Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2023 – 11:09 PM EDT

PDB ID	:	6N96
Title	:	Methylmalonyl-CoA decarboxylase in complex with 2-sulfonate-propionyl-oxa(dethia)-CoA
Authors	:	Stunkard, L.M.; Dixon, A.D.; Huth, T.J.; Lohman, J.R.
Deposited on	:	2018-11-30
Resolution	:	1.70 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 1.70 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15313 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.

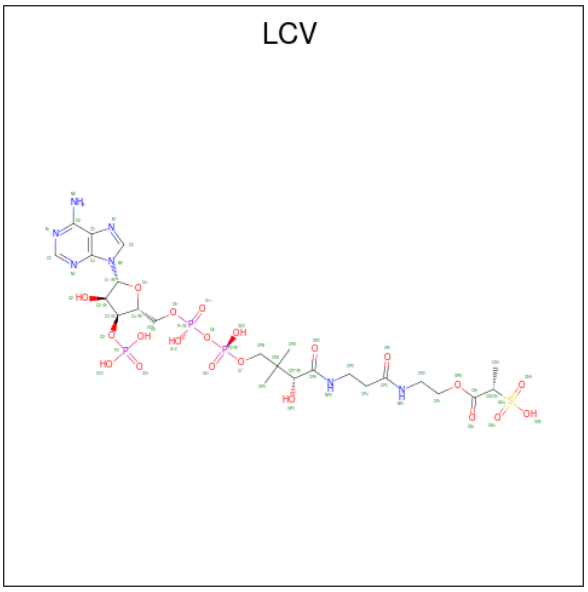
- Molecule 1 is a protein called Methylmalonyl-CoA decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	18	0
			2161	1382	373	393	13			
1	B	260	Total	C	N	O	S	0	12	0
			2114	1351	360	391	12			
1	C	260	Total	C	N	O	S	0	8	0
			2091	1339	360	380	12			
1	D	260	Total	C	N	O	S	0	11	0
			2096	1341	358	385	12			
1	E	260	Total	C	N	O	S	0	11	0
			2099	1344	357	385	13			
1	F	260	Total	C	N	O	S	0	20	0
			2131	1370	360	388	13			

There are 6 discrepancies between the modelled and reference sequences:

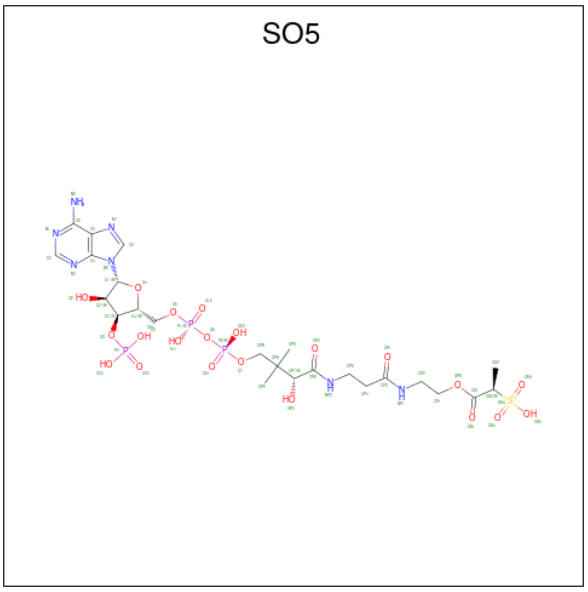
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	engineered mutation	UNP P52045
B	2	ALA	SER	engineered mutation	UNP P52045
C	2	ALA	SER	engineered mutation	UNP P52045
D	2	ALA	SER	engineered mutation	UNP P52045
E	2	ALA	SER	engineered mutation	UNP P52045
F	2	ALA	SER	engineered mutation	UNP P52045

- Molecule 2 is (2 {S})-1-[2-[3-[[(2 {R})-4-[[[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-4-oxidanyl-3-phosphonooxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-3,3-dimethyl-2-oxidanyl-butanoyl]amino]propanoylamino]ethoxy]-1-oxidanylidene-propane-2-sulfonic acid (three-letter code: LCV) (formula: $C_{24}H_{40}N_7O_{21}P_3S$).



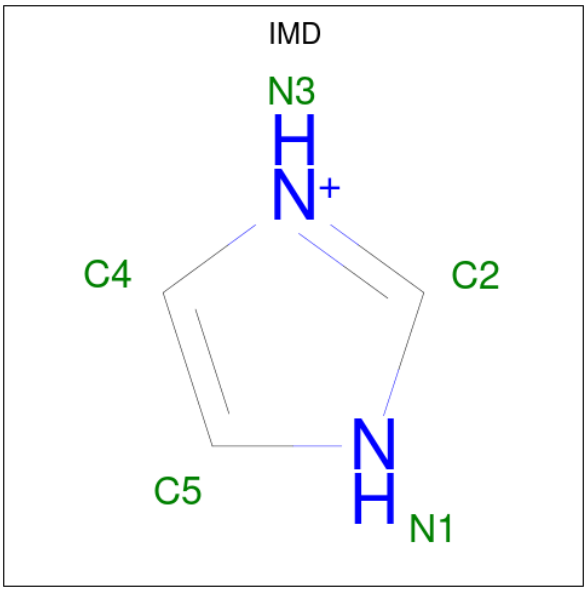
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O P S 56 24 7 21 3 1	0	1
2	B	1	Total C N O P S 56 24 7 21 3 1	0	1
2	C	1	Total C N O P S 56 24 7 21 3 1	0	1
2	C	1	Total C N O P 31 10 5 13 3	0	1
2	D	1	Total C N O P S 56 24 7 21 3 1	0	1
2	E	1	Total C N O P S 56 24 7 21 3 1	0	1
2	F	1	Total C N O P S 56 24 7 21 3 1	0	1
2	F	1	Total C N O P 31 10 5 13 3	0	1

- Molecule 3 is (2 {R})-1-[2-[3-[[(2 {R})-4-[[[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-4-oxidanyl-3-phosphonooxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-3,3-dimethyl-2-oxidanyl-butanoyl]amino]propanoylamino]ethoxy]-1-oxidanylidene-propane-2-sulfonic acid (three-letter code: SO5) (formula: $C_{24}H_{40}N_7O_{21}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	1
			56	24	7	21	3	1		
3	B	1	Total	C	N	O	P	S	0	1
			56	24	7	21	3	1		
3	C	1	Total	C	N	O	P	S	0	1
			56	24	7	21	3	1		
3	D	1	Total	C	N	O	P	S	0	1
			56	24	7	21	3	1		
3	E	1	Total	C	N	O	P	S	0	1
			56	24	7	21	3	1		
3	F	1	Total	C	N	O	P	S	0	1
			56	24	7	21	3	1		

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C N 5 3 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	314	Total O 330 330	0	17
5	B	282	Total O 291 291	0	10
5	C	295	Total O 308 308	0	15
5	D	305	Total O 320 320	0	15
5	E	292	Total O 307 307	0	14
5	F	316	Total O 326 326	0	14

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	87.15Å 114.66Å 192.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 1.70	Depositor
% Data completeness (in resolution range)	88.2 (29.96-1.70)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.151 , 0.184	Depositor
Wilson B-factor (Å^2)	14.2	Xtriage
Anisotropy	0.050	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15313	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	LCV	C	303[A]	-	28,33,58	1.21	3 (10%)	35,52,88	1.59	7 (20%)
2	LCV	B	301[B]	-	48,58,58	1.25	2 (4%)	61,88,88	1.65	9 (14%)
2	LCV	F	301[B]	-	48,58,58	1.47	4 (8%)	61,88,88	3.48	17 (27%)
2	LCV	D	301[B]	-	48,58,58	1.17	5 (10%)	61,88,88	1.57	8 (13%)
3	SO5	A	302[A]	-	48,58,58	1.12	3 (6%)	61,88,88	1.54	9 (14%)
2	LCV	C	301[B]	-	48,58,58	1.19	4 (8%)	61,88,88	1.37	8 (13%)
2	LCV	F	303[A]	-	28,33,58	1.15	3 (10%)	35,52,88	1.73	6 (17%)
2	LCV	A	301[B]	-	48,58,58	1.14	4 (8%)	61,88,88	3.15	13 (21%)
3	SO5	B	302[A]	-	48,58,58	1.22	2 (4%)	61,88,88	3.52	13 (21%)
3	SO5	D	302[A]	-	48,58,58	1.14	4 (8%)	61,88,88	1.74	10 (16%)
3	SO5	E	302[A]	-	48,58,58	1.17	3 (6%)	61,88,88	2.88	13 (21%)
3	SO5	F	302[A]	-	48,58,58	1.37	4 (8%)	61,88,88	1.86	10 (16%)
3	SO5	C	302[A]	-	48,58,58	1.16	3 (6%)	61,88,88	1.68	8 (13%)
2	LCV	E	301[B]	-	48,58,58	1.21	3 (6%)	61,88,88	2.82	13 (21%)
4	IMD	D	303	-	3,5,5	0.24	0	4,5,5	0.70	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	LCV	C	303[A]	-	-	5/17/37/77	0/3/3/3
2	LCV	B	301[B]	-	-	3/56/77/77	0/3/3/3
2	LCV	F	301[B]	-	-	10/56/77/77	0/3/3/3
2	LCV	D	301[B]	-	-	3/56/77/77	0/3/3/3
3	SO5	A	302[A]	-	-	3/56/77/77	0/3/3/3
2	LCV	C	301[B]	-	-	2/56/77/77	0/3/3/3
2	LCV	F	303[A]	-	-	6/17/37/77	0/3/3/3
2	LCV	A	301[B]	-	-	7/56/77/77	0/3/3/3
3	SO5	B	302[A]	-	-	6/56/77/77	0/3/3/3
3	SO5	D	302[A]	-	-	3/56/77/77	0/3/3/3
3	SO5	E	302[A]	-	-	7/56/77/77	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO5	F	302[A]	-	-	2/56/77/77	0/3/3/3
3	SO5	C	302[A]	-	-	0/56/77/77	0/3/3/3
2	LCV	E	301[B]	-	-	9/56/77/77	0/3/3/3
4	IMD	D	303	-	-	-	0/1/1/1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301[B]	LCV	CS2-CS1	-6.04	1.45	1.52
3	F	302[A]	SO5	OPS-CS1	5.85	1.45	1.33
3	B	302[A]	SO5	OPS-CS1	5.59	1.44	1.33
2	B	301[B]	LCV	OPS-CS1	5.50	1.44	1.33
2	F	301[B]	LCV	OPS-CS1	5.42	1.44	1.33
3	E	302[A]	SO5	OPS-CS1	5.34	1.44	1.33
2	E	301[B]	LCV	OPS-CS1	5.15	1.43	1.33
3	F	302[A]	SO5	CS2-CS1	-4.98	1.46	1.52
2	A	301[B]	LCV	OPS-CS1	4.92	1.43	1.33
3	C	302[A]	SO5	OPS-CS1	4.86	1.43	1.33
2	D	301[B]	LCV	OPS-CS1	4.85	1.43	1.33
2	C	301[B]	LCV	OPS-CS1	4.85	1.43	1.33
3	A	302[A]	SO5	OPS-CS1	4.75	1.43	1.33
3	D	302[A]	SO5	OPS-CS1	4.65	1.42	1.33
2	E	301[B]	LCV	CS2-CS1	-3.57	1.48	1.52
2	B	301[B]	LCV	CS2-CS1	-3.42	1.48	1.52
2	F	303[A]	LCV	C5-C4	3.20	1.49	1.40
2	C	303[A]	LCV	C2-N3	3.00	1.36	1.32
2	C	303[A]	LCV	C5-C4	2.96	1.48	1.40
3	C	302[A]	SO5	O4'-C1'	2.96	1.45	1.41
2	C	301[B]	LCV	O4'-C1'	2.95	1.45	1.41
3	B	302[A]	SO5	CS2-CS1	-2.80	1.49	1.52
2	F	303[A]	LCV	C2-N3	2.66	1.36	1.32
2	D	301[B]	LCV	CS2-CS1	-2.44	1.49	1.52
2	F	303[A]	LCV	C8-N7	2.42	1.39	1.34
2	A	301[B]	LCV	CS2-CS1	-2.42	1.49	1.52
2	D	301[B]	LCV	C2-N3	2.42	1.36	1.32
2	C	303[A]	LCV	C2'-C1'	-2.41	1.50	1.53
3	D	302[A]	SO5	C2-N3	2.38	1.35	1.32
3	E	302[A]	SO5	CS2-CS1	-2.37	1.49	1.52
3	C	302[A]	SO5	C5-C4	2.33	1.47	1.40
2	F	301[B]	LCV	C5-C4	2.33	1.47	1.40
2	C	301[B]	LCV	C5-C4	2.33	1.47	1.40
3	F	302[A]	SO5	C5-C4	2.32	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301[B]	LCV	P3-O3'	2.25	1.63	1.59
3	D	302[A]	SO5	P3-O3'	2.19	1.63	1.59
2	D	301[B]	LCV	P3-O3'	2.19	1.63	1.59
2	D	301[B]	LCV	C5-C4	2.17	1.46	1.40
3	D	302[A]	SO5	C5-C4	2.17	1.46	1.40
3	A	302[A]	SO5	P3-O3'	2.16	1.63	1.59
2	C	301[B]	LCV	CS2-CS1	-2.11	1.50	1.52
2	A	301[B]	LCV	C5-C4	2.10	1.46	1.40
2	F	301[B]	LCV	O4'-C1'	2.08	1.44	1.41
2	E	301[B]	LCV	C5-C4	2.07	1.46	1.40
3	E	302[A]	SO5	C5-C4	2.07	1.46	1.40
3	A	302[A]	SO5	C5-C4	2.06	1.46	1.40
3	F	302[A]	SO5	O4'-C1'	2.05	1.43	1.41

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301[B]	LCV	CP8-CPA-CPB	-13.77	85.78	108.23
3	B	302[A]	SO5	CP8-CPA-CPB	-13.60	86.04	108.23
2	A	301[B]	LCV	CP8-CPA-CPB	-13.36	86.45	108.23
2	F	301[B]	LCV	CP8-CPA-CP7	-13.27	85.81	108.82
3	E	302[A]	SO5	CP8-CPA-CPB	-13.14	86.80	108.23
2	E	301[B]	LCV	CP8-CPA-CPB	-13.09	86.89	108.23
3	B	302[A]	SO5	CP8-CPA-CP7	-12.56	87.04	108.82
3	B	302[A]	SO5	CP8-CPA-CP9	-10.88	87.00	109.17
3	F	302[A]	SO5	OS4-SS4-CS2	-10.65	102.34	109.43
3	B	302[A]	SO5	CP9-CPA-CPB	10.53	125.41	108.23
2	A	301[B]	LCV	CP8-CPA-CP7	-10.31	90.94	108.82
2	A	301[B]	LCV	CP8-CPA-CP9	-9.85	89.10	109.17
2	F	301[B]	LCV	CP9-CPA-CP7	9.79	125.79	108.82
2	E	301[B]	LCV	CP8-CPA-CP7	-9.15	92.96	108.82
3	E	302[A]	SO5	CP8-CPA-CP7	-9.15	92.96	108.82
2	F	301[B]	LCV	O56-SS4-CS2	-8.92	103.49	109.43
2	F	301[B]	LCV	CP8-CPA-CP9	-8.70	91.43	109.17
3	D	302[A]	SO5	O56-SS4-CS2	-8.58	103.71	109.43
2	A	301[B]	LCV	CP9-CPA-CPB	8.54	122.17	108.23
3	C	302[A]	SO5	O56-SS4-CS2	-8.37	103.86	109.43
3	B	302[A]	SO5	OS4-SS4-CS2	-8.13	104.02	109.43
2	E	301[B]	LCV	CP9-CPA-CP7	7.87	122.47	108.82
3	E	302[A]	SO5	CP9-CPA-CP7	7.86	122.44	108.82
2	E	301[B]	LCV	CP8-CPA-CP9	-6.68	95.55	109.17
3	E	302[A]	SO5	CP8-CPA-CP9	-6.67	95.58	109.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302[A]	SO5	OS4-SS4-CS2	-6.48	105.11	109.43
2	B	301[B]	LCV	O56-SS4-CS2	-6.15	105.34	109.43
2	D	301[B]	LCV	OS4-SS4-CS2	-6.09	105.37	109.43
2	F	303[A]	LCV	P1-O6-P2	-5.84	112.78	132.83
2	A	301[B]	LCV	O56-SS4-CS2	-5.74	105.61	109.43
2	C	301[B]	LCV	OS4-SS4-CS2	-5.35	105.87	109.43
2	A	301[B]	LCV	CP9-CPA-CP7	5.00	117.49	108.82
2	B	301[B]	LCV	OS4-SS4-CS2	4.92	112.71	109.43
3	C	302[A]	SO5	OS4-SS4-CS2	-4.76	106.26	109.43
2	E	301[B]	LCV	CP9-CPA-CPB	4.63	115.78	108.23
3	E	302[A]	SO5	CP9-CPA-CPB	4.62	115.78	108.23
3	E	302[A]	SO5	O56-SS4-CS2	4.51	112.44	109.43
3	B	302[A]	SO5	O56-SS4-CS2	4.51	112.43	109.43
2	F	301[B]	LCV	P1-O6-P2	-4.29	118.09	132.83
3	E	302[A]	SO5	OP3-CP7-CPA	-4.29	100.16	110.25
2	E	301[B]	LCV	OP3-CP7-CPA	-4.27	100.19	110.25
3	E	302[A]	SO5	N3-C2-N1	-4.00	122.43	128.68
2	E	301[B]	LCV	N3-C2-N1	-3.98	122.46	128.68
2	D	301[B]	LCV	O56-SS4-CS2	3.83	111.98	109.43
2	D	301[B]	LCV	CP5-CP4-CP3	-3.81	106.02	112.36
2	C	303[A]	LCV	C1'-N9-C4	-3.78	120.00	126.64
2	A	301[B]	LCV	OP3-CP7-CPA	-3.78	101.36	110.25
3	D	302[A]	SO5	CP5-CP4-CP3	-3.77	106.08	112.36
2	D	301[B]	LCV	N3-C2-N1	-3.77	122.79	128.68
2	F	303[A]	LCV	C4-C5-N7	-3.76	105.48	109.40
3	D	302[A]	SO5	N3-C2-N1	-3.75	122.82	128.68
2	C	303[A]	LCV	N3-C2-N1	-3.63	123.01	128.68
3	B	302[A]	SO5	N3-C2-N1	-3.60	123.05	128.68
2	B	301[B]	LCV	N3-C2-N1	-3.59	123.07	128.68
3	F	302[A]	SO5	P1-O6-P2	-3.54	120.68	132.83
2	F	301[B]	LCV	N3-C2-N1	-3.44	123.30	128.68
3	F	302[A]	SO5	N3-C2-N1	-3.44	123.30	128.68
2	C	303[A]	LCV	O3'-C3'-C2'	-3.43	99.23	111.68
3	B	302[A]	SO5	CP9-CPA-CP7	3.38	114.68	108.82
2	F	301[B]	LCV	OS1-CS1-CS2	3.30	127.56	124.44
2	A	301[B]	LCV	N3-C2-N1	-3.20	123.67	128.68
3	D	302[A]	SO5	OS4-SS4-CS2	3.18	111.55	109.43
3	D	302[A]	SO5	P1-O6-P2	-3.18	121.93	132.83
2	D	301[B]	LCV	P1-O6-P2	-3.17	121.94	132.83
3	A	302[A]	SO5	N3-C2-N1	-3.17	123.73	128.68
2	C	301[B]	LCV	N3-C2-N1	-3.15	123.76	128.68
3	C	302[A]	SO5	N3-C2-N1	-3.12	123.81	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301[B]	LCV	OS4-SS4-CS2	3.04	111.46	109.43
2	E	301[B]	LCV	P1-O6-P2	-3.02	122.45	132.83
3	E	302[A]	SO5	P1-O6-P2	-3.01	122.50	132.83
2	F	303[A]	LCV	N3-C2-N1	-2.97	124.04	128.68
3	D	302[A]	SO5	CP9-CPA-CP7	2.90	113.85	108.82
2	D	301[B]	LCV	CP9-CPA-CP7	2.84	113.75	108.82
2	F	301[B]	LCV	CP5-CP4-CP3	-2.82	107.66	112.36
3	B	302[A]	SO5	OP3-CP7-CPA	-2.78	103.71	110.25
2	C	303[A]	LCV	O22-P2-O6	2.77	113.93	104.64
2	A	301[B]	LCV	P1-O6-P2	-2.75	123.38	132.83
3	A	302[A]	SO5	OP3-CP7-CPA	-2.74	103.79	110.25
2	F	303[A]	LCV	C1'-N9-C4	-2.74	121.82	126.64
3	A	302[A]	SO5	CP9-CPA-CP7	2.74	113.57	108.82
3	D	302[A]	SO5	N6-C6-N1	2.72	124.22	118.57
2	D	301[B]	LCV	N6-C6-N1	2.70	124.18	118.57
2	B	301[B]	LCV	OP3-CP7-CPA	-2.69	103.92	110.25
2	A	301[B]	LCV	O33-P3-O32	2.67	117.84	107.64
3	A	302[A]	SO5	P1-O6-P2	-2.66	123.70	132.83
2	C	303[A]	LCV	C2-N1-C6	2.65	123.29	118.75
3	C	302[A]	SO5	OPS-CS1-OS1	-2.61	119.19	124.13
3	A	302[A]	SO5	CP5-CP4-CP3	-2.59	108.04	112.36
3	E	302[A]	SO5	OS4-SS4-O56	-2.57	106.38	116.52
3	F	302[A]	SO5	O7-CPB-CPA	-2.53	106.47	110.55
3	B	302[A]	SO5	C1'-N9-C4	-2.51	122.23	126.64
3	A	302[A]	SO5	O56-SS4-CS2	2.51	111.10	109.43
2	B	301[B]	LCV	OS4-SS4-O56	-2.48	106.74	116.52
2	E	301[B]	LCV	O56-SS4-CS2	2.46	111.07	109.43
2	A	301[B]	LCV	CP5-CP4-CP3	-2.44	108.29	112.36
2	B	301[B]	LCV	C1'-N9-C4	-2.41	122.41	126.64
2	F	303[A]	LCV	O22-P2-O7	2.40	116.81	107.64
2	C	301[B]	LCV	OPS-CS1-OS1	-2.40	119.59	124.13
2	F	301[B]	LCV	O4'-C1'-C2'	-2.38	103.45	106.93
3	A	302[A]	SO5	O3'-P3-O33	-2.37	100.24	109.39
3	F	302[A]	SO5	O4'-C1'-C2'	-2.37	103.46	106.93
2	C	301[B]	LCV	C4-C5-N7	-2.37	106.93	109.40
3	C	302[A]	SO5	C4-C5-N7	-2.36	106.94	109.40
2	F	301[B]	LCV	OP3-CP7-CPA	-2.35	104.72	110.25
2	B	301[B]	LCV	N6-C6-N1	2.34	123.43	118.57
2	E	301[B]	LCV	OS4-SS4-O56	-2.33	107.33	116.52
2	E	301[B]	LCV	CP2-NP1-CP3	-2.33	118.52	122.84
3	B	302[A]	SO5	N6-C6-N1	2.32	123.39	118.57
2	F	301[B]	LCV	C4-C5-N7	-2.32	106.98	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301[B]	LCV	OS1-CS1-CS2	-2.31	122.26	124.44
3	F	302[A]	SO5	C4-C5-N7	-2.31	106.99	109.40
2	A	301[B]	LCV	O3'-P3-O31	-2.31	100.47	109.39
2	E	301[B]	LCV	CP5-CP4-CP3	-2.29	108.54	112.36
2	F	303[A]	LCV	O7-P2-O21	-2.28	101.74	110.68
2	F	301[B]	LCV	O5'-C5'-C4'	-2.28	101.14	108.99
3	E	302[A]	SO5	CP2-NP1-CP3	-2.28	118.61	122.84
3	E	302[A]	SO5	C2-N1-C6	2.27	122.63	118.75
3	C	302[A]	SO5	C2-N1-C6	2.27	122.63	118.75
2	C	301[B]	LCV	C2-N1-C6	2.26	122.62	118.75
2	E	301[B]	LCV	C2-N1-C6	2.25	122.60	118.75
3	F	302[A]	SO5	O5'-C5'-C4'	-2.24	101.28	108.99
3	F	302[A]	SO5	CP9-CPA-CP7	2.21	112.65	108.82
2	B	301[B]	LCV	CP9-CPA-CP7	2.20	112.63	108.82
3	C	302[A]	SO5	C5'-C4'-C3'	-2.19	107.13	114.40
3	F	302[A]	SO5	O56-SS4-CS2	-2.19	107.97	109.43
2	C	301[B]	LCV	C5'-C4'-C3'	-2.18	107.16	114.40
3	E	302[A]	SO5	CP5-CP4-CP3	-2.18	108.72	112.36
2	D	301[B]	LCV	C1'-N9-C4	-2.18	122.81	126.64
3	A	302[A]	SO5	O32-P3-O33	2.18	119.20	110.68
3	D	302[A]	SO5	C1'-N9-C4	-2.17	122.82	126.64
2	C	303[A]	LCV	C4-C5-N7	-2.16	107.15	109.40
3	D	302[A]	SO5	O32-P3-O31	2.15	115.86	107.64
3	F	302[A]	SO5	CP5-CP4-CP3	-2.15	108.78	112.36
2	F	301[B]	LCV	OPS-CS1-OS1	-2.14	120.08	124.13
2	B	301[B]	LCV	C2'-C3'-C4'	2.13	107.01	103.22
3	B	302[A]	SO5	P1-O6-P2	-2.10	125.61	132.83
3	C	302[A]	SO5	C1'-N9-C4	-2.09	122.97	126.64
2	A	301[B]	LCV	OS4-SS4-O56	-2.09	108.28	116.52
2	C	301[B]	LCV	C1'-N9-C4	-2.07	123.00	126.64
2	C	303[A]	LCV	O3'-P3-O31	-2.07	101.40	109.39
2	F	301[B]	LCV	CP9-CPA-CPB	2.07	111.61	108.23
3	D	302[A]	SO5	OPS-CS1-OS1	-2.05	120.25	124.13
3	B	302[A]	SO5	CP1-OPS-CS1	2.04	120.90	116.58
2	F	301[B]	LCV	CP2-NP1-CP3	-2.01	119.11	122.84

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301[B]	LCV	OPS-CS1-CS2-CS3
2	A	301[B]	LCV	CP6-CP7-CPA-CP9

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Mol	Chain	Res	Type	Atoms
2	A	301[B]	LCV	OP3-CP7-CPA-CP9
2	A	301[B]	LCV	CP7-CPA-CPB-O7
2	B	301[B]	LCV	OPS-CS1-CS2-CS3
2	B	301[B]	LCV	C3'-O3'-P3-O33
2	C	303[A]	LCV	C5'-O5'-P1-O6
2	C	303[A]	LCV	C5'-O5'-P1-O12
2	E	301[B]	LCV	OPS-CS1-CS2-CS3
2	E	301[B]	LCV	CP6-CP7-CPA-CP9
2	E	301[B]	LCV	OP3-CP7-CPA-CP9
2	E	301[B]	LCV	CP7-CPA-CPB-O7
2	E	301[B]	LCV	C5'-O5'-P1-O6
2	E	301[B]	LCV	C5'-O5'-P1-O11
2	F	301[B]	LCV	CS3-CS2-SS4-OS5
2	F	301[B]	LCV	CP6-CP7-CPA-CP9
2	F	301[B]	LCV	CP6-CP7-CPA-CPB
2	F	301[B]	LCV	OP3-CP7-CPA-CP9
2	F	301[B]	LCV	CP7-CPA-CPB-O7
2	F	303[A]	LCV	C5'-O5'-P1-O11
2	F	303[A]	LCV	C5'-O5'-P1-O12
2	F	303[A]	LCV	C3'-O3'-P3-O33
3	B	302[A]	SO5	CP6-CP7-CPA-CP9
3	B	302[A]	SO5	OP3-CP7-CPA-CP9
3	B	302[A]	SO5	CP7-CPA-CPB-O7
3	D	302[A]	SO5	C3'-O3'-P3-O33
3	E	302[A]	SO5	CP6-CP7-CPA-CP9
3	E	302[A]	SO5	OP3-CP7-CPA-CP9
3	E	302[A]	SO5	CP7-CPA-CPB-O7
3	E	302[A]	SO5	C5'-O5'-P1-O12
3	F	302[A]	SO5	C5'-O5'-P1-O12
2	E	301[B]	LCV	CP8-CPA-CPB-O7
2	F	301[B]	LCV	CP8-CPA-CPB-O7
3	B	302[A]	SO5	CP9-CPA-CPB-O7
3	E	302[A]	SO5	CP8-CPA-CPB-O7
2	C	301[B]	LCV	OPS-CS1-CS2-CS3
2	D	301[B]	LCV	OPS-CS1-CS2-CS3
2	F	301[B]	LCV	OPS-CS1-CS2-CS3
2	F	301[B]	LCV	P1-O6-P2-O7
2	F	303[A]	LCV	P2-O6-P1-O5'
2	B	301[B]	LCV	C3'-O3'-P3-O31
2	F	303[A]	LCV	C3'-O3'-P3-O31
3	A	302[A]	SO5	C3'-O3'-P3-O33
2	A	301[B]	LCV	C3'-O3'-P3-O32

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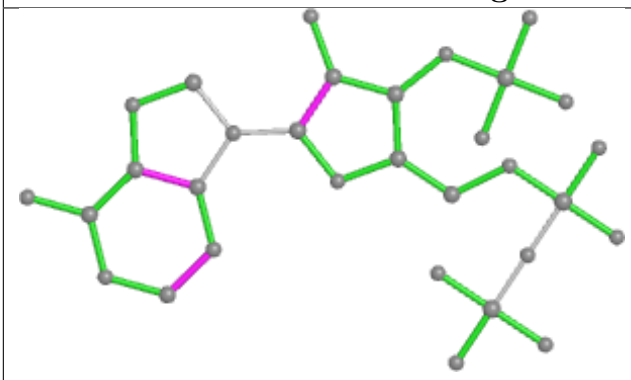
Mol	Chain	Res	Type	Atoms
2	D	301[B]	LCV	C3'-O3'-P3-O32
3	D	302[A]	SO5	C3'-O3'-P3-O32
3	E	302[A]	SO5	C5'-O5'-P1-O6
2	C	303[A]	LCV	C5'-O5'-P1-O11
2	E	301[B]	LCV	OP3-CP7-CPA-CPB
2	F	301[B]	LCV	OP3-CP7-CPA-CPB
3	E	302[A]	SO5	OP3-CP7-CPA-CPB
2	A	301[B]	LCV	OS1-CS1-CS2-CS3
2	A	301[B]	LCV	CP8-CPA-CPB-O7
2	C	303[A]	LCV	O4'-C4'-C5'-O5'
2	E	301[B]	LCV	OS1-CS1-CS2-CS3
2	C	303[A]	LCV	C3'-C4'-C5'-O5'
3	B	302[A]	SO5	CP6-CP7-CPA-CP8
2	D	301[B]	LCV	C3'-O3'-P3-O33
2	F	303[A]	LCV	C5'-O5'-P1-O6
3	A	302[A]	SO5	CPB-O7-P2-O6
3	A	302[A]	SO5	C3'-O3'-P3-O31
3	F	302[A]	SO5	C5'-O5'-P1-O6
2	F	301[B]	LCV	CPB-O7-P2-O22
3	B	302[A]	SO5	C5'-O5'-P1-O12
3	D	302[A]	SO5	C5'-O5'-P1-O12
2	C	301[B]	LCV	CP9-CPA-CPB-O7

There are no ring outliers.

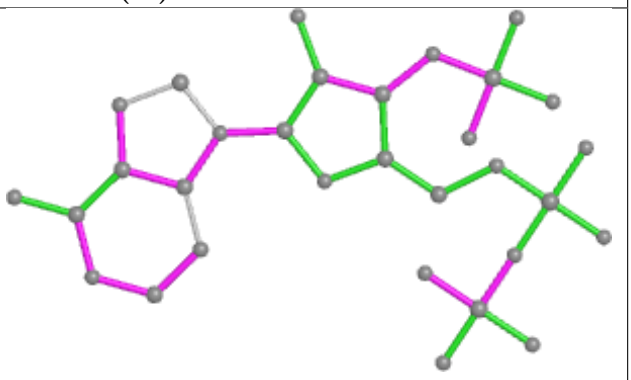
No monomer is involved in short contacts.

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.

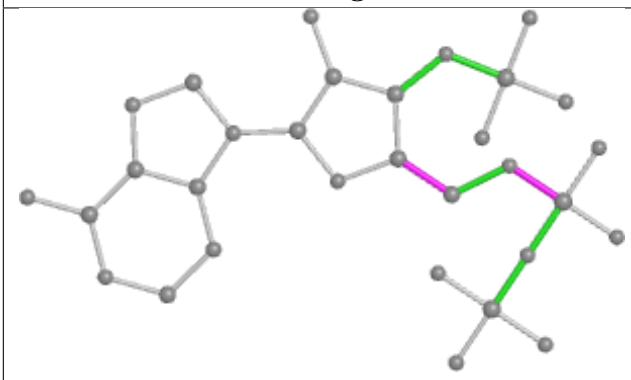
Ligand LCV C 303 (A)



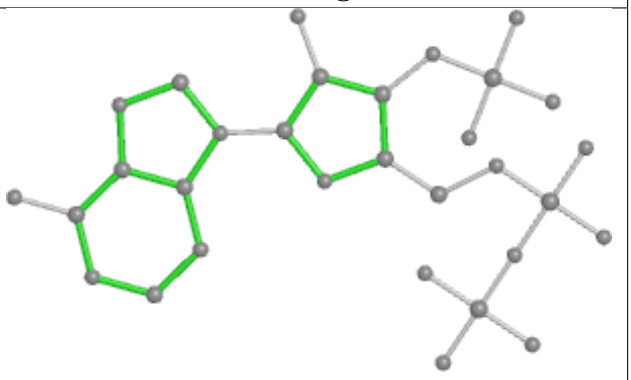
Bond lengths



Bond angles

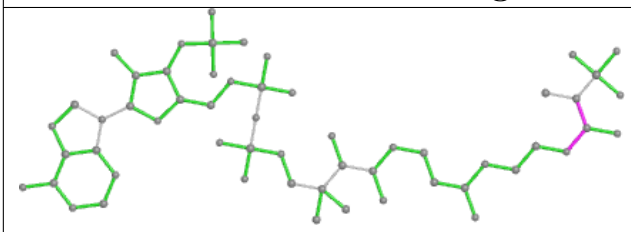


Torsions

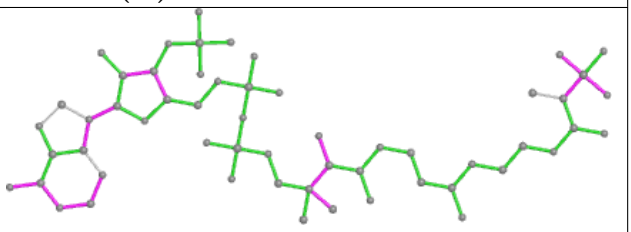


Rings

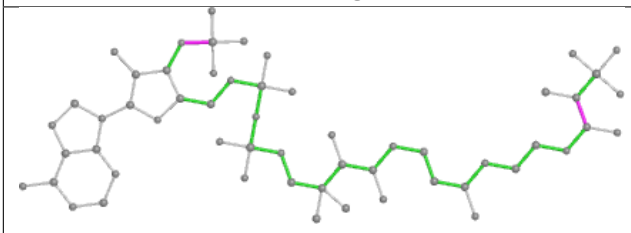
Ligand LCV B 301 (B)



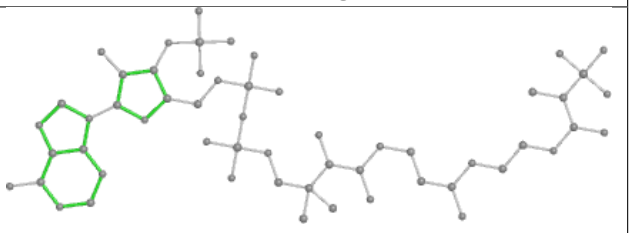
Bond lengths



Bond angles

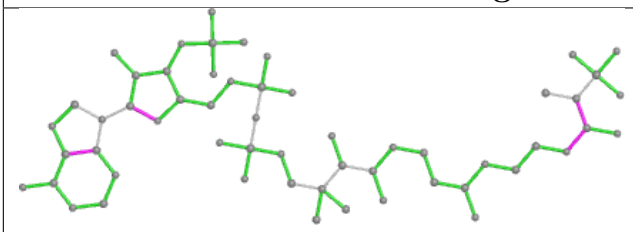


Torsions

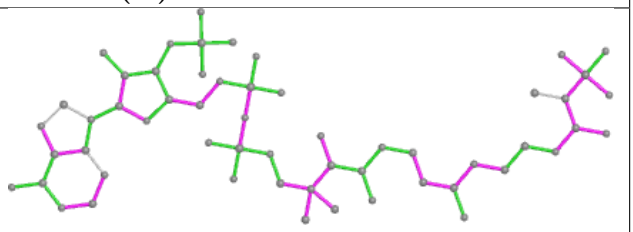


Rings

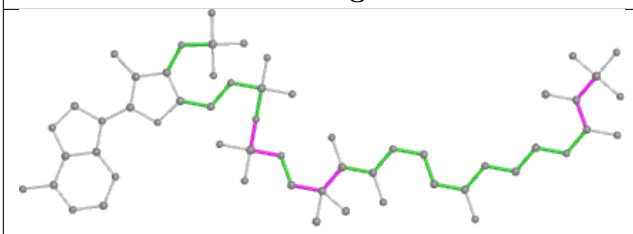
Ligand LCV F 301 (B)



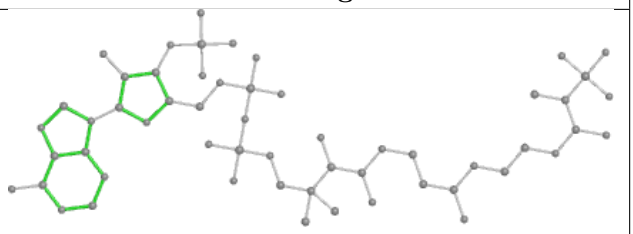
Bond lengths



Bond angles

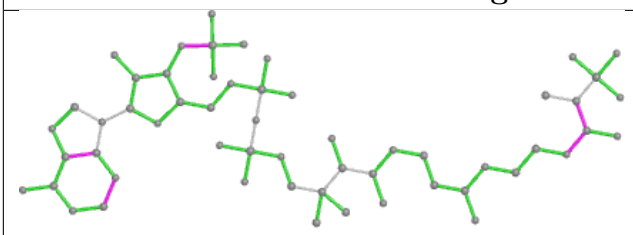


Torsions

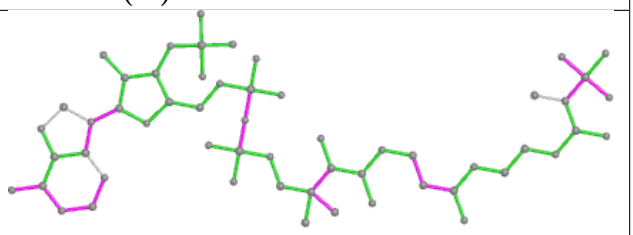


Rings

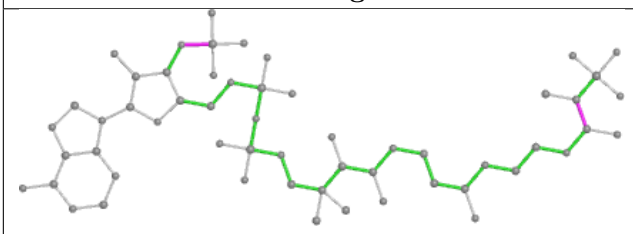
Ligand LCV D 301 (B)



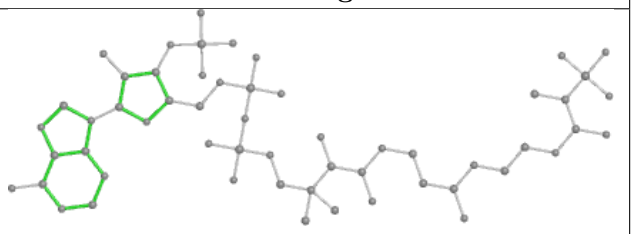
Bond lengths



Bond angles

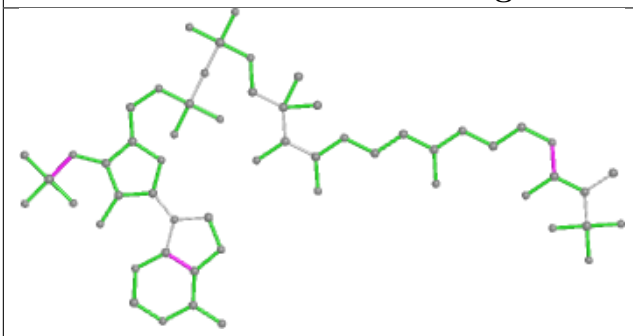


Torsions

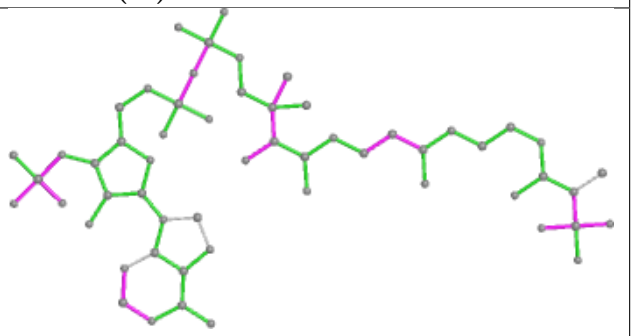


Rings

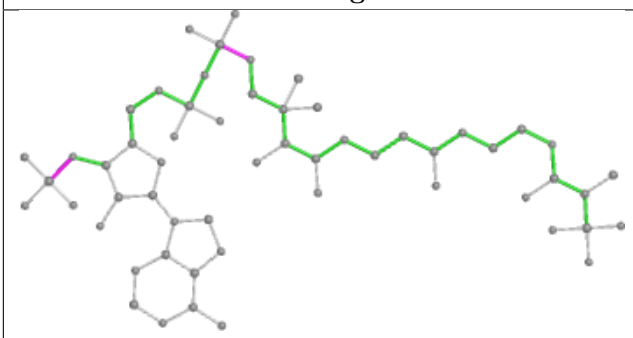
Ligand SO5 A 302 (A)



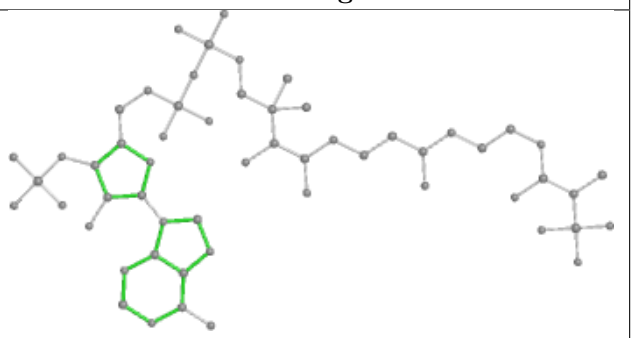
Bond lengths



Bond angles

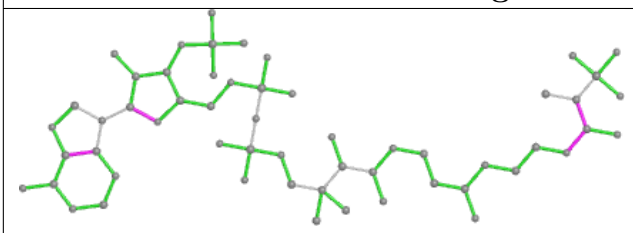


Torsions

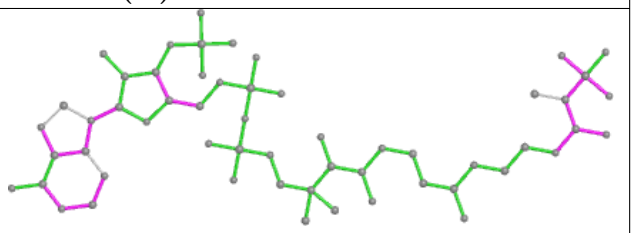


Rings

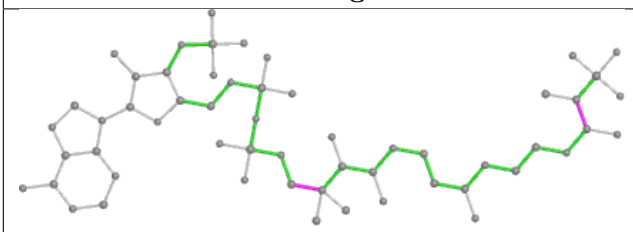
Ligand LCV C 301 (B)



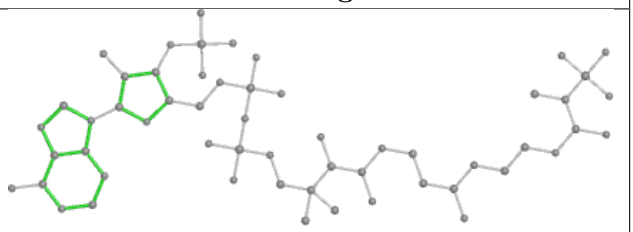
Bond lengths



Bond angles

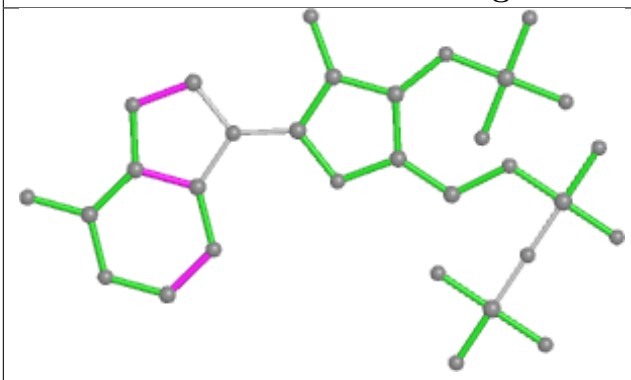


Torsions

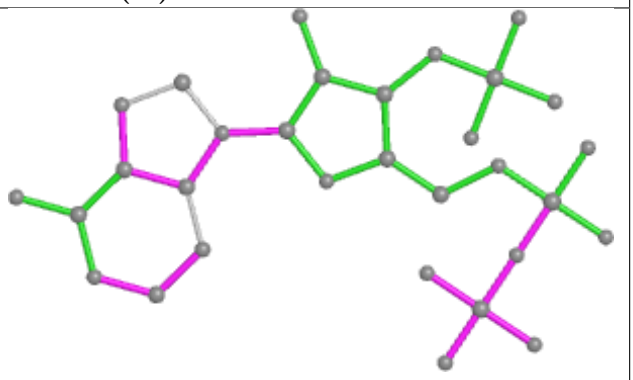


Rings

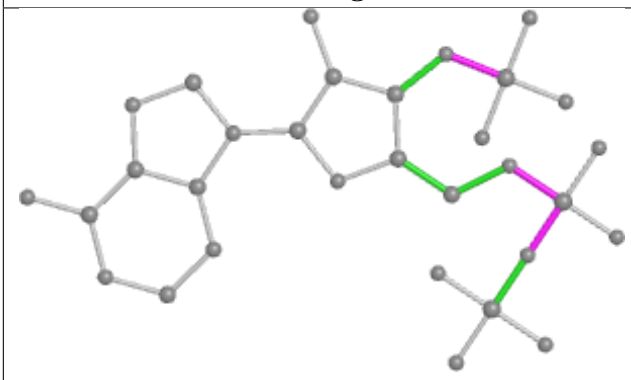
Ligand LCV F 303 (A)



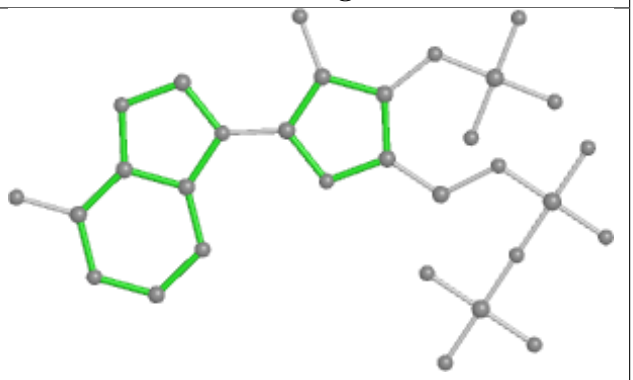
Bond lengths



Bond angles

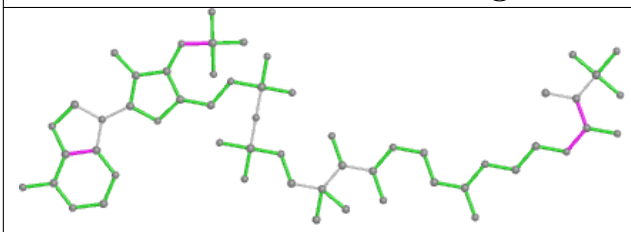


Torsions

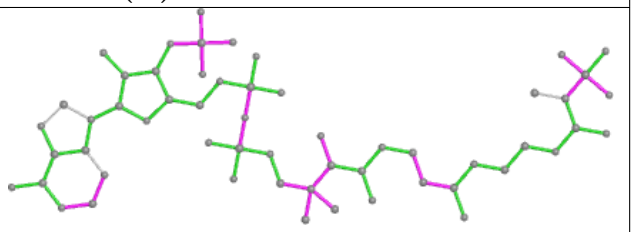


Rings

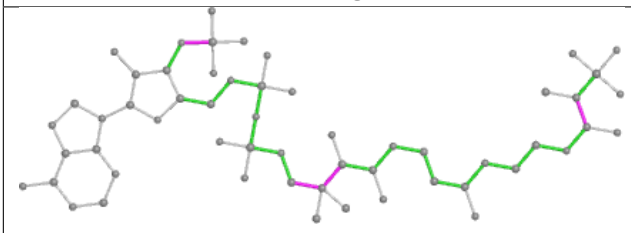
Ligand LCV A 301 (B)



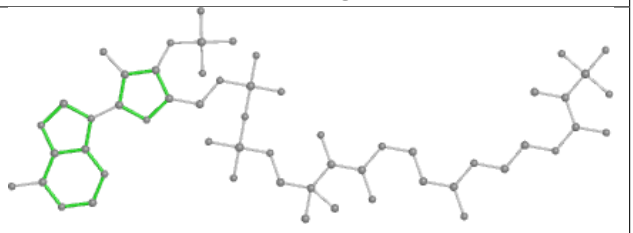
Bond lengths



Bond angles

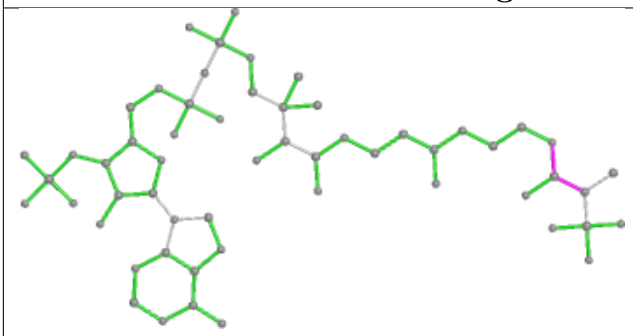


Torsions

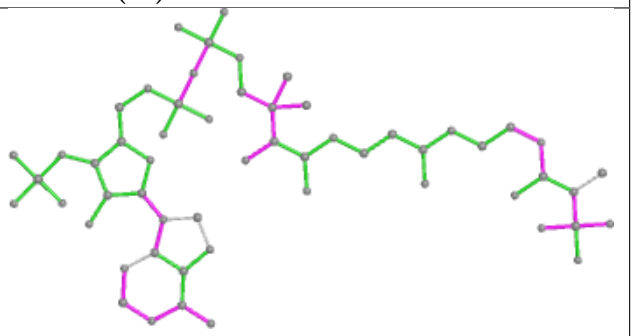


Rings

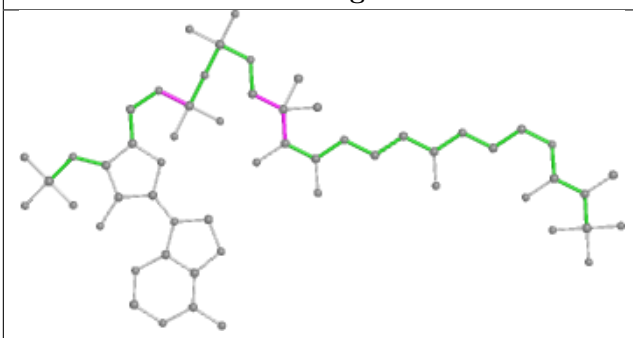
Ligand SO5 B 302 (A)



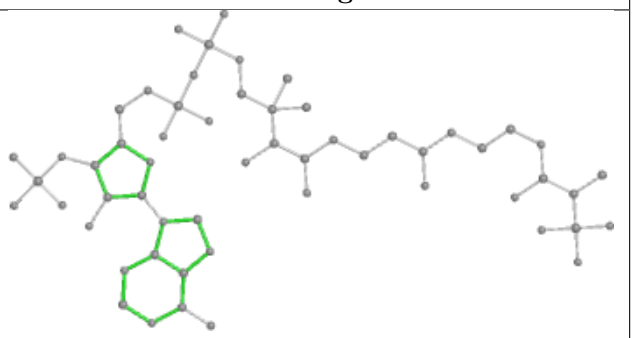
Bond lengths



Bond angles

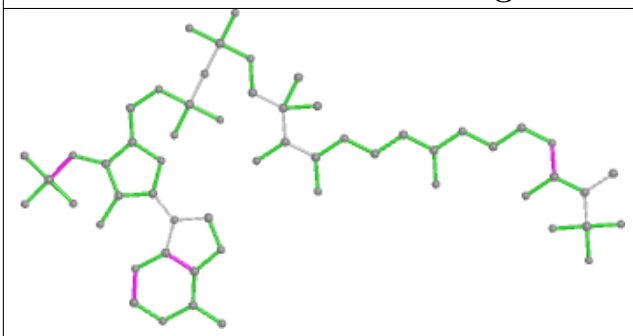


Torsions

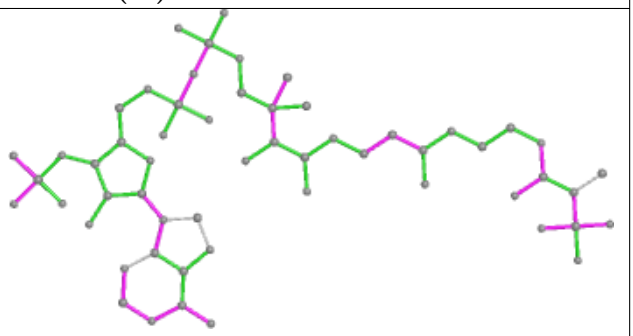


Rings

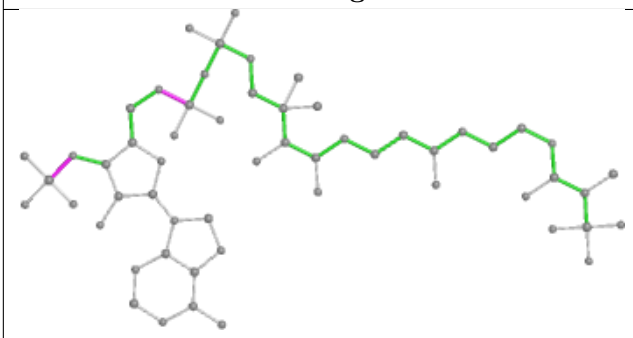
Ligand SO5 D 302 (A)



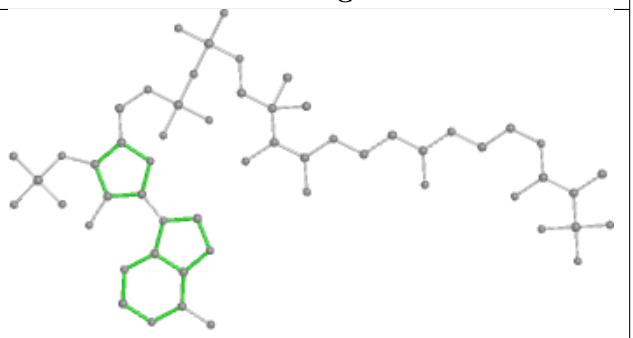
Bond lengths



Bond angles

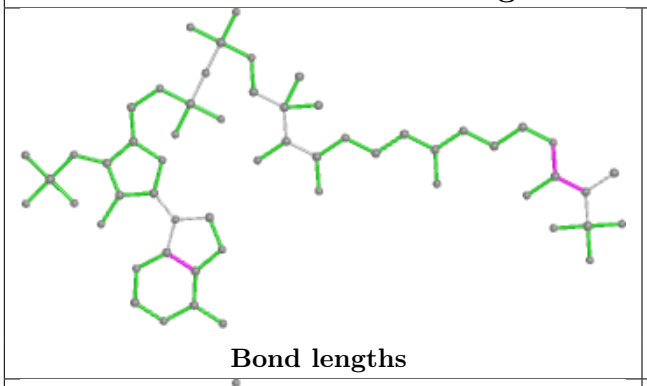


Torsions

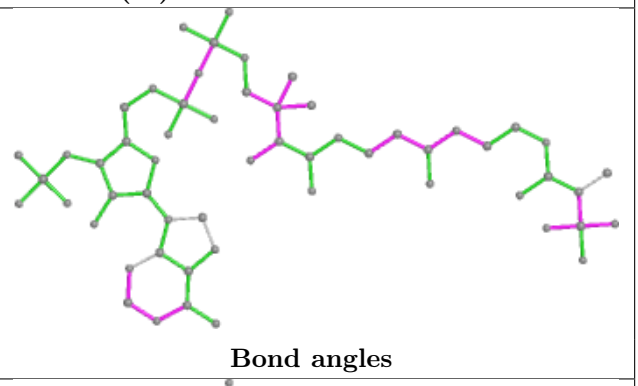


Rings

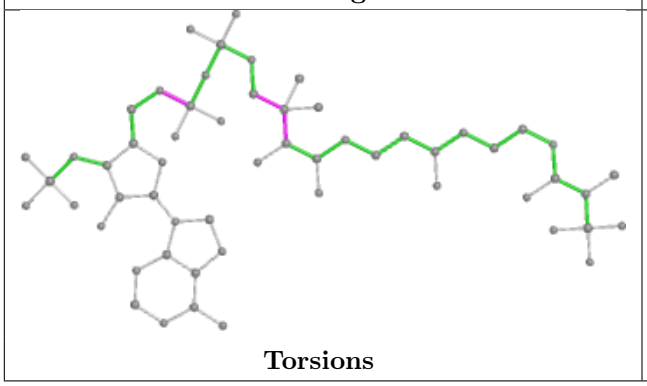
Ligand SO5 E 302 (A)



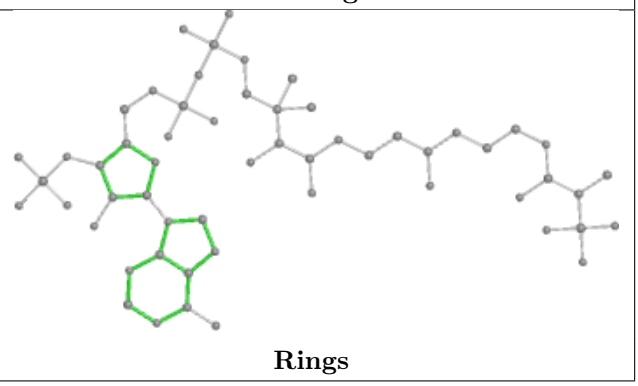
Bond lengths



Bond angles

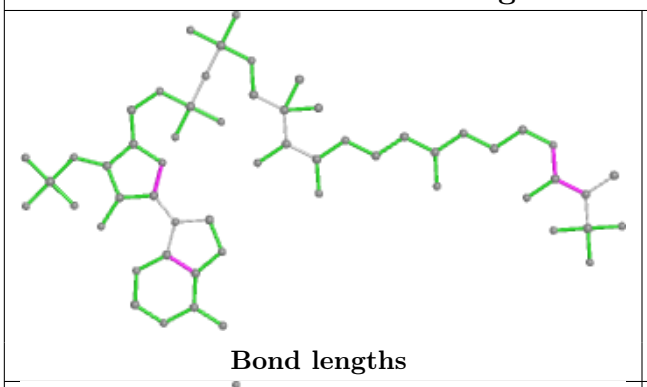


Torsions

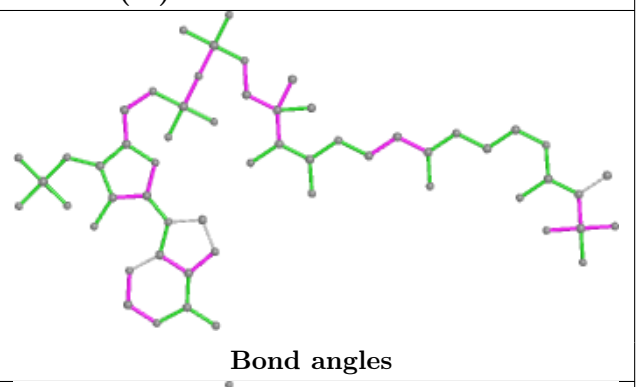


Rings

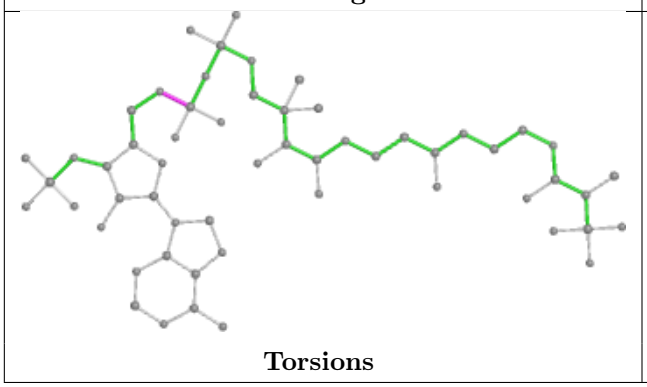
Ligand SO5 F 302 (A)



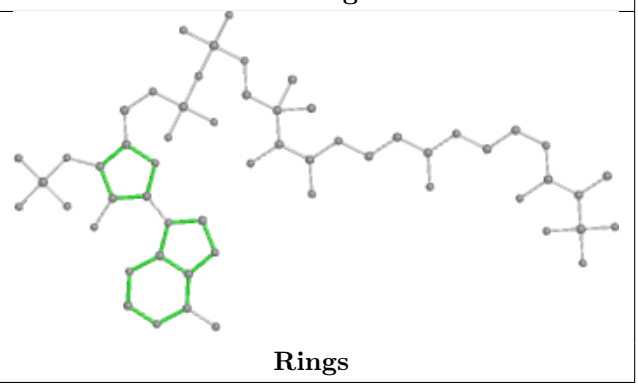
Bond lengths



Bond angles

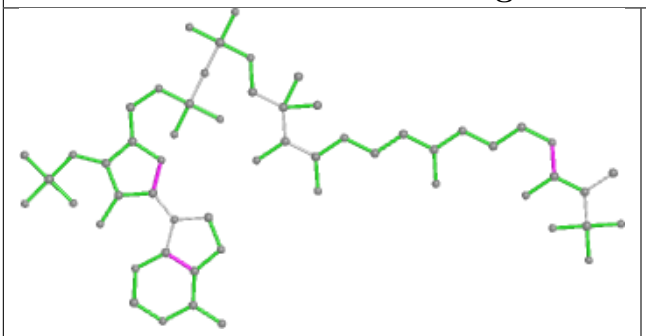


Torsions

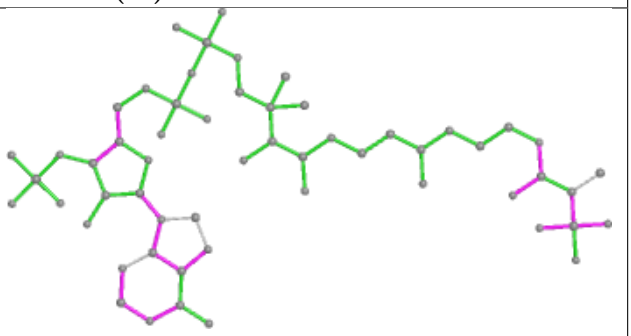


Rings

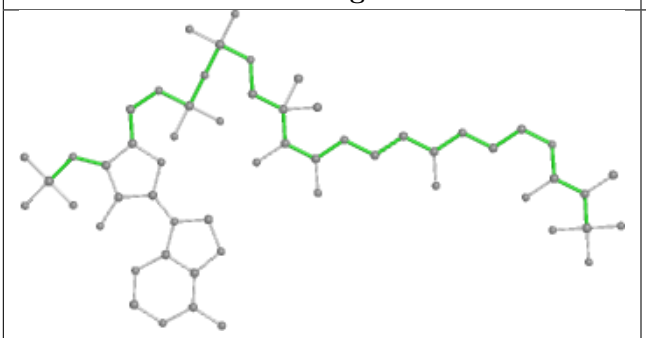
Ligand SO5 C 302 (A)



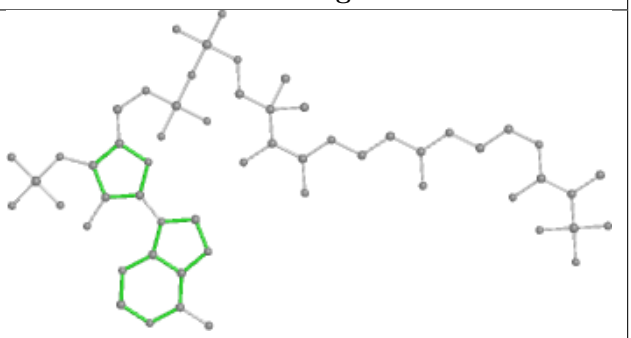
Bond lengths



Bond angles

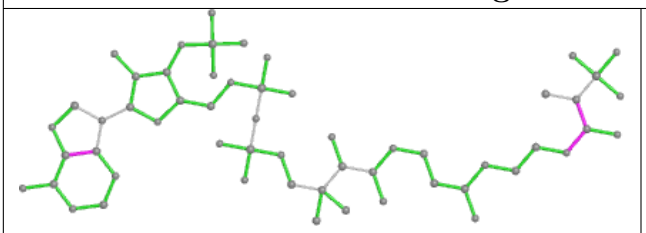


Torsions

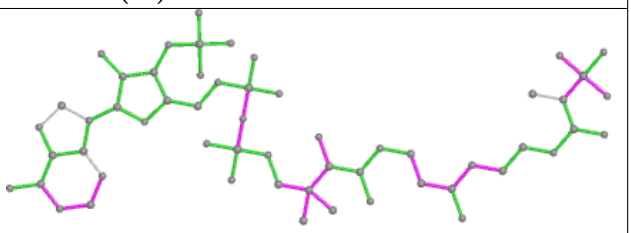


Rings

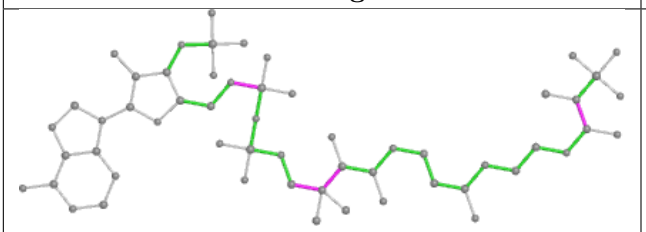
Ligand LCV E 301 (B)



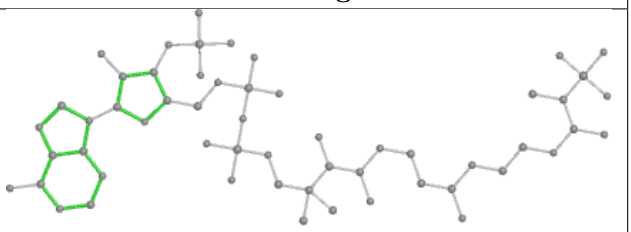
Bond lengths



Bond angles



Torsions



Rings

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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