-CAR	3.98	1.54	1.45
4	A	603	PKS	OAH-CAC	3.96	1.41	1.35
2	A	601	FAD	C10-N10	3.92	1.45	1.37
2	F	601	FAD	C8-C7	3.91	1.50	1.40
2	D	602	FAD	C8-C7	3.91	1.50	1.40
2	C	702	FAD	C8-C7	3.91	1.50	1.40
2	B	601	FAD	C8-C7	3.91	1.50	1.40
4	B	603	PKS	CAK-CAE	3.81	1.54	1.51
2	D	602	FAD	C10-N10	3.71	1.45	1.37
4	B	603	PKS	CAQ-CAR	3.62	1.53	1.45
2	C	702	FAD	C10-N10	3.52	1.45	1.37
2	E	601	FAD	C10-N10	3.52	1.45	1.37
4	A	603	PKS	CAQ-CAR	3.52	1.53	1.45
4	F	603	PKS	CAQ-CAR	3.43	1.53	1.45
2	A	601	FAD	C4X-N5	3.27	1.37	1.30
2	F	601	FAD	C4X-N5	3.20	1.37	1.30
2	D	602	FAD	C4X-N5	3.17	1.36	1.30
2	F	601	FAD	C10-N10	3.17	1.44	1.37
2	C	702	FAD	C1'-C2'	3.14	1.57	1.52
2	B	601	FAD	C10-N10	3.10	1.44	1.37
2	A	601	FAD	C4X-C10	3.08	1.53	1.44
4	B	603	PKS	CAC-NAD	2.97	1.38	1.33
4	C	703	PKS	CAA-CAF	-2.93	1.36	1.40
2	B	601	FAD	C5A-C4A	2.93	1.48	1.40
2	D	602	FAD	C5A-C4A	2.89	1.48	1.40
2	E	601	FAD	C4X-N5	2.87	1.36	1.30
2	A	601	FAD	C5A-C4A	2.85	1.48	1.40
2	C	702	FAD	C4X-N5	2.84	1.36	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	PKS	CAA-CAF	-2.78	1.37	1.40
4	D	604	PKS	CAB-CAC	2.76	1.43	1.38
2	C	702	FAD	C5A-C4A	2.76	1.48	1.40
4	A	603	PKS	CAF-CAE	2.75	1.42	1.39
2	E	601	FAD	C5A-C4A	2.75	1.48	1.40
2	B	601	FAD	C9A-N10	2.68	1.45	1.41
2	F	601	FAD	C5A-C4A	2.67	1.48	1.40
2	C	702	FAD	C4-N3	-2.63	1.34	1.38
4	B	603	PKS	OAG-CAA	2.61	1.41	1.36
2	F	601	FAD	C4-N3	-2.58	1.34	1.38
4	A	603	PKS	CAL-CAM	2.56	1.39	1.33
2	A	601	FAD	C9A-N10	2.55	1.45	1.41
2	B	601	FAD	C4X-N5	2.55	1.35	1.30
2	A	601	FAD	C10-N1	2.53	1.38	1.33
2	A	601	FAD	O4B-C1B	2.51	1.44	1.41
4	E	603	PKS	CAB-CAC	2.50	1.42	1.38
4	B	603	PKS	CAL-CAM	2.43	1.38	1.33
2	C	702	FAD	C4X-C10	2.42	1.51	1.44
4	E	603	PKS	OAH-CAC	2.42	1.39	1.35
4	D	604	PKS	CAK-CAL	2.42	1.56	1.50
4	E	603	PKS	OAG-CAA	2.41	1.41	1.36
4	D	604	PKS	CAT-CAR	2.40	1.55	1.50
2	B	601	FAD	C4X-C10	2.38	1.51	1.44
4	D	604	PKS	CAA-CAF	-2.38	1.37	1.40
2	B	601	FAD	C2A-N3A	2.37	1.35	1.32
2	E	601	FAD	C4X-C10	2.34	1.51	1.44
2	D	602	FAD	C10-N1	2.30	1.37	1.33
4	A	603	PKS	CAC-NAD	2.30	1.37	1.33
4	E	603	PKS	CAK-CAL	2.28	1.55	1.50
2	C	702	FAD	C9A-N10	2.27	1.45	1.41
4	C	703	PKS	OAG-CAA	2.25	1.41	1.36
4	E	603	PKS	CAT-CAR	2.25	1.55	1.50
4	C	703	PKS	CAS-CAR	2.24	1.41	1.34
4	C	703	PKS	CAL-CAM	2.23	1.38	1.33
2	F	601	FAD	C2A-N3A	2.22	1.35	1.32
4	F	603	PKS	CAB-CAC	2.21	1.42	1.38
2	E	601	FAD	C4-N3	-2.20	1.34	1.38
4	C	703	PKS	CAT-CAR	2.19	1.55	1.50
4	D	604	PKS	CAL-CAM	2.18	1.38	1.33
4	D	604	PKS	CAC-NAD	2.15	1.36	1.33
2	C	702	FAD	C2A-N3A	2.14	1.35	1.32
4	E	603	PKS	CAL-CAM	2.13	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	PKS	CAT-CAR	2.13	1.55	1.50
2	F	601	FAD	C6A-C5A	2.11	1.51	1.43
2	D	602	FAD	C2A-N3A	2.11	1.35	1.32
2	F	601	FAD	C4X-C10	2.09	1.50	1.44
2	C	702	FAD	C5X-N5	-2.09	1.35	1.39
2	A	601	FAD	C6A-C5A	2.09	1.51	1.43
2	D	602	FAD	C4X-C10	2.09	1.50	1.44
4	B	603	PKS	CAA-CAF	-2.08	1.37	1.40
4	A	603	PKS	CAZ-CAW	2.07	1.54	1.50
2	B	601	FAD	C10-N1	2.07	1.37	1.33
2	C	702	FAD	C10-N1	2.05	1.37	1.33
2	B	601	FAD	C6A-C5A	2.04	1.50	1.43
4	A	603	PKS	CAT-CAR	2.03	1.55	1.50
4	F	603	PKS	CAA-CAF	-2.02	1.37	1.40
2	C	702	FAD	C2'-C3'	2.02	1.57	1.53

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	603	PKS	CAN-CAP-CAQ	-8.90	110.35	124.18
4	C	703	PKS	CAP-CAQ-CAR	-7.07	115.20	125.89
4	E	603	PKS	CAP-CAQ-CAR	-6.63	115.87	125.89
4	B	603	PKS	CAN-CAP-CAQ	-6.15	114.63	124.18
4	F	603	PKS	CAK-CAL-CAM	-6.15	117.71	127.24
4	F	603	PKS	CAN-CAP-CAQ	-5.85	115.10	124.18
4	E	603	PKS	CAE-CAK-CAL	-5.67	103.23	112.18
4	B	603	PKS	CAE-CAK-CAL	-5.46	103.56	112.18
4	B	603	PKS	CAK-CAL-CAM	-5.08	119.36	127.24
4	F	603	PKS	CAP-CAQ-CAR	-4.62	118.90	125.89
4	A	603	PKS	CAJ-CAF-CAA	-4.39	115.67	120.84
4	A	603	PKS	CAE-CAK-CAL	-4.35	105.30	112.18
2	E	601	FAD	N3A-C2A-N1A	-4.35	121.89	128.68
4	A	603	PKS	CAF-CAE-NAD	-4.34	119.28	123.87
4	D	604	PKS	CAE-CAK-CAL	-4.25	105.46	112.18
4	F	603	PKS	CAB-CAC-NAD	-4.22	119.16	124.08
4	F	603	PKS	CAE-CAK-CAL	-4.18	105.58	112.18
2	F	601	FAD	C4A-C5A-N7A	-4.06	105.17	109.40
4	D	604	PKS	CAA-CAF-CAE	4.02	119.47	116.51
4	C	703	PKS	CAB-CAC-NAD	-4.00	119.42	124.08
2	F	601	FAD	C4-C4X-N5	3.99	123.91	118.23
4	E	603	PKS	CAK-CAL-CAM	-3.88	121.22	127.24
2	A	601	FAD	C7M-C7-C8	3.76	128.44	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	FAD	C4X-C10-N1	-3.75	116.02	124.73
4	D	604	PKS	CAK-CAL-CAM	-3.73	121.46	127.24
2	B	601	FAD	O4-C4-C4X	-3.72	116.72	126.60
4	E	603	PKS	CAA-CAF-CAE	3.71	119.25	116.51
2	D	602	FAD	C4X-C10-N1	-3.69	116.18	124.73
2	C	702	FAD	C4X-C10-N1	-3.68	116.18	124.73
2	A	601	FAD	C4A-C5A-N7A	-3.63	105.62	109.40
4	C	703	PKS	CAN-CAP-CAQ	-3.61	118.57	124.18
2	A	601	FAD	C4X-C10-N1	-3.60	116.37	124.73
4	C	703	PKS	CAF-CAE-NAD	-3.59	120.07	123.87
2	E	601	FAD	C1B-N9A-C4A	-3.51	120.47	126.64
4	B	603	PKS	CAB-CAC-NAD	-3.51	119.99	124.08
2	B	601	FAD	C4X-C10-N1	-3.47	116.67	124.73
4	D	604	PKS	CAN-CAP-CAQ	-3.46	118.81	124.18
2	A	601	FAD	C7M-C7-C6	-3.46	113.10	119.49
2	C	702	FAD	C4A-C5A-N7A	-3.42	105.84	109.40
2	F	601	FAD	C4X-C10-N1	-3.40	116.85	124.73
4	A	603	PKS	CAO-CAM-CAN	3.37	122.73	114.88
4	A	603	PKS	CAJ-CAF-CAE	3.35	125.61	122.69
2	F	601	FAD	C3B-C2B-C1B	3.33	106.00	100.98
2	C	702	FAD	C9A-N10-C10	-3.32	115.59	120.77
2	A	601	FAD	N3-C2-N1	3.28	125.82	119.38
4	D	604	PKS	CAP-CAQ-CAR	-3.27	120.95	125.89
4	B	603	PKS	CAA-CAF-CAE	3.24	118.90	116.51
2	A	601	FAD	N3A-C2A-N1A	-3.24	123.61	128.68
2	D	602	FAD	N3A-C2A-N1A	-3.14	123.77	128.68
2	B	601	FAD	C3B-C2B-C1B	3.03	105.55	100.98
4	D	604	PKS	CAF-CAE-NAD	-3.03	120.67	123.87
4	E	603	PKS	CAF-CAE-NAD	-3.03	120.67	123.87
2	B	601	FAD	C4A-C5A-N7A	-3.03	106.25	109.40
2	F	601	FAD	C9A-N10-C10	-3.02	116.07	120.77
4	C	703	PKS	CAN-CAM-CAL	-3.00	112.71	121.06
4	A	603	PKS	CAA-CAF-CAE	2.99	118.72	116.51
4	B	603	PKS	CAO-CAM-CAN	2.99	121.85	114.88
2	A	601	FAD	C4-N3-C2	-2.97	120.15	125.64
4	B	603	PKS	CAZ-CAW-CAX	-2.97	115.65	123.48
2	C	702	FAD	C1'-C2'-C3'	2.94	118.00	109.79
2	E	601	FAD	C2A-N1A-C6A	2.91	123.72	118.75
4	C	703	PKS	CAT-CAR-CAQ	-2.89	113.53	118.08
4	A	603	PKS	CAN-CAM-CAL	-2.88	113.04	121.06
2	B	601	FAD	C4-N3-C2	-2.88	120.32	125.64
2	E	601	FAD	C4-N3-C2	-2.88	120.32	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	703	PKS	CAJ-CAF-CAE	-2.87	120.18	122.69
2	D	602	FAD	C4-C4X-N5	2.85	122.29	118.23
2	D	602	FAD	C10-N1-C2	2.82	122.55	116.90
4	C	703	PKS	CAA-CAF-CAE	2.82	118.59	116.51
2	A	601	FAD	C1B-N9A-C4A	-2.82	121.69	126.64
4	F	603	PKS	CAO-CAM-CAN	2.81	121.44	114.88
2	C	702	FAD	N3A-C2A-N1A	-2.81	124.29	128.68
4	B	603	PKS	CAZ-CAW-CAV	2.80	121.93	115.85
4	A	603	PKS	CAP-CAQ-CAR	-2.80	121.66	125.89
2	F	601	FAD	N3A-C2A-N1A	-2.80	124.31	128.68
2	B	601	FAD	N3-C2-N1	2.77	124.83	119.38
2	C	702	FAD	C4'-C3'-C2'	2.74	119.06	113.36
4	C	703	PKS	CAC-NAD-CAE	2.74	121.55	117.64
4	C	703	PKS	CAO-CAM-CAN	2.73	121.25	114.88
2	F	601	FAD	C9A-C5X-N5	-2.72	119.47	122.43
2	C	702	FAD	C4X-C10-N10	2.69	120.41	116.48
2	C	702	FAD	C10-N1-C2	2.68	122.26	116.90
2	F	601	FAD	C10-N1-C2	2.68	122.26	116.90
4	F	603	PKS	CAF-CAE-NAD	-2.67	121.05	123.87
4	E	603	PKS	CAO-CAM-CAN	2.66	121.08	114.88
2	B	601	FAD	O2'-C2'-C3'	-2.65	102.65	109.10
2	F	601	FAD	C10-C4X-N5	-2.64	119.25	124.86
4	A	603	PKS	CAB-CAC-NAD	-2.63	121.01	124.08
2	A	601	FAD	O2-C2-N3	-2.62	113.55	118.65
2	E	601	FAD	C10-N1-C2	2.61	122.12	116.90
2	D	602	FAD	C4-N3-C2	-2.60	120.83	125.64
2	E	601	FAD	O4B-C4B-C3B	2.59	110.23	105.11
2	D	602	FAD	C4X-C4-N3	2.57	119.72	113.19
2	A	601	FAD	N10-C10-N1	2.57	125.73	118.35
2	E	601	FAD	C4-C4X-N5	2.54	121.85	118.23
2	B	601	FAD	C9A-N10-C10	-2.53	116.83	120.77
2	B	601	FAD	N3A-C2A-N1A	-2.50	124.77	128.68
2	D	602	FAD	C3B-C2B-C1B	2.49	104.73	100.98
2	B	601	FAD	N10-C10-N1	2.48	125.49	118.35
2	D	602	FAD	O4-C4-C4X	-2.48	120.02	126.60
2	E	601	FAD	C4X-C4-N3	2.46	119.44	113.19
2	C	702	FAD	O4'-C4'-C3'	2.45	115.06	109.10
2	E	601	FAD	N3-C2-N1	2.44	124.17	119.38
2	A	601	FAD	C4X-C4-N3	2.43	119.37	113.19
2	C	702	FAD	C5X-C9A-N10	2.43	120.46	117.95
2	D	602	FAD	O2B-C2B-C1B	-2.38	102.05	110.85
4	A	603	PKS	CAT-CAR-CAQ	2.38	121.83	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	602	FAD	N10-C10-N1	2.38	125.19	118.35
4	C	703	PKS	CAK-CAE-NAD	2.36	120.89	116.25
2	D	602	FAD	C9A-C5X-N5	-2.33	119.90	122.43
2	F	601	FAD	C4X-C4-N3	2.33	119.11	113.19
4	A	603	PKS	CAC-NAD-CAE	2.33	120.97	117.64
4	F	603	PKS	CAC-NAD-CAE	2.32	120.97	117.64
2	E	601	FAD	C4A-C5A-N7A	-2.29	107.01	109.40
2	A	601	FAD	O4-C4-C4X	-2.28	120.56	126.60
2	B	601	FAD	C4X-C4-N3	2.26	118.93	113.19
2	A	601	FAD	C4-C4X-N5	2.25	121.44	118.23
2	D	602	FAD	C1'-N10-C9A	-2.25	116.76	120.51
4	E	603	PKS	CAU-CAS-CAR	-2.22	119.63	126.67
2	B	601	FAD	O4-C4-N3	2.21	124.35	120.12
2	B	601	FAD	C6-C5X-C9A	2.19	122.03	118.94
2	E	601	FAD	C5X-N5-C4X	2.18	121.70	118.07
2	E	601	FAD	C10-C4X-N5	-2.18	120.23	124.86
2	E	601	FAD	O4-C4-C4X	-2.17	120.83	126.60
2	E	601	FAD	N10-C10-N1	2.15	124.54	118.35
2	F	601	FAD	C4-N3-C2	-2.14	121.68	125.64
2	D	602	FAD	C4A-C5A-N7A	-2.14	107.17	109.40
2	A	601	FAD	C2A-N1A-C6A	2.13	122.40	118.75
2	D	602	FAD	C10-C4X-N5	-2.13	120.34	124.86
4	A	603	PKS	OBA-CAV-CAU	-2.09	104.67	108.10
4	B	603	PKS	CAP-CAQ-CAR	-2.08	122.75	125.89
4	A	603	PKS	CBB-CAU-CAS	-2.07	106.60	110.05
2	D	602	FAD	C9A-N10-C10	-2.07	117.55	120.77
4	B	603	PKS	CAF-CAE-NAD	-2.05	121.70	123.87
4	A	603	PKS	CAZ-CAW-CAX	-2.05	118.08	123.48
2	D	602	FAD	N6A-C6A-N1A	2.05	122.82	118.57
4	D	604	PKS	CAJ-CAF-CAE	-2.04	120.91	122.69
4	E	603	PKS	CAJ-CAF-CAE	-2.04	120.91	122.69
2	A	601	FAD	C5A-C6A-N6A	2.04	123.45	120.35
2	C	702	FAD	C6-C5X-C9A	2.04	121.82	118.94
4	C	703	PKS	OAH-CAC-CAB	2.04	124.48	118.09
2	A	601	FAD	C10-C4X-N5	-2.03	120.55	124.86
4	A	603	PKS	CAY-CAX-CAW	-2.02	121.76	126.52
2	D	602	FAD	N3-C2-N1	2.02	123.35	119.38
2	D	602	FAD	O2P-P-O1P	2.01	122.19	112.24
4	C	703	PKS	CAZ-CAW-CAV	2.01	120.21	115.85
2	E	601	FAD	C4X-C10-N10	2.00	119.41	116.48
2	A	601	FAD	O3'-C3'-C4'	2.00	113.65	108.81

There are no chirality outliers.

All (189) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C1'-C2'-C3'-O3'
2	A	601	FAD	C1'-C2'-C3'-C4'
2	A	601	FAD	O4'-C4'-C5'-O5'
2	B	601	FAD	C5B-O5B-PA-O2A
2	B	601	FAD	C1'-C2'-C3'-O3'
2	B	601	FAD	C1'-C2'-C3'-C4'
2	B	601	FAD	O4'-C4'-C5'-O5'
2	C	702	FAD	O4'-C4'-C5'-O5'
2	C	702	FAD	PA-O3P-P-O5'
2	D	602	FAD	O4'-C4'-C5'-O5'
2	D	602	FAD	C5'-O5'-P-O1P
2	D	602	FAD	C5'-O5'-P-O2P
2	E	601	FAD	C5'-O5'-P-O3P
4	A	603	PKS	CAU-CAV-CAW-CAZ
4	A	603	PKS	CAP-CAQ-CAR-CAS
4	A	603	PKS	CAP-CAQ-CAR-CAT
4	C	703	PKS	CAU-CAV-CAW-CAZ
4	C	703	PKS	CAO-CAM-CAN-CAP
4	D	604	PKS	OBA-CAV-CAW-CAZ
4	D	604	PKS	CAU-CAV-CAW-CAX
4	D	604	PKS	CAU-CAV-CAW-CAZ
4	D	604	PKS	CAP-CAQ-CAR-CAS
4	D	604	PKS	CAP-CAQ-CAR-CAT
4	E	603	PKS	NAD-CAC-OAH-CAI
4	E	603	PKS	CAS-CAU-CAV-CAW
4	E	603	PKS	CAM-CAN-CAP-CAQ
4	E	603	PKS	CAO-CAM-CAN-CAP
4	E	603	PKS	CAL-CAM-CAN-CAP
4	F	603	PKS	OBA-CAV-CAW-CAZ
4	F	603	PKS	CAU-CAV-CAW-CAX
4	F	603	PKS	CAU-CAV-CAW-CAZ
4	F	603	PKS	CAP-CAQ-CAR-CAS
4	F	603	PKS	CAP-CAQ-CAR-CAT
4	F	603	PKS	CAM-CAN-CAP-CAQ
7	A	607	GOL	O1-C1-C2-C3
7	A	607	GOL	C1-C2-C3-O3
7	A	608	GOL	O1-C1-C2-C3
7	A	608	GOL	C1-C2-C3-O3
7	D	601	GOL	O1-C1-C2-C3
7	D	607	GOL	O1-C1-C2-O2
7	D	607	GOL	C1-C2-C3-O3
7	E	608	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	E	603	PKS	CAB-CAC-OAH-CAI
4	F	603	PKS	CAB-CAC-OAH-CAI
4	B	603	PKS	NAD-CAC-OAH-CAI
4	F	603	PKS	NAD-CAC-OAH-CAI
2	B	601	FAD	O2'-C2'-C3'-O3'
2	B	601	FAD	O2'-C2'-C3'-C4'
6	A	605	1PE	OH4-C13-C23-OH3
4	A	603	PKS	CAL-CAM-CAN-CAP
4	C	703	PKS	CAL-CAM-CAN-CAP
4	A	603	PKS	CAO-CAM-CAN-CAP
5	C	701	PGE	O2-C3-C4-O3
6	C	705	1PE	OH6-C15-C25-OH5
6	D	605	1PE	OH4-C13-C23-OH3
6	C	705	1PE	OH5-C14-C24-OH4
6	D	605	1PE	OH6-C15-C25-OH5
6	D	605	1PE	OH5-C14-C24-OH4
6	E	605	1PE	OH6-C15-C25-OH5
4	B	603	PKS	CAB-CAC-OAH-CAI
4	C	703	PKS	CAB-CAC-OAH-CAI
4	B	603	PKS	CAP-CAQ-CAR-CAT
4	C	703	PKS	CAP-CAQ-CAR-CAT
4	B	603	PKS	CAP-CAQ-CAR-CAS
4	C	703	PKS	CAP-CAQ-CAR-CAS
6	F	604	1PE	OH4-C13-C23-OH3
6	F	604	1PE	OH5-C14-C24-OH4
7	E	608	GOL	O1-C1-C2-O2
2	A	601	FAD	O2'-C2'-C3'-O3'
6	B	604	1PE	OH4-C13-C23-OH3
5	A	604	PGE	O1-C1-C2-O2
5	E	604	PGE	O1-C1-C2-O2
6	E	605	1PE	OH2-C12-C22-OH3
6	F	604	1PE	OH2-C12-C22-OH3
4	C	703	PKS	NAD-CAC-OAH-CAI
6	F	604	1PE	OH6-C15-C25-OH5
6	E	605	1PE	OH5-C14-C24-OH4
2	C	702	FAD	C2'-C3'-C4'-C5'
6	D	605	1PE	OH2-C12-C22-OH3
6	D	605	1PE	OH7-C16-C26-OH6
6	F	604	1PE	OH7-C16-C26-OH6
2	C	702	FAD	C2'-C3'-C4'-O4'
5	E	604	PGE	O2-C3-C4-O3
7	D	601	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	D	607	GOL	O1-C1-C2-C3
7	E	608	GOL	O1-C1-C2-C3
5	C	701	PGE	O1-C1-C2-O2
5	C	704	PGE	O2-C3-C4-O3
6	B	604	1PE	OH6-C15-C25-OH5
2	E	601	FAD	O4'-C4'-C5'-O5'
7	A	607	GOL	O2-C2-C3-O3
7	A	608	GOL	O1-C1-C2-O2
7	D	601	GOL	O2-C2-C3-O3
7	E	608	GOL	O2-C2-C3-O3
5	E	604	PGE	O3-C5-C6-O4
6	A	605	1PE	OH2-C12-C22-OH3
6	C	705	1PE	OH2-C12-C22-OH3
6	E	605	1PE	C13-C23-OH3-C22
2	D	602	FAD	C3'-C4'-C5'-O5'
2	E	601	FAD	C3'-C4'-C5'-O5'
5	C	704	PGE	O3-C5-C6-O4
7	A	607	GOL	O1-C1-C2-O2
7	A	608	GOL	O2-C2-C3-O3
7	D	601	GOL	O1-C1-C2-O2
7	D	607	GOL	O2-C2-C3-O3
2	B	601	FAD	O4B-C4B-C5B-O5B
4	A	603	PKS	NAD-CAC-OAH-CAI
2	C	702	FAD	O3'-C3'-C4'-C5'
5	C	704	PGE	C6-C5-O3-C4
4	A	603	PKS	CAB-CAC-OAH-CAI
2	D	602	FAD	PA-O3P-P-O5'
6	B	604	1PE	C23-C13-OH4-C24
5	A	604	PGE	C6-C5-O3-C4
6	E	605	1PE	C25-C15-OH6-C26
6	F	604	1PE	C16-C26-OH6-C15
6	B	604	1PE	C15-C25-OH5-C14
4	C	703	PKS	CAM-CAN-CAP-CAQ
6	A	605	1PE	C16-C26-OH6-C15
6	D	605	1PE	C16-C26-OH6-C15
6	B	604	1PE	C12-C22-OH3-C23
6	E	605	1PE	C14-C24-OH4-C13
6	B	604	1PE	C25-C15-OH6-C26
2	C	702	FAD	O3'-C3'-C4'-O4'
2	D	602	FAD	P-O3P-PA-O1A
4	E	603	PKS	CAP-CAQ-CAR-CAT
4	E	603	PKS	CAP-CAQ-CAR-CAS

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Mol	Chain	Res	Type	Atoms
6	C	705	1PE	C25-C15-OH6-C26
6	D	605	1PE	C14-C24-OH4-C13
6	E	605	1PE	C24-C14-OH5-C25
6	E	605	1PE	C16-C26-OH6-C15
6	F	604	1PE	C14-C24-OH4-C13
2	A	601	FAD	O2'-C2'-C3'-C4'
6	B	604	1PE	C24-C14-OH5-C25
2	B	601	FAD	C5'-O5'-P-O2P
4	A	603	PKS	CAU-CAV-CAW-CAX
5	C	701	PGE	C3-C4-O3-C5
6	C	705	1PE	C16-C26-OH6-C15
6	A	605	1PE	C14-C24-OH4-C13
6	A	605	1PE	OH6-C15-C25-OH5
6	E	605	1PE	OH7-C16-C26-OH6
6	F	604	1PE	C15-C25-OH5-C14
2	C	702	FAD	O2'-C2'-C3'-C4'
6	B	604	1PE	C13-C23-OH3-C22
6	E	605	1PE	C12-C22-OH3-C23
6	D	605	1PE	C13-C23-OH3-C22
6	F	604	1PE	C24-C14-OH5-C25
5	C	701	PGE	C6-C5-O3-C4
4	D	604	PKS	NAD-CAC-OAH-CAI
2	D	602	FAD	C2'-C1'-N10-C10
6	E	605	1PE	C23-C13-OH4-C24
6	D	605	1PE	C24-C14-OH5-C25
2	F	601	FAD	O4B-C4B-C5B-O5B
2	F	601	FAD	PA-O3P-P-O5'
6	A	605	1PE	OH5-C14-C24-OH4
5	A	604	PGE	O3-C5-C6-O4
5	A	604	PGE	C3-C4-O3-C5
2	B	601	FAD	C3B-C4B-C5B-O5B
6	C	705	1PE	OH4-C13-C23-OH3
6	C	705	1PE	C24-C14-OH5-C25
4	D	604	PKS	CBB-CAU-CAV-OBA
4	E	603	PKS	CBB-CAU-CAV-OBA
2	A	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C5B-O5B-PA-O3P
2	D	602	FAD	C5'-O5'-P-O3P
6	F	604	1PE	C13-C23-OH3-C22
6	E	605	1PE	OH4-C13-C23-OH3
2	D	602	FAD	P-O3P-PA-O2A
6	A	605	1PE	C25-C15-OH6-C26

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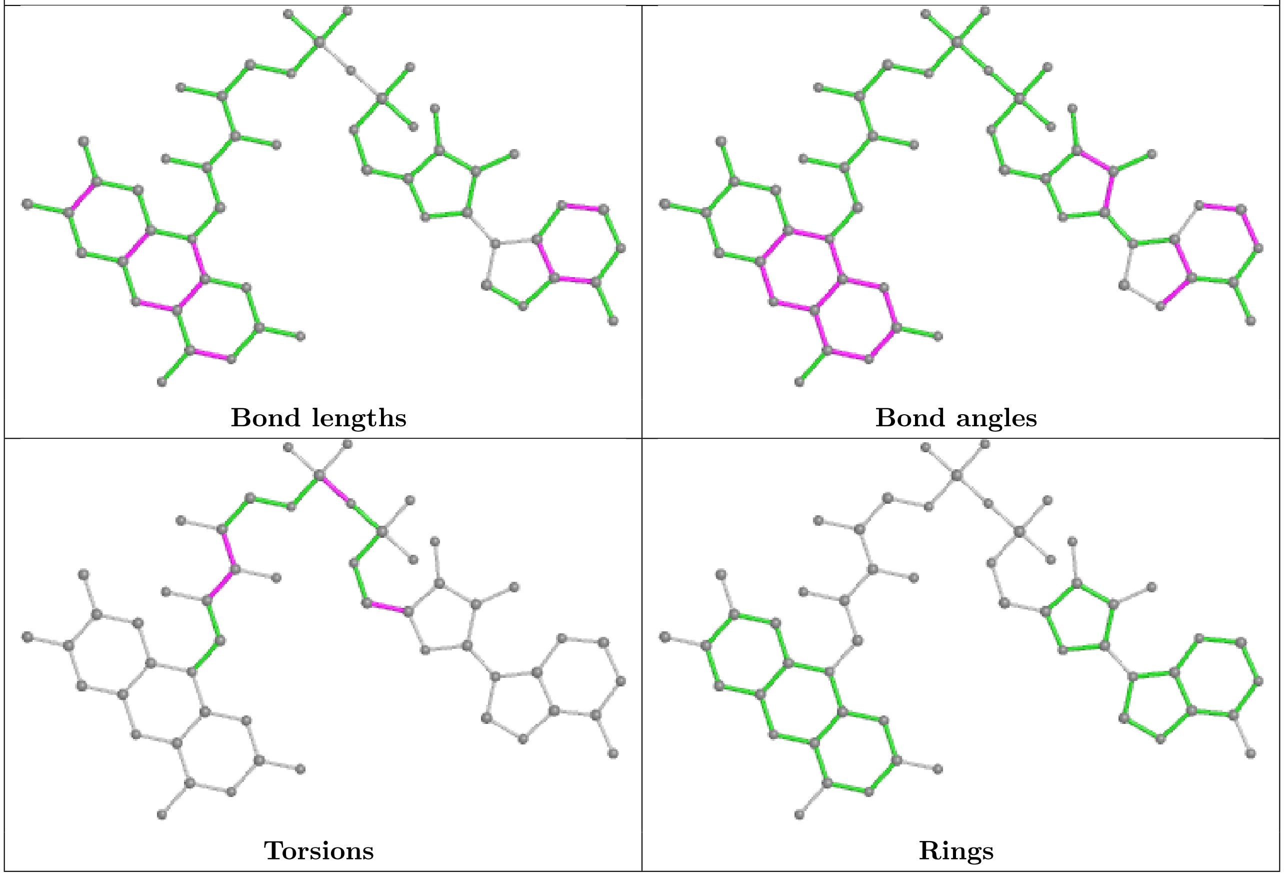
Mol	Chain	Res	Type	Atoms
6	B	604	1PE	OH5-C14-C24-OH4
4	D	604	PKS	CAB-CAC-OAH-CAI
4	A	603	PKS	OBA-CAV-CAW-CAZ
4	C	703	PKS	OBA-CAV-CAW-CAZ
4	E	603	PKS	OBA-CAV-CAW-CAZ
2	A	601	FAD	C3'-C4'-C5'-O5'
2	B	601	FAD	C5B-O5B-PA-O1A
2	B	601	FAD	C3'-C4'-C5'-O5'
2	B	601	FAD	C5'-O5'-P-O1P
4	C	703	PKS	CAU-CAV-CAW-CAX
4	D	604	PKS	CAS-CAU-CAV-CAW
2	C	702	FAD	O4B-C4B-C5B-O5B
2	D	602	FAD	O4B-C4B-C5B-O5B
2	E	601	FAD	O4B-C4B-C5B-O5B
2	F	601	FAD	O3'-C3'-C4'-C5'
5	A	604	PGE	O2-C3-C4-O3
2	F	601	FAD	C1'-C2'-C3'-O3'
6	B	604	1PE	C16-C26-OH6-C15
4	C	703	PKS	OBA-CAV-CAW-CAX
4	D	604	PKS	OBA-CAV-CAW-CAX
4	F	603	PKS	OBA-CAV-CAW-CAX

There are no ring outliers.

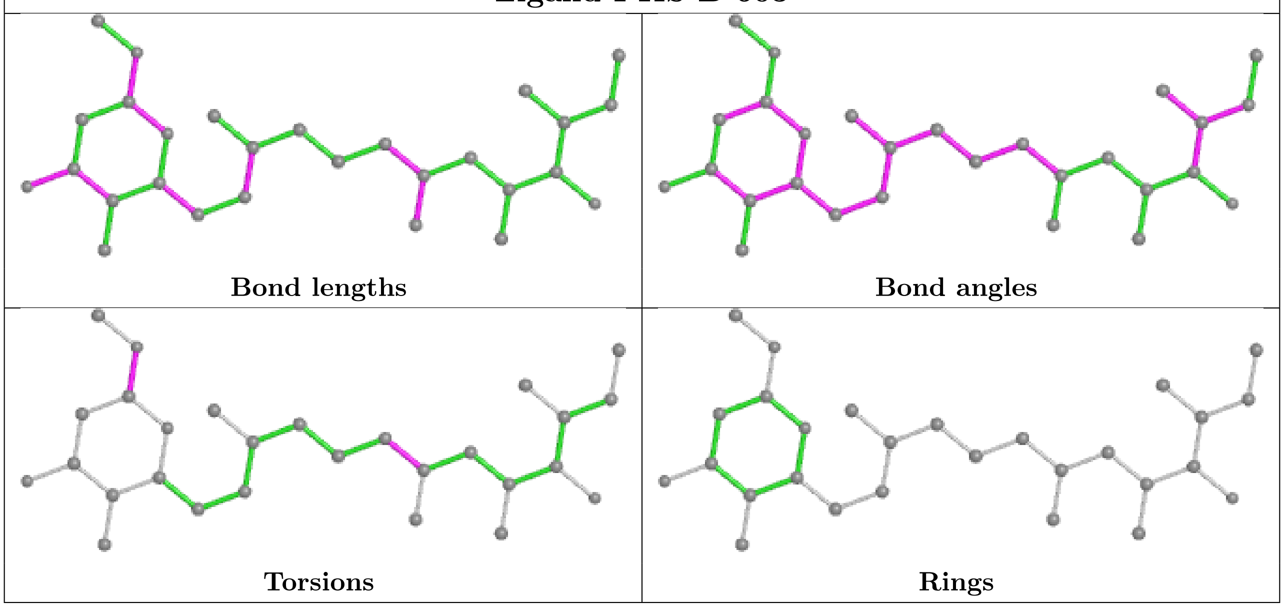
No monomer is involved in short contacts.

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.

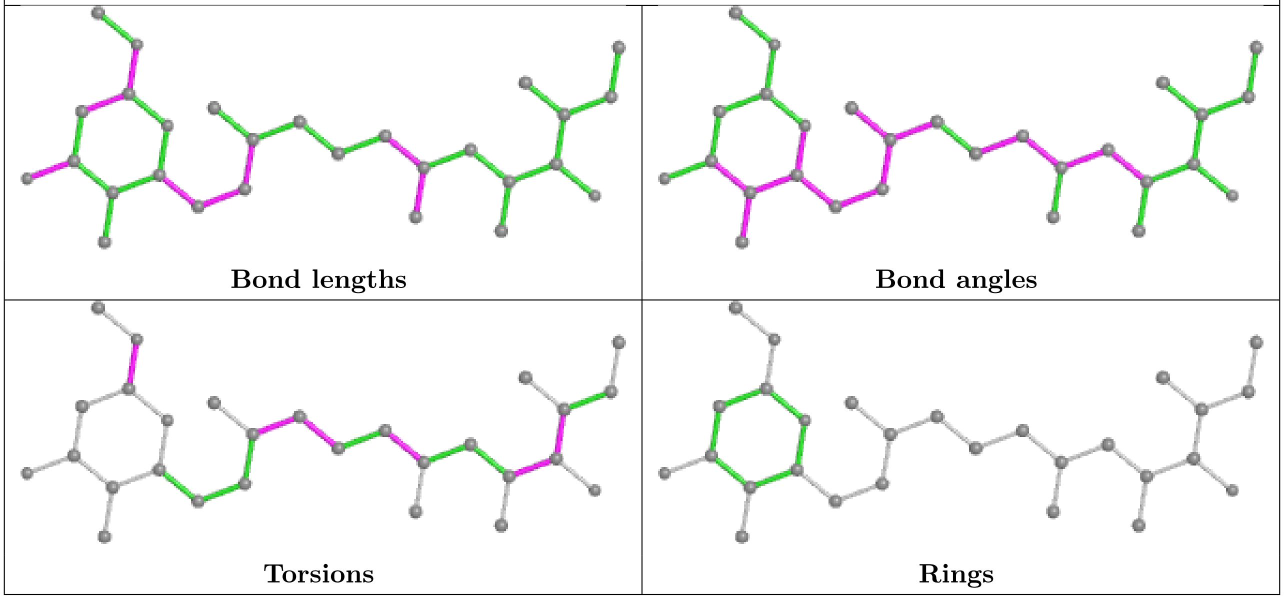
Ligand FAD F 601



Ligand PKS B 603



Ligand PKS E 603



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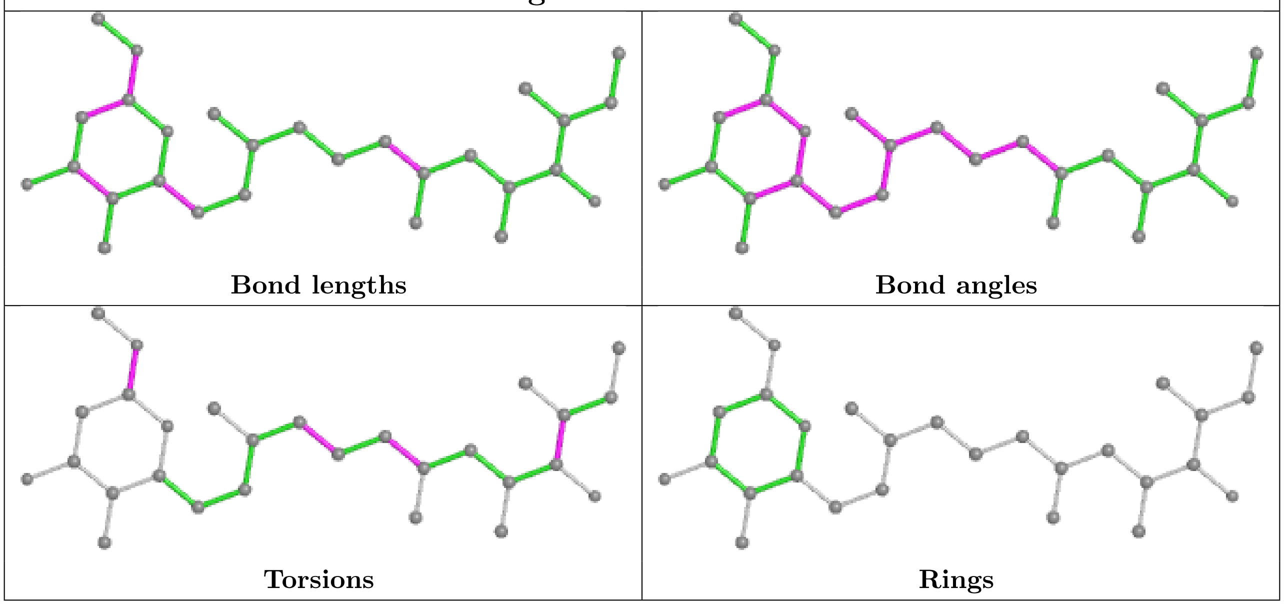

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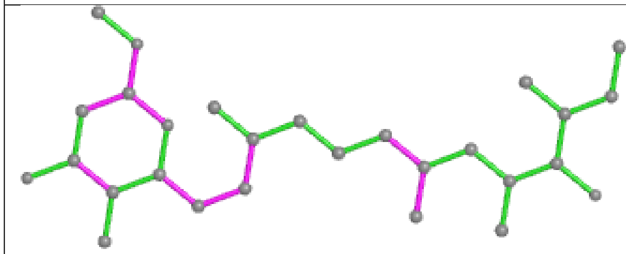
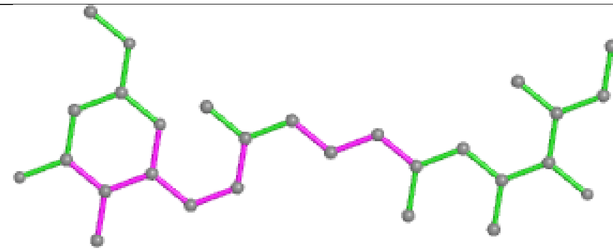
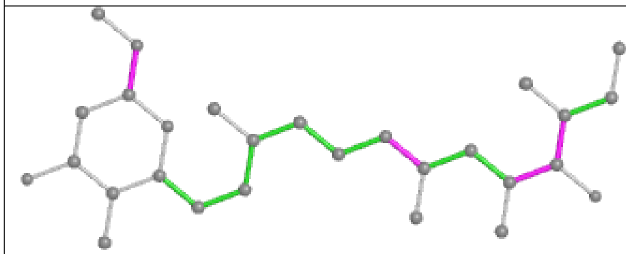
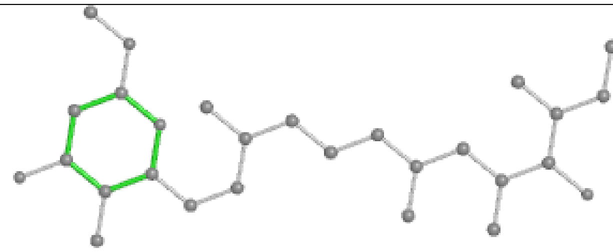
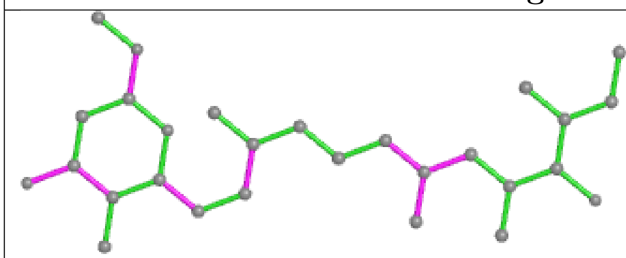
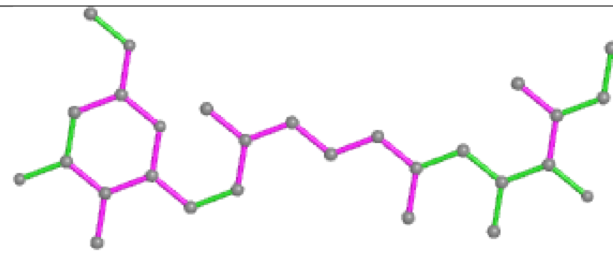
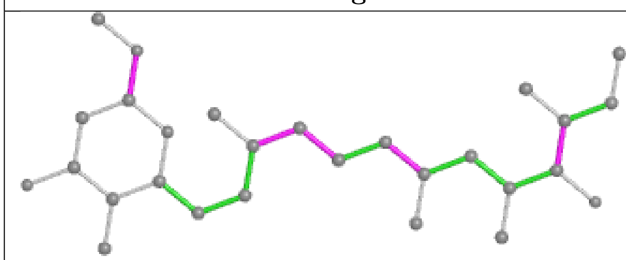
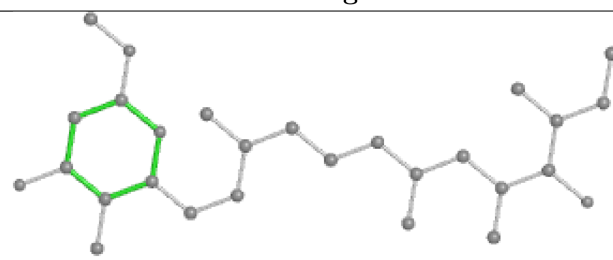
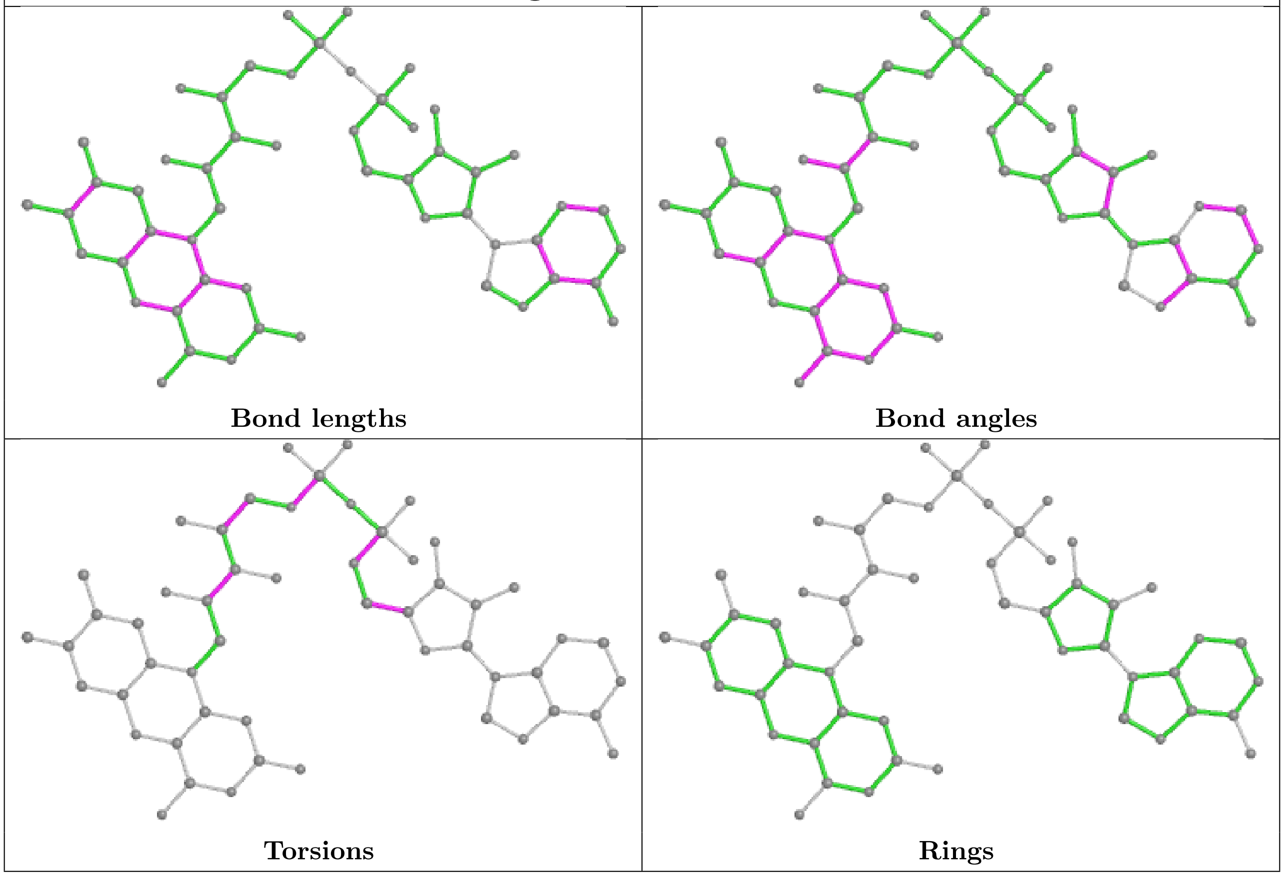
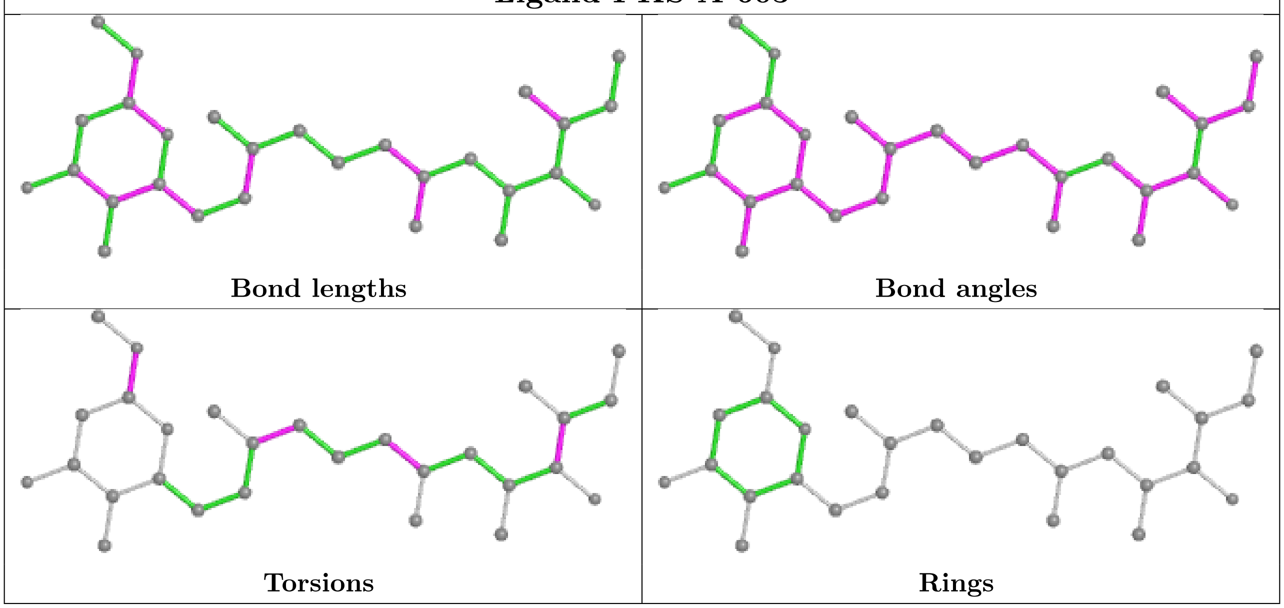
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PKS C 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

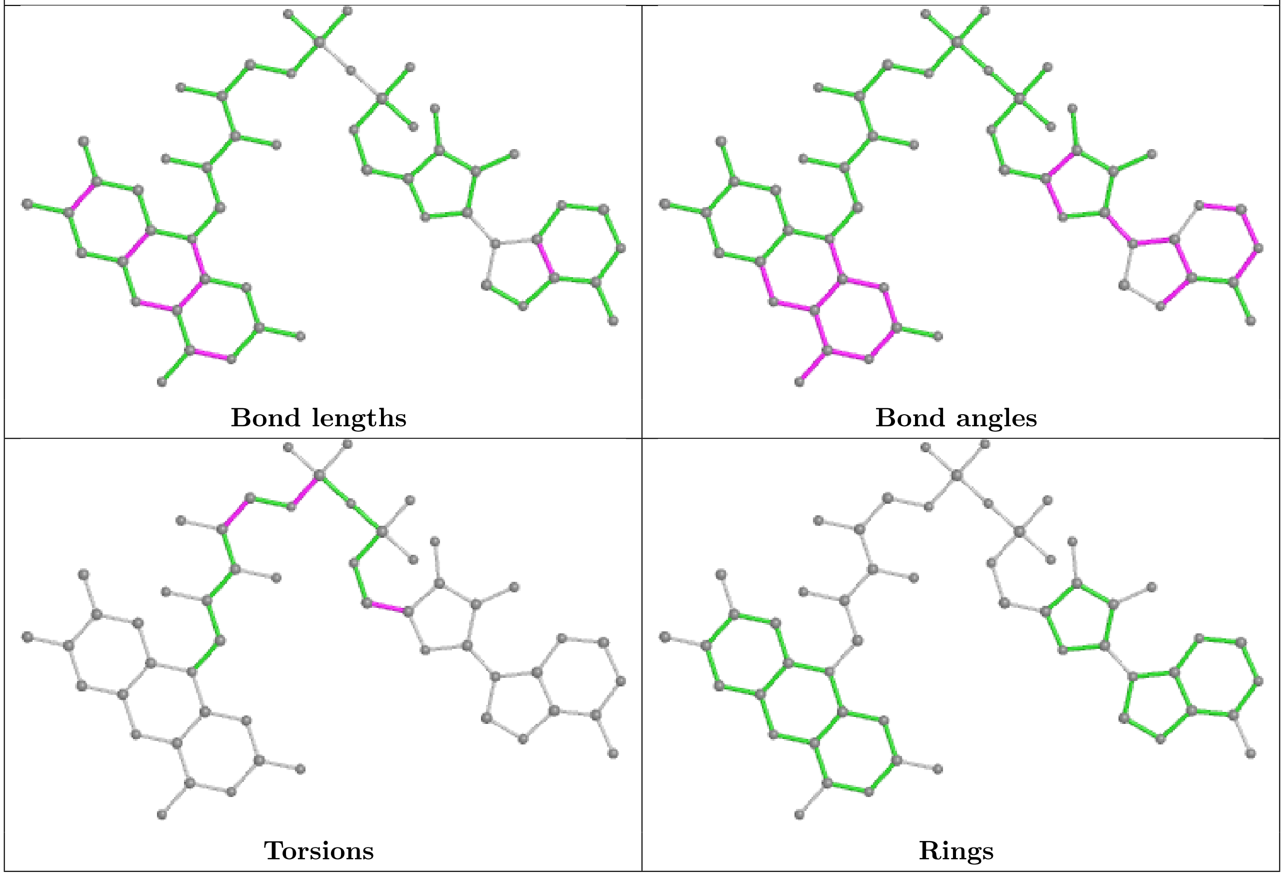
Ligand FAD B 601



Ligand PKS A 603



Ligand FAD E 601



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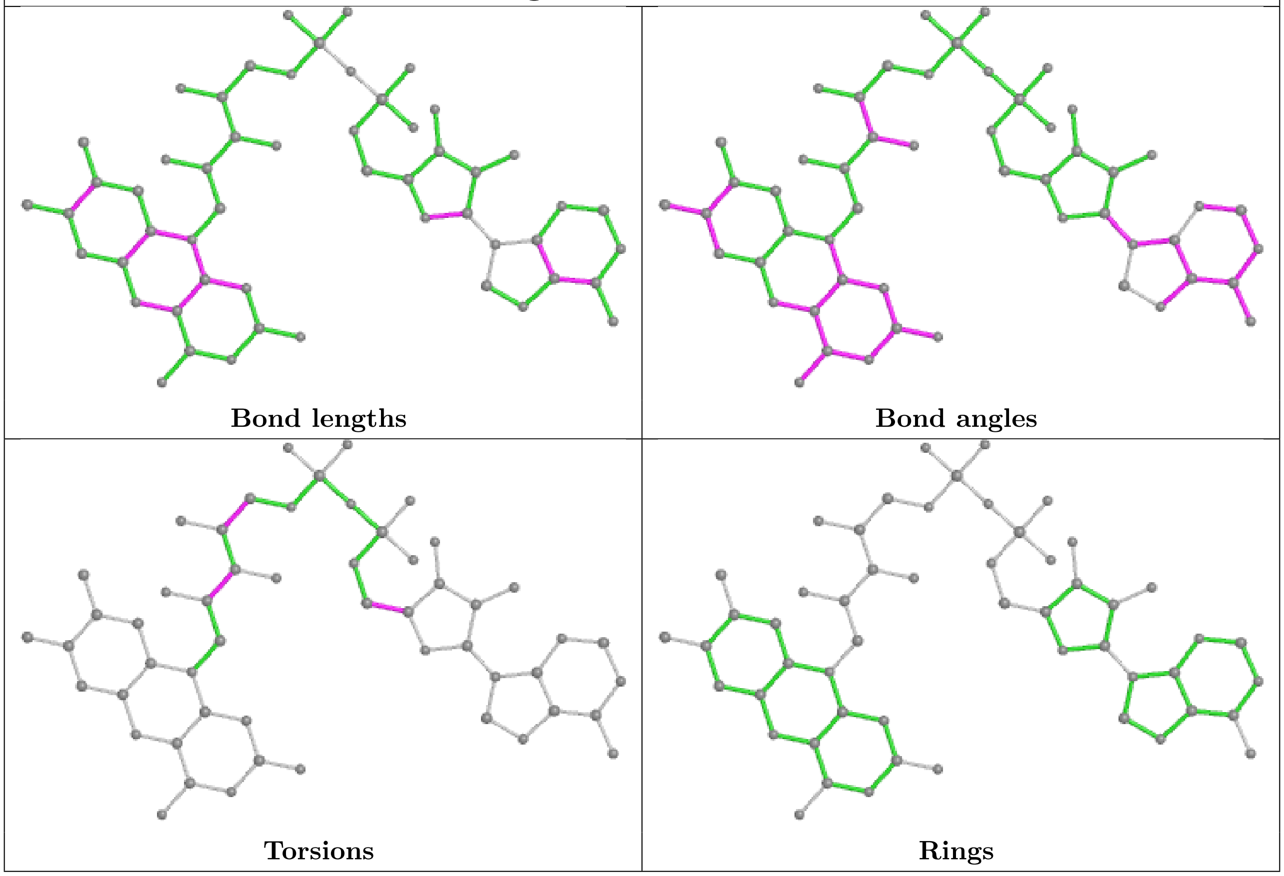

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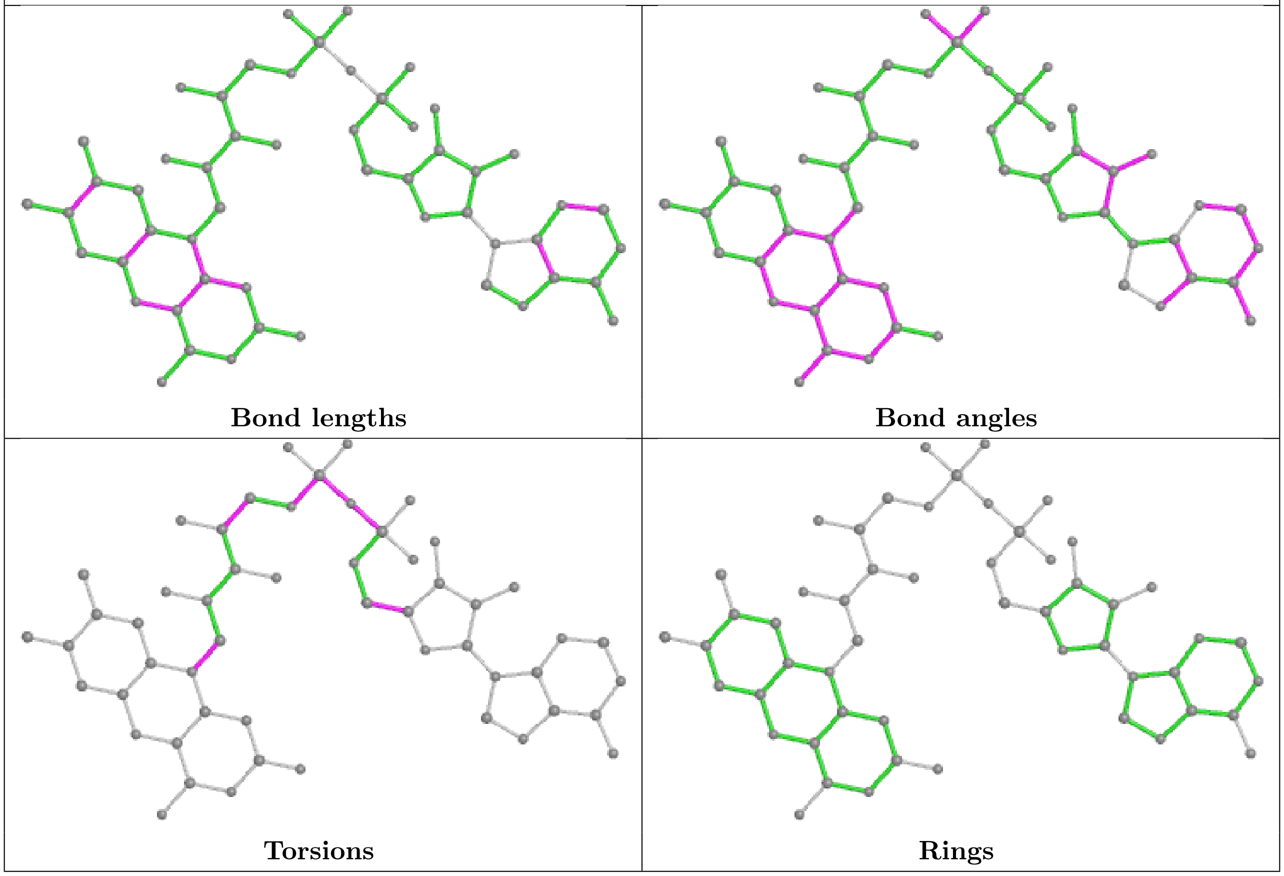
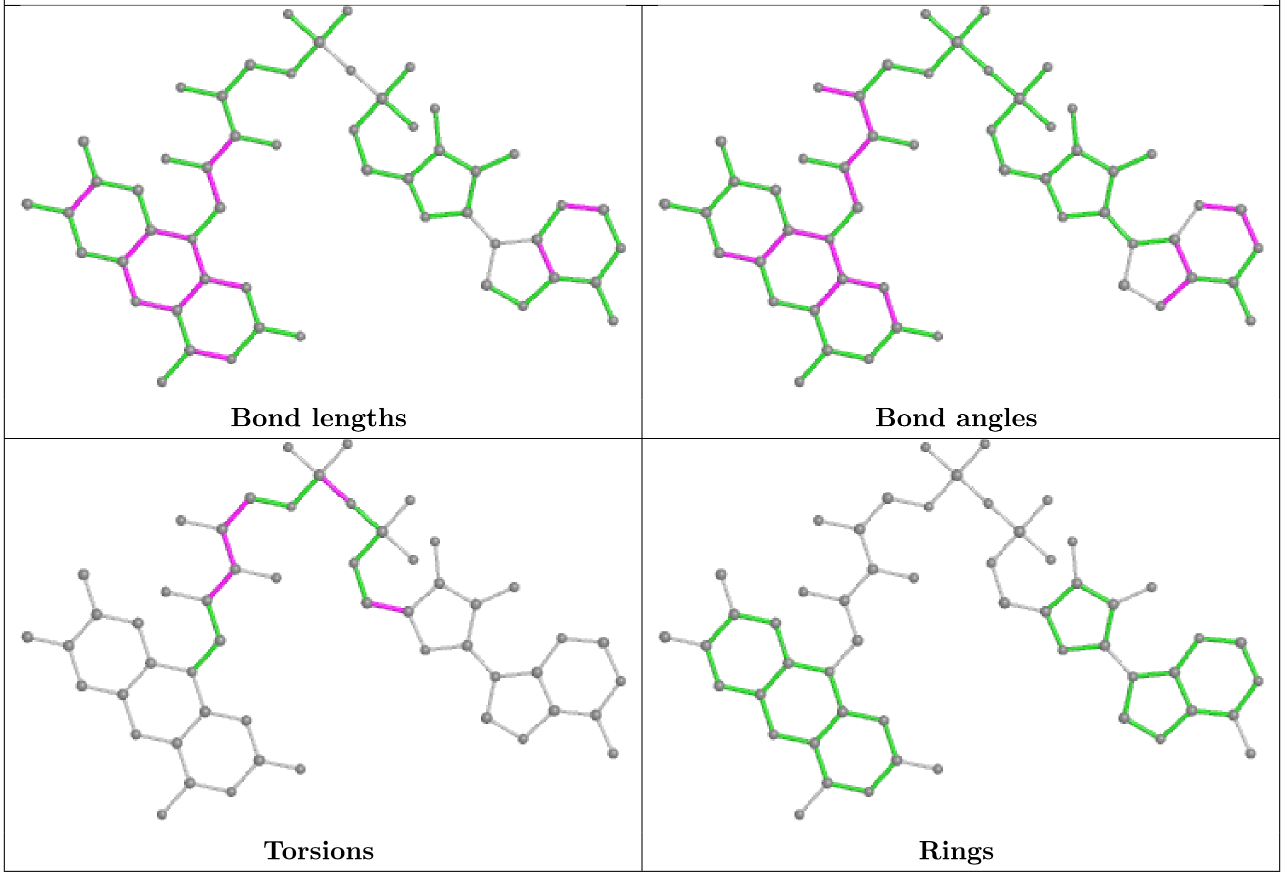


Ligand FAD C 702



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 (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.