Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 04:31 AM EDT

PDB ID	:	6NHG
Title	:	Rhodobacter sphaeroides Mitochondrial respiratory chain complex
Authors	:	Xia, D.; Zhou, F.; Esser, L.
Deposited on	:	2018-12-21
Resolution	:	2.80 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 2.80 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 20 unique types of molecules in this entry. The entry contains 33542 atoms, of which 16676 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 Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	446	6799	2161	3341	609	668	20	0	0	0

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	425	6328	1998	3147	564	612	7	0	0	0

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	378	6056	2013	3053	471	501	18	0	0	0

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	241	3778	1225	1859	330	349	15	0	0	0

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
5	E	196	3015	957	1497	263	290	8	0	0	0

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
6	F	105	1816	576	905	166	167	2	0	0	0

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	75	Total	C	H	N	O	S	0	0	0
			1261	410	633	118	99	1			

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	H	67	Total	C	H	N	O	S	0	0	0
			1075	332	527	99	112	5			

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
9	I	34	Total	C	H	N	O	S	0	0	0
			509	149	265	51	43	1			

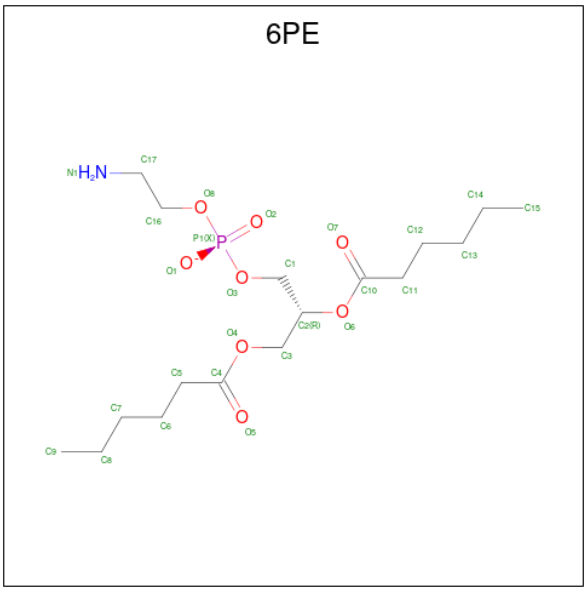
- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	61	Total	C	H	N	O	0	0	0
			1004	329	502	87	86			

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 10.

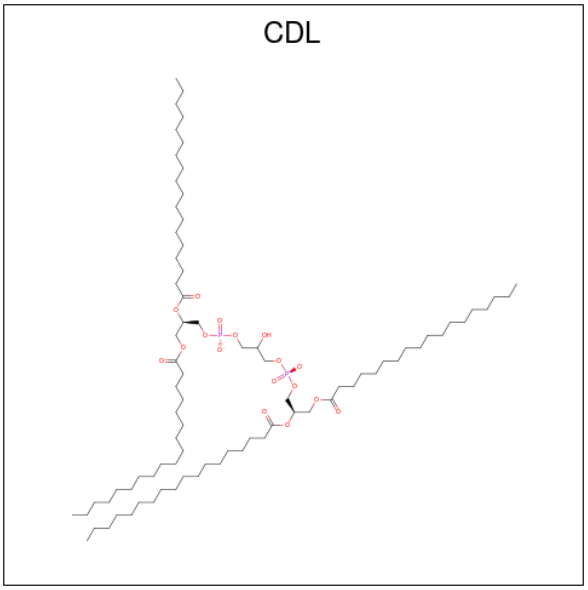
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	52	Total	C	H	N	O	0	0	0
			865	288	435	77	65			

- Molecule 12 is 1,2-DIHEXANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 6PE) (formula: $C_{17}H_{33}NO_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	A	1	Total	C	H	N	O	P	0	0
			60	17	33	1	8	1		
12	K	1	Total	C	H	N	O	P	0	0
			60	17	33	1	8	1		

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	H	O	P	0	0
			124	41	64	17	2		
13	D	1	Total	C	H	O	P	0	0
			124	41	64	17	2		

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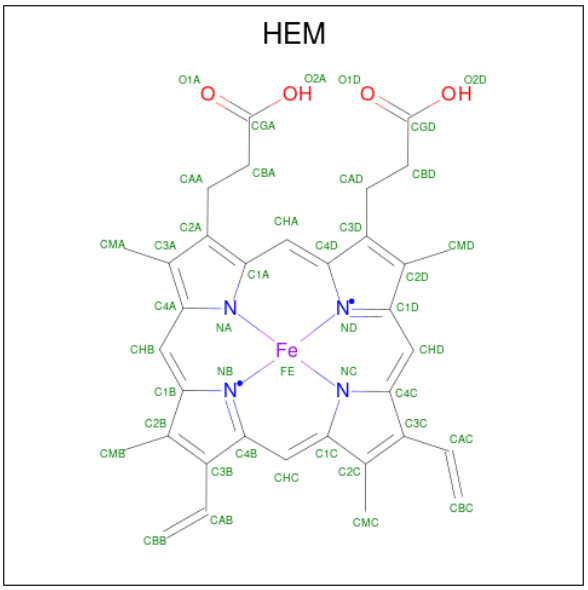
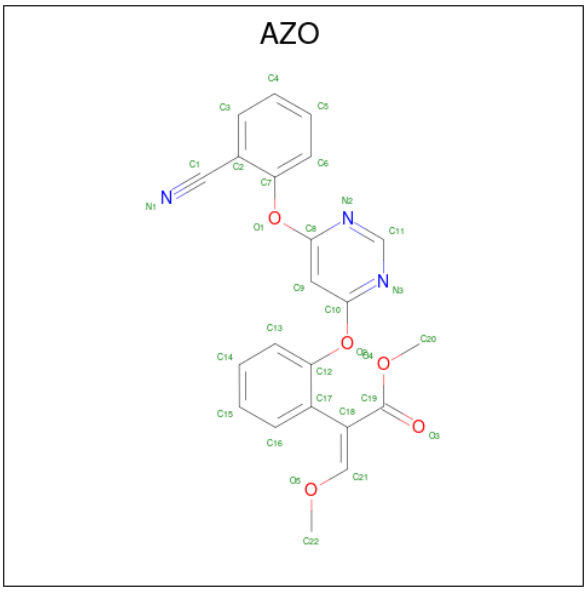
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	G	1	Total	C	H	O	P	0	0
			124	41	64	17	2		

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



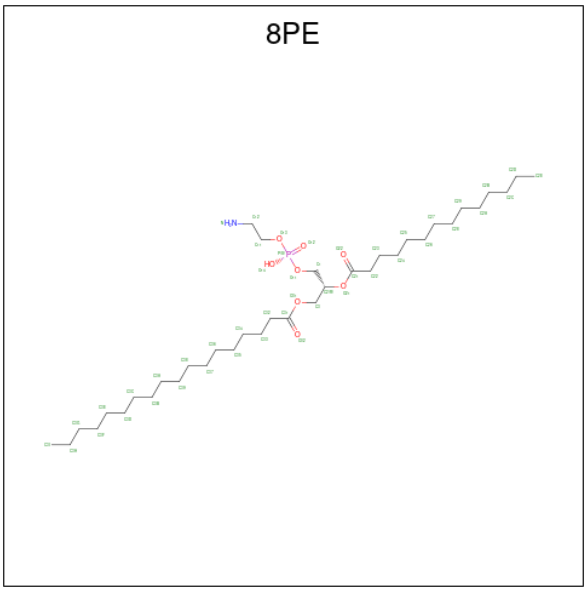
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
14	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 15 is METHYL (2Z)-2-(2-{[6-(2-CYANOPHENOXY)PYRIMIDIN-4-YL]OXY}PHENYL)-3-METHOXYACRYLATE (three-letter code: AZO) (formula: $C_{22}H_{17}N_3O_5$).



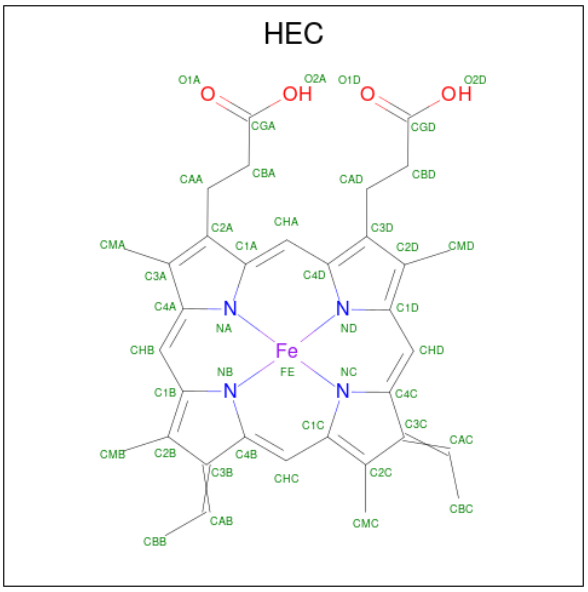
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	H	N	O	0	0
			47	22	17	3	5		

- Molecule 16 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (three-letter code: 8PE) (formula: $C_{37}H_{74}NO_8P$).



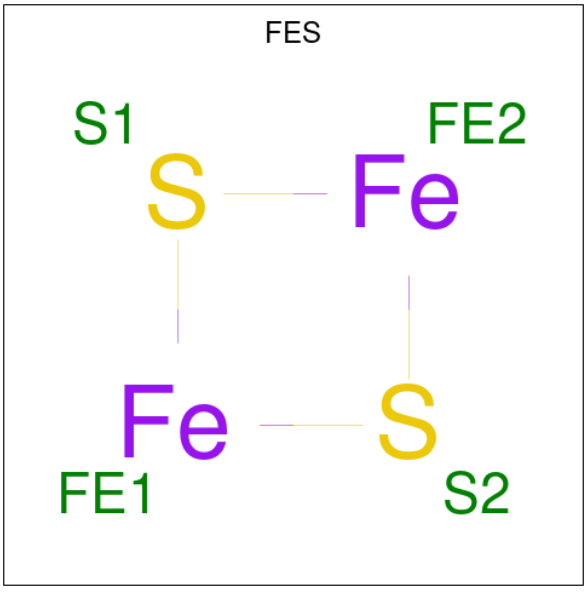
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
16	C	1	Total	C	H	N	O	P	0	0
			120	37	73	1	8	1		

- Molecule 17 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



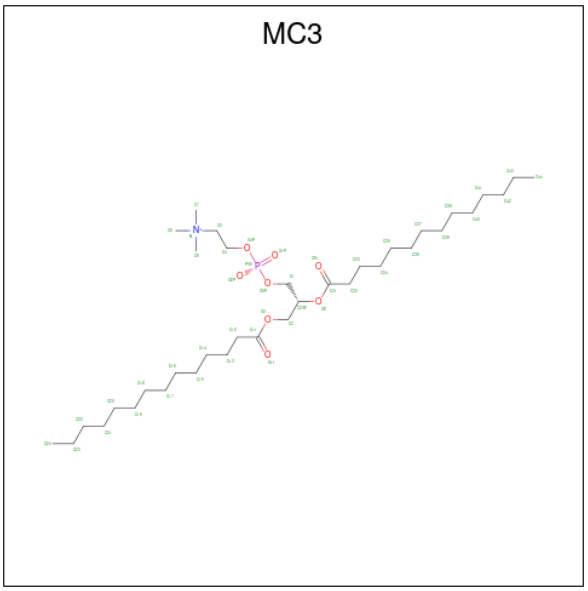
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
17	D	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	E	1	Total	Fe	S		0	0
			4	2	2			

- Molecule 19 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: MC3) (formula: $C_{36}H_{72}NO_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
19	J	1	Total	C	H	N	O	P	0	0
			118	36	72	1	8	1		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	O	0	0
			1	1		
20	B	23	Total	O	0	0
			23	23		
20	C	1	Total	O	0	0
			1	1		
20	F	6	Total	O	0	0
			6	6		
20	G	2	Total	O	0	0
			2	2		
20	I	1	Total	O	0	0
			1	1		

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	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	154.18Å 154.18Å 598.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.80	Depositor
% Data completeness (in resolution range)	98.7 (29.87-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.80Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.251 , 0.289	Depositor
Wilson B-factor (Å^2)	67.6	Xtriage
Anisotropy	0.243	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	33542	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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

12 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	$\#\|Z\| > 2$
13	CDL	G	101	-	59,59,99	1.28	6 (10%)	65,71,111	1.00	4 (6%)
15	AZO	C	1003	-	32,32,32	0.66	0	42,42,42	1.63	8 (19%)
18	FES	E	1001	5	0,4,4	-	-	-		
19	MC3	J	101	-	45,45,45	1.37	3 (6%)	51,53,53	0.97	5 (9%)
13	CDL	A	502	-	59,59,99	1.26	7 (11%)	65,71,111	1.09	4 (6%)
14	HEM	C	1002	3	41,50,50	1.46	5 (12%)	45,82,82	1.39	6 (13%)
12	6PE	K	101	-	26,26,26	1.77	8 (30%)	29,31,31	1.14	2 (6%)
13	CDL	D	1002	-	59,59,99	1.26	5 (8%)	65,71,111	1.18	5 (7%)
14	HEM	C	1001	3	41,50,50	1.49	6 (14%)	45,82,82	1.43	6 (13%)
17	HEC	D	1001	4	32,50,50	2.15	4 (12%)	24,82,82	1.36	1 (4%)
12	6PE	A	501	-	26,26,26	1.74	8 (30%)	29,31,31	1.11	2 (6%)
16	8PE	C	1004	-	46,46,46	1.62	6 (13%)	49,51,51	1.07	4 (8%)

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
13	CDL	G	101	-	-	17/70/70/110	-
15	AZO	C	1003	-	-	2/23/23/23	0/3/3/3
18	FES	E	1001	5	-	-	0/1/1/1
19	MC3	J	101	-	-	24/49/49/49	-
13	CDL	A	502	-	-	25/70/70/110	-
14	HEM	C	1002	3	-	3/12/54/54	-
12	6PE	K	101	-	-	12/30/30/30	-
13	CDL	D	1002	-	-	32/70/70/110	-
14	HEM	C	1001	3	-	4/12/54/54	-
17	HEC	D	1001	4	-	3/10/54/54	-
12	6PE	A	501	-	-	13/30/30/30	-
16	8PE	C	1004	-	-	22/50/50/50	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	D	1001	HEC	C2B-C3B	-6.35	1.34	1.40
17	D	1001	HEC	C3D-C2D	5.43	1.53	1.37
17	D	1001	HEC	C3C-C2C	-5.37	1.35	1.40
19	J	101	MC3	P-O4P	4.87	1.79	1.59
16	C	1004	8PE	P-O11	4.81	1.78	1.59
13	G	101	CDL	OA8-CA7	4.13	1.45	1.33
14	C	1001	HEM	C3C-C2C	-4.11	1.34	1.40
12	K	101	6PE	P1-O3	4.09	1.75	1.59
13	D	1002	CDL	OA6-CA5	4.06	1.45	1.34
13	G	101	CDL	OA6-CA5	4.02	1.45	1.34
13	A	502	CDL	OA6-CA5	4.02	1.45	1.34
13	D	1002	CDL	OA8-CA7	4.00	1.45	1.33
13	A	502	CDL	OA8-CA7	3.97	1.44	1.33
14	C	1002	HEM	C3C-C2C	-3.77	1.35	1.40
14	C	1001	HEM	C3C-CAC	3.62	1.55	1.47
12	A	501	6PE	P1-O8	3.61	1.73	1.59
14	C	1002	HEM	C3C-CAC	3.57	1.55	1.47
13	G	101	CDL	OB8-CB7	3.57	1.43	1.33
12	A	501	6PE	P1-O3	3.56	1.73	1.59
16	C	1004	8PE	C3-C2	3.48	1.61	1.50
13	D	1002	CDL	OB8-CB7	3.47	1.43	1.33
13	A	502	CDL	OB8-CB7	3.47	1.43	1.33
12	A	501	6PE	C3-C2	3.36	1.61	1.50
12	K	101	6PE	P1-O8	3.35	1.72	1.59
16	C	1004	8PE	P-O13	3.33	1.72	1.59
16	C	1004	8PE	C1-C2	3.28	1.60	1.50
13	D	1002	CDL	OB6-CB5	3.23	1.43	1.34
12	K	101	6PE	C3-C2	3.23	1.60	1.50
13	G	101	CDL	OB6-CB5	3.23	1.43	1.34
13	A	502	CDL	OB6-CB5	3.11	1.43	1.34
14	C	1001	HEM	CAB-C3B	2.99	1.55	1.47
14	C	1002	HEM	CAB-C3B	2.96	1.55	1.47
19	J	101	MC3	C1-C2	2.78	1.59	1.50
16	C	1004	8PE	C32-C31	2.52	1.58	1.50
12	K	101	6PE	O4-C4	2.47	1.40	1.33
12	A	501	6PE	C5-C4	2.45	1.57	1.50
16	C	1004	8PE	C33-C32	2.42	1.61	1.52
12	K	101	6PE	C5-C4	2.41	1.57	1.50
12	A	501	6PE	O4-C4	2.38	1.40	1.33
12	K	101	6PE	C1-C2	2.35	1.57	1.50
12	K	101	6PE	C11-C10	2.34	1.57	1.50
12	K	101	6PE	O6-C10	2.32	1.40	1.34
19	J	101	MC3	P-O3P	2.30	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	502	CDL	OA6-CA4	-2.27	1.40	1.46
13	G	101	CDL	OA6-CA4	-2.26	1.40	1.46
14	C	1002	HEM	FE-NB	2.26	2.08	1.96
12	A	501	6PE	C1-C2	2.23	1.57	1.50
12	A	501	6PE	C11-C10	2.22	1.57	1.50
14	C	1002	HEM	CMB-C2B	2.14	1.55	1.50
12	A	501	6PE	O6-C10	2.14	1.40	1.34
13	D	1002	CDL	C11-CA5	2.12	1.56	1.50
14	C	1001	HEM	CAA-C2A	2.08	1.55	1.52
13	A	502	CDL	C11-CA5	2.04	1.56	1.50
14	C	1001	HEM	CMB-C2B	2.04	1.55	1.50
17	D	1001	HEC	CAD-C3D	2.03	1.55	1.52
13	G	101	CDL	C11-CA5	2.02	1.56	1.50
13	A	502	CDL	C31-CA7	2.02	1.56	1.50
14	C	1001	HEM	CMD-C2D	2.01	1.55	1.50

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	1003	AZO	C11-N3-C10	5.83	118.86	114.48
13	D	1002	CDL	OA6-CA5-C11	4.55	121.32	111.50
13	A	502	CDL	OB6-CB5-C51	4.14	120.42	111.50
13	G	101	CDL	OB6-CB5-C51	3.88	119.87	111.50
16	C	1004	8PE	O21-C21-C22	3.82	119.72	111.50
13	D	1002	CDL	OB6-CB5-C51	3.65	119.36	111.50
13	A	502	CDL	OA6-CA5-C11	3.49	119.03	111.50
15	C	1003	AZO	C11-N2-C8	3.35	117.00	114.48
12	K	101	6PE	O6-C10-C11	3.32	118.65	111.50
13	G	101	CDL	OA6-CA5-C11	3.29	118.59	111.50
19	J	101	MC3	O2P-P-O1P	3.28	128.46	112.24
15	C	1003	AZO	C9-C10-N3	-3.24	120.01	124.57
17	D	1001	HEC	CMC-C2C-C1C	-3.21	123.54	128.46
14	C	1002	HEM	C4D-ND-C1D	3.10	108.27	105.07
16	C	1004	8PE	O31-C31-C32	3.05	121.48	111.91
15	C	1003	AZO	C20-O4-C19	3.00	121.53	115.86
14	C	1001	HEM	C4D-ND-C1D	2.98	108.15	105.07
14	C	1002	HEM	C4B-CHC-C1C	2.92	126.41	122.56
14	C	1001	HEM	C1B-NB-C4B	2.85	108.02	105.07
14	C	1001	HEM	C4B-CHC-C1C	2.81	126.26	122.56
16	C	1004	8PE	O31-C31-O32	-2.73	116.71	123.59
14	C	1001	HEM	C4C-CHD-C1D	2.69	126.11	122.56
15	C	1003	AZO	N2-C11-N3	-2.67	124.43	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	D	1002	CDL	OA8-CA7-C31	2.65	120.21	111.91
14	C	1001	HEM	CBA-CAA-C2A	-2.60	108.19	112.62
12	A	501	6PE	O6-C10-C11	2.56	117.02	111.50
13	A	502	CDL	OA8-CA7-C31	2.54	119.89	111.91
14	C	1002	HEM	CBD-CAD-C3D	-2.54	105.57	112.63
13	D	1002	CDL	OB8-CB7-C71	2.51	119.80	111.91
14	C	1002	HEM	C1B-NB-C4B	2.51	107.66	105.07
15	C	1003	AZO	C7-C2-C1	2.41	121.91	119.57
13	A	502	CDL	OB8-CB7-C71	2.40	119.43	111.91
13	G	101	CDL	OB8-CB7-C71	2.39	119.41	111.91
14	C	1002	HEM	C4C-CHD-C1D	2.36	125.67	122.56
15	C	1003	AZO	O2-C10-N3	2.33	123.95	118.64
13	G	101	CDL	OA8-CA7-C31	2.33	119.21	111.91
12	A	501	6PE	O4-C3-C2	2.32	115.18	108.43
12	K	101	6PE	O4-C3-C2	2.25	114.98	108.43
14	C	1001	HEM	C3D-C4D-ND	-2.21	107.71	110.17
14	C	1002	HEM	C3D-C4D-ND	-2.21	107.71	110.17
15	C	1003	AZO	C21-C18-C19	2.20	121.44	117.41
19	J	101	MC3	O2-C31-O31	-2.19	118.41	123.70
16	C	1004	8PE	O31-C3-C2	2.18	114.78	108.43
19	J	101	MC3	O3-C11-O11	-2.14	118.20	123.59
19	J	101	MC3	O4P-P-O1P	-2.12	100.79	109.07
19	J	101	MC3	O2-C31-C32	2.05	115.92	111.50
13	D	1002	CDL	OA6-CA4-CA6	2.02	115.73	108.40

There are no chirality outliers.

All (157) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	501	6PE	C1-O3-P1-O2
12	A	501	6PE	C1-O3-P1-O8
12	A	501	6PE	C11-C10-O6-C2
12	K	101	6PE	C16-O8-P1-O1
12	K	101	6PE	C16-O8-P1-O2
12	K	101	6PE	O8-C16-C17-N1
13	A	502	CDL	CB2-OB2-PB2-OB3
13	A	502	CDL	C51-CB5-OB6-CB4
13	D	1002	CDL	O1-C1-CA2-OA2
13	D	1002	CDL	CA3-OA5-PA1-OA3
13	D	1002	CDL	OA7-CA5-OA6-CA4
13	D	1002	CDL	CB2-OB2-PB2-OB3
13	D	1002	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
13	G	101	CDL	OA6-CA4-CA6-OA8
16	C	1004	8PE	C1-O11-P-O14
16	C	1004	8PE	O13-C11-C12-N
19	J	101	MC3	C1-O3P-P-O1P
16	C	1004	8PE	O32-C31-O31-C3
12	K	101	6PE	C5-C4-O4-C3
12	K	101	6PE	O5-C4-O4-C3
13	A	502	CDL	OB7-CB5-OB6-CB4
13	D	1002	CDL	C31-CA7-OA8-CA6
16	C	1004	8PE	C32-C31-O31-C3
13	D	1002	CDL	C11-CA5-OA6-CA4
19	J	101	MC3	C12-C11-O3-C3
12	A	501	6PE	O7-C10-O6-C2
13	D	1002	CDL	OB9-CB7-OB8-CB6
13	A	502	CDL	O1-C1-CB2-OB2
13	D	1002	CDL	O1-C1-CB2-OB2
13	D	1002	CDL	C71-CB7-OB8-CB6
13	D	1002	CDL	OA9-CA7-OA8-CA6
19	J	101	MC3	O11-C11-O3-C3
13	A	502	CDL	CA2-C1-CB2-OB2
13	D	1002	CDL	CB2-C1-CA2-OA2
13	A	502	CDL	C31-CA7-OA8-CA6
12	A	501	6PE	C10-C11-C12-C13
13	G	101	CDL	CA7-C31-C32-C33
12	A	501	6PE	O5-C4-O4-C3
13	A	502	CDL	OA9-CA7-OA8-CA6
19	J	101	MC3	C32-C31-O2-C2
12	K	101	6PE	C16-O8-P1-O3
13	D	1002	CDL	CA3-OA5-PA1-OA2
13	D	1002	CDL	CB3-OB5-PB2-OB2
13	G	101	CDL	CB2-OB2-PB2-OB5
19	J	101	MC3	C1-O3P-P-O4P
19	J	101	MC3	C13-C14-C15-C16
13	D	1002	CDL	C51-CB5-OB6-CB4
13	A	502	CDL	C12-C13-C14-C15
19	J	101	MC3	C32-C33-C34-C35
13	D	1002	CDL	OB7-CB5-OB6-CB4
19	J	101	MC3	C36-C37-C38-C39
13	G	101	CDL	O1-C1-CB2-OB2
12	A	501	6PE	C4-C5-C6-C7
13	A	502	CDL	CB7-C71-C72-C73
16	C	1004	8PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
16	C	1004	8PE	C3B-C3C-C3D-C3E
13	G	101	CDL	C52-C53-C54-C55
13	G	101	CDL	C12-C13-C14-C15
12	K	101	6PE	O7-C10-O6-C2
19	J	101	MC3	C35-C36-C37-C38
13	A	502	CDL	OA7-CA5-OA6-CA4
12	A	501	6PE	C5-C4-O4-C3
13	D	1002	CDL	C72-C73-C74-C75
13	D	1002	CDL	C51-C52-C53-C54
13	D	1002	CDL	CB5-C51-C52-C53
13	D	1002	CDL	C31-C32-C33-C34
12	K	101	6PE	C11-C10-O6-C2
13	A	502	CDL	C11-CA5-OA6-CA4
16	C	1004	8PE	C22-C21-O21-C2
12	A	501	6PE	O6-C2-C3-O4
16	C	1004	8PE	C2-C3-O31-C31
16	C	1004	8PE	C26-C27-C28-C29
19	J	101	MC3	O31-C31-O2-C2
13	D	1002	CDL	CB2-OB2-PB2-OB5
16	C	1004	8PE	C1-O11-P-O13
13	D	1002	CDL	C12-C13-C14-C15
13	A	502	CDL	C51-C52-C53-C54
16	C	1004	8PE	C3A-C3B-C3C-C3D
19	J	101	MC3	C41-C42-C43-C44
19	J	101	MC3	C31-C32-C33-C34
13	D	1002	CDL	CA2-C1-CB2-OB2
16	C	1004	8PE	C35-C36-C37-C38
19	J	101	MC3	C14-C15-C16-C17
13	A	502	CDL	C14-C15-C16-C17
19	J	101	MC3	C37-C38-C39-C40
16	C	1004	8PE	C3D-C3E-C3F-C3G
19	J	101	MC3	C33-C34-C35-C36
13	A	502	CDL	C74-C75-C76-C77
19	J	101	MC3	C34-C35-C36-C37
13	A	502	CDL	OB5-CB3-CB4-CB6
19	J	101	MC3	O3P-C1-C2-C3
14	C	1001	HEM	C3D-CAD-CBD-CGD
12	A	501	6PE	C1-C2-C3-O4
16	C	1004	8PE	C1-C2-C3-O31
13	A	502	CDL	CB2-OB2-PB2-OB5
19	J	101	MC3	O3P-C1-C2-O2
13	G	101	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
13	G	101	CDL	C11-C12-C13-C14
13	G	101	CDL	C14-C15-C16-C17
16	C	1004	8PE	C25-C26-C27-C28
13	G	101	CDL	OB7-CB5-OB6-CB4
12	K	101	6PE	C2-C1-O3-P1
13	G	101	CDL	CA3-CA4-CA6-OA8
16	C	1004	8PE	C24-C25-C26-C27
12	A	501	6PE	C2-C1-O3-P1
13	A	502	CDL	CB2-OB2-PB2-OB4
13	D	1002	CDL	CA3-OA5-PA1-OA4
13	D	1002	CDL	CB2-OB2-PB2-OB4
13	G	101	CDL	CB2-OB2-PB2-OB4
16	C	1004	8PE	C1-O11-P-O12
19	J	101	MC3	C1-O3P-P-O2P
16	C	1004	8PE	C3E-C3F-C3G-C3H
13	A	502	CDL	OB5-CB3-CB4-OB6
19	J	101	MC3	C38-C39-C40-C41
19	J	101	MC3	O4P-C4-C5-N
16	C	1004	8PE	O21-C2-C3-O31
13	D	1002	CDL	CA6-CA4-OA6-CA5
13	D	1002	CDL	CB6-CB4-OB6-CB5
19	J	101	MC3	O2-C2-C3-O3
19	J	101	MC3	C1-C2-C3-O3
13	A	502	CDL	OA6-CA4-CA6-OA8
13	G	101	CDL	C73-C74-C75-C76
13	A	502	CDL	CA3-CA4-CA6-OA8
13	D	1002	CDL	CA3-CA4-CA6-OA8
13	D	1002	CDL	OA5-CA3-CA4-OA6
13	A	502	CDL	OA5-CA3-CA4-CA6
12	K	101	6PE	O6-C2-C3-O4
13	G	101	CDL	OB9-CB7-OB8-CB6
14	C	1002	HEM	CAA-CBA-CGA-O1A
12	K	101	6PE	C1-C2-C3-O4
13	A	502	CDL	C71-C72-C73-C74
17	D	1001	HEC	CAA-CBA-CGA-O2A
13	G	101	CDL	C71-CB7-OB8-CB6
16	C	1004	8PE	C11-O13-P-O11
17	D	1001	HEC	CAA-CBA-CGA-O1A
12	A	501	6PE	O3-C1-C2-C3
14	C	1001	HEM	CAD-CBD-CGD-O1D
13	A	502	CDL	C52-C51-CB5-OB6
15	C	1003	AZO	N1-C1-C2-C7

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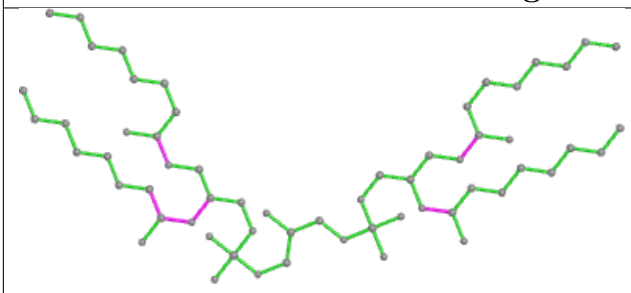
Mol	Chain	Res	Type	Atoms
14	C	1002	HEM	CAA-CBA-CGA-O2A
15	C	1003	AZO	C12-C17-C18-C21
13	D	1002	CDL	C14-C15-C16-C17
13	G	101	CDL	OA7-CA5-OA6-CA4
14	C	1001	HEM	CAA-CBA-CGA-O2A
16	C	1004	8PE	C29-C2A-C2B-C2C
13	D	1002	CDL	CB3-OB5-PB2-OB3
13	G	101	CDL	CB2-OB2-PB2-OB3
16	C	1004	8PE	C11-O13-P-O12
12	A	501	6PE	O7-C10-C11-C12
13	A	502	CDL	C52-C51-CB5-OB7
19	J	101	MC3	O2-C31-C32-C33
14	C	1001	HEM	CAD-CBD-CGD-O2D
13	D	1002	CDL	C52-C51-CB5-OB6
14	C	1002	HEM	CAD-CBD-CGD-O2D
17	D	1001	HEC	CAD-CBD-CGD-O1D
12	K	101	6PE	C4-C5-C6-C7
13	A	502	CDL	C11-C12-C13-C14

There are no ring outliers.

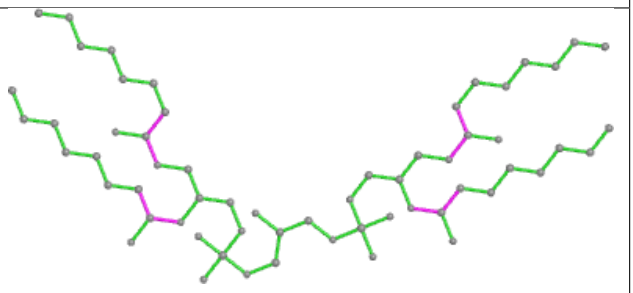
No monomer is involved in short contacts.

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.

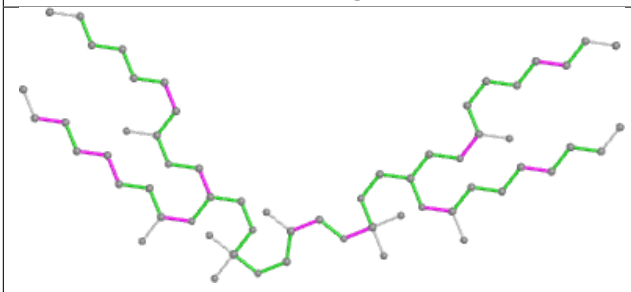
Ligand CDL G 101



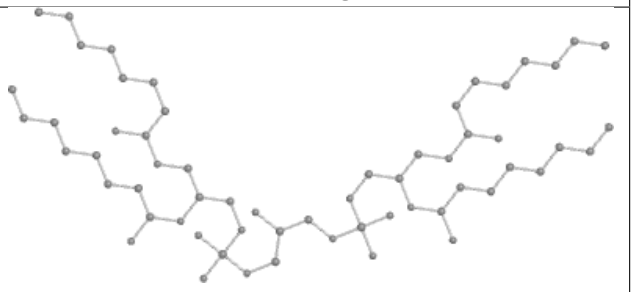
Bond lengths



Bond angles

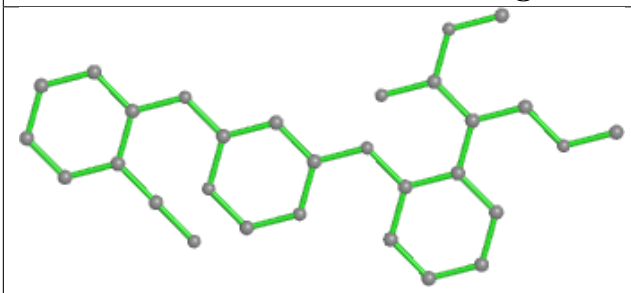


Torsions

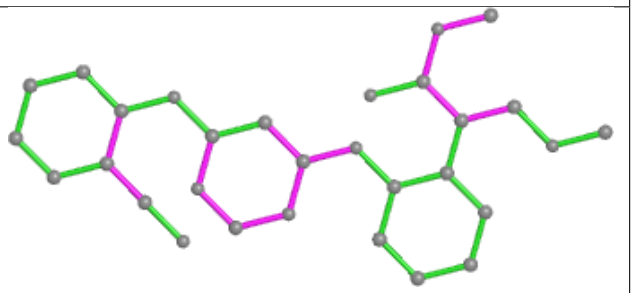


Rings

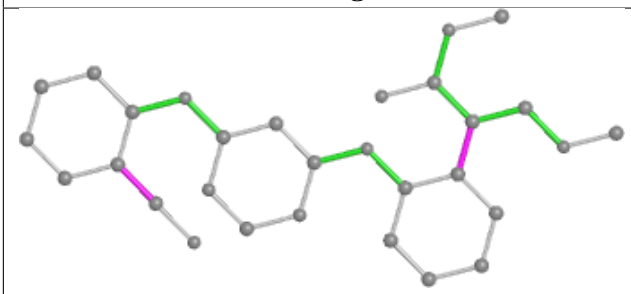
Ligand AZO C 1003



Bond lengths



Bond angles



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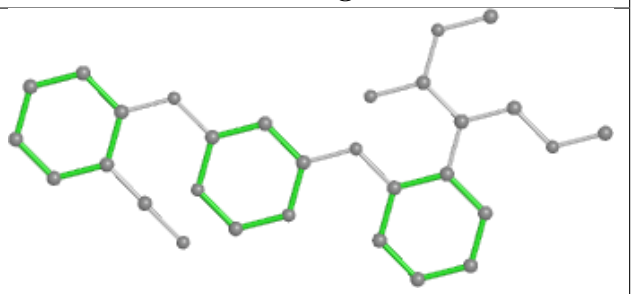
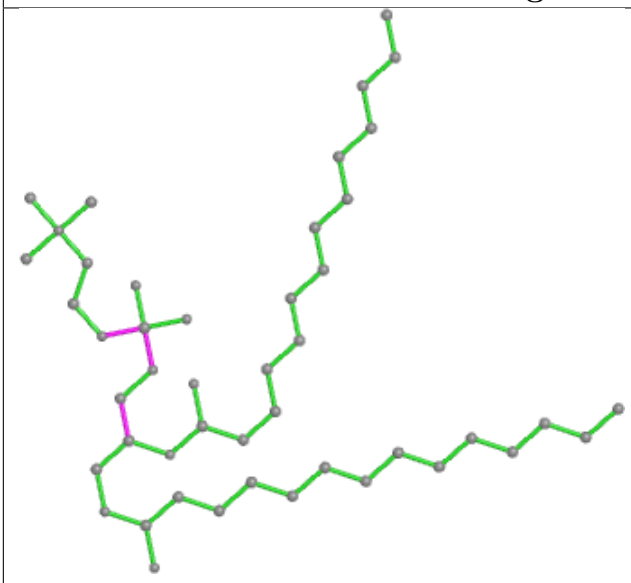
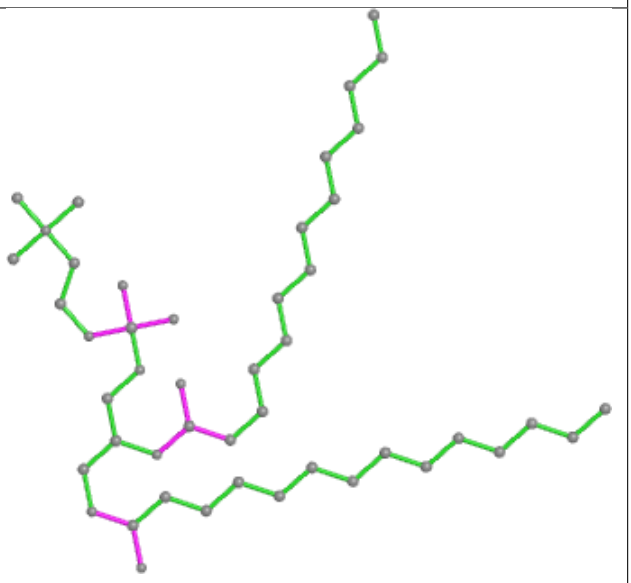


Rings

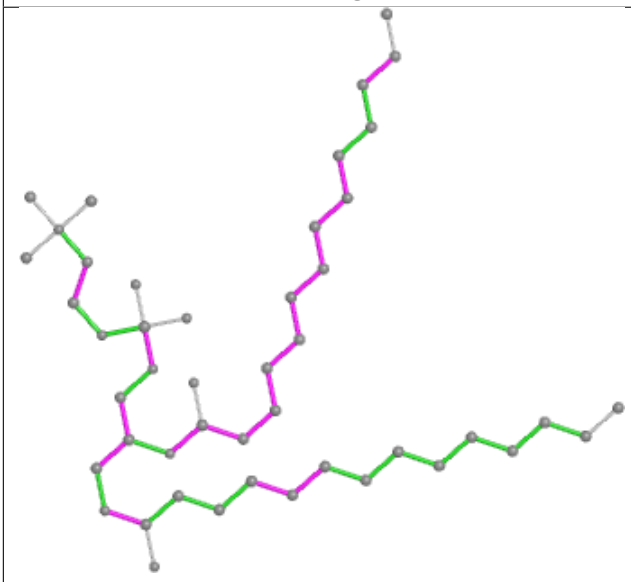
Ligand MC3 J 101



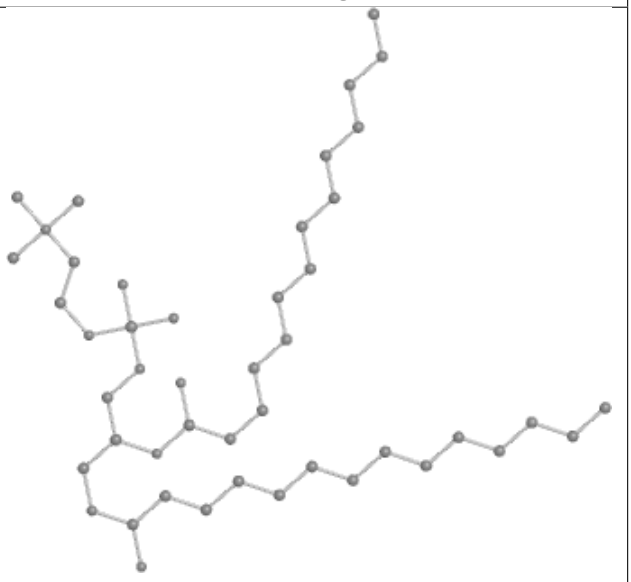
Bond lengths



Bond angles

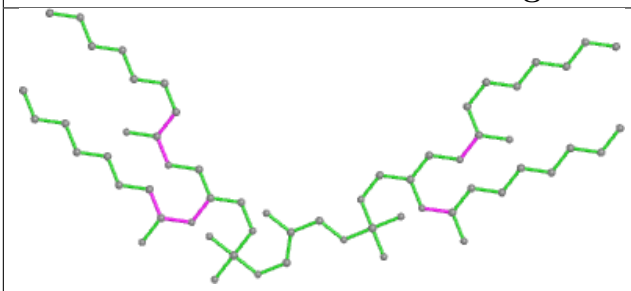


Torsions

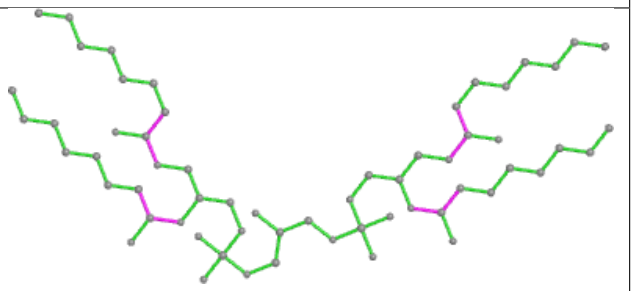


Rings

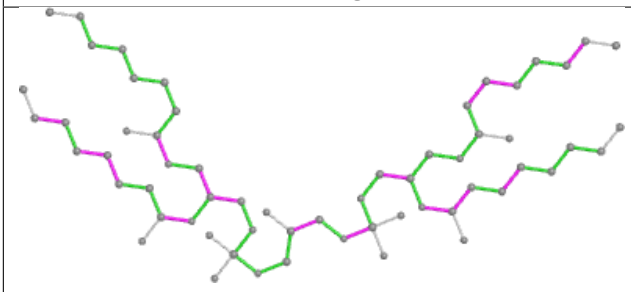
Ligand CDL A 502



Bond lengths



Bond angles



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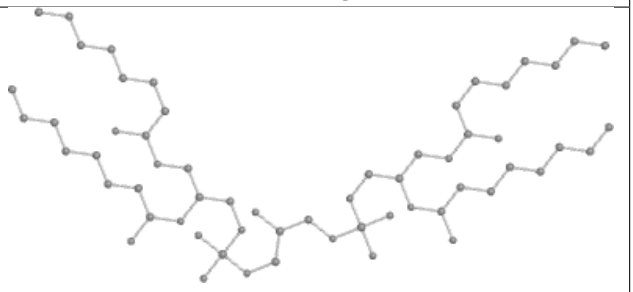
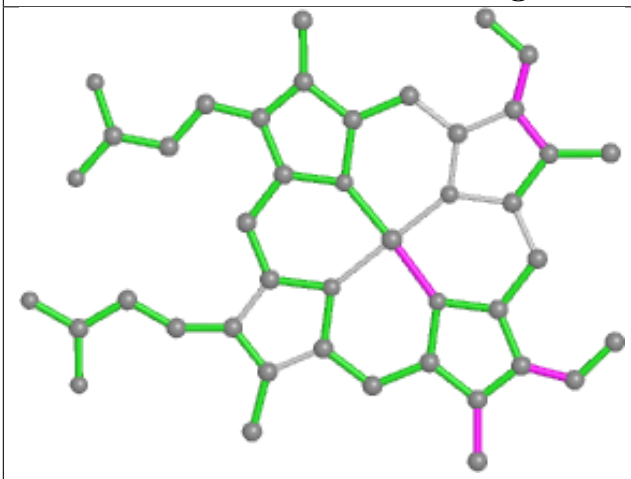
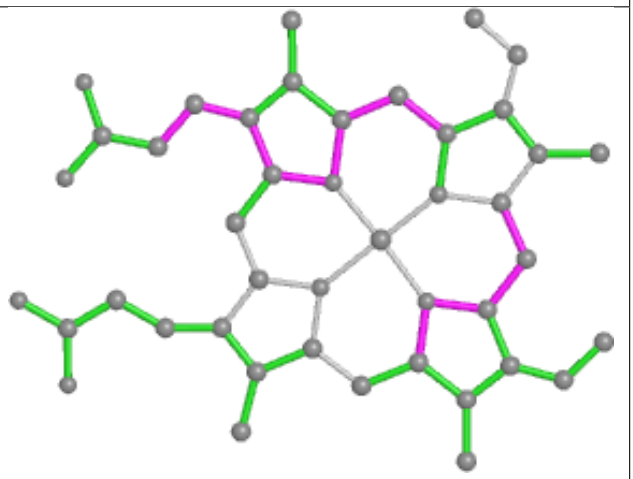


Rings

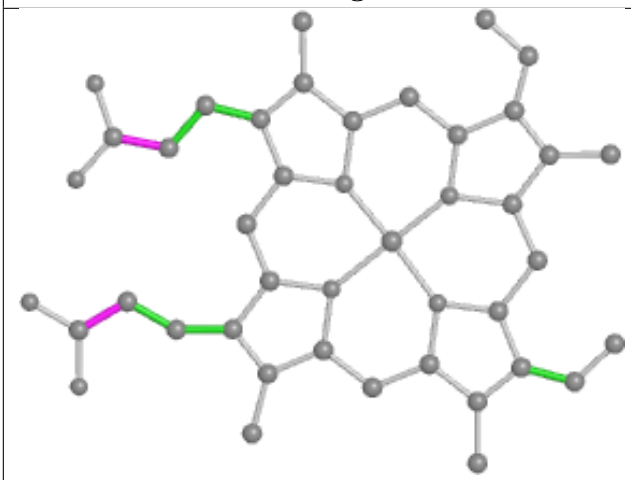
Ligand HEM C 1002



Bond lengths



Bond angles



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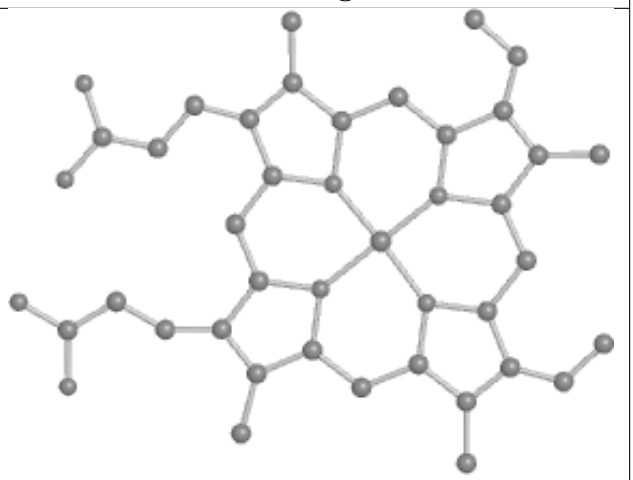
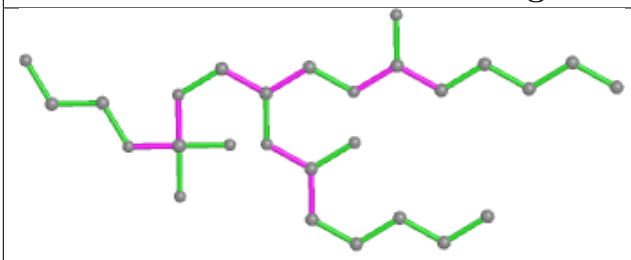
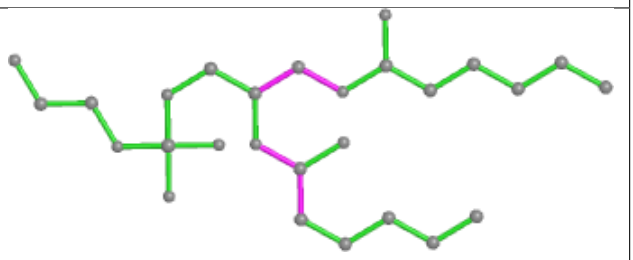


Rings

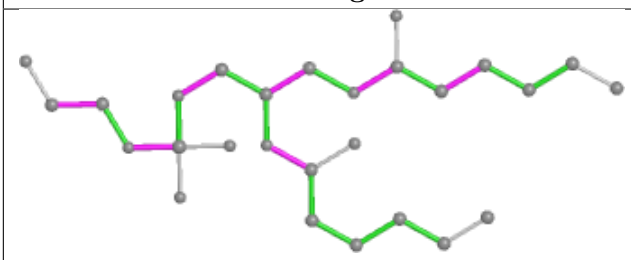
Ligand 6PE K 101



Bond lengths



Bond angles



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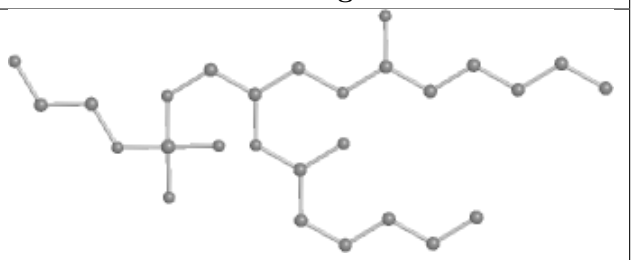
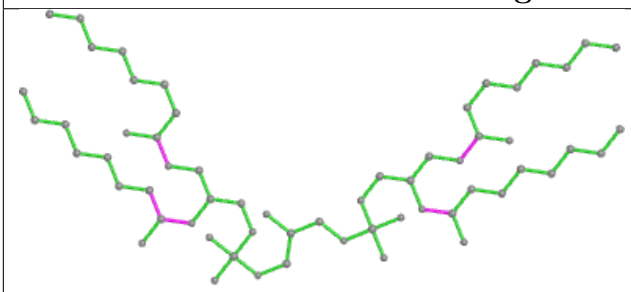
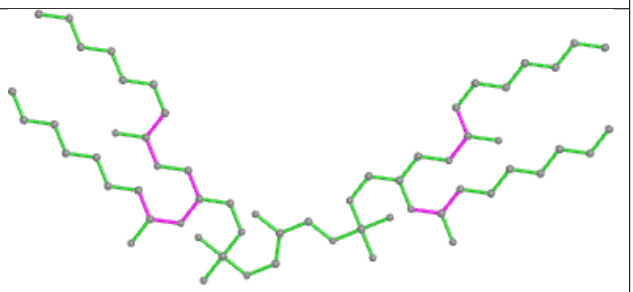


Rings

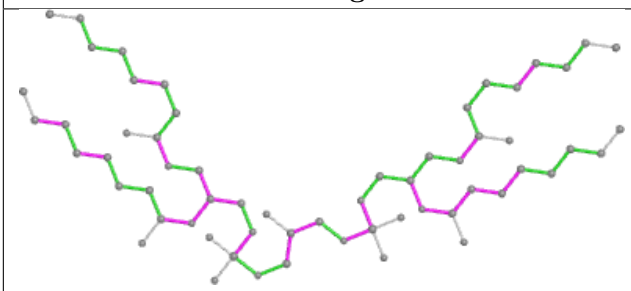
Ligand CDL D 1002



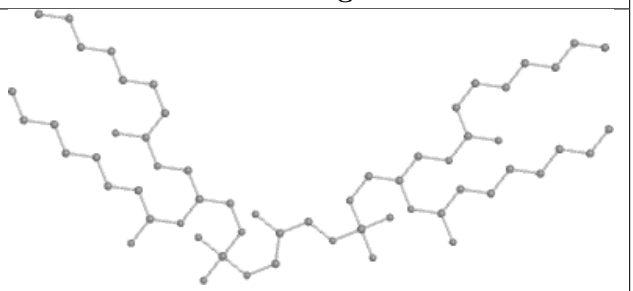
Bond lengths



Bond angles

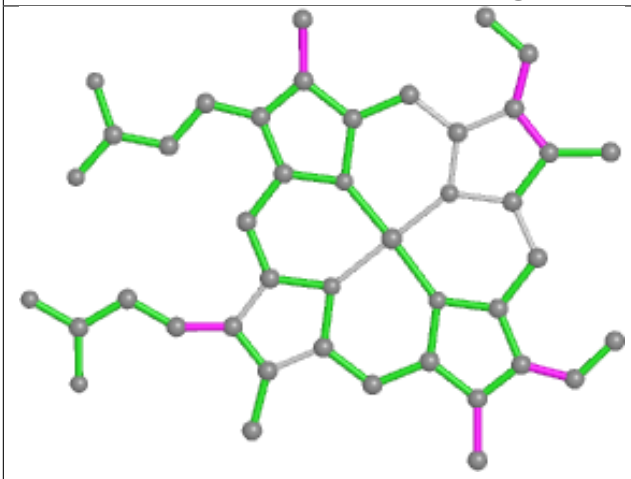


Torsions

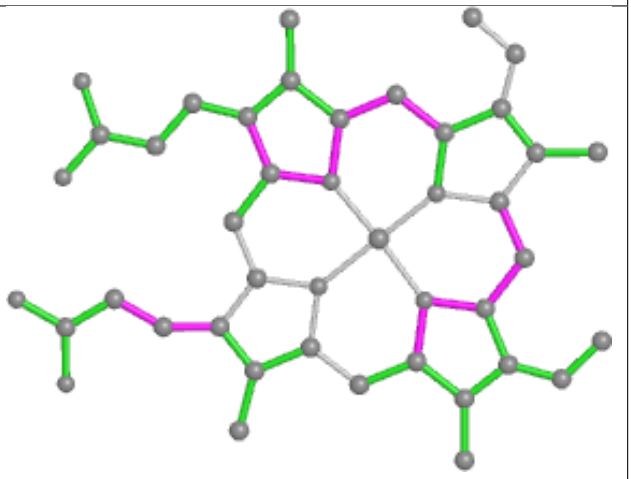


Rings

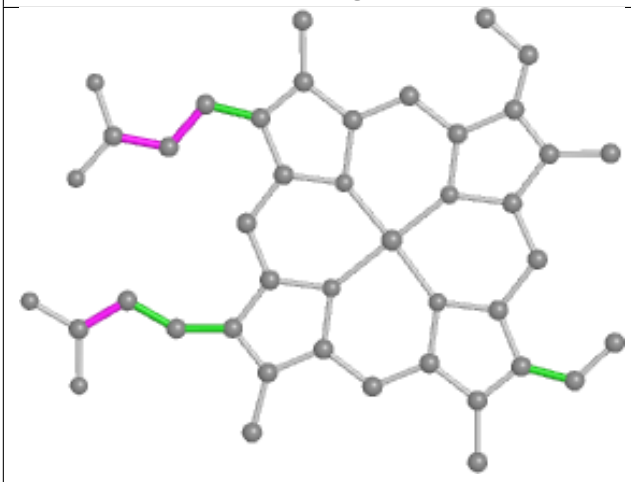
Ligand HEM C 1001



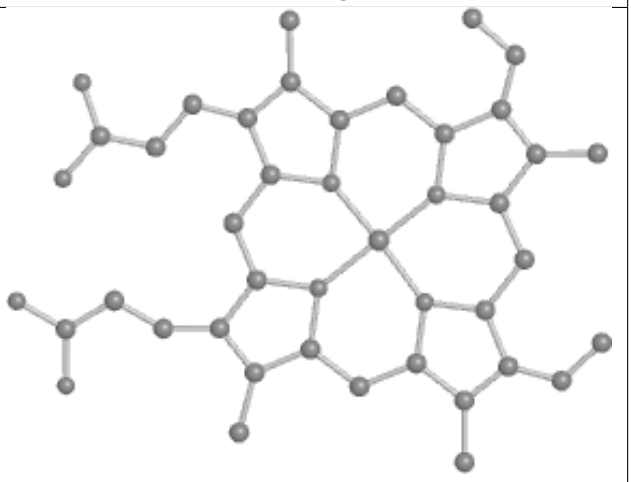
Bond lengths



Bond angles

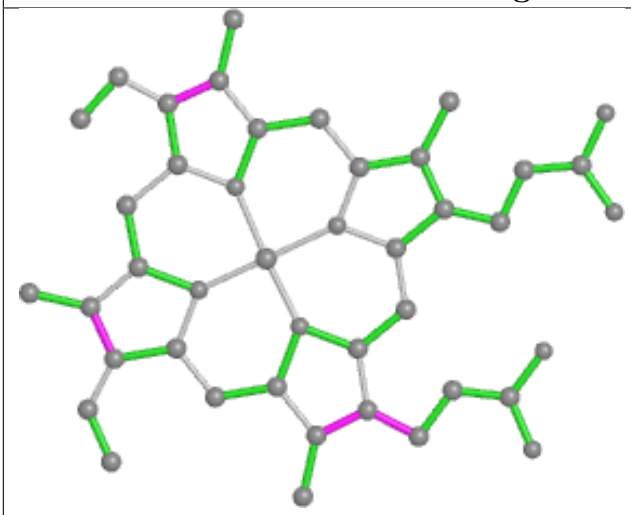


Torsions

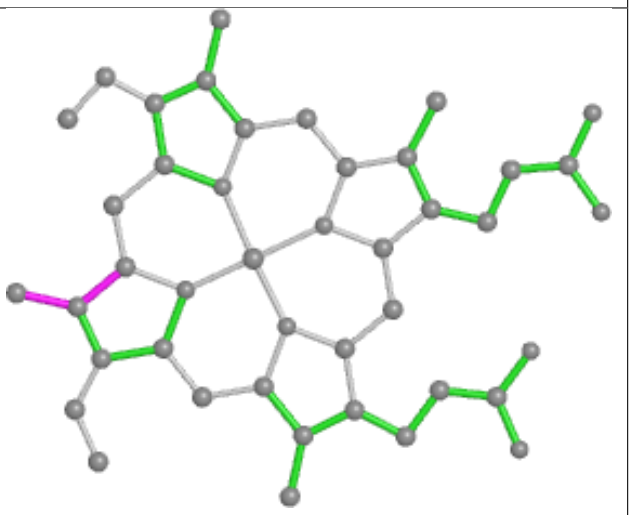


Rings

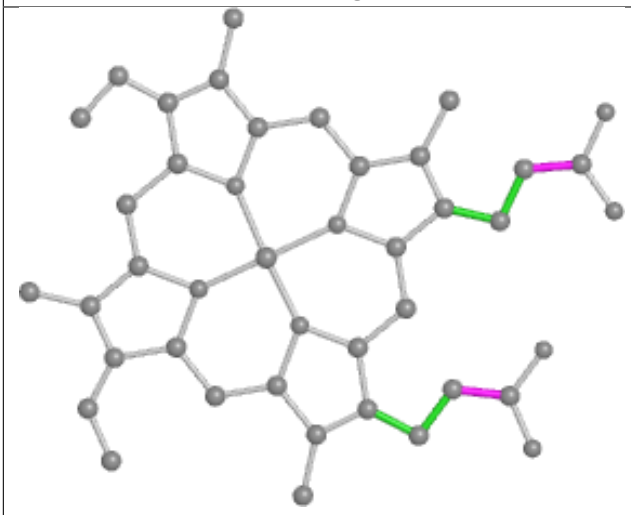
Ligand HEC D 1001



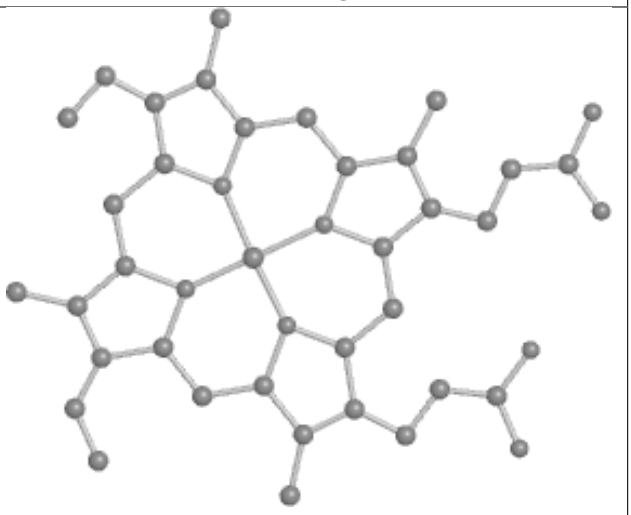
Bond lengths



Bond angles

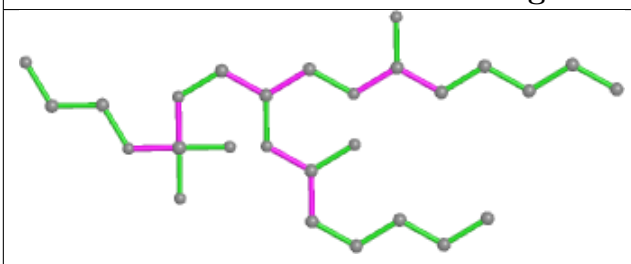


Torsions

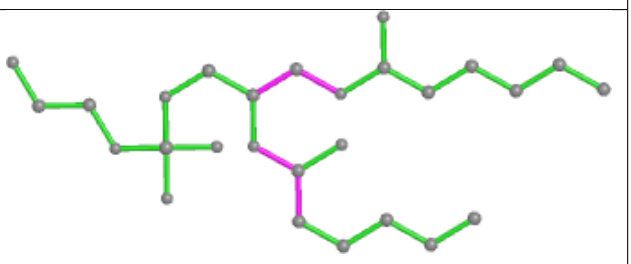


Rings

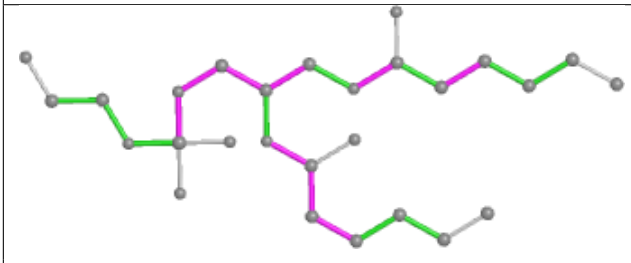
Ligand 6PE A 501



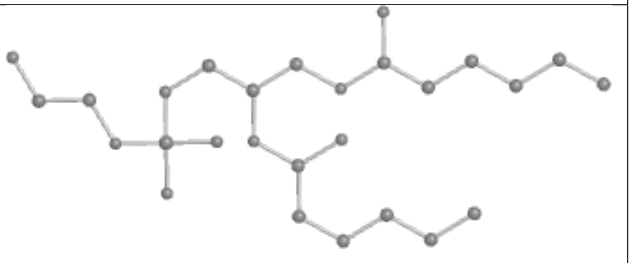
Bond lengths



Bond angles

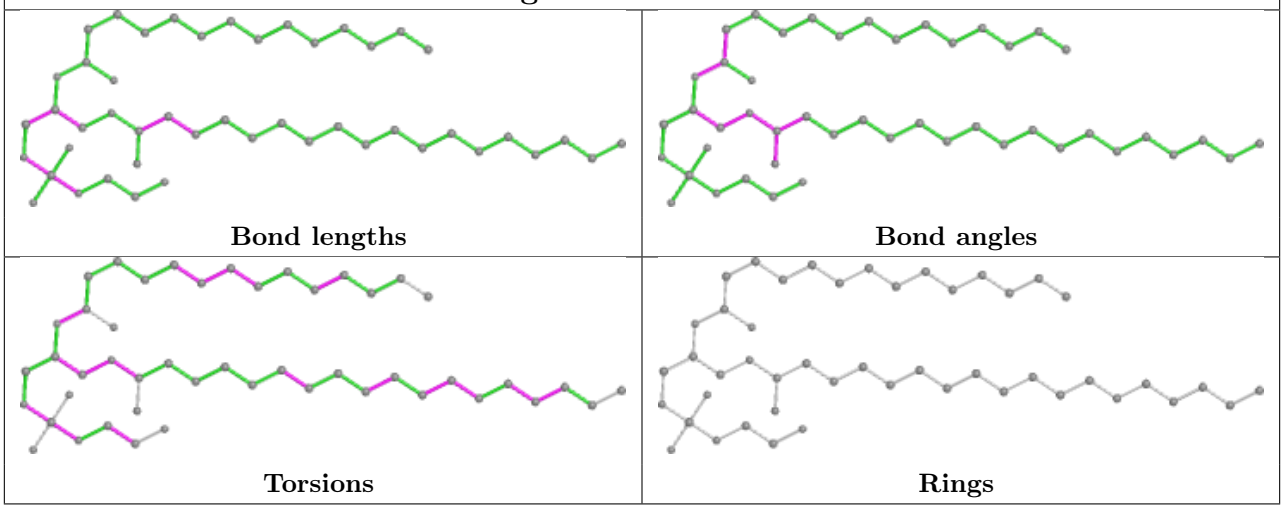


Torsions



Rings

Ligand 8PE C 1004



4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

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

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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