wwPDB X-ray Structure Validation Summary Report (i)

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 wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) 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			

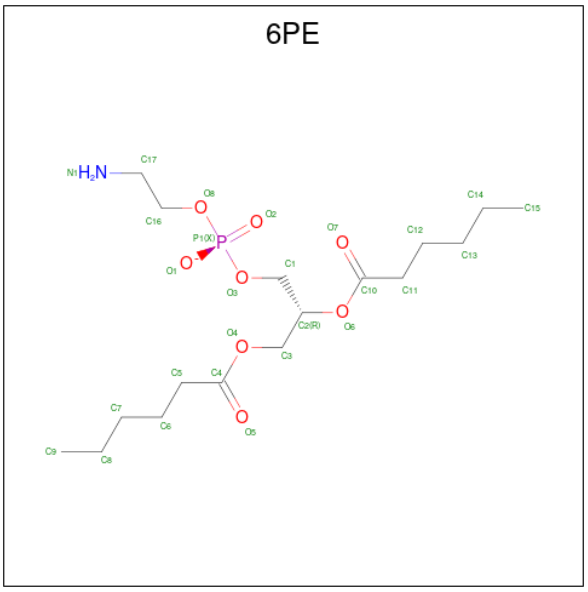
- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

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.

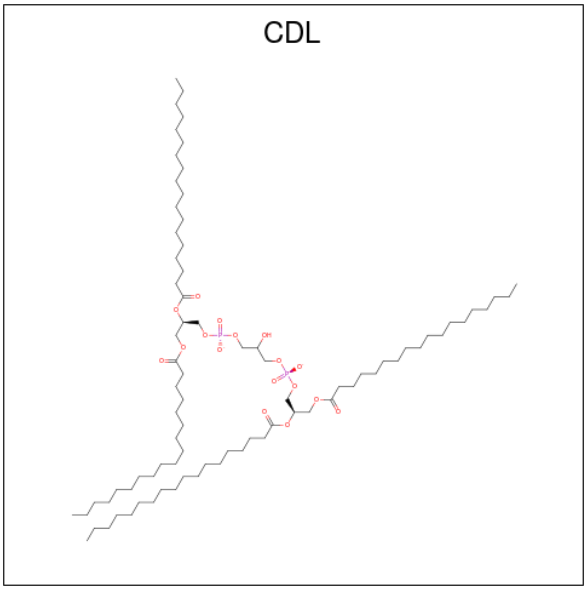
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	52	Total	C	H	N	O	0	0	0
			865	288	435	77	65			

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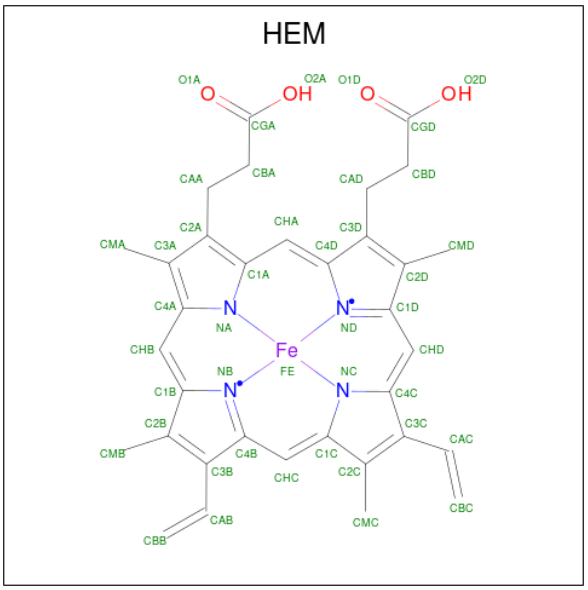
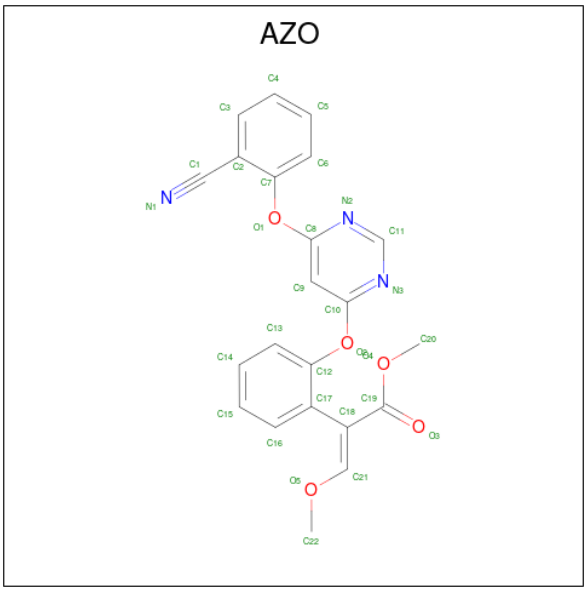
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	G	1	Total	C	H	O	P	0	0
			124	41	64	17	2		

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



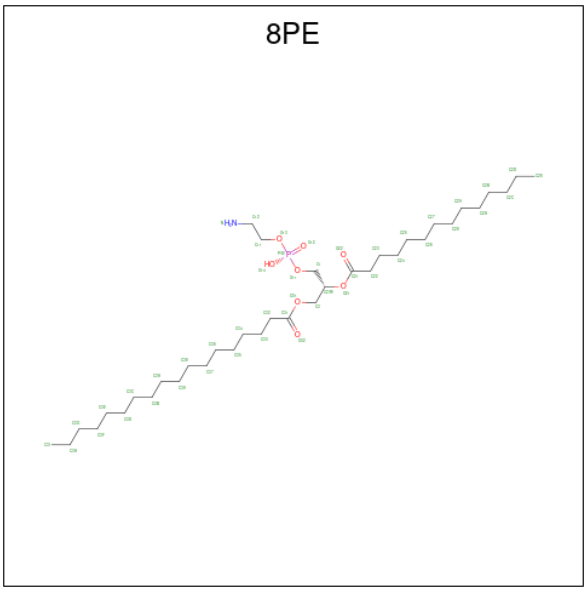
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
14	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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



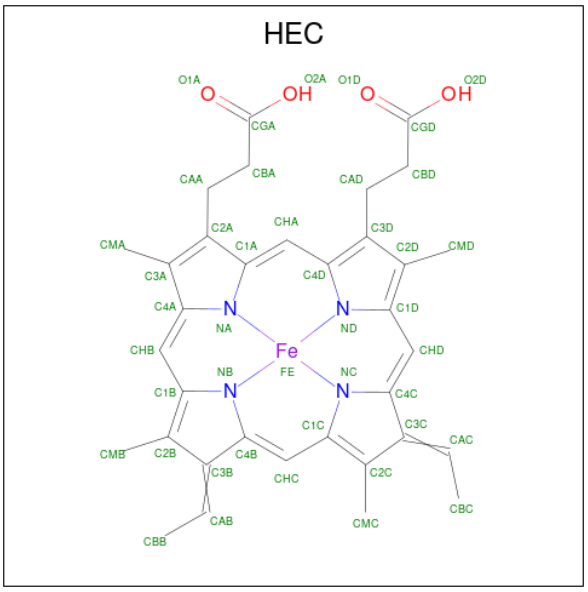
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	H	N	O	0	0
			47	22	17	3	5		

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



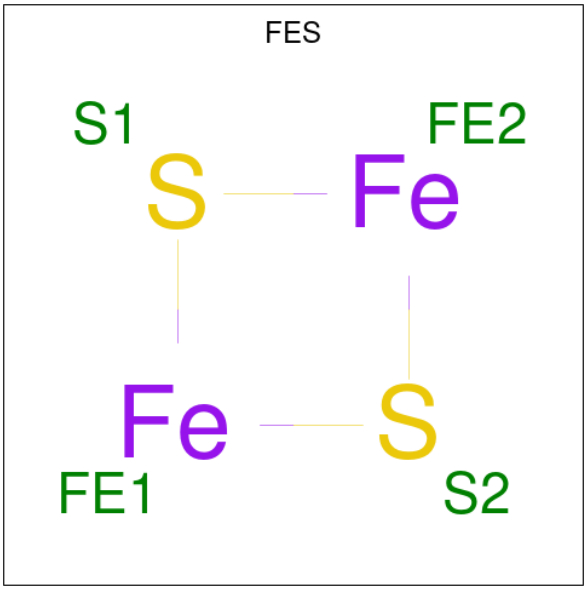
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
16	C	1	Total	C	H	N	O	P	0	0
			120	37	73	1	8	1		

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



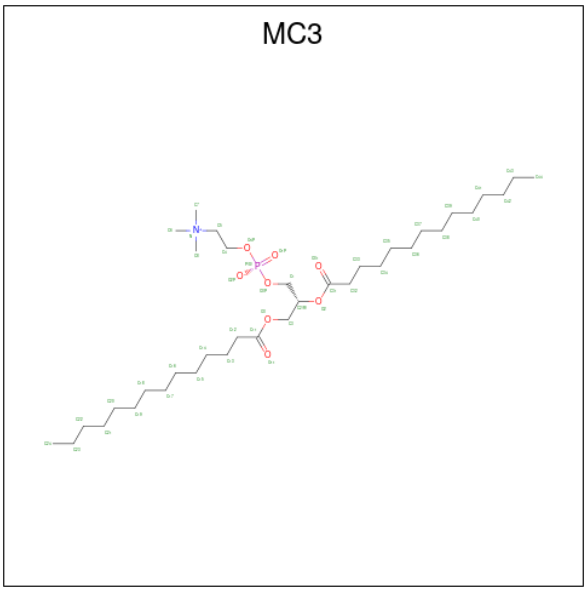
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
17	D	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

- 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	-

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 157 torsion outliers are listed below:

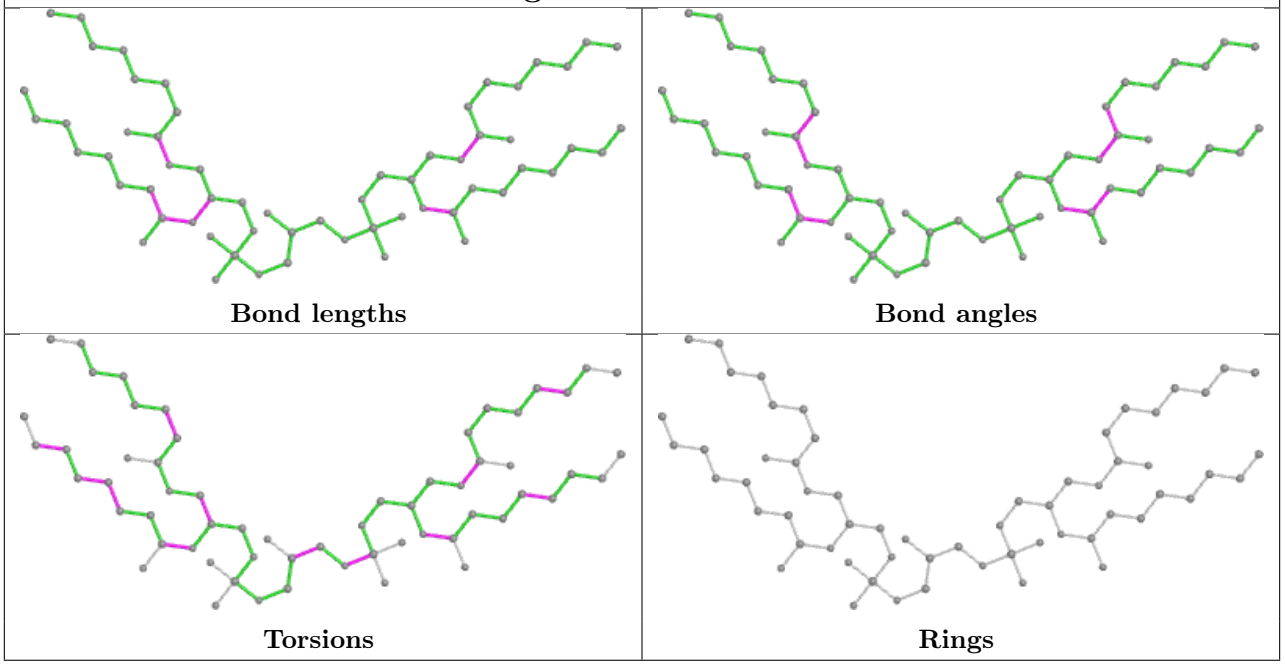
Mol	Chain	Res	Type	Atoms
12	A	501	6PE	C1-O3-P1-O2
12	A	501	6PE	C1-O3-P1-O8
12	A	501	6PE	C11-C10-O6-C2
12	K	101	6PE	C16-O8-P1-O1
12	K	101	6PE	C16-O8-P1-O2

There are no ring outliers.

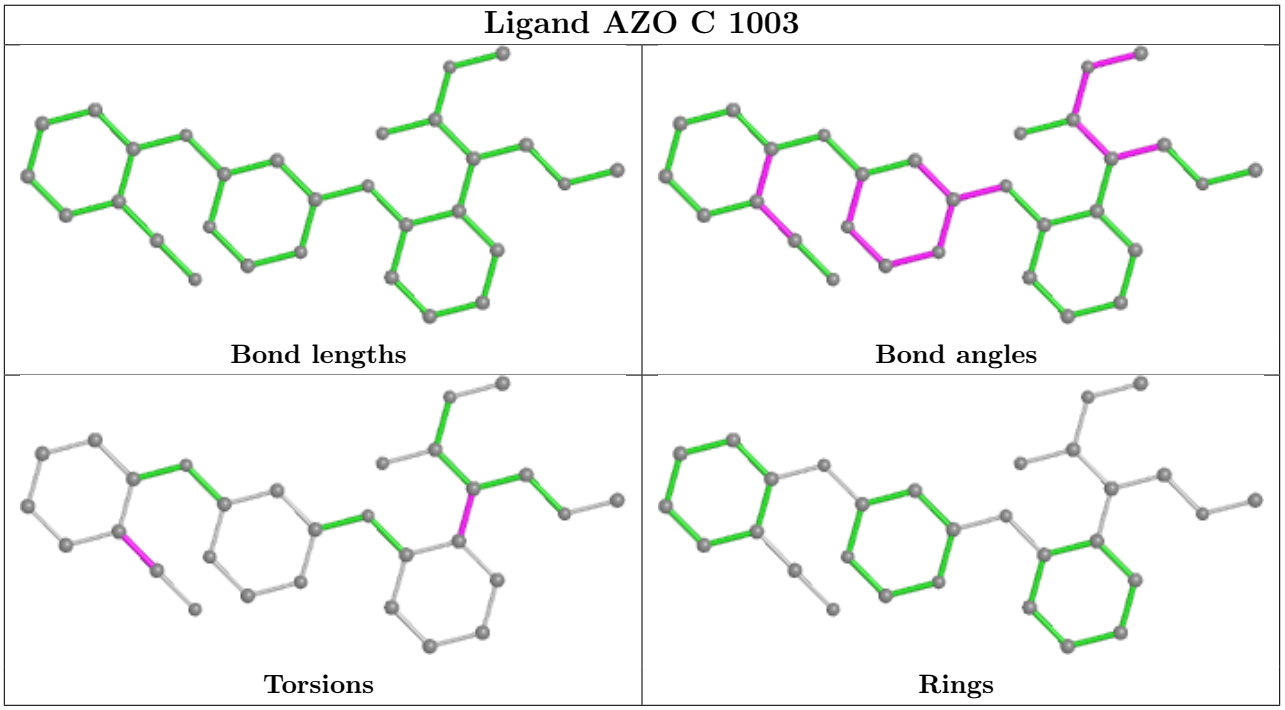
No monomer is involved in short contacts.

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.

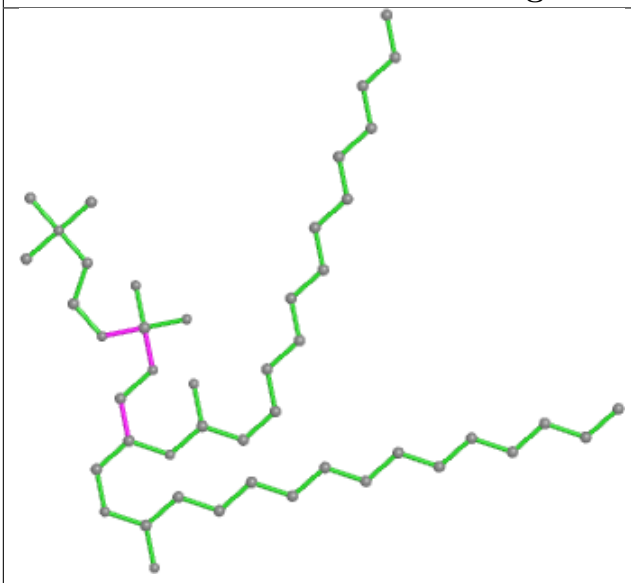
Ligand CDL G 101



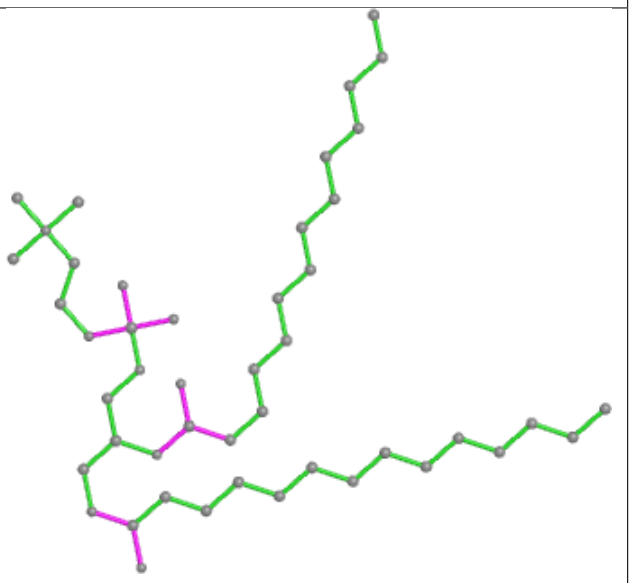
Ligand AZO C 1003



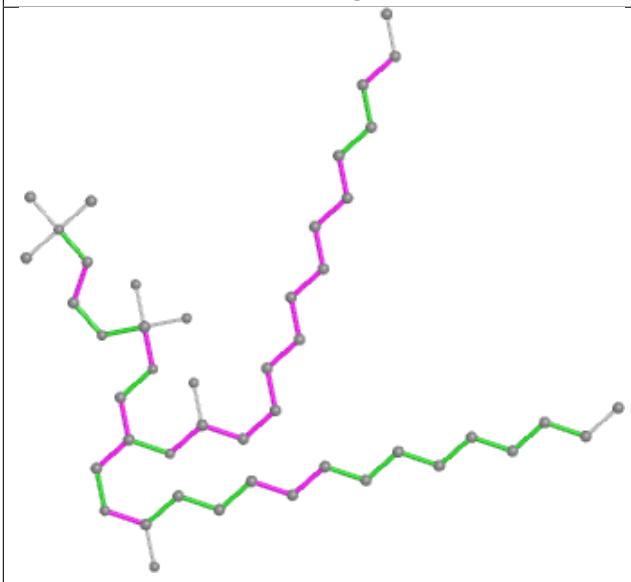
Ligand MC3 J 101



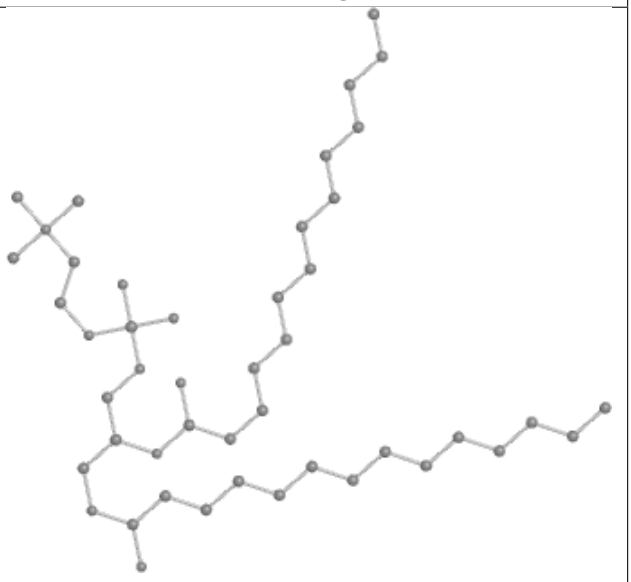
Bond lengths



Bond angles

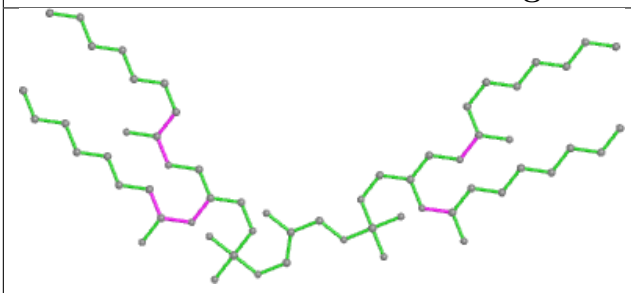


Torsions

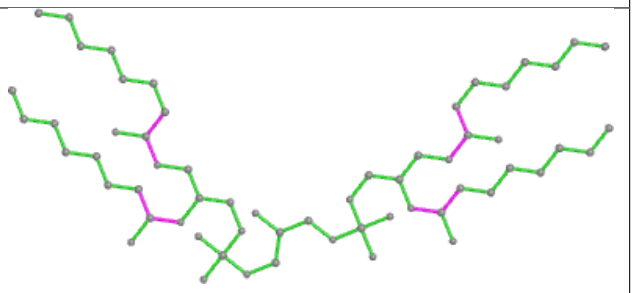


Rings

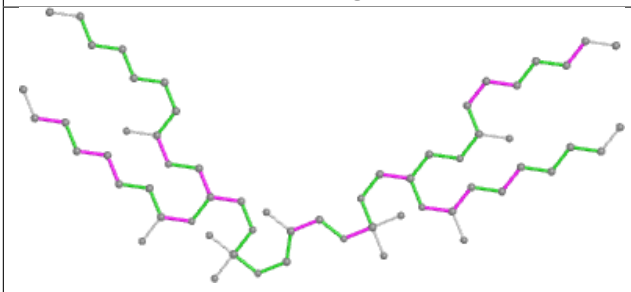
Ligand CDL A 502



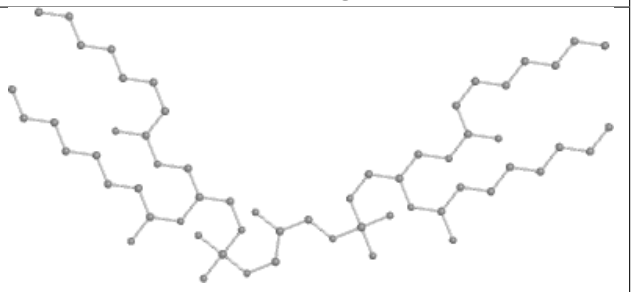
Bond lengths



Bond angles

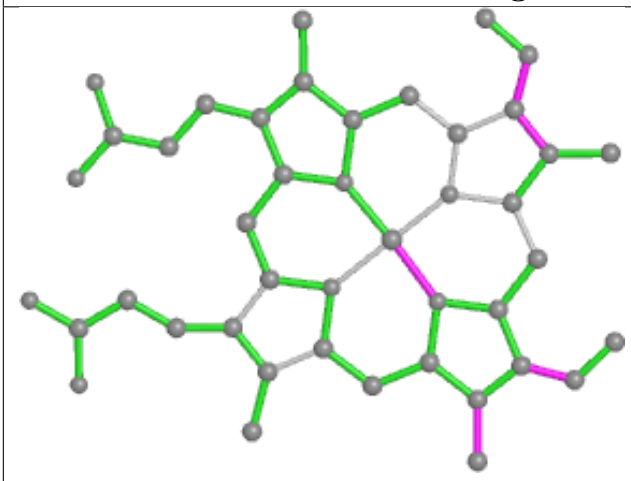


Torsions

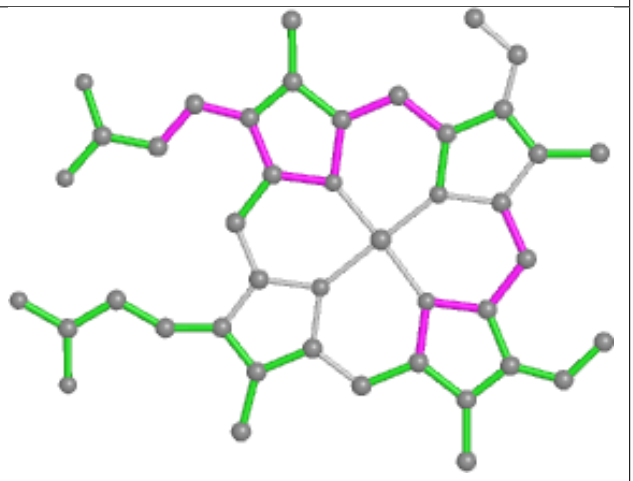


Rings

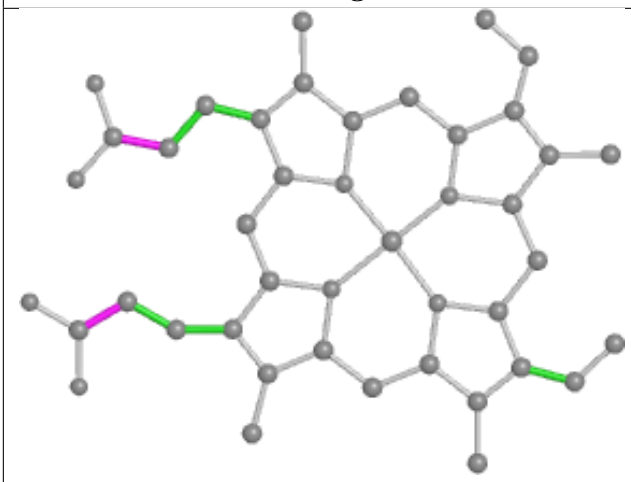
Ligand HEM C 1002



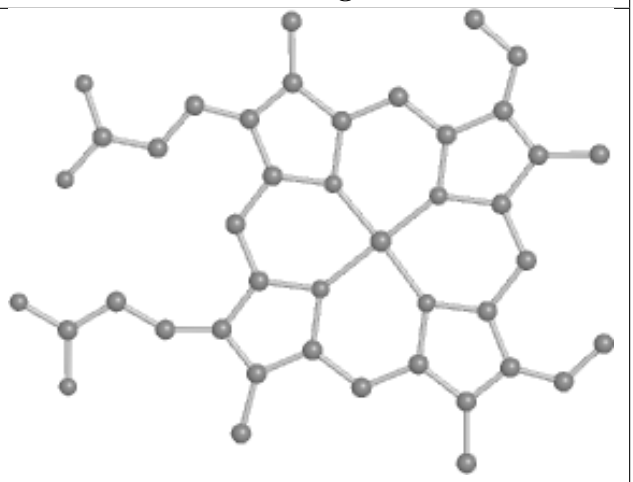
Bond lengths



Bond angles

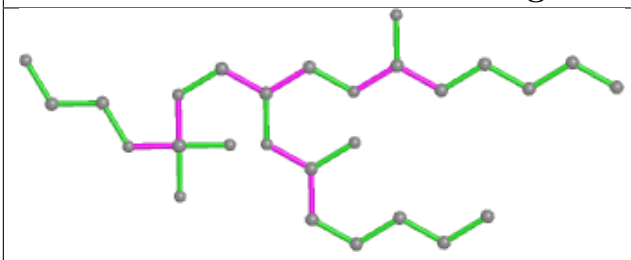


Torsions

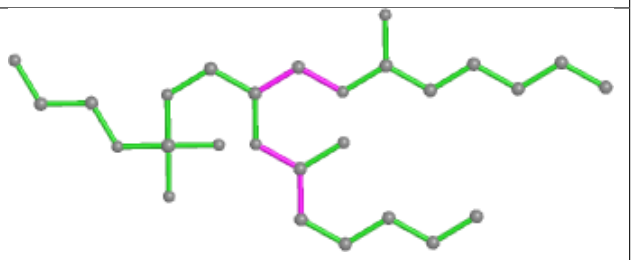


Rings

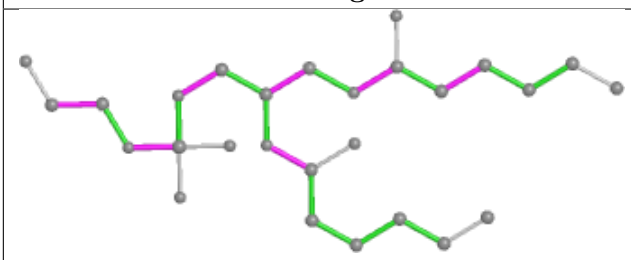
Ligand 6PE K 101



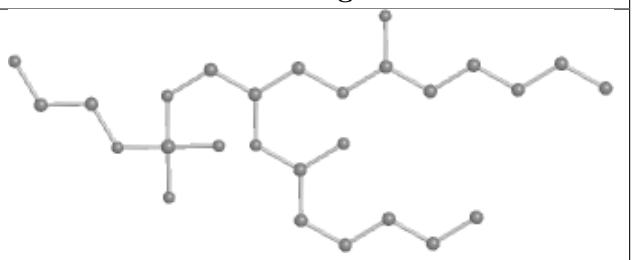
Bond lengths



Bond angles

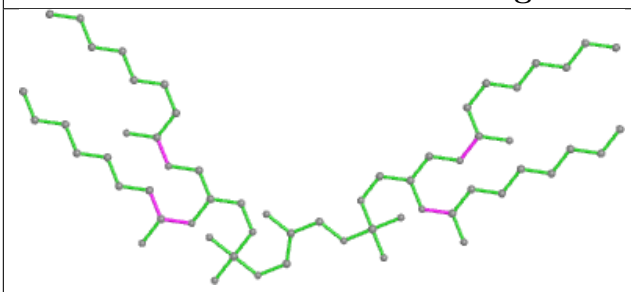


Torsions

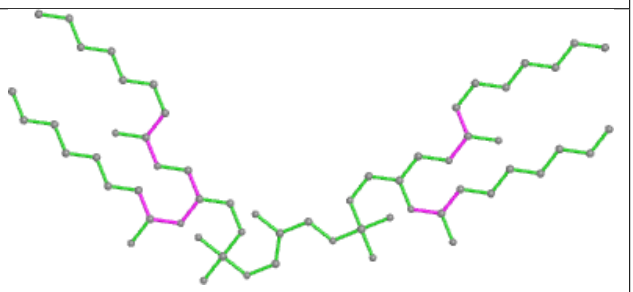


Rings

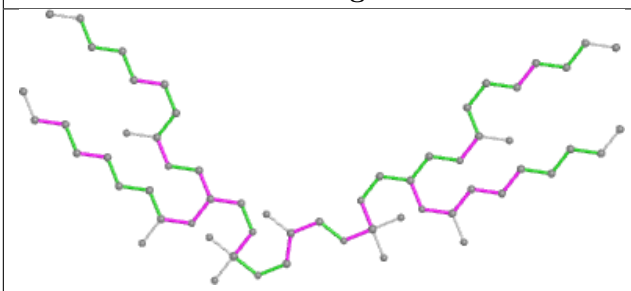
Ligand CDL D 1002



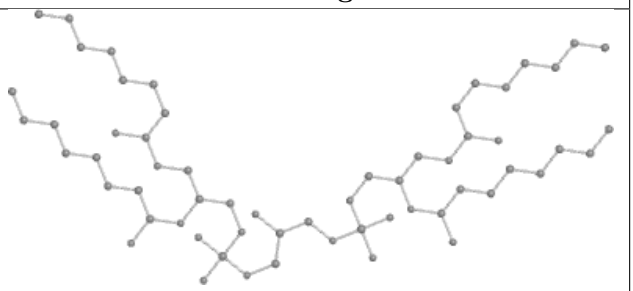
Bond lengths



Bond angles

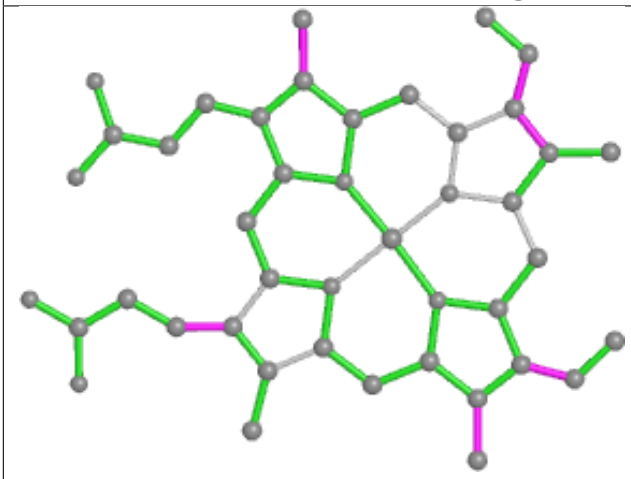


Torsions

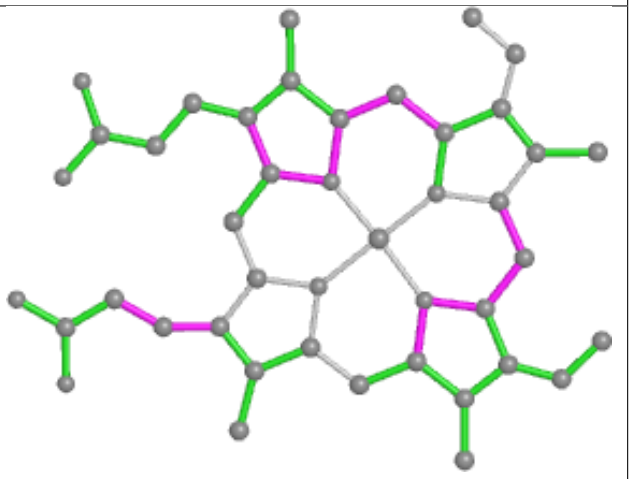


Rings

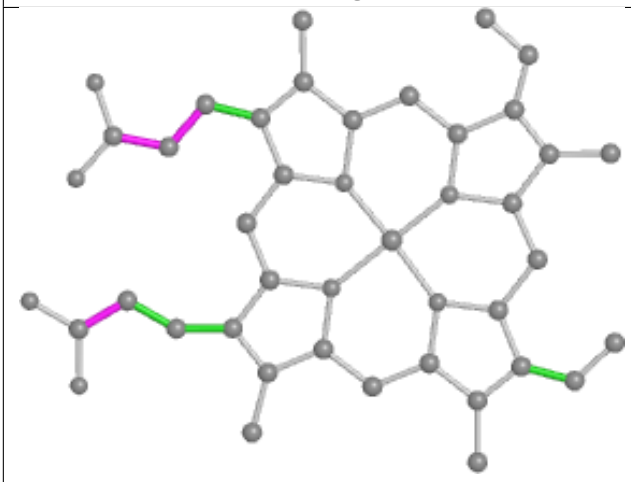
Ligand HEM C 1001



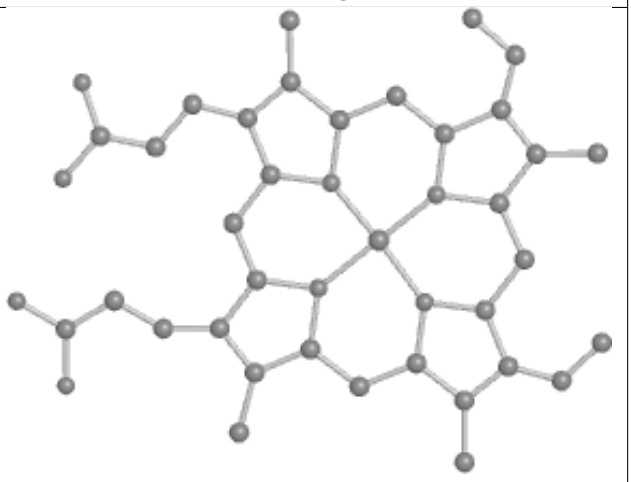
Bond lengths



Bond angles

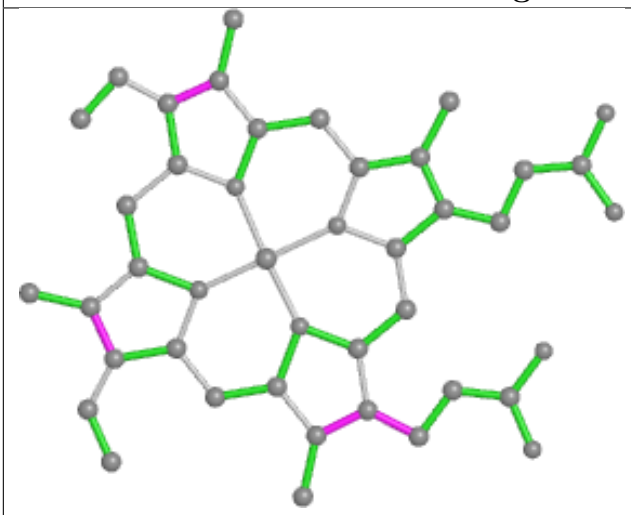


Torsions

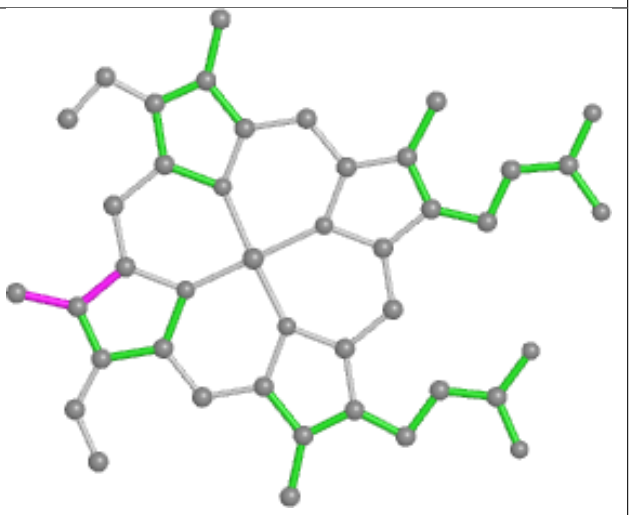


Rings

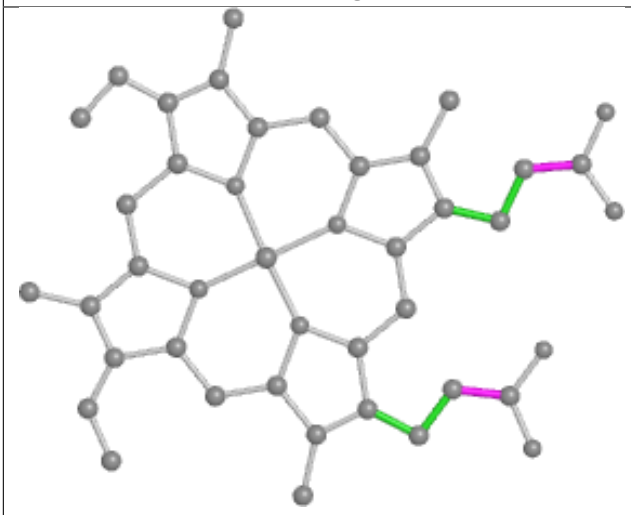
Ligand HEC D 1001



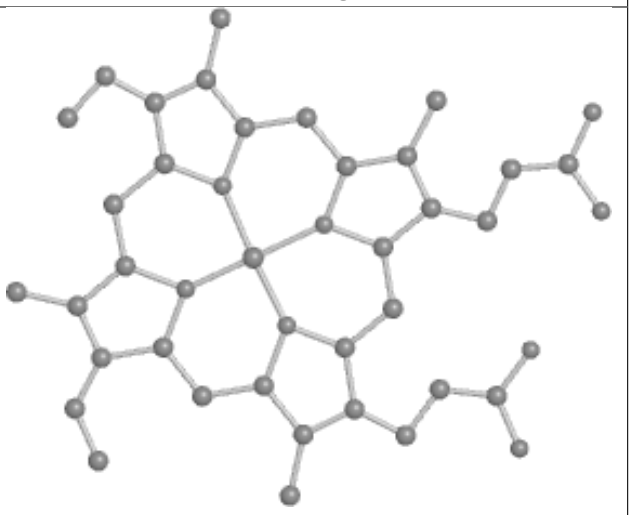
Bond lengths



Bond angles

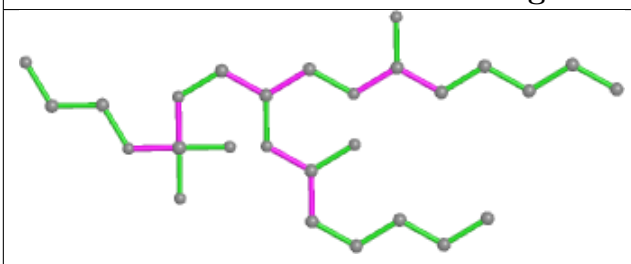


Torsions

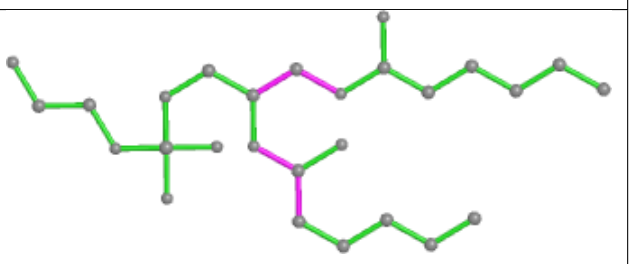


Rings

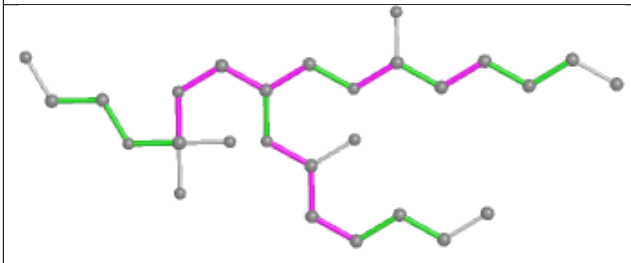
Ligand 6PE A 501



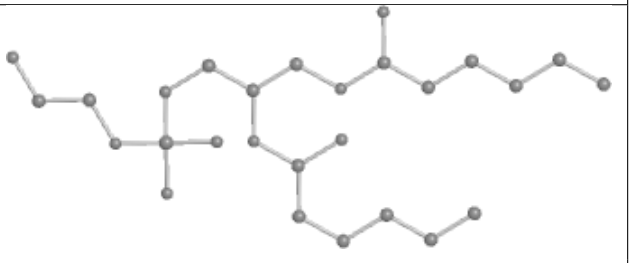
Bond lengths



Bond angles

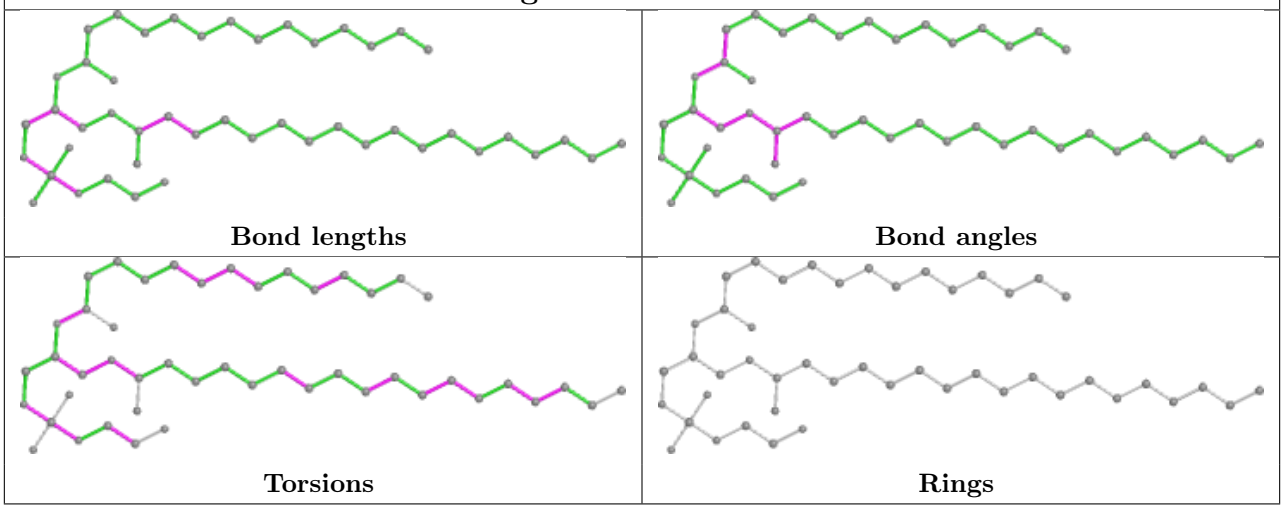


Torsions



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.