wwPDB X-ray Structure Validation Summary Report (i)

Nov 28, 2023 – 08:17 pm GMT

PDB ID	:	1DXR
Title	:	Photosynthetic reaction center from Rhodopseudomonas viridis - His L168 Phe mutant (terbutryn complex)
Authors	:	Lancaster, C.R.D.; Bibikova, M.; Sabatino, P.; Oesterhelt, D.; Michel, H.
Deposited on	:	2000-01-15
Resolution	:	2.00 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:

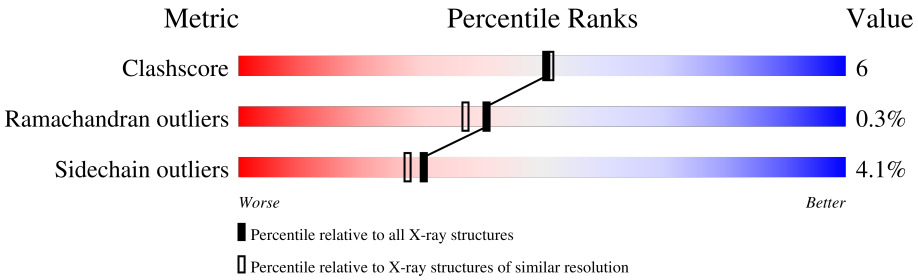
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	336	89% 9% ••
2	H	258	86% 11% •
3	L	273	89% 10% •
4	M	323	87% 12% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	BCB	L	400	X	-	-	-
8	BCB	L	401	X	-	-	-
8	BCB	M	400	X	-	-	-
8	BCB	M	401	X	-	-	-
9	BPB	M	402	X	-	-	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 10777 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 PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	332	2636	1658	474	486	18	39	4	0

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER H SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	258	2018	1292	344	380	2	118	0	0

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER L SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	273	2172	1462	348	355	7	13	0	0

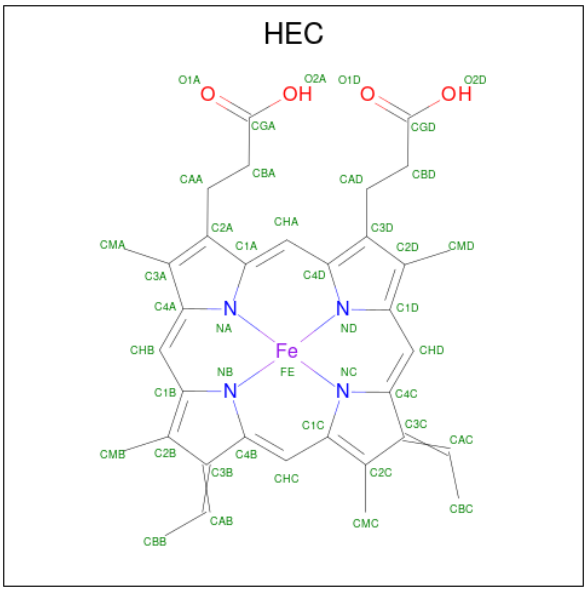
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	168	PHE	HIS	engineered mutation	UNP P06009

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER M SUBUNIT.

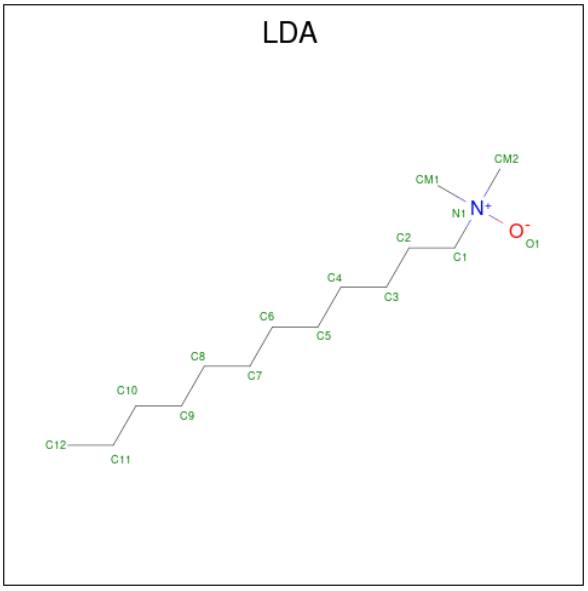
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	M	323	2569	1710	421	425	13	15	2	0

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



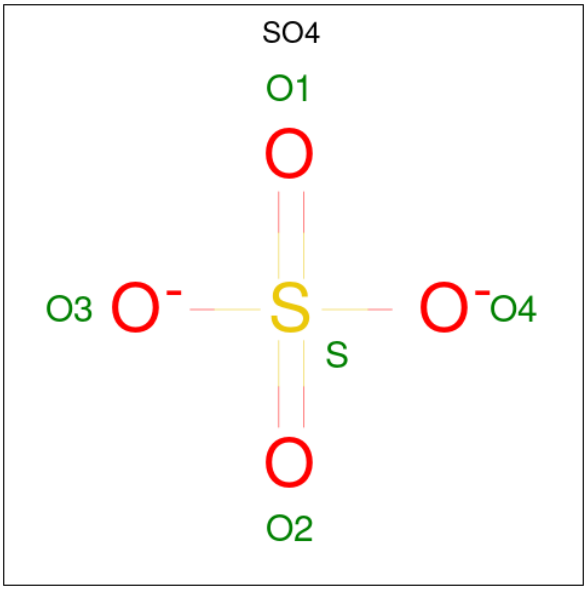
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



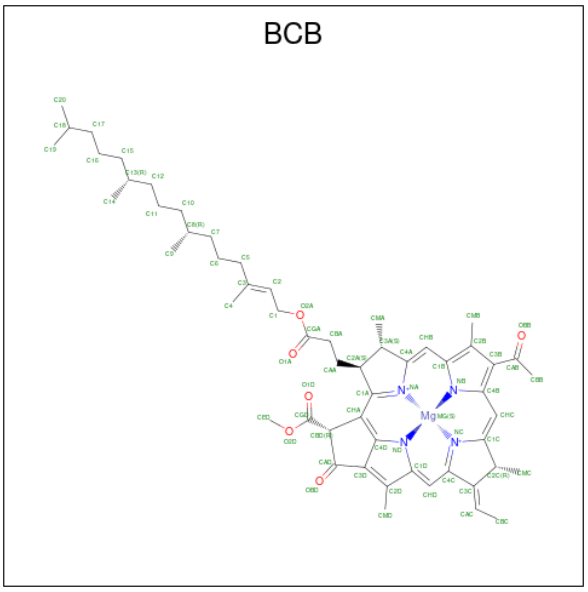
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total C N O 16 14 1 1	0	0
6	H	1	Total C N O 16 14 1 1	0	0
6	L	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	3	0
6	M	1	Total C N O 16 14 1 1	4	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



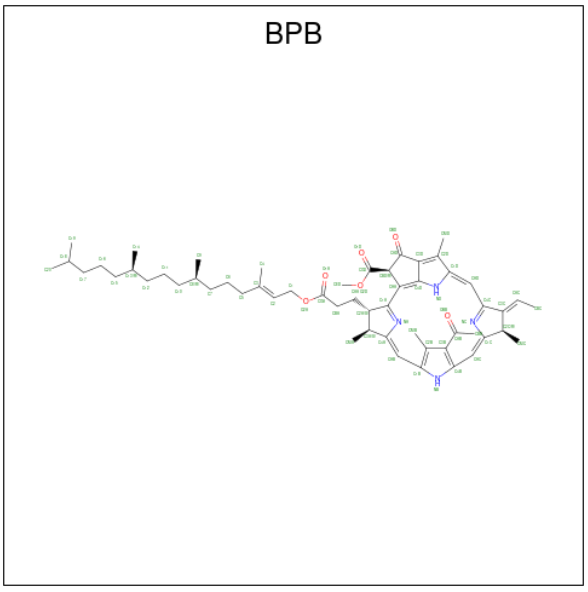
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0
7	M	1	Total O S 5 4 1	0	0

- Molecule 8 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 9 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).

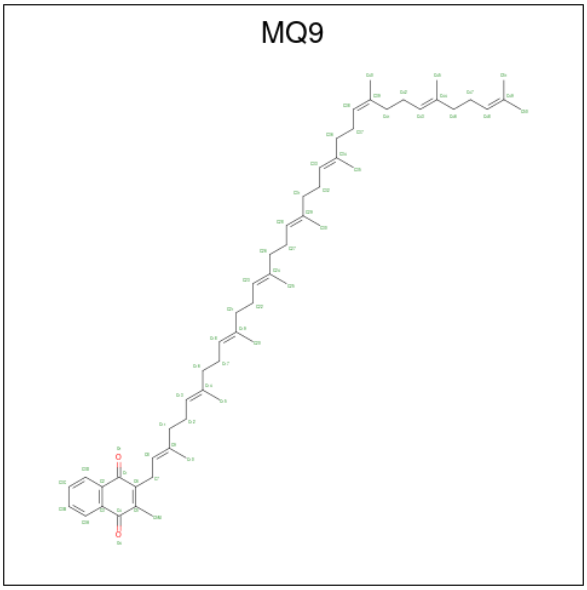


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	1	Total C N O 65 55 4 6	0	0
9	M	1	Total C N O 65 55 4 6	7	0

- Molecule 10 is FE (II) ION (three-letter code: FE2) (formula: Fe).

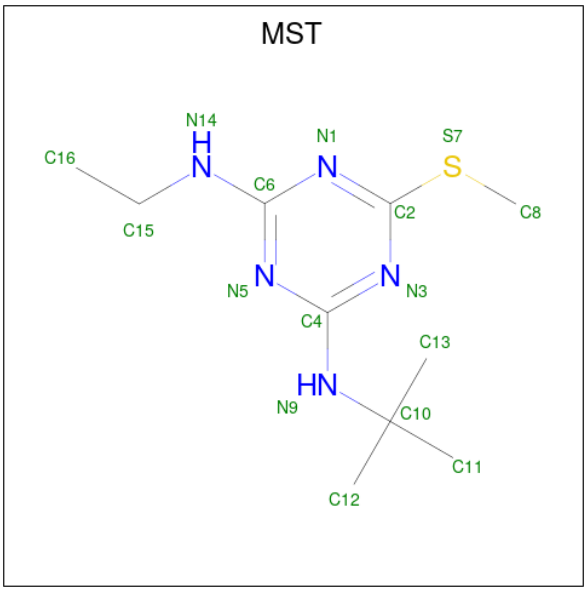
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total Fe 1 1	0	0

- Molecule 11 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$).



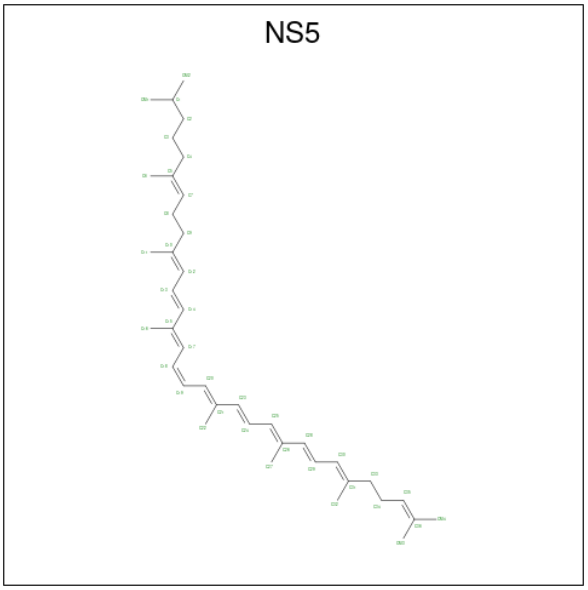
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	1	Total C O 58 56 2	0	0

- Molecule 12 is 2-T-BUTYLAMINO-4-ETHYLAMINO-6-METHYLTHIO-S-TRIAZINE (three-letter code: MST) (formula: $C_{10}H_{19}N_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	L	1	Total C N S 16 10 5 1	0	0

- Molecule 13 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: $C_{40}H_{60}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total C 40 40	14	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	222	Total O 222 222	0	0
14	H	146	Total O 146 146	0	0
14	H	1	Total O 1 1	0	0
14	H	2	Total O 2 2	0	0
14	H	1	Total O 1 1	0	0
14	L	88	Total O 88 88	0	0
14	L	1	Total O 1 1	0	0
14	M	120	Total O 120 120	0	0
14	M	1	Total O 1 1	0	0
14	M	1	Total O 1 1	0	0
14	M	1	Total O 1 1	0	0
14	M	1	Total O 1 1	0	0

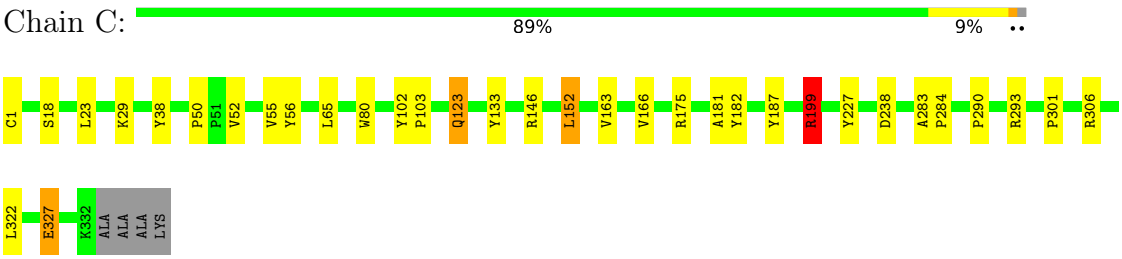
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

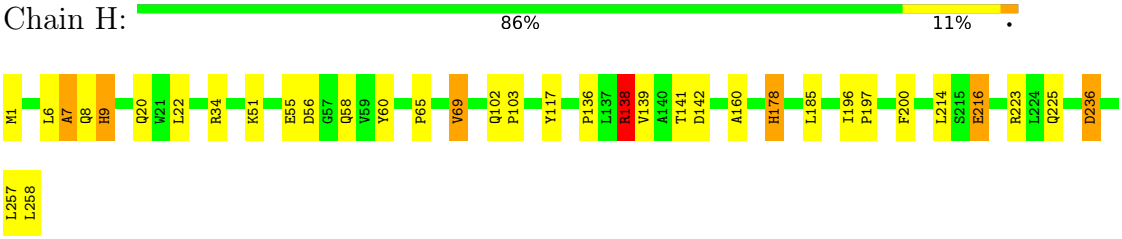
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT

Chain C:



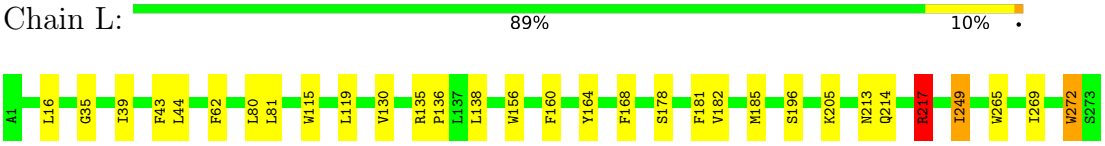
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER H SUBUNIT

Chain H:



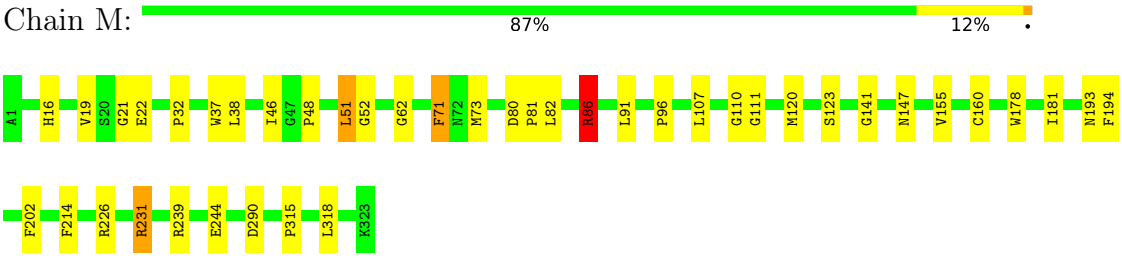
• Molecule 3: PHOTOSYNTHETIC REACTION CENTER L SUBUNIT

Chain L:



• Molecule 4: PHOTOSYNTHETIC REACTION CENTER M SUBUNIT

Chain M:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	223.50Å 223.50Å 113.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	97.5 (10.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.194 , 0.218	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10777	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, BCB, BPB, HEC, FME, MST, LDA, FE2, NS5, MQ9

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	C	0.49	0/2703	0.60	2/3683 (0.1%)
2	H	0.52	0/2055	0.65	1/2807 (0.0%)
3	L	0.54	0/2260	0.56	0/3085
4	M	0.52	0/2673	0.58	1/3655 (0.0%)
All	All	0.52	0/9691	0.60	4/13230 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	4
2	H	0	4
3	L	0	2
4	M	0	2
All	All	0	12

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	199[A]	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	C	199[B]	ARG	NE-CZ-NH2	-6.46	117.07	120.30
4	M	231	ARG	NE-CZ-NH2	-6.35	117.12	120.30
2	H	138	ARG	NE-CZ-NH2	-5.52	117.54	120.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	187	TYR	Sidechain
1	C	199[A]	ARG	Sidechain
1	C	227	TYR	Sidechain
1	C	327	GLU	Mainchain
2	H	8	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2636	0	2599	19	0
2	H	2018	0	2020	21	0
3	L	2172	0	2100	34	0
4	M	2569	0	2464	27	0
5	C	172	0	120	4	0
6	H	32	0	62	3	0
6	L	16	0	31	4	0
6	M	48	0	93	2	0
7	H	5	0	0	0	0
7	M	15	0	0	1	0
8	L	132	0	144	8	0
8	M	132	0	144	14	0
9	L	65	0	74	3	0
9	M	65	0	74	7	0
10	L	1	0	0	0	0
11	L	58	0	80	1	0
12	L	16	0	19	0	0
13	M	40	0	60	2	0
14	C	222	0	0	0	0
14	H	150	0	0	0	0
14	L	89	0	0	2	0
14	M	124	0	0	2	0
All	All	10777	0	10084	113	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 113 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:402:BPB:HHC	9:M:402:BPB:HBBB	1.46	0.94
8:M:400:BCB:HBB2	8:M:400:BCB:HHC	1.50	0.91
3:L:62:PHE:HD2	6:L:1274:LDA:HM11	1.48	0.77
3:L:185:MET:SD	8:M:400:BCB:H41	2.29	0.73
2:H:65:PRO:HG3	6:H:1260:LDA:H72	1.70	0.72

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	334/336 (99%)	327 (98%)	7 (2%)	0	100	100
2	H	256/258 (99%)	245 (96%)	9 (4%)	2 (1%)	19	13
3	L	271/273 (99%)	265 (98%)	6 (2%)	0	100	100
4	M	323/323 (100%)	314 (97%)	8 (2%)	1 (0%)	41	37
All	All	1184/1190 (100%)	1151 (97%)	30 (2%)	3 (0%)	41	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	7	ALA
2	H	9	HIS
4	M	193	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	284/282 (101%)	273 (96%)	11 (4%)	32 30
2	H	212/212 (100%)	200 (94%)	12 (6%)	20 16
3	L	218/218 (100%)	211 (97%)	7 (3%)	39 38
4	M	251/249 (101%)	240 (96%)	11 (4%)	28 25
All	All	965/961 (100%)	924 (96%)	41 (4%)	30 27

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	249	ILE
4	M	86	ARG
3	L	272	TRP
4	M	37	TRP
4	M	181	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	302	GLN
2	H	102	GLN
3	L	183	ASN
3	L	214	GLN
4	M	147	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	FME	H	1	2	8,9,10	0.59	0	7,9,11	2.30	2 (28%)

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	FME	H	1	2	-	2/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	FME	O1-CN-N	-4.26	114.05	125.27
2	H	1	FME	CA-N-CN	-3.35	117.68	122.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FME	O1-CN-N-CA
2	H	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	BCB	M	401	8,4	63,74,74	1.25	8 (12%)	74,115,115	2.19	15 (20%)
6	LDA	M	1326	-	12,15,15	2.29	1 (8%)	14,17,17	0.56	0
5	HEC	C	401	1	32,50,50	1.50	2 (6%)	24,82,82	1.38	3 (12%)
5	HEC	C	403	1	32,50,50	1.56	3 (9%)	24,82,82	1.81	6 (25%)
6	LDA	H	1259	-	12,15,15	2.20	1 (8%)	14,17,17	0.59	0
6	LDA	M	1325	-	12,15,15	2.31	1 (8%)	14,17,17	0.57	0
7	SO4	M	1328	-	4,4,4	1.03	0	6,6,6	0.53	0
12	MST	L	502	-	16,16,16	1.22	1 (6%)	22,22,22	1.41	2 (9%)
6	LDA	H	1260	-	12,15,15	2.35	1 (8%)	14,17,17	0.49	0
6	LDA	M	1324	-	12,15,15	1.84	1 (8%)	14,17,17	0.58	0
8	BCB	L	400	8,3	63,74,74	1.38	9 (14%)	74,115,115	1.97	16 (21%)
5	HEC	C	404	1	32,50,50	1.64	3 (9%)	24,82,82	1.41	3 (12%)
9	BPB	M	402	-	49,70,70	1.27	6 (12%)	47,101,101	2.29	9 (19%)
8	BCB	L	401	3	63,74,74	1.52	9 (14%)	74,115,115	1.86	9 (12%)
7	SO4	H	1261	-	4,4,4	0.55	0	6,6,6	0.38	0
6	LDA	L	1274	-	12,15,15	2.24	1 (8%)	14,17,17	0.46	0
9	BPB	L	402	-	49,70,70	1.22	5 (10%)	47,101,101	2.37	9 (19%)
11	MQ9	L	501	-	59,59,59	1.66	21 (35%)	72,75,75	1.40	12 (16%)
7	SO4	M	1329	-	4,4,4	1.38	0	6,6,6	0.80	0
7	SO4	M	1327	-	4,4,4	1.15	0	6,6,6	0.42	0
8	BCB	M	400	4	63,74,74	1.51	9 (14%)	74,115,115	2.03	12 (16%)
13	NS5	M	600	-	39,39,39	0.87	2 (5%)	44,46,46	1.13	4 (9%)
5	HEC	C	402	1	32,50,50	1.55	3 (9%)	24,82,82	1.26	2 (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
8	BCB	M	401	8,4	3/3/21/26	8/37/137/137	-
6	LDA	M	1326	-	-	2/13/13/13	-
5	HEC	C	401	1	-	2/10/54/54	-
5	HEC	C	403	1	-	0/10/54/54	-
6	LDA	H	1259	-	-	5/13/13/13	-
6	LDA	M	1325	-	-	3/13/13/13	-
12	MST	L	502	-	-	0/10/10/10	0/1/1/1
6	LDA	H	1260	-	-	4/13/13/13	-
6	LDA	M	1324	-	-	3/13/13/13	-
8	BCB	L	400	8,3	3/3/21/26	6/37/137/137	-
5	HEC	C	404	1	-	2/10/54/54	-
9	BPB	M	402	-	1/1/18/23	2/37/105/105	0/5/6/6
8	BCB	L	401	3	2/2/21/26	3/37/137/137	-
6	LDA	L	1274	-	-	3/13/13/13	-
9	BPB	L	402	-	-	3/37/105/105	0/5/6/6
11	MQ9	L	501	-	-	4/53/73/73	0/2/2/2
8	BCB	M	400	4	2/2/21/26	4/37/137/137	-
13	NS5	M	600	-	-	11/43/43/43	-
5	HEC	C	402	1	-	4/10/54/54	-

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	1260	LDA	O1-N1	-8.11	1.23	1.42
6	M	1326	LDA	O1-N1	-7.93	1.23	1.42
6	M	1325	LDA	O1-N1	-7.78	1.24	1.42
6	L	1274	LDA	O1-N1	-7.62	1.24	1.42
6	H	1259	LDA	O1-N1	-7.55	1.24	1.42

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	402	BPB	O2D-CGD-CBD	11.31	125.33	111.00
9	L	402	BPB	O2D-CGD-CBD	10.35	124.11	111.00
8	M	400	BCB	C4A-NA-C1A	9.06	110.78	106.71
8	M	401	BCB	C4A-NA-C1A	8.33	110.45	106.71
8	L	400	BCB	C4A-NA-C1A	7.80	110.21	106.71

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	L	400	BCB	NC
8	L	400	BCB	NA
8	L	400	BCB	ND
8	L	401	BCB	NC
8	L	401	BCB	NA

5 of 69 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	M	401	BCB	CHA-CBD-CGD-O1D
8	M	401	BCB	CHA-CBD-CGD-O2D
8	M	401	BCB	CAD-CBD-CGD-O1D
8	M	401	BCB	CAD-CBD-CGD-O2D
9	L	402	BPB	O2A-C1-C2-C3

There are no ring outliers.

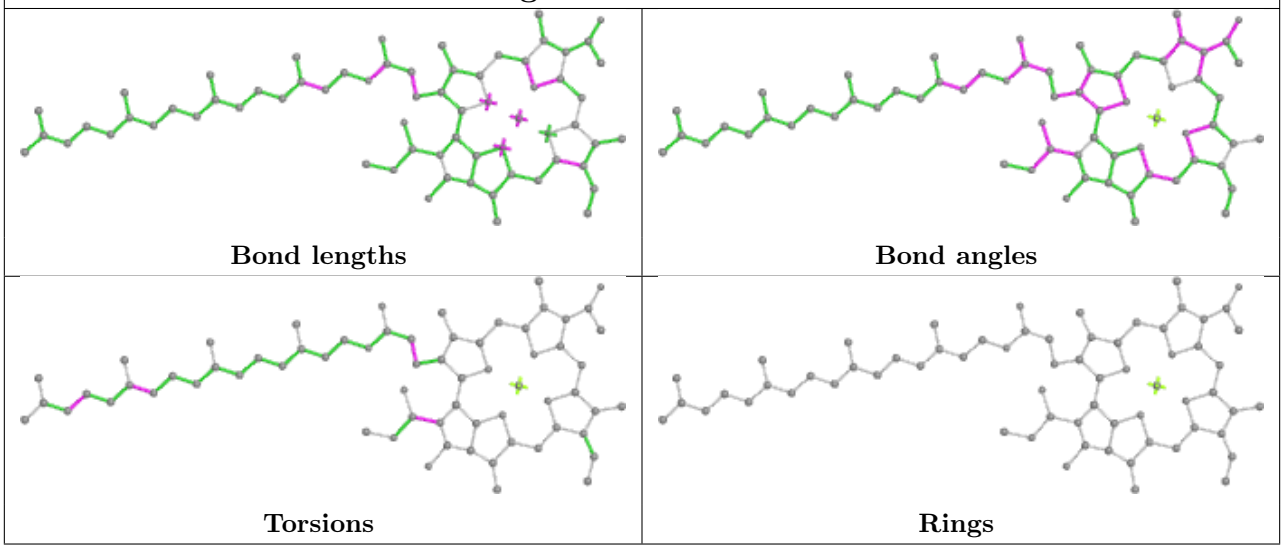
15 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	401	BCB	7	0
6	M	1326	LDA	1	0
5	C	401	HEC	1	0
6	H	1260	LDA	3	0
6	M	1324	LDA	1	0
8	L	400	BCB	5	0
9	M	402	BPB	7	0
8	L	401	BCB	4	0
6	L	1274	LDA	4	0
9	L	402	BPB	3	0
11	L	501	MQ9	1	0
7	M	1329	SO4	1	0
8	M	400	BCB	8	0
13	M	600	NS5	2	0
5	C	402	HEC	3	0

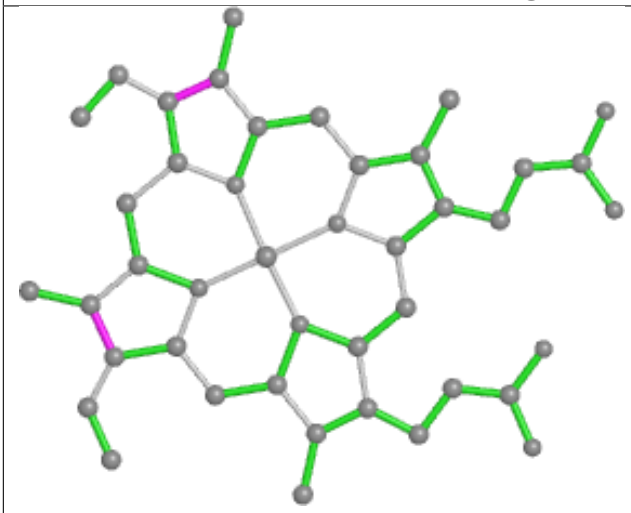
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

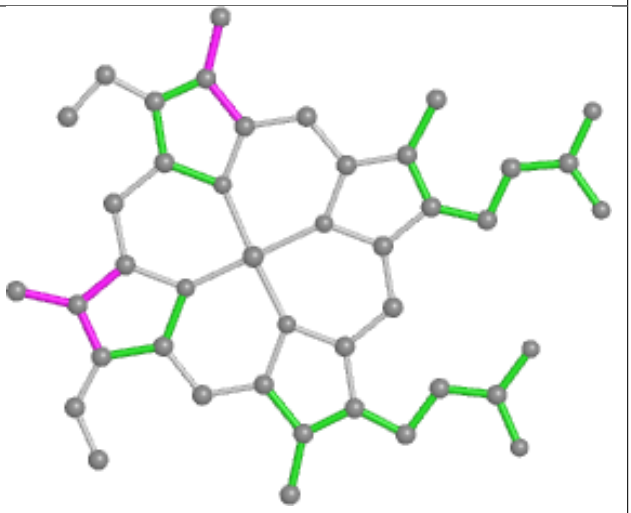
Ligand BCB M 401



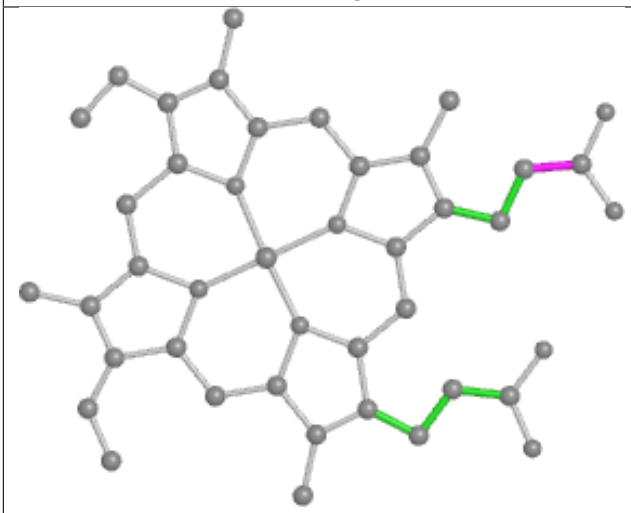
Ligand HEC C 401



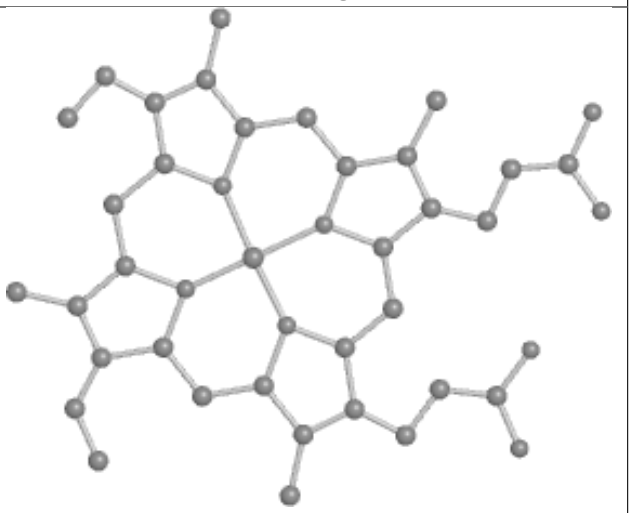
Bond lengths



Bond angles

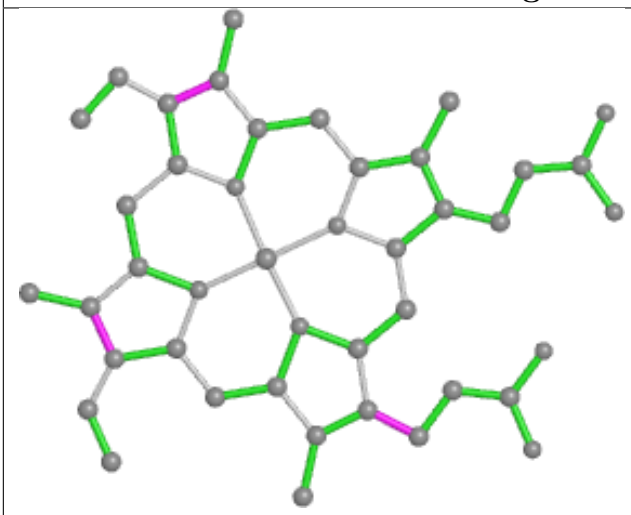


Torsions



Rings

Ligand HEC C 403



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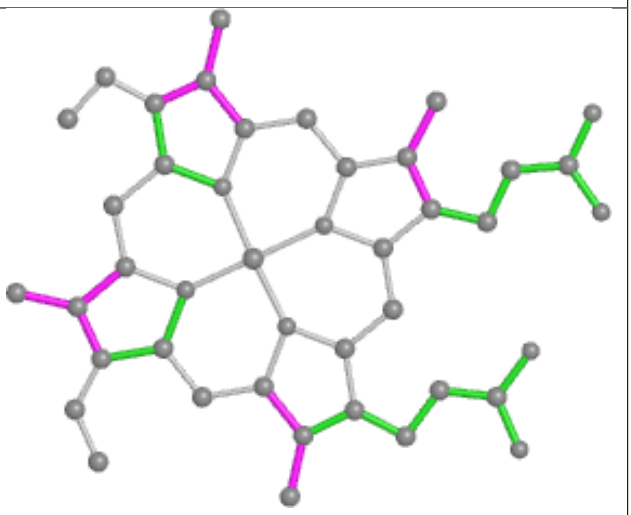

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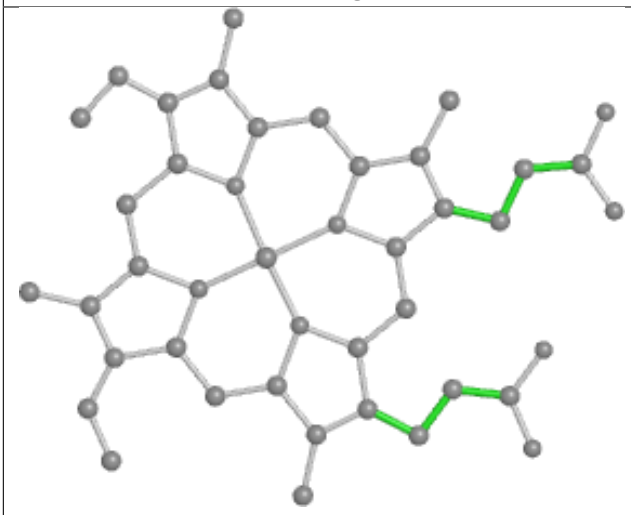

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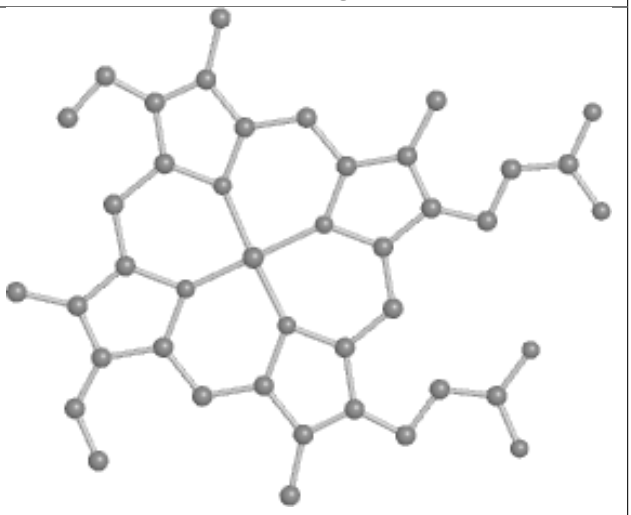
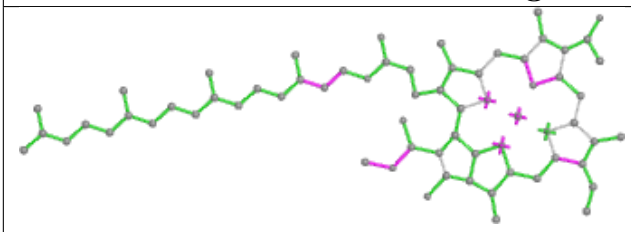


Rings

Ligand BCB L 400



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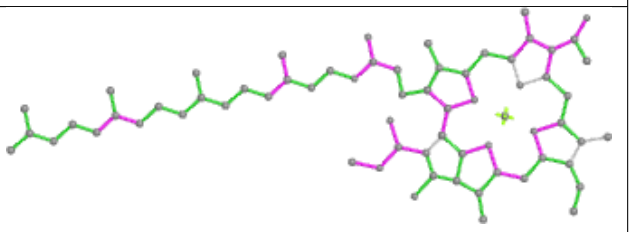
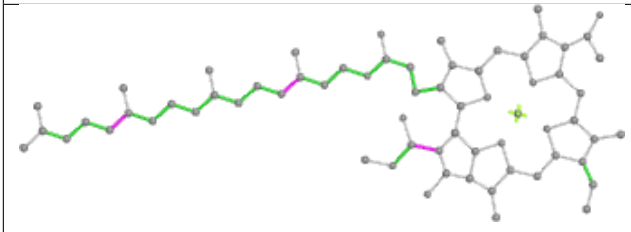


Bond angles



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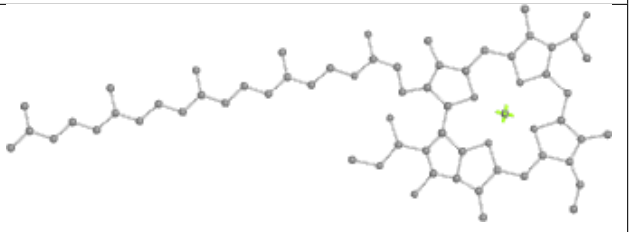
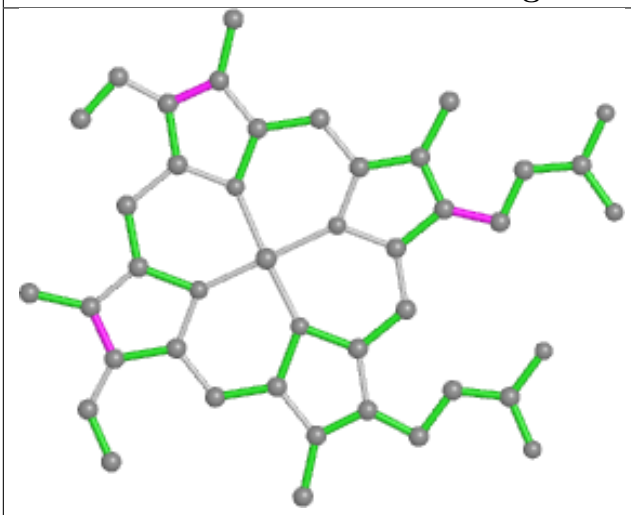


Rings

Ligand HEC C 404



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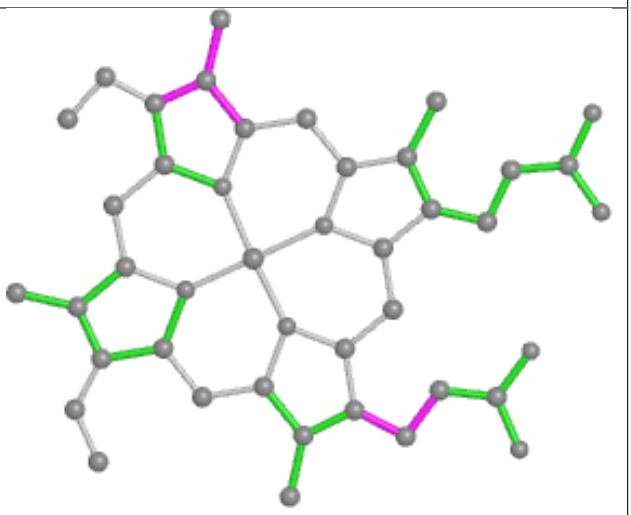
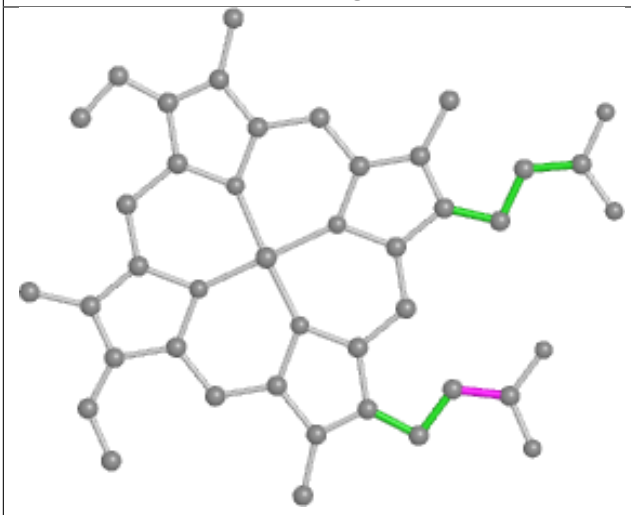


Bond angles



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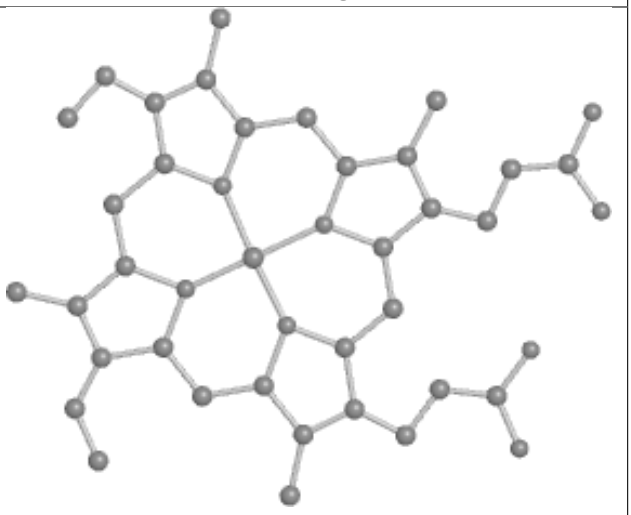
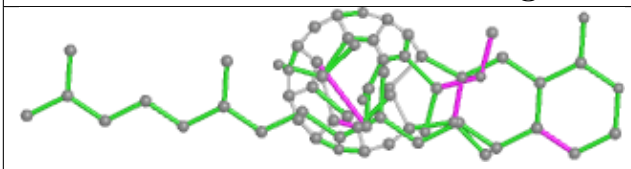


Rings

Ligand BPB M 402



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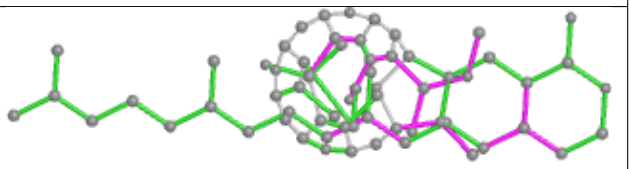

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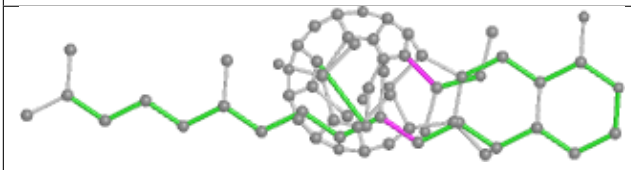

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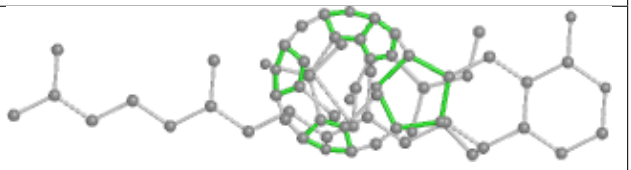
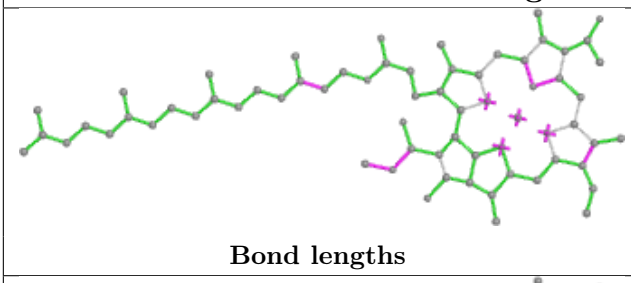
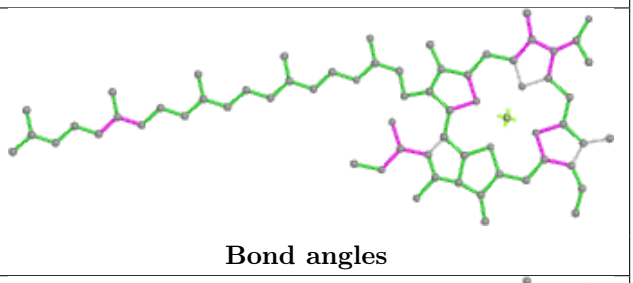


Rings

Ligand BCB L 401


Bond lengths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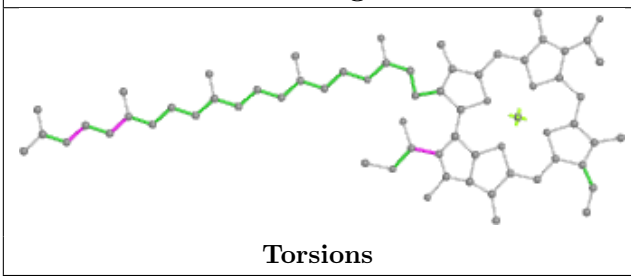
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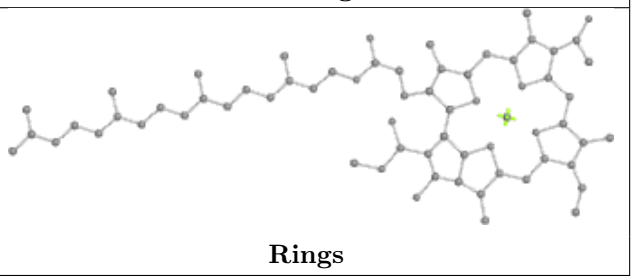
Rings

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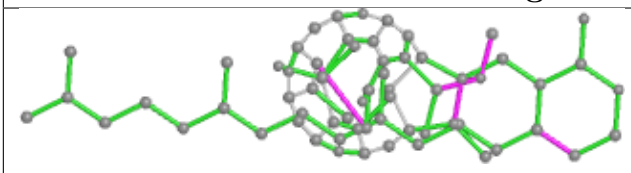
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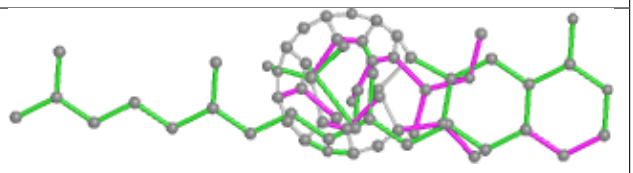
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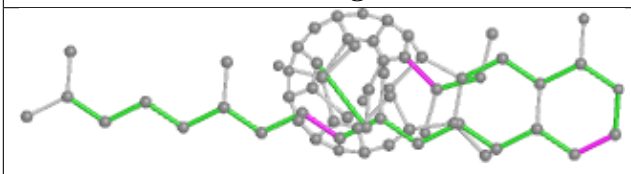
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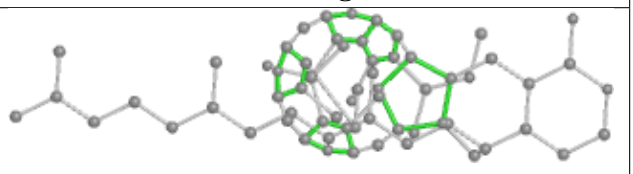
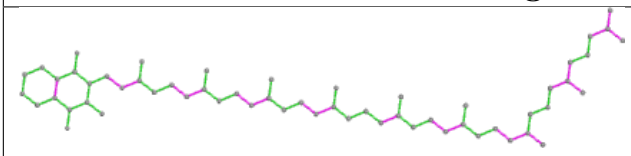

Rings

Ligand MQ9 L 501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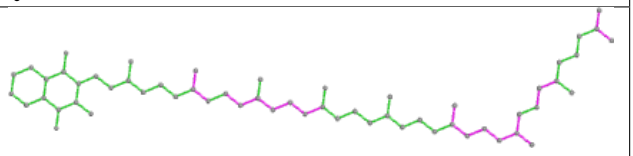
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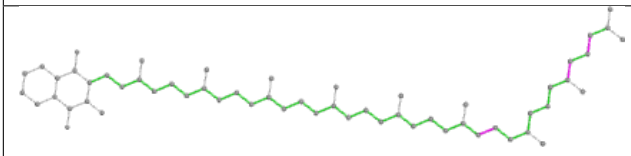
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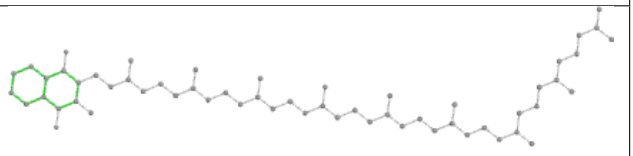
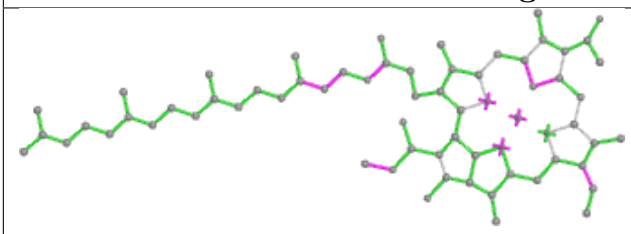
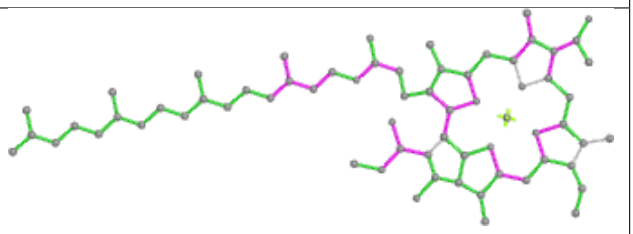

Rings

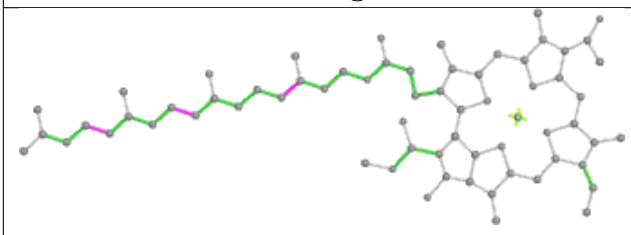
Ligand BCB M 400



Bond lengths



Bond angles



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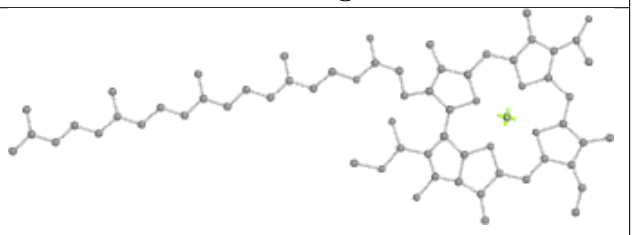
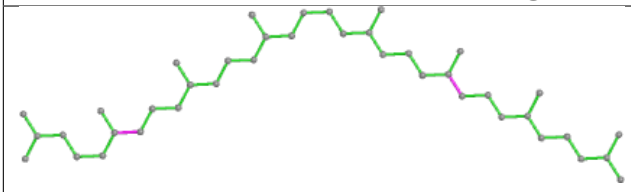
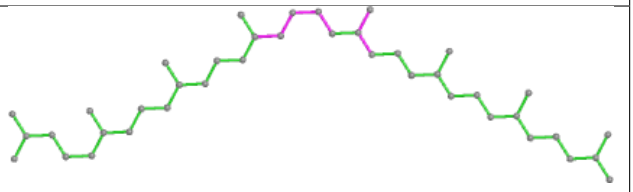


Rings

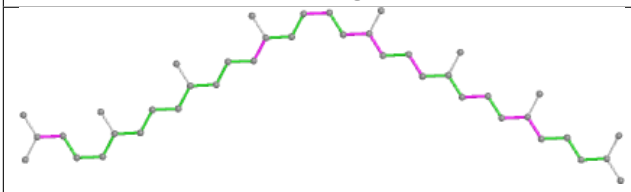
Ligand NS5 M 600



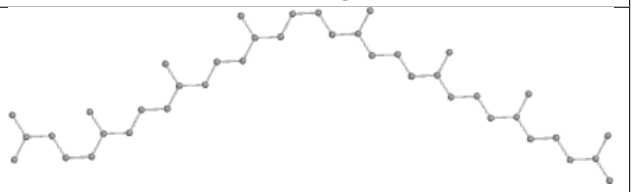
Bond lengths



Bond angles

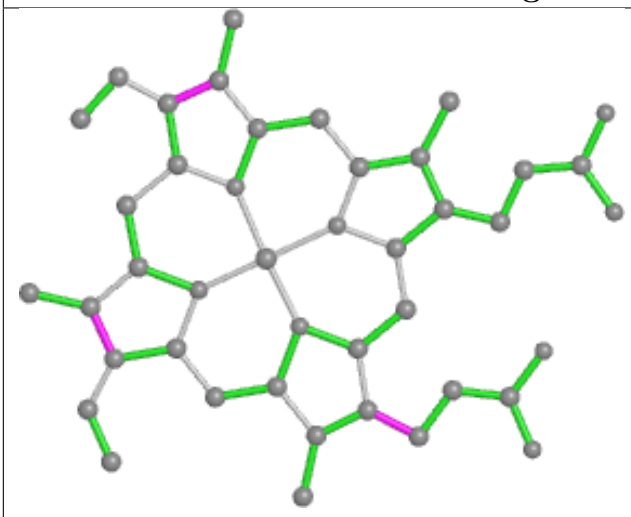


Torsions

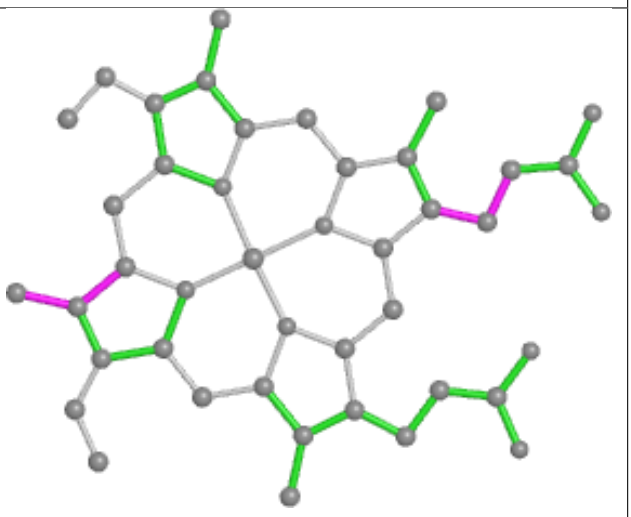


Rings

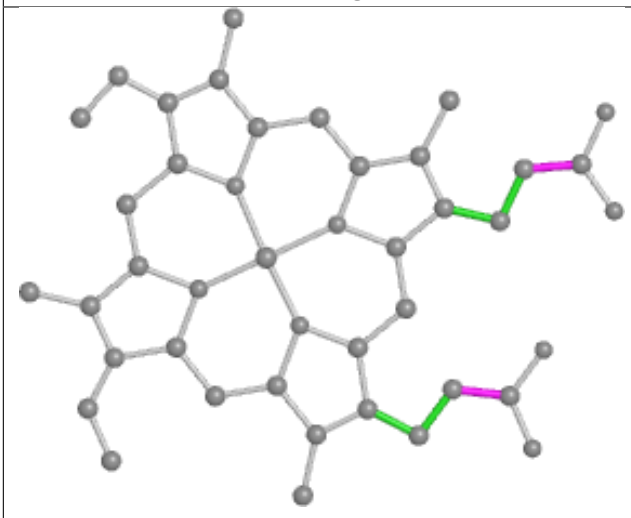
Ligand HEC C 402



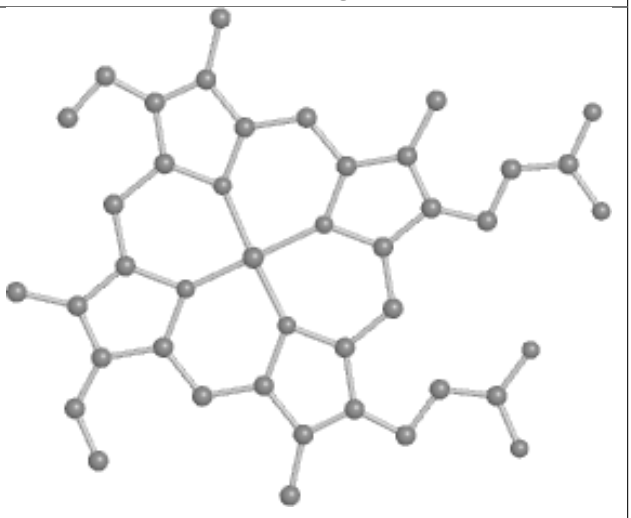
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.