wwPDB EM Validation Summary Report (i)

Apr 2, 2025 – 02:56 am BST

PDB ID	:	6HWH / pdb_00006hwh
EMDB ID	:	EMD-0289
Title	:	Structure of a functional obligate respiratory supercomplex from Mycobacterium smegmatis
Authors	:	Wiseman, B.; Nitharwal, R.G.; Fedotovskaya, O.; Schafer, J.; Guo, H.; Kuang, Q.; Benlekbir, S.; Sjostrand, D.; Adelroth, P.; Rubinstein, J.L.; Brzezinski, P.; Hogbom, M.
Deposited on	:	2018-10-12
Resolution	:	3.30 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
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 (i)) were used in the production of this report:

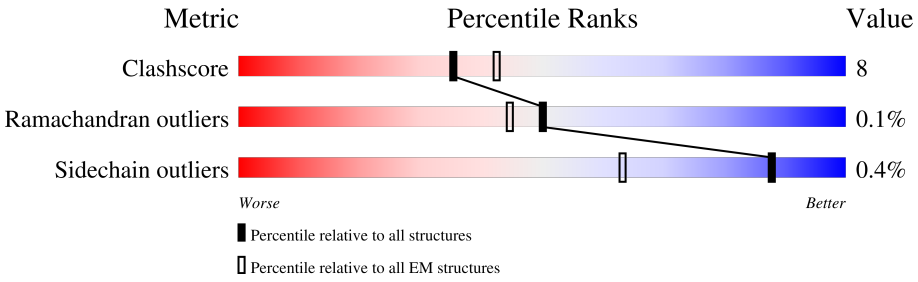
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	408	83% 10% 7%
1	B	408	79% 14% 7%
2	C	74	99% .
2	G	74	100%
3	D	65	100%
3	H	65	100%
4	E	20	100%
4	I	20	100%
5	F	35	97% .

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Mol	Chain	Length	Quality of chain
5	J	35	97%
6	K	268	10% 89%
6	M	268	11% 89%
6	i	268	59% 40%
6	j	268	60% 40%
7	L	341	69% 14% 18%
7	P	341	69% 13% 18%
8	N	79	63% 5% 32%
8	R	79	65% 32%
9	O	157	80% 10% 10%
9	T	157	83% 8% 10%
10	Q	583	77% 17% 6%
10	V	583	78% 16% 6%
11	S	139	86% 14%
11	X	139	90% 10%
12	W	203	80% 10% 9%
12	Z	203	82% 9% 9%
13	Y	554	86% 11%
13	b	554	97%

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
14	FES	B	501	-	-	X	-
18	HAS	Q	801	X	-	-	-
18	HAS	Q	802	X	-	-	-
18	HAS	V	801	X	-	-	-
18	HAS	V	802	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	HEC	V	804	-	-	X	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 40632 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Ubiquinol-cytochrome c reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	380	Total	C	N	O	S	0	0
			2960	1914	500	535	11		
1	B	380	Total	C	N	O	S	0	0
			2960	1914	500	535	11		

- Molecule 2 is a protein called Co-purified unknown transmembrane helices built as polyALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	74	Total	C	N	O	0	0
			370	222	74	74		
2	C	74	Total	C	N	O	0	0
			370	222	74	74		

- Molecule 3 is a protein called Co-purified unknown transmembrane helices built as polyALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	65	Total	C	N	O	0	0
			325	195	65	65		
3	D	65	Total	C	N	O	0	0
			325	195	65	65		

- Molecule 4 is a protein called Co-purified unknown peptide built as polyALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	20	Total	C	N	O	0	0
			100	60	20	20		
4	E	20	Total	C	N	O	0	0
			100	60	20	20		

- Molecule 5 is a protein called Co-purified unknown peptide built as polyALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	35	Total	C	N	O	0	0
			175	105	35	35		
5	F	35	Total	C	N	O	0	0
			175	105	35	35		

- Molecule 6 is a protein called Cytochrome bc1 complex cytochrome c subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	30	Total	C	N	O	S	0	0
			211	139	35	33	4		
6	K	30	Total	C	N	O	S	0	0
			211	139	35	33	4		
6	i	162	Total	C	N	O		0	0
			648	324	162	162			
6	j	162	Total	C	N	O		0	0
			648	324	162	162			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	281	Total	C	N	O	S	0	0
			2236	1450	368	409	9		
7	L	281	Total	C	N	O	S	0	0
			2236	1450	368	409	9		

- Molecule 8 is a protein called MSMEG_4693.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	54	Total	C	N	O	S	0	0
			415	276	67	70	2		
8	N	54	Total	C	N	O	S	0	0
			415	276	67	70	2		

- Molecule 9 is a protein called Uncharacterized protein MSMEG_4692/MSMEI_4575.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	142	Total	C	N	O	S	0	0
			1019	644	173	200	2		
9	O	142	Total	C	N	O	S	0	0
			1019	644	173	200	2		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	550	Total	C	N	O	S	0	0
			4354	2927	695	709	23		
10	Q	550	Total	C	N	O	S	0	0
			4354	2927	695	709	23		

- Molecule 11 is a protein called Cytochrome c oxidase polypeptide 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		
11	S	139	Total	C	N	O	S	0	0
			1077	719	167	188	3		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	184	Total	C	N	O	S	0	0
			1441	967	229	238	7		
12	W	184	Total	C	N	O	S	0	0
			1441	967	229	238	7		

- Molecule 13 is a protein called Ubiquinol-cytochrome C reductase QcrB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	b	536	Total	C	N	O	S	0	0
			4190	2757	712	703	18		
13	Y	536	Total	C	N	O	S	0	0
			4190	2757	712	703	18		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	547	ASP	-	expression tag	UNP I7FGS8
b	548	TYR	-	expression tag	UNP I7FGS8
b	549	LYS	-	expression tag	UNP I7FGS8
b	550	ASP	-	expression tag	UNP I7FGS8
b	551	ASP	-	expression tag	UNP I7FGS8
b	552	ASP	-	expression tag	UNP I7FGS8
b	553	ASP	-	expression tag	UNP I7FGS8
b	554	LYS	-	expression tag	UNP I7FGS8
Y	547	ASP	-	expression tag	UNP I7FGS8
Y	548	TYR	-	expression tag	UNP I7FGS8
Y	549	LYS	-	expression tag	UNP I7FGS8

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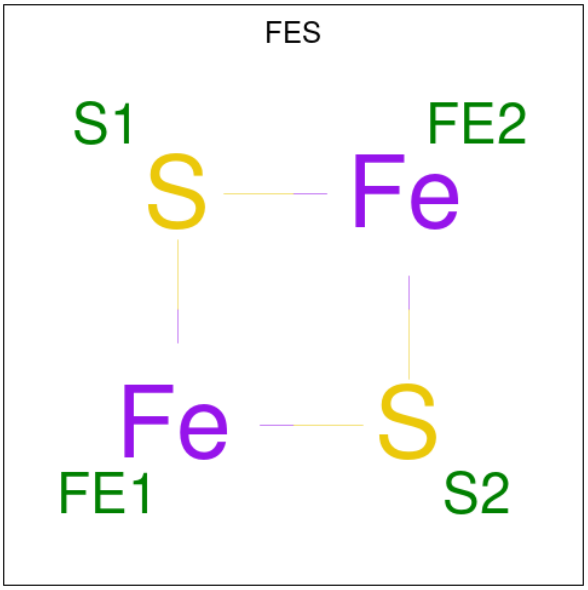
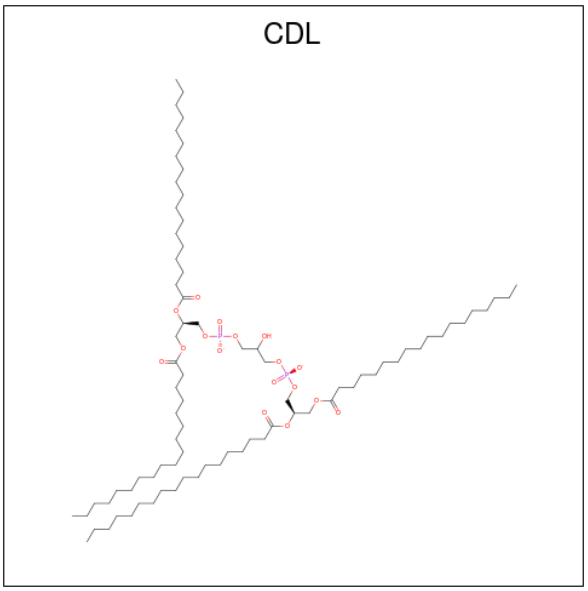
Chain	Residue	Modelled	Actual	Comment	Reference
Y	550	ASP	-	expression tag	UNP I7FGS8
Y	551	ASP	-	expression tag	UNP I7FGS8
Y	552	ASP	-	expression tag	UNP I7FGS8
Y	553	ASP	-	expression tag	UNP I7FGS8
Y	554	LYS	-	expression tag	UNP I7FGS8

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



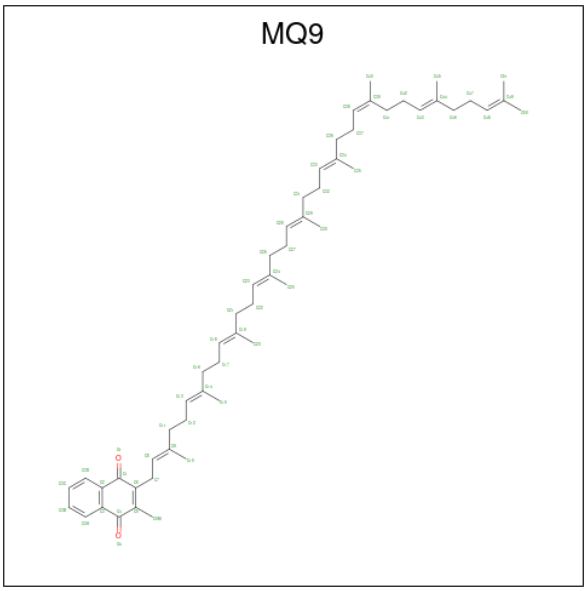
Mol	Chain	Residues	Atoms	AltConf
14	A	1	Total Fe S 4 2 2	0
14	B	1	Total Fe S 4 2 2	0

- Molecule 15 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
15	M	1	Total	C	O	P	0
			100	81	17	2	
15	V	1	Total	C	O	P	0
			87	68	17	2	
15	b	1	Total	C	O	P	0
			92	73	17	2	
15	b	1	Total	C	O	P	0
			91	72	17	2	
15	K	1	Total	C	O	P	0
			100	81	17	2	
15	Q	1	Total	C	O	P	0
			87	68	17	2	
15	Y	1	Total	C	O	P	0
			91	72	17	2	
15	Y	1	Total	C	O	P	0
			92	73	17	2	

- Molecule 16 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$).

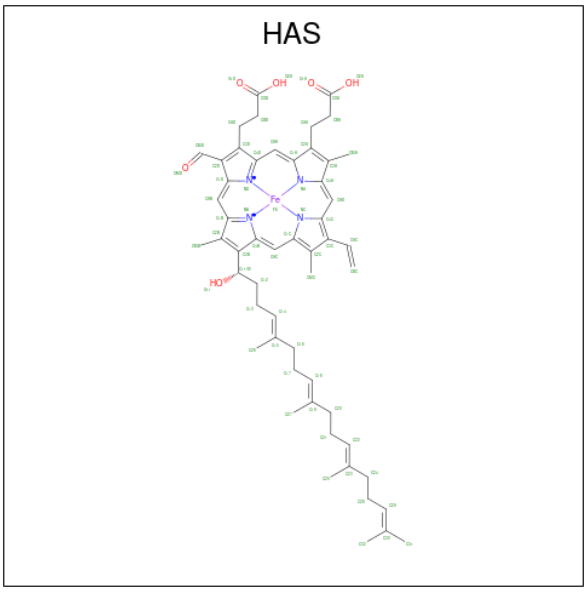


Mol	Chain	Residues	Atoms	AltConf
16	M	1	Total C O 58 56 2	0
16	b	1	Total C O 58 56 2	0
16	Y	1	Total C O 58 56 2	0
16	Y	1	Total C O 58 56 2	0

- Molecule 17 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

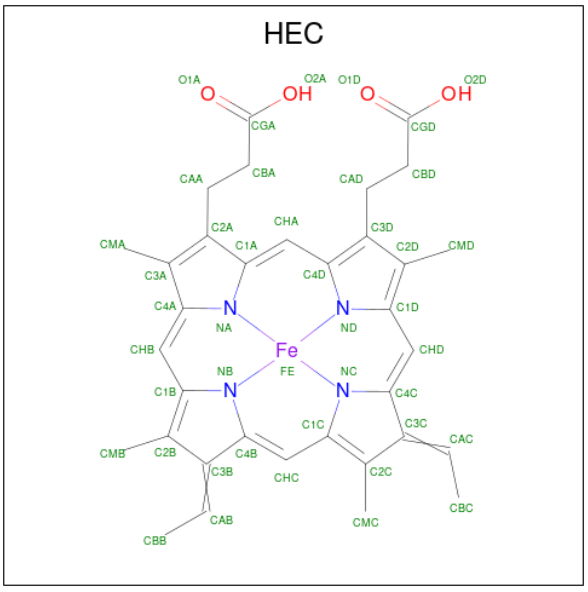
Mol	Chain	Residues	Atoms	AltConf
17	P	2	Total Cu 2 2	0
17	V	1	Total Cu 1 1	0
17	L	2	Total Cu 2 2	0
17	Q	1	Total Cu 1 1	0

- Molecule 18 is HEME-AS (CCD ID: HAS) (formula: $C_{54}H_{64}FeN_4O_6$).



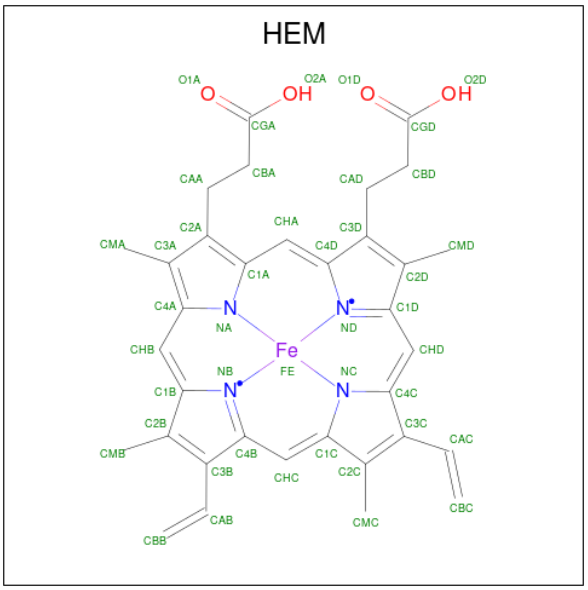
Mol	Chain	Residues	Atoms					AltConf
18	V	1	Total	C	Fe	N	O	0
			65	54	1	4	6	
18	V	1	Total	C	Fe	N	O	0
			65	54	1	4	6	
18	Q	1	Total	C	Fe	N	O	0
			65	54	1	4	6	
18	Q	1	Total	C	Fe	N	O	0
			65	54	1	4	6	

- Molecule 19 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
19	V	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
19	i	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
19	j	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
19	j	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 20 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



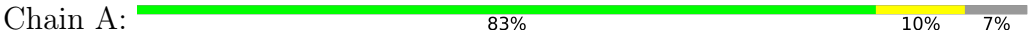
Mol	Chain	Residues	Atoms					AltConf
20	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	b	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	Y	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
20	Y	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

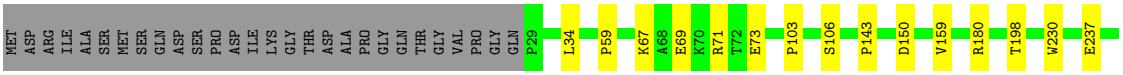
3 Residue-property plots (i)

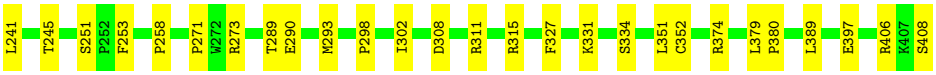
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

• Molecule 1: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain A:

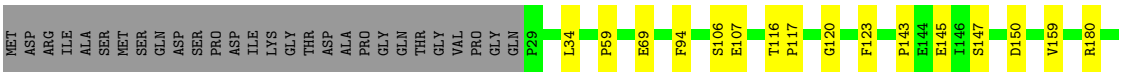


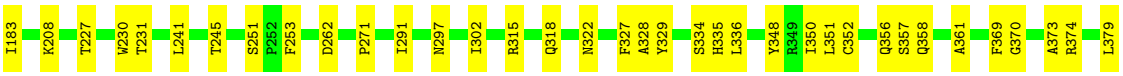


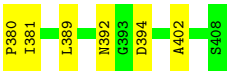


• Molecule 1: Ubiquinol-cytochrome c reductase iron-sulfur subunit

Chain B:

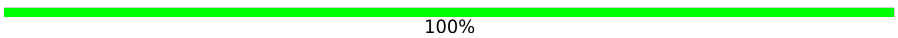






• Molecule 2: Co-purified unknown transmembrane helices built as polyALA

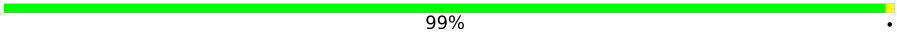
Chain G:



There are no outlier residues recorded for this chain.

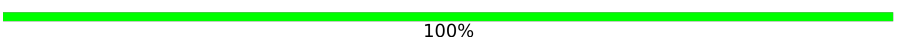
• Molecule 2: Co-purified unknown transmembrane helices built as polyALA

Chain C:



• Molecule 3: Co-purified unknown transmembrane helices built as polyALA

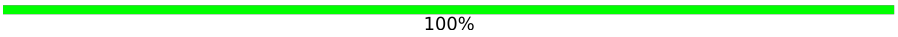
Chain H:



There are no outlier residues recorded for this chain.

• Molecule 3: Co-purified unknown transmembrane helices built as polyALA

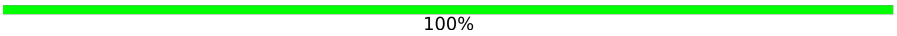
Chain D:



There are no outlier residues recorded for this chain.

• Molecule 4: Co-purified unknown peptide built as polyALA

Chain I:



There are no outlier residues recorded for this chain.

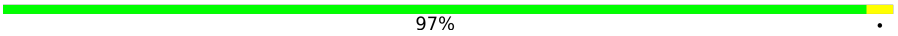
• Molecule 4: Co-purified unknown peptide built as polyALA

Chain E:

There are no outlier residues recorded for this chain.

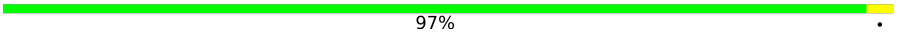
• Molecule 5: Co-purified unknown peptide built as polyALA

Chain J:



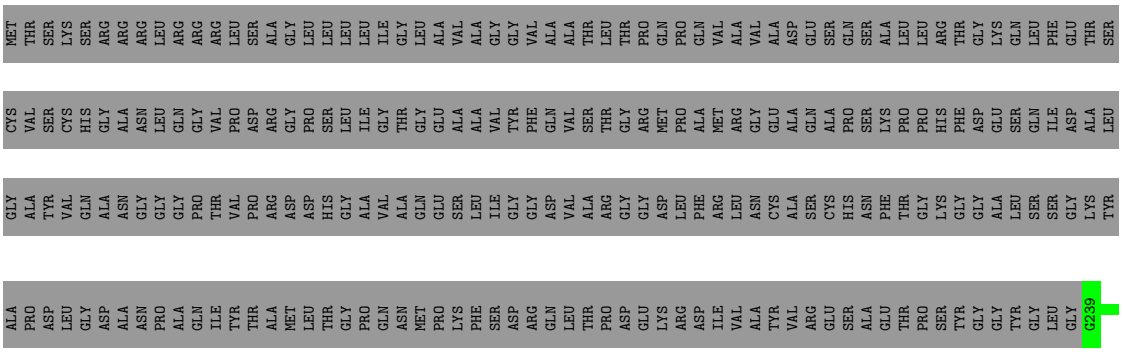
• Molecule 5: Co-purified unknown peptide built as polyALA

Chain F:



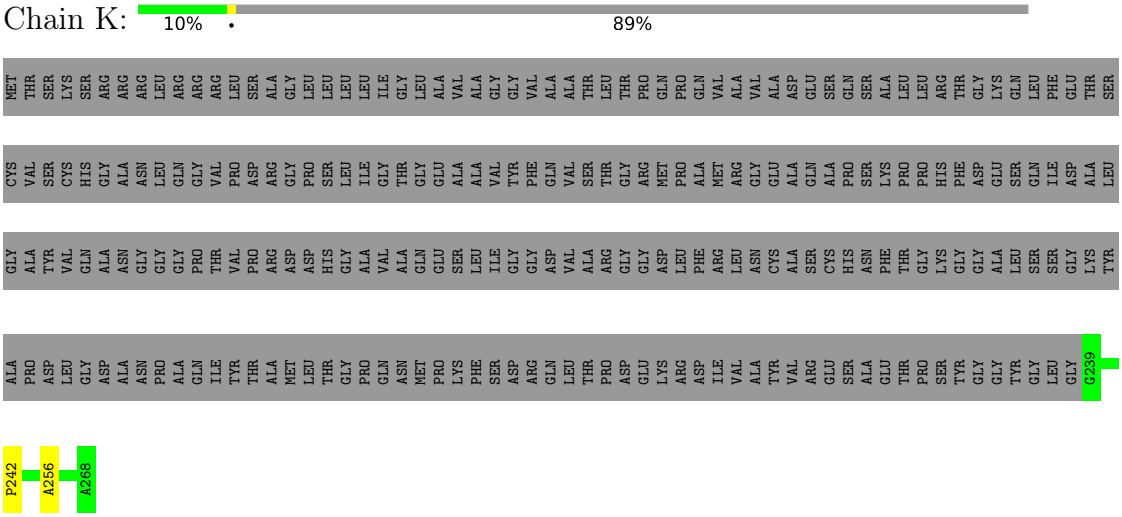
• Molecule 6: Cytochrome bc1 complex cytochrome c subunit

Chain M:



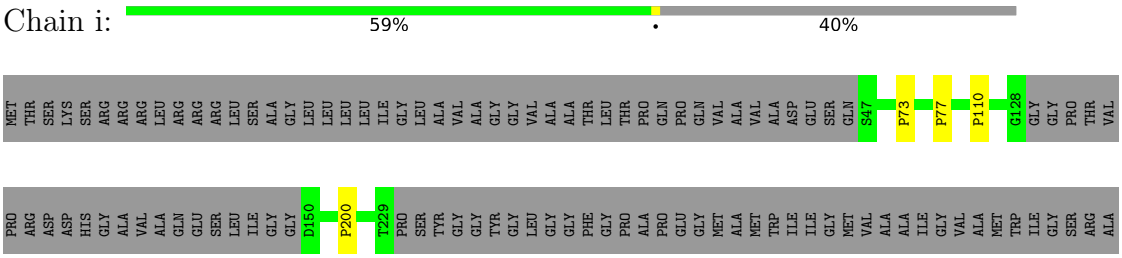
• Molecule 6: Cytochrome bc1 complex cytochrome c subunit

Chain K:



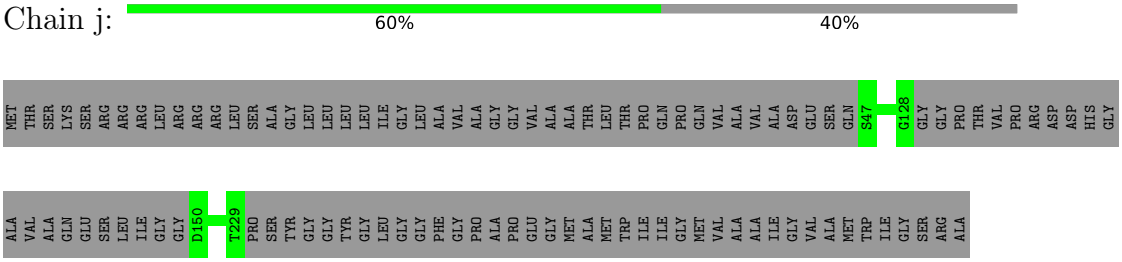
• Molecule 6: Cytochrome bc1 complex cytochrome c subunit

Chain i:



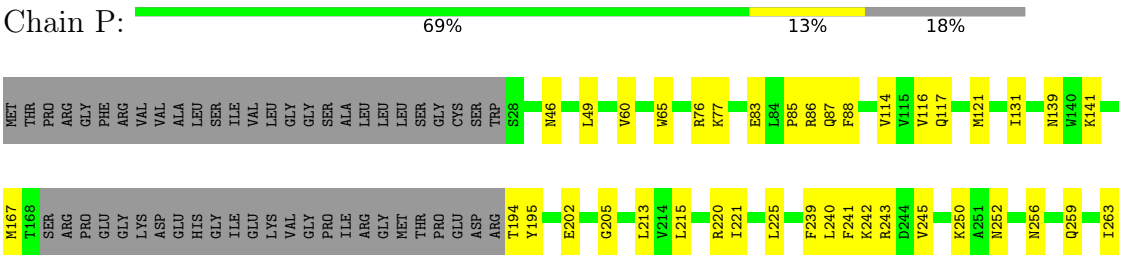
• Molecule 6: Cytochrome bc1 complex cytochrome c subunit

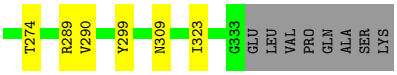
Chain j:



• Molecule 7: Cytochrome c oxidase subunit 2

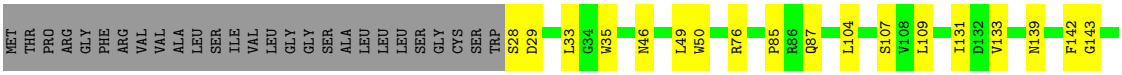
Chain P:

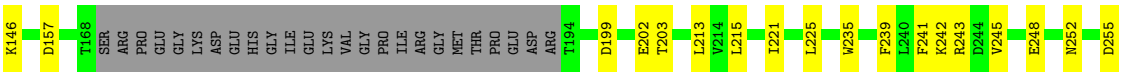


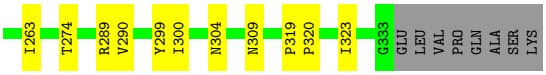


• Molecule 7: Cytochrome c oxidase subunit 2

Chain L:







• Molecule 8: MSMEG_4693

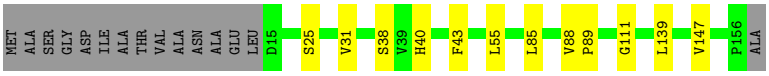
Chain R:

• Molecule 8: MSMEG_4693

Chain N:

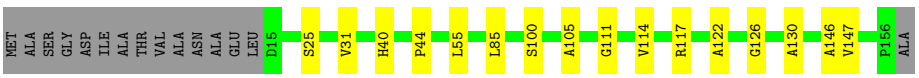
• Molecule 9: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain T:



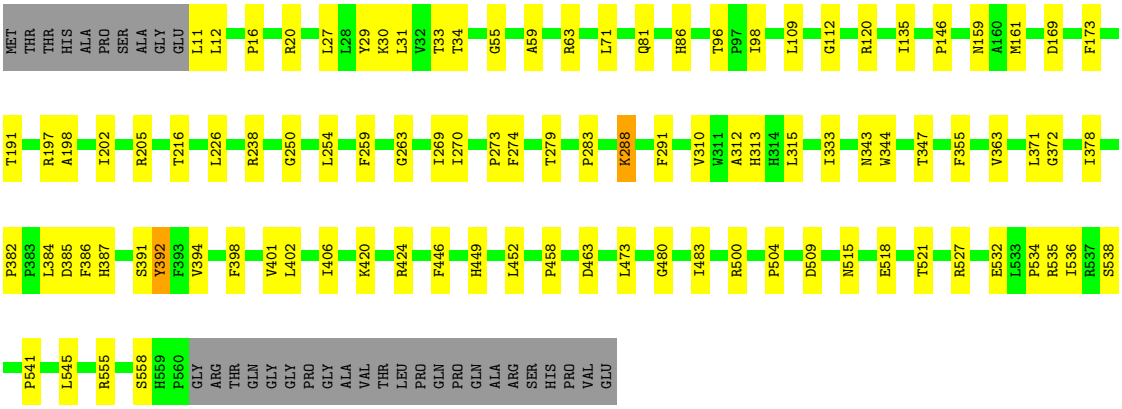
• Molecule 9: Uncharacterized protein MSMEG_4692/MSMEI_4575

Chain O:



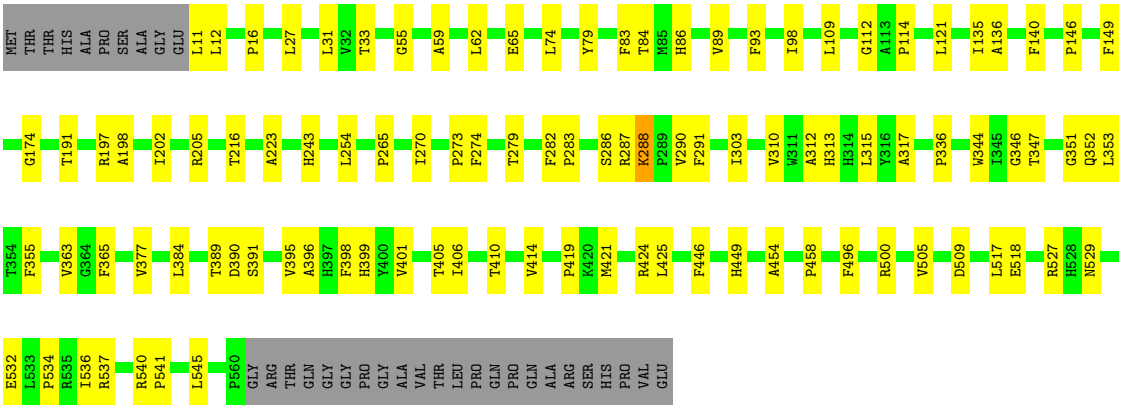
• Molecule 10: Cytochrome c oxidase subunit 1

Chain V:



• Molecule 10: Cytochrome c oxidase subunit 1

Chain Q:

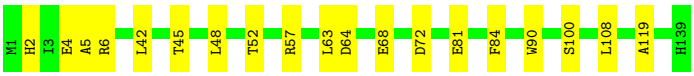


• Molecule 11: Cytochrome c oxidase polypeptide 4

Chain X:

• Molecule 11: Cytochrome c oxidase polypeptide 4

Chain S:

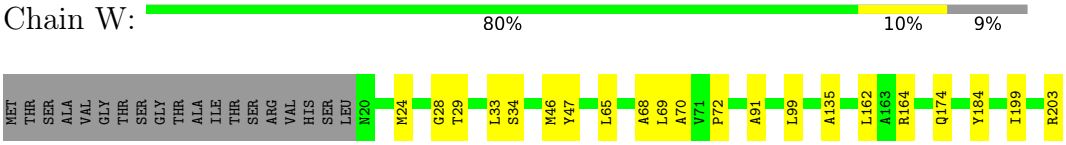


• Molecule 12: Cytochrome c oxidase subunit 3

Chain Z:

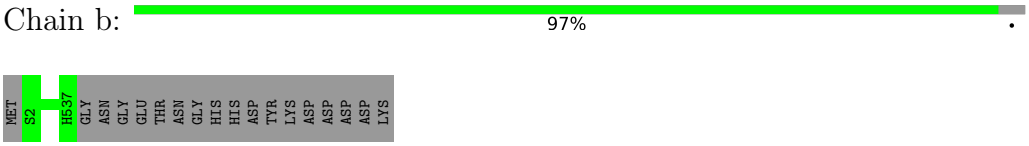
• Molecule 12: Cytochrome c oxidase subunit 3

Chain W:



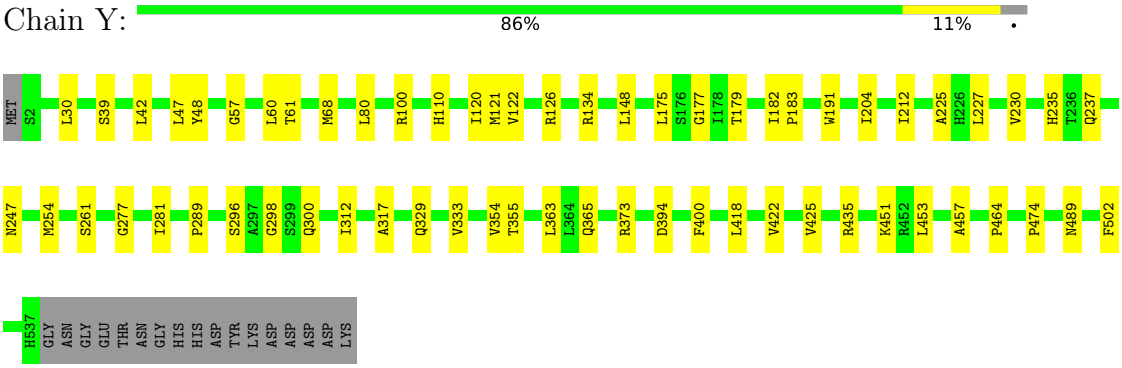
• Molecule 13: Ubiquinol-cytochrome C reductase QcrB

Chain b:



• Molecule 13: Ubiquinol-cytochrome C reductase QcrB

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	104198	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, CDL, HAS, FES, MQ9, HEM, CU

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	A	0.35	0/3039	0.59	0/4120
1	B	0.40	0/3039	0.61	0/4120
6	K	0.42	0/217	0.56	0/293
6	M	0.41	0/217	0.52	0/293
6	i	0.73	0/646	0.91	0/804
6	j	0.66	0/646	0.97	0/804
7	L	0.44	0/2297	0.63	0/3126
7	P	0.38	0/2297	0.59	0/3126
8	N	0.32	0/430	0.65	0/591
8	R	0.29	0/430	0.63	0/591
9	O	0.38	0/1037	0.57	0/1416
9	T	0.35	0/1037	0.57	0/1416
10	Q	0.51	0/4515	0.68	0/6176
10	V	0.48	0/4515	0.67	0/6176
11	S	0.46	0/1112	0.62	0/1524
11	X	0.42	0/1112	0.59	0/1524
12	W	0.45	0/1488	0.58	0/2032
12	Z	0.40	0/1488	0.56	0/2032
13	Y	0.46	0/4324	0.62	0/5897
13	b	0.41	0/4324	0.61	0/5897
All	All	0.44	0/38210	0.63	0/51958

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	2960	0	2963	27	0
1	B	2960	0	2965	45	0
2	C	370	0	80	1	0
2	G	370	0	80	0	0
3	D	325	0	67	0	0
3	H	325	0	67	0	0
4	E	100	0	23	0	0
4	I	100	0	23	0	0
5	F	175	0	38	1	0
5	J	175	0	41	1	0
6	K	211	0	212	2	0
6	M	211	0	212	1	0
6	i	648	0	182	0	0
6	j	648	0	185	0	0
7	L	2236	0	2189	29	0
7	P	2236	0	2189	28	0
8	N	415	0	424	4	0
8	R	415	0	424	3	0
9	O	1019	0	1030	11	0
9	T	1019	0	1030	10	0
10	Q	4354	0	4342	69	0
10	V	4354	0	4341	84	0
11	S	1077	0	1058	20	0
11	X	1077	0	1058	12	0
12	W	1441	0	1439	18	0
12	Z	1441	0	1439	12	0
13	Y	4190	0	4211	45	0
13	b	4190	0	4211	0	0
14	A	4	0	0	0	0
14	B	4	0	0	2	0
15	K	100	0	154	6	0
15	M	100	0	154	4	0
15	Q	87	0	118	3	0
15	V	87	0	118	2	0
15	Y	183	0	266	9	0
15	b	183	0	266	0	0
16	M	58	0	80	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Y	116	0	160	10	0
16	b	58	0	80	0	0
17	L	2	0	0	0	0
17	P	2	0	0	0	0
17	Q	1	0	0	0	0
17	V	1	0	0	0	0
18	Q	130	0	124	6	0
18	V	130	0	124	7	0
19	V	43	0	32	22	0
19	i	43	0	32	0	0
19	j	86	0	63	0	0
20	Y	86	0	60	6	0
20	b	86	0	60	0	0
All	All	40632	0	38414	391	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 8.

The worst 5 of 391 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)
10:V:161:MET:CG	19:V:804:HEC:HBC2	1.36	1.53
10:V:161:MET:CB	19:V:804:HEC:HBC2	1.58	1.31
10:V:161:MET:CG	19:V:804:HEC:CBC	2.15	1.23
10:V:161:MET:HG2	19:V:804:HEC:CBC	1.73	1.19
10:V:161:MET:O	19:V:804:HEC:HBC1	1.46	1.16

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 PDB entries followed by that with respect to all EM entries.

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	A	378/408 (93%)	335 (89%)	43 (11%)	0	100	100
1	B	378/408 (93%)	335 (89%)	43 (11%)	0	100	100
6	K	28/268 (10%)	27 (96%)	1 (4%)	0	100	100
6	M	28/268 (10%)	26 (93%)	2 (7%)	0	100	100
6	i	158/268 (59%)	143 (90%)	11 (7%)	4 (2%)	4	24
6	j	158/268 (59%)	145 (92%)	13 (8%)	0	100	100
7	L	277/341 (81%)	234 (84%)	43 (16%)	0	100	100
7	P	277/341 (81%)	236 (85%)	41 (15%)	0	100	100
8	N	52/79 (66%)	41 (79%)	11 (21%)	0	100	100
8	R	52/79 (66%)	44 (85%)	8 (15%)	0	100	100
9	O	140/157 (89%)	130 (93%)	10 (7%)	0	100	100
9	T	140/157 (89%)	129 (92%)	11 (8%)	0	100	100
10	Q	548/583 (94%)	504 (92%)	44 (8%)	0	100	100
10	V	548/583 (94%)	504 (92%)	44 (8%)	0	100	100
11	S	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
11	X	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
12	W	182/203 (90%)	166 (91%)	16 (9%)	0	100	100
12	Z	182/203 (90%)	169 (93%)	13 (7%)	0	100	100
13	Y	534/554 (96%)	489 (92%)	45 (8%)	0	100	100
13	b	534/554 (96%)	486 (91%)	48 (9%)	0	100	100
All	All	4868/6000 (81%)	4405 (90%)	459 (9%)	4 (0%)	50	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	i	73	PRO
6	i	77	PRO
6	i	110	PRO
6	i	200	PRO

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 PDB entries followed by that with respect to all EM entries.

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	A	310/333 (93%)	310 (100%)	0	100 100
1	B	310/333 (93%)	310 (100%)	0	100 100
6	K	18/197 (9%)	18 (100%)	0	100 100
6	M	18/197 (9%)	18 (100%)	0	100 100
7	L	239/288 (83%)	237 (99%)	2 (1%)	79 87
7	P	239/288 (83%)	236 (99%)	3 (1%)	65 79
8	N	44/59 (75%)	44 (100%)	0	100 100
8	R	44/59 (75%)	44 (100%)	0	100 100
9	O	105/114 (92%)	105 (100%)	0	100 100
9	T	105/114 (92%)	105 (100%)	0	100 100
10	Q	456/481 (95%)	452 (99%)	4 (1%)	75 85
10	V	456/481 (95%)	451 (99%)	5 (1%)	70 82
11	S	106/106 (100%)	106 (100%)	0	100 100
11	X	106/106 (100%)	106 (100%)	0	100 100
12	W	146/161 (91%)	146 (100%)	0	100 100
12	Z	146/161 (91%)	146 (100%)	0	100 100
13	Y	431/446 (97%)	430 (100%)	1 (0%)	92 95
13	b	431/446 (97%)	431 (100%)	0	100 100
All	All	3710/4370 (85%)	3695 (100%)	15 (0%)	88 93

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	V	527	ARG
10	Q	527	ARG
7	L	76	ARG
13	Y	60	LEU
10	Q	353	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
13	b	365	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 6 are monoatomic - leaving 26 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	$\#\|Z\| > 2$
15	CDL	Q	804	-	86,86,99	1.23	8 (9%)	92,98,111	1.06	4 (4%)
19	HEC	j	301	6	32,50,50	2.26	12 (37%)	24,82,82	1.92	3 (12%)
15	CDL	K	301	-	99,99,99	1.19	8 (8%)	105,111,111	0.97	4 (3%)
18	HAS	Q	801	10	69,72,72	1.23	7 (10%)	73,109,109	1.39	10 (13%)
16	MQ9	M	302	-	59,59,59	1.02	4 (6%)	72,75,75	1.40	11 (15%)
14	FES	A	501	1	0,4,4	-	-	-		
16	MQ9	b	605	-	59,59,59	0.93	1 (1%)	72,75,75	1.52	15 (20%)
18	HAS	Q	802	10	69,72,72	1.29	8 (11%)	73,109,109	1.37	6 (8%)
16	MQ9	Y	606	-	59,59,59	1.24	7 (11%)	72,75,75	1.47	11 (15%)
15	CDL	M	301	-	99,99,99	1.19	8 (8%)	105,111,111	0.97	4 (3%)
19	HEC	V	804	-	32,50,50	2.25	12 (37%)	24,82,82	1.93	3 (12%)
19	HEC	j	302	-	32,50,50	2.24	12 (37%)	24,82,82	1.92	3 (12%)
20	HEM	b	601	13	41,50,50	1.44	7 (17%)	45,82,82	2.49	17 (37%)
20	HEM	Y	602	13	41,50,50	1.47	7 (17%)	45,82,82	2.05	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	HEM	Y	601	13	41,50,50	1.38	6 (14%)	45,82,82	1.97	12 (26%)
19	HEC	i	301	-	32,50,50	2.25	12 (37%)	24,82,82	1.93	3 (12%)
15	CDL	Y	603	-	90,90,99	1.19	8 (8%)	96,102,111	1.03	5 (5%)
14	FES	B	501	1	0,4,4	-	-	-		
18	HAS	V	802	10	69,72,72	1.23	7 (10%)	73,109,109	1.33	7 (9%)
15	CDL	b	604	-	90,90,99	1.21	8 (8%)	96,102,111	0.97	4 (4%)
18	HAS	V	801	10	69,72,72	1.24	6 (8%)	73,109,109	1.45	13 (17%)
20	HEM	b	602	13	41,50,50	1.45	7 (17%)	45,82,82	2.48	15 (33%)
16	MQ9	Y	605	-	59,59,59	0.88	1 (1%)	72,75,75	1.50	12 (16%)
15	CDL	V	805	-	86,86,99	1.23	9 (10%)	92,98,111	1.01	4 (4%)
15	CDL	Y	604	-	91,91,99	1.18	7 (7%)	97,103,111	1.04	5 (5%)
15	CDL	b	603	-	91,91,99	1.18	6 (6%)	97,103,111	1.08	4 (4%)

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
15	CDL	Q	804	-	-	47/97/97/110	-
19	HEC	j	301	6	-	3/10/54/54	-
15	CDL	K	301	-	-	56/110/110/110	-
18	HAS	Q	801	10	1/1/8/18	7/40/82/82	-
16	MQ9	M	302	-	-	8/53/73/73	0/2/2/2
16	MQ9	b	605	-	-	15/53/73/73	0/2/2/2
14	FES	A	501	1	-	-	0/1/1/1
18	HAS	Q	802	10	1/1/8/18	11/40/82/82	-
16	MQ9	Y	606	-	-	9/53/73/73	0/2/2/2
15	CDL	M	301	-	-	55/110/110/110	-
19	HEC	V	804	-	-	3/10/54/54	-
19	HEC	j	302	-	-	3/10/54/54	-
20	HEM	b	601	13	-	10/12/54/54	-
20	HEM	Y	602	13	-	4/12/54/54	-
20	HEM	Y	601	13	-	5/12/54/54	-
19	HEC	i	301	-	-	3/10/54/54	-
15	CDL	Y	603	-	-	56/101/101/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FES	B	501	1	-	-	0/1/1/1
18	HAS	V	802	10	1/1/8/18	11/40/82/82	-
15	CDL	b	604	-	-	55/101/101/110	-
18	HAS	V	801	10	1/1/8/18	11/40/82/82	-
20	HEM	b	602	13	-	5/12/54/54	-
16	MQ9	Y	605	-	-	16/53/73/73	0/2/2/2
15	CDL	V	805	-	-	46/97/97/110	-
15	CDL	Y	604	-	-	61/102/102/110	-
15	CDL	b	603	-	-	44/102/102/110	-

The worst 5 of 178 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	j	301	HEC	C2B-C3B	6.07	1.47	1.40
19	j	301	HEC	C3C-C2C	6.05	1.47	1.40
19	V	804	HEC	C2B-C3B	6.04	1.47	1.40
19	i	301	HEC	C2B-C3B	6.03	1.47	1.40
19	j	302	HEC	C2B-C3B	6.00	1.47	1.40

The worst 5 of 187 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	b	602	HEM	CBA-CAA-C2A	8.62	127.33	112.62
20	b	601	HEM	CBA-CAA-C2A	7.56	125.52	112.62
19	V	804	HEC	C1D-C2D-C3D	-6.10	102.75	107.00
19	i	301	HEC	C1D-C2D-C3D	-6.07	102.77	107.00
19	j	302	HEC	C1D-C2D-C3D	-6.06	102.78	107.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	V	801	HAS	NA
18	V	802	HAS	NA
18	Q	801	HAS	NA
18	Q	802	HAS	NA

5 of 544 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	M	301	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
15	M	301	CDL	CA2-OA2-PA1-OA4
15	M	301	CDL	CA3-OA5-PA1-OA3
15	V	805	CDL	CA2-OA2-PA1-OA3
15	V	805	CDL	CB2-OB2-PB2-OB3

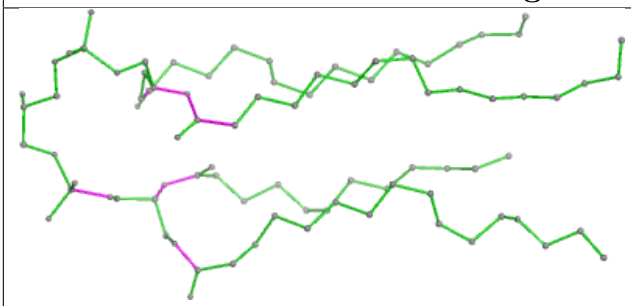
There are no ring outliers.

17 monomers are involved in 79 short contacts:

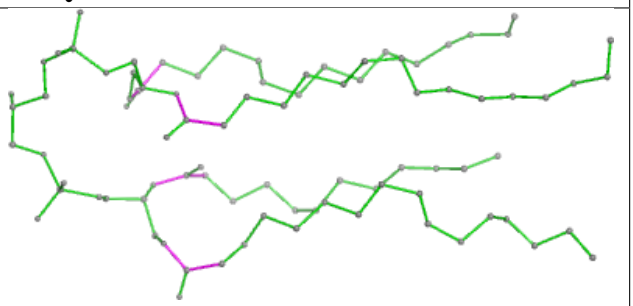
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Q	804	CDL	3	0
15	K	301	CDL	6	0
18	Q	801	HAS	3	0
16	M	302	MQ9	4	0
18	Q	802	HAS	3	0
16	Y	606	MQ9	4	0
15	M	301	CDL	4	0
19	V	804	HEC	22	0
20	Y	602	HEM	5	0
20	Y	601	HEM	1	0
15	Y	603	CDL	4	0
14	B	501	FES	2	0
18	V	802	HAS	2	0
18	V	801	HAS	5	0
16	Y	605	MQ9	6	0
15	V	805	CDL	2	0
15	Y	604	CDL	8	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.

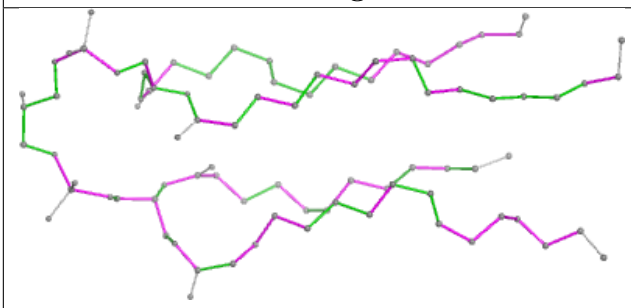
Ligand CDL Q 804



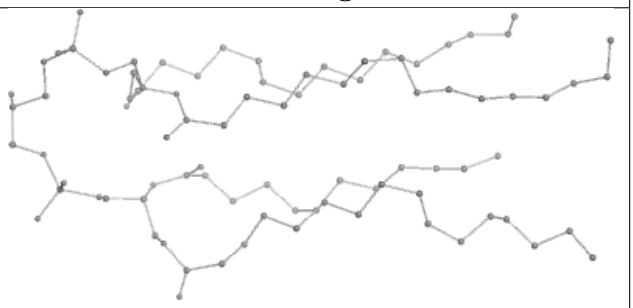
Bond lengths



Bond angles

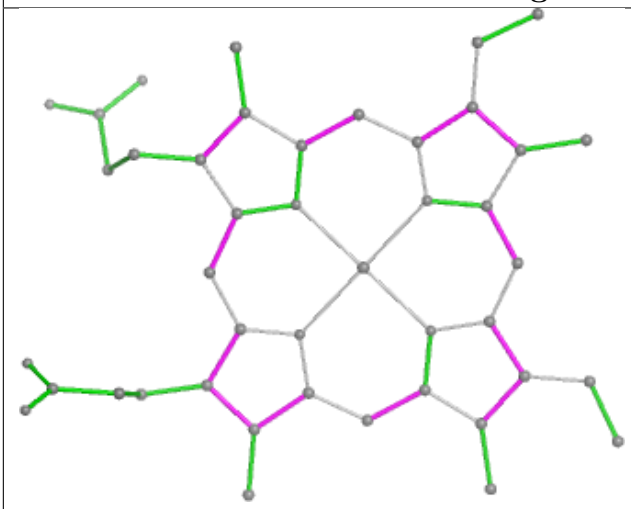


Torsions



Rings

Ligand HEC j 301



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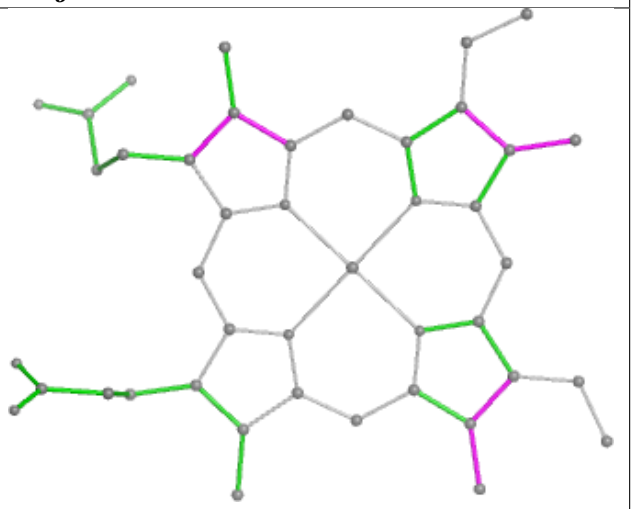
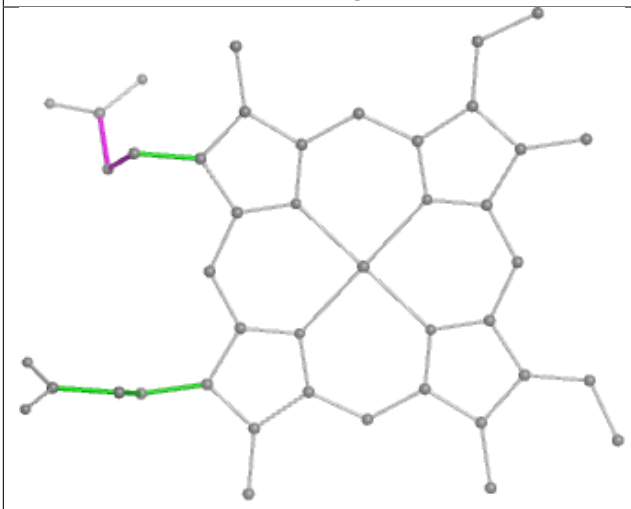


Bond angles



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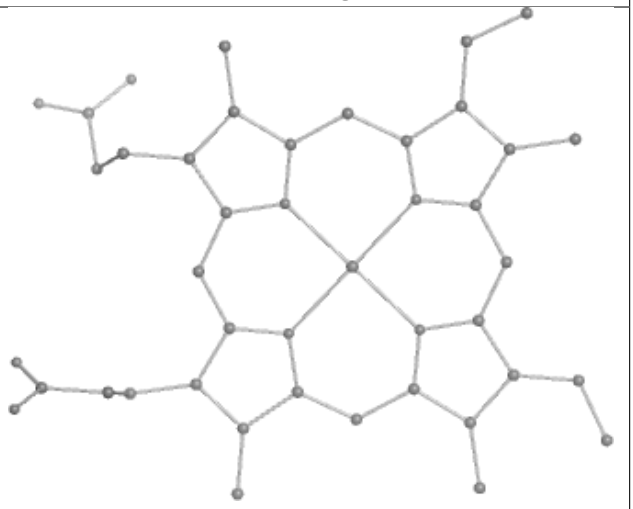
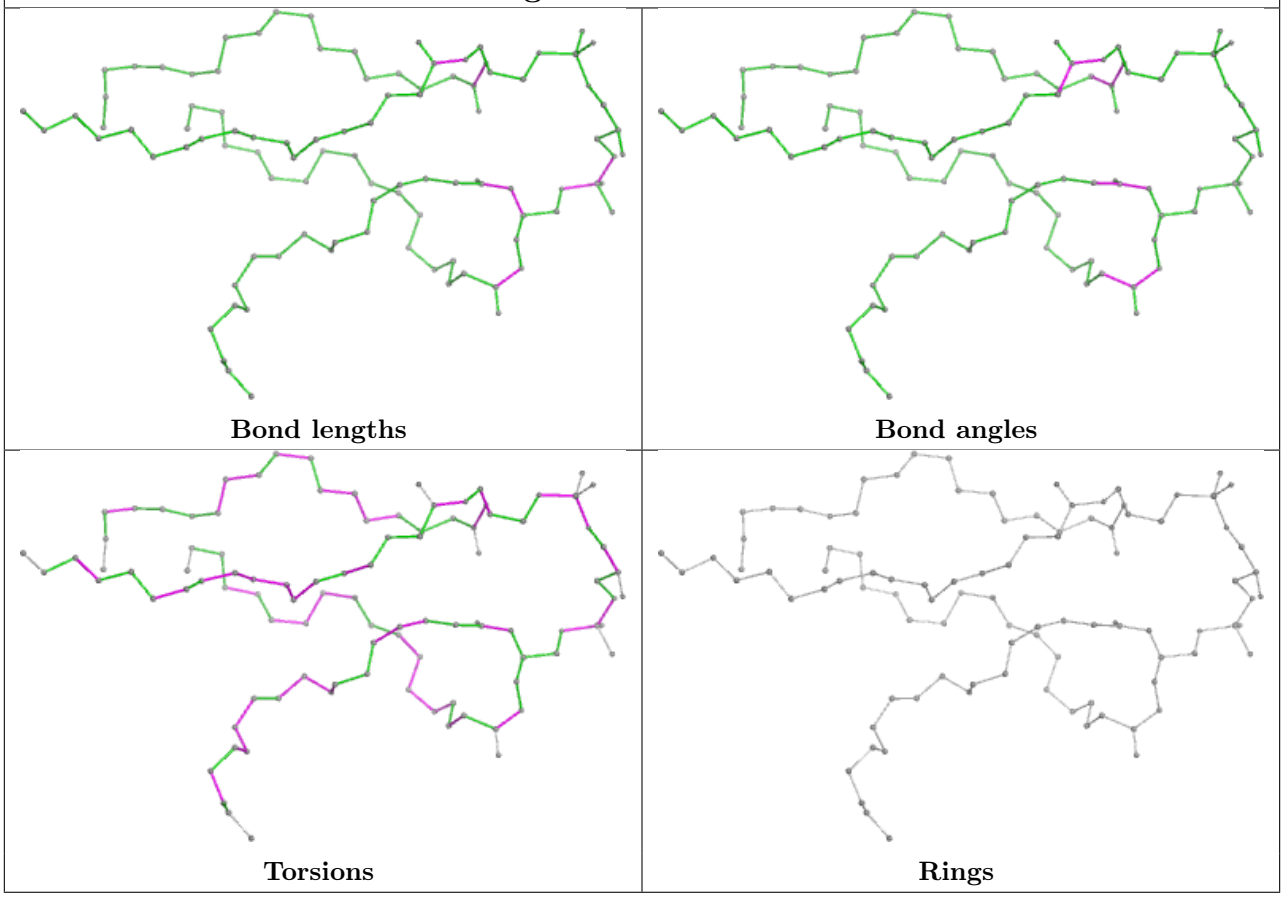
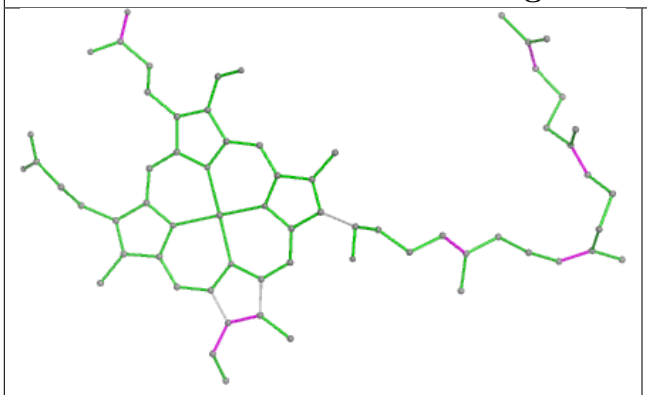


Rings

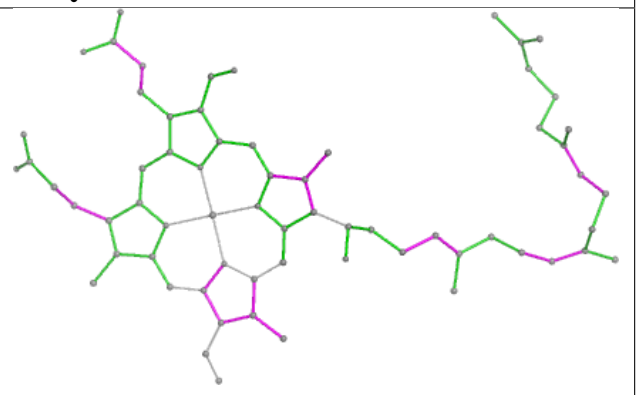
Ligand CDL K 301



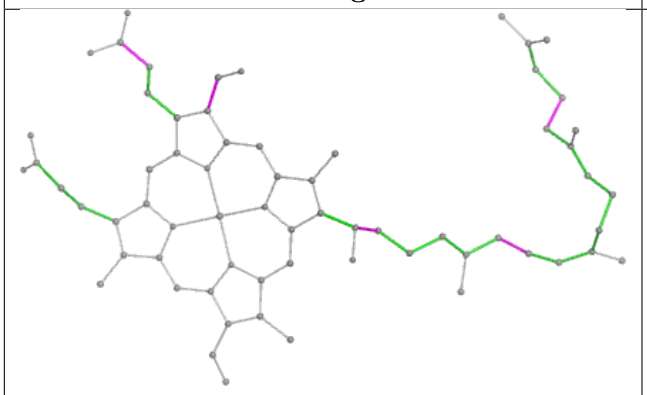
Ligand HAS Q 801



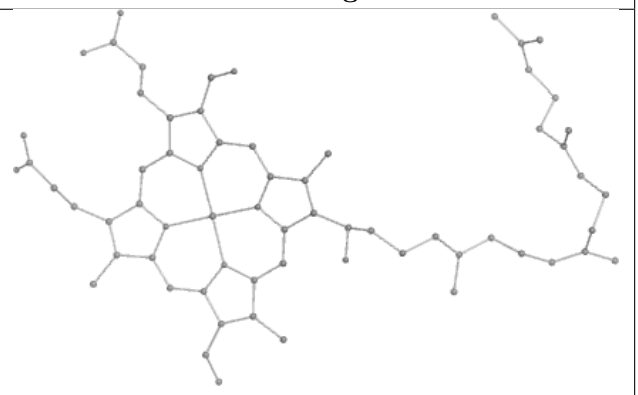
Bond lengths



Bond angles

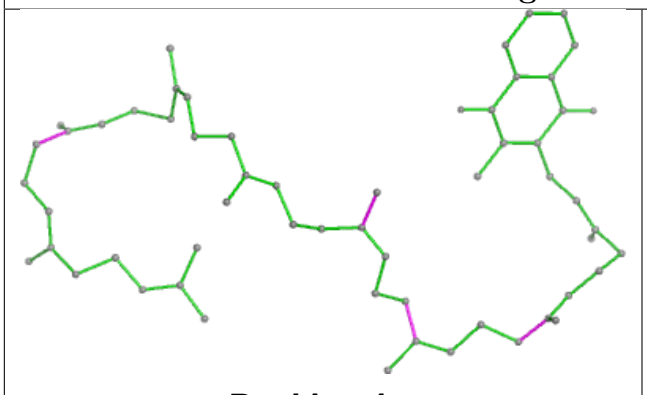


Torsions

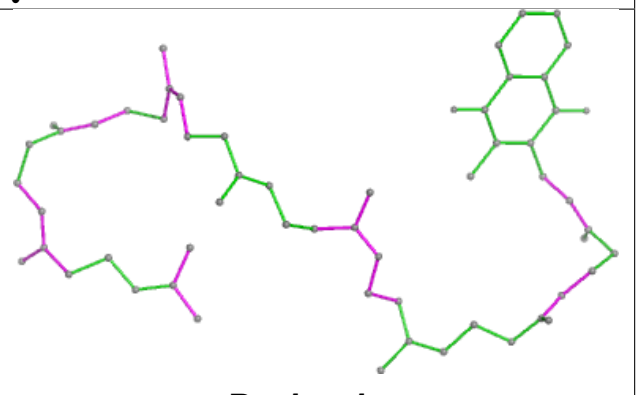


Rings

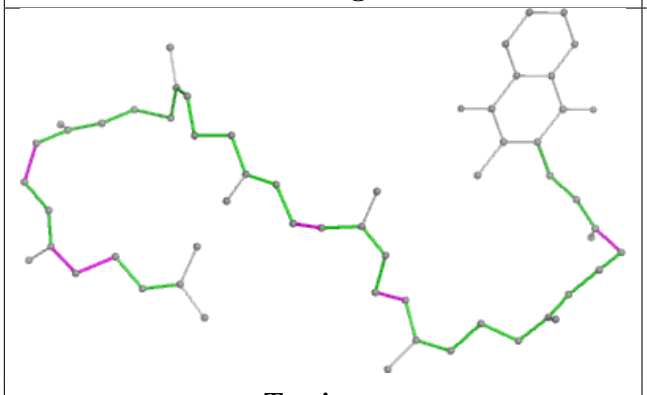
Ligand MQ9 M 302



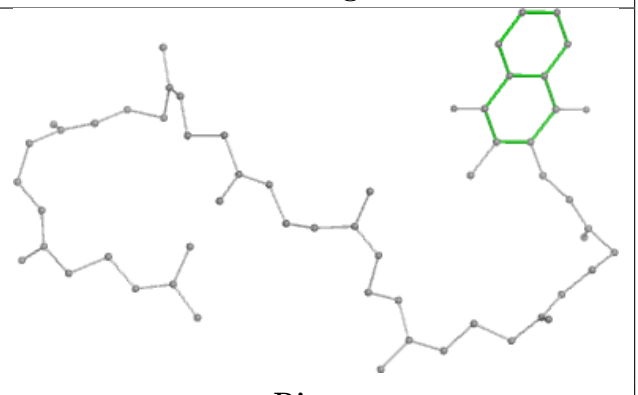
Bond lengths



Bond angles

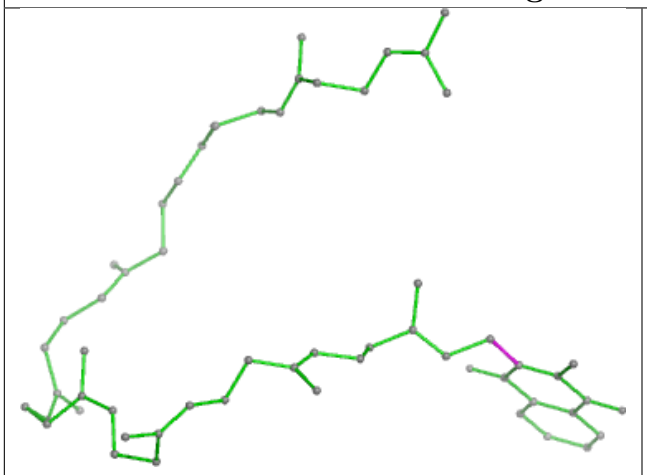


Torsions

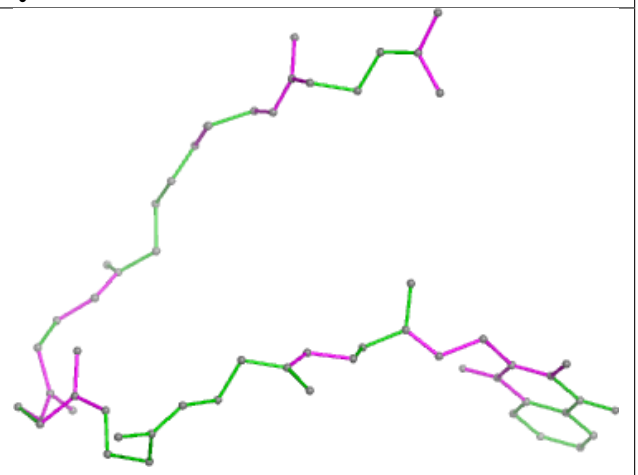


Rings

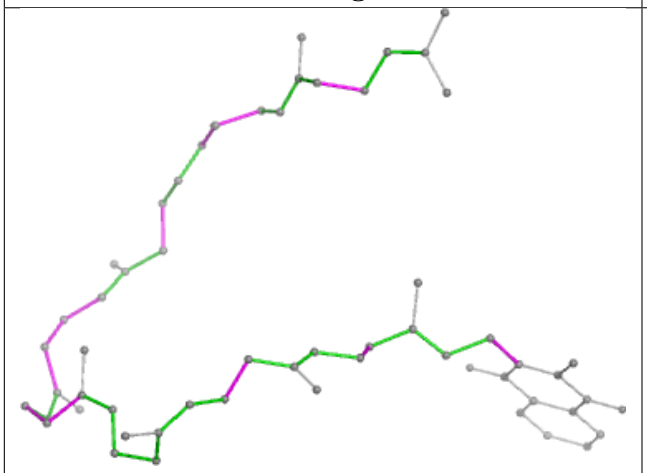
Ligand MQ9 b 605



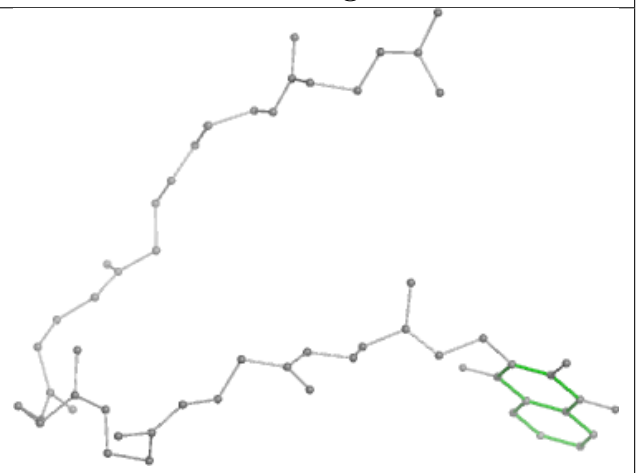
Bond lengths



Bond angles

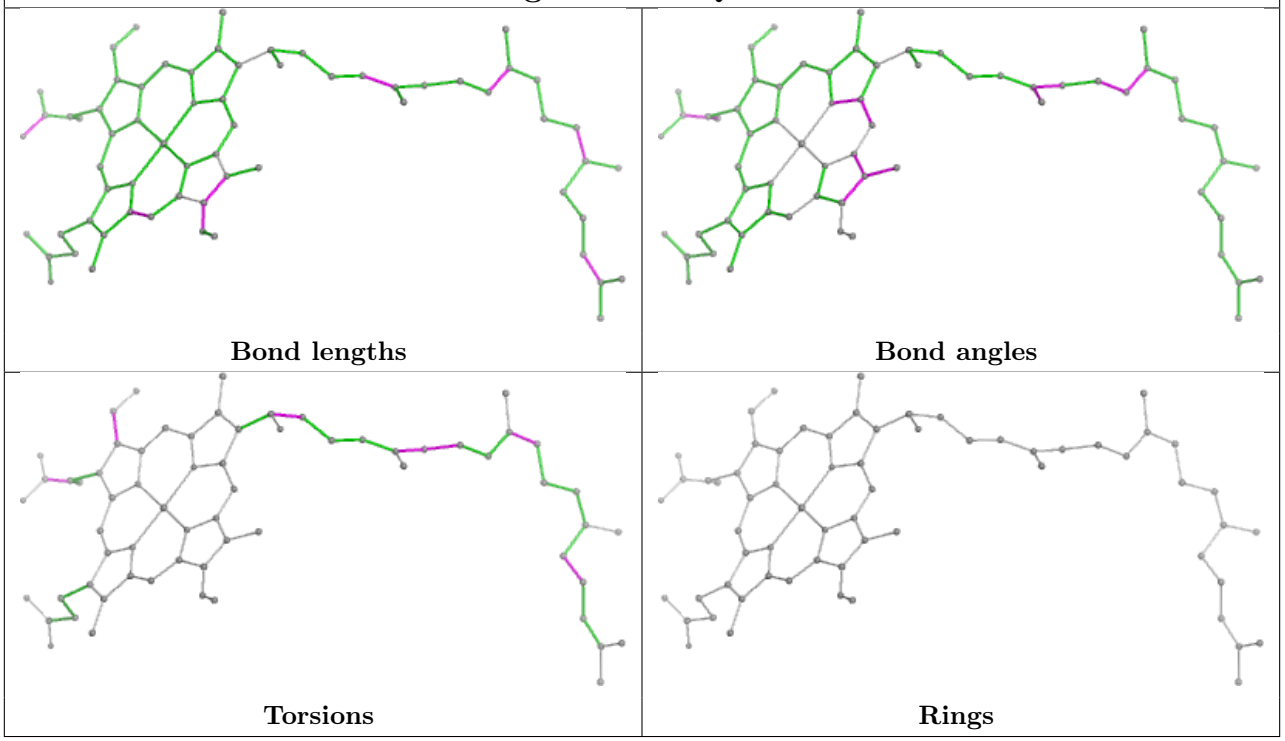


Torsions

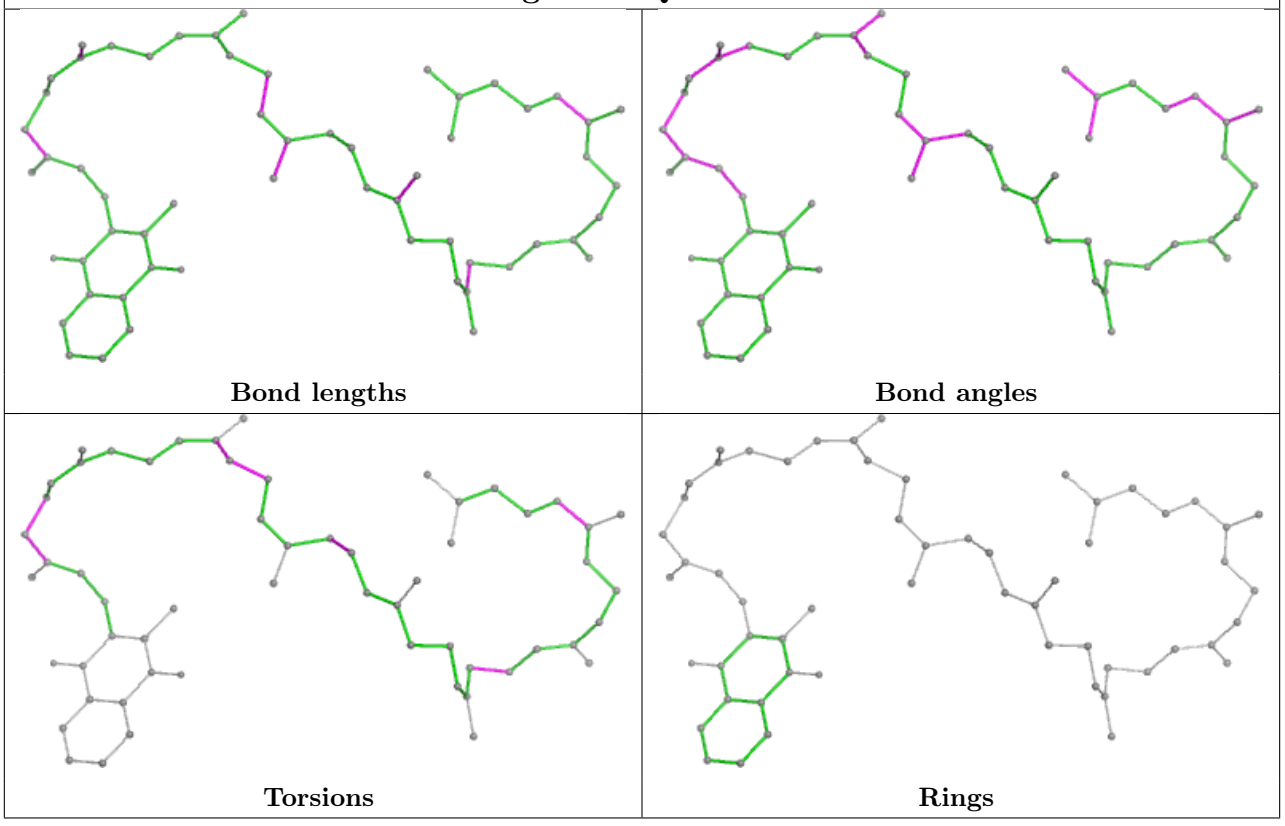


Rings

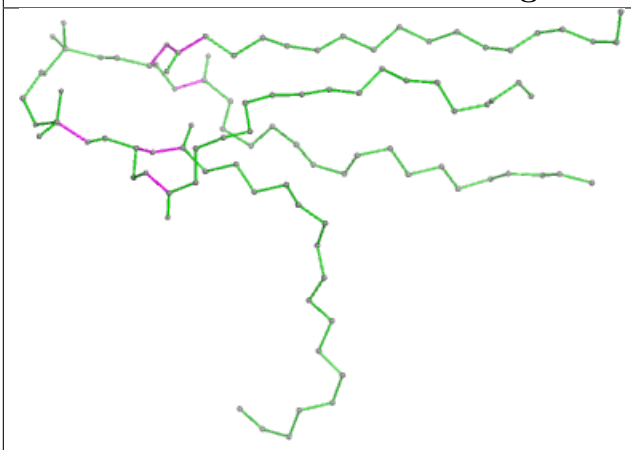
Ligand HAS Q 802



Ligand MQ9 Y 606



Ligand CDL M 301



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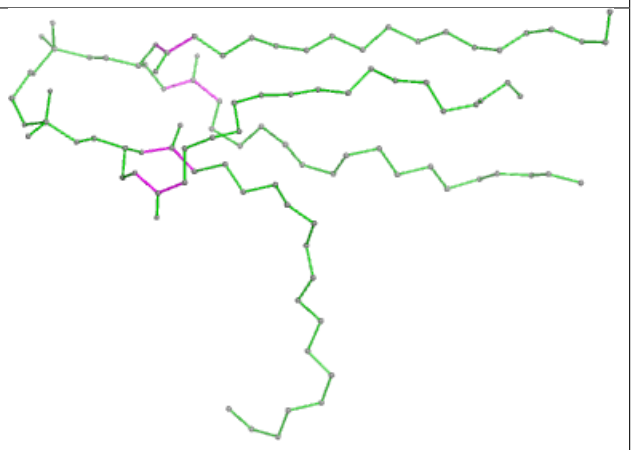
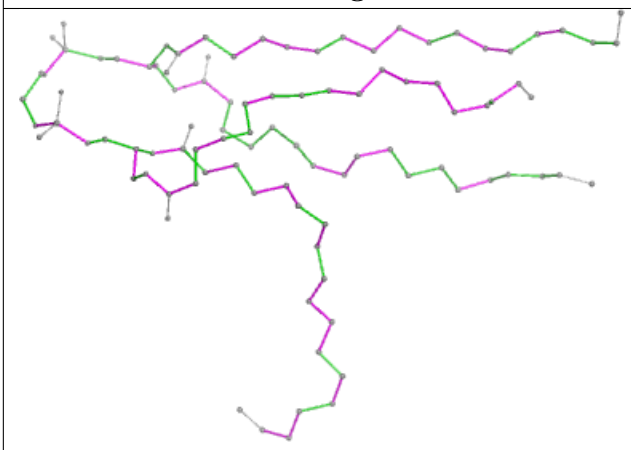


Bond angles



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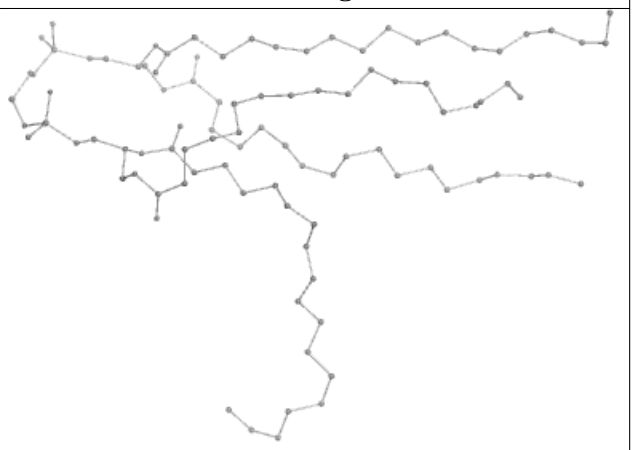
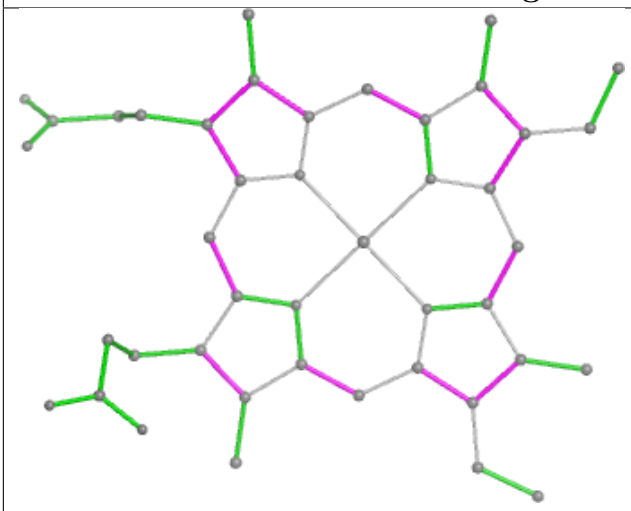


Rings

Ligand HEC V 804



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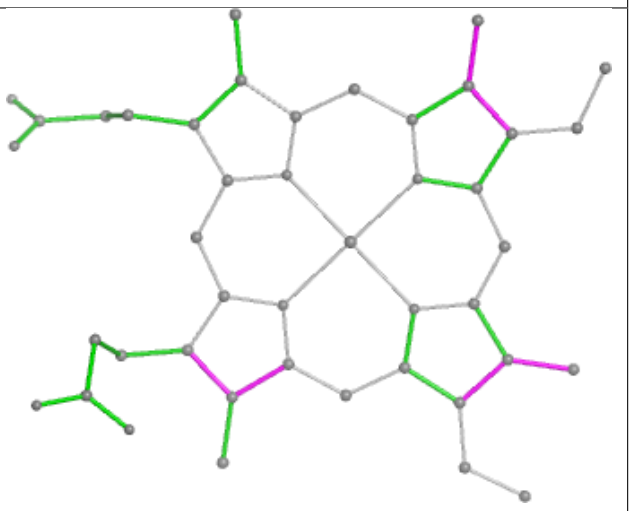
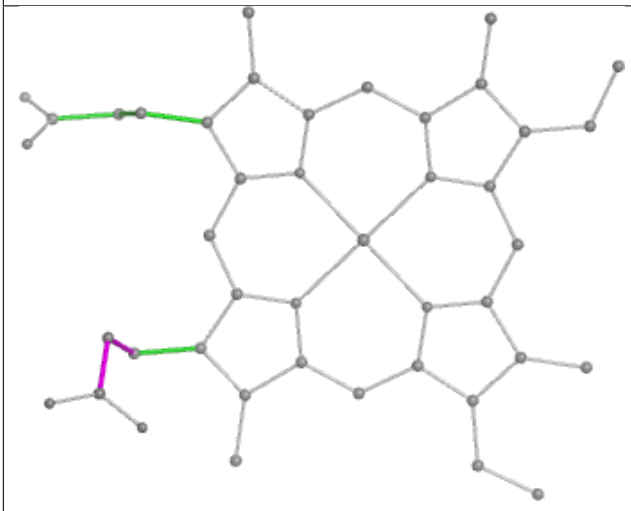


Bond angles



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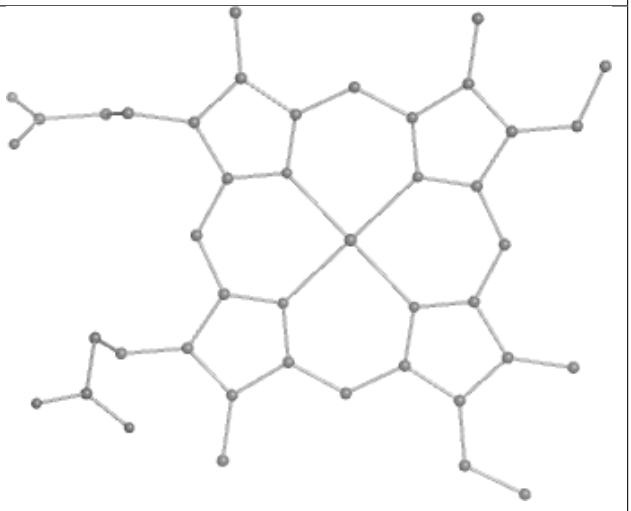
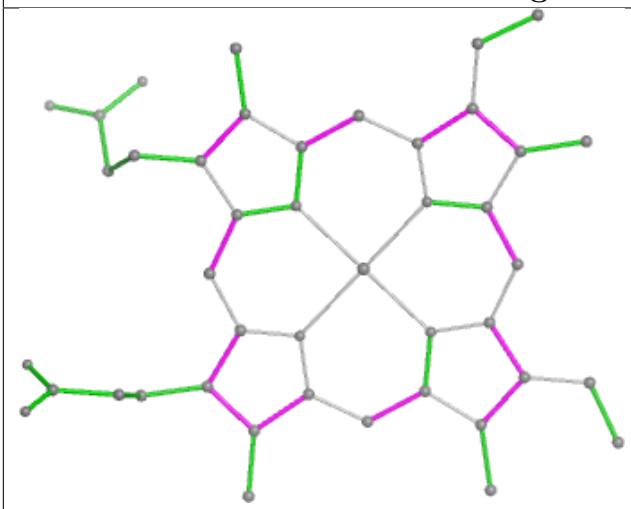


Rings

Ligand HEC j 302



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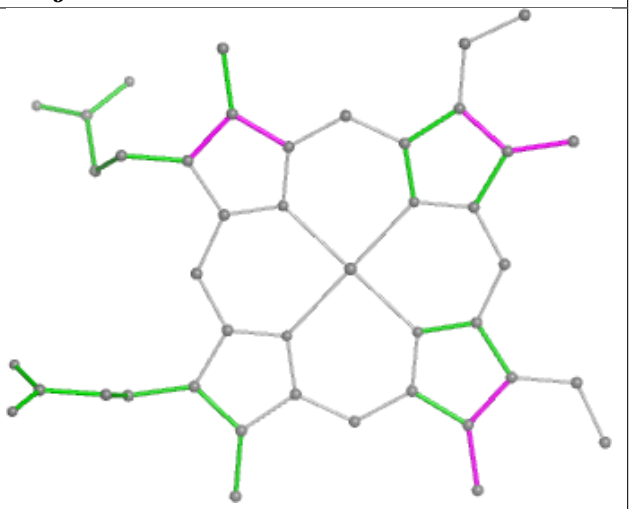
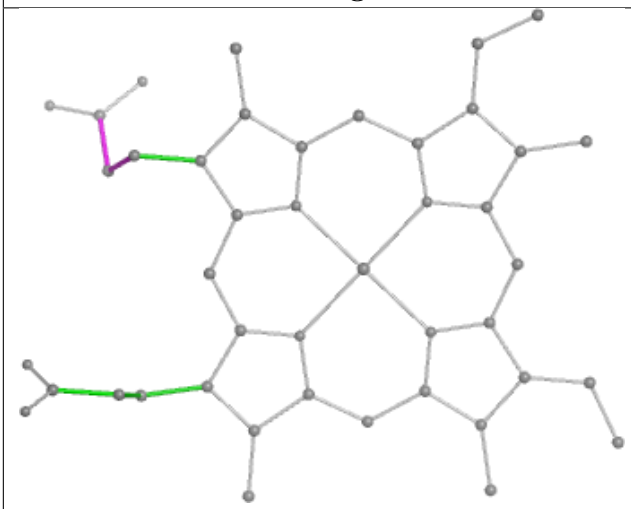
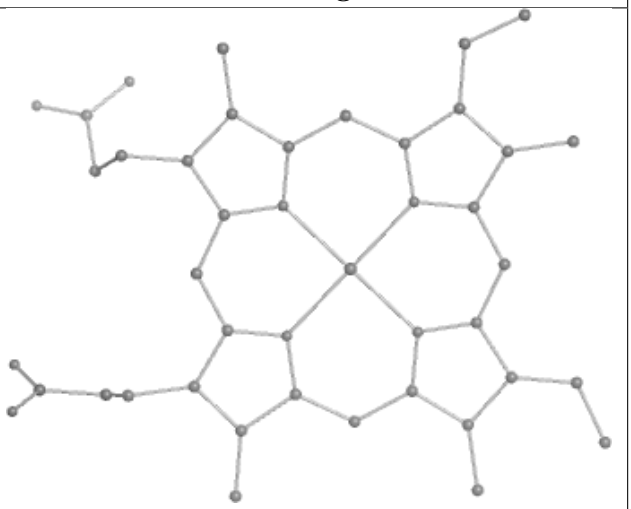


Bond angles

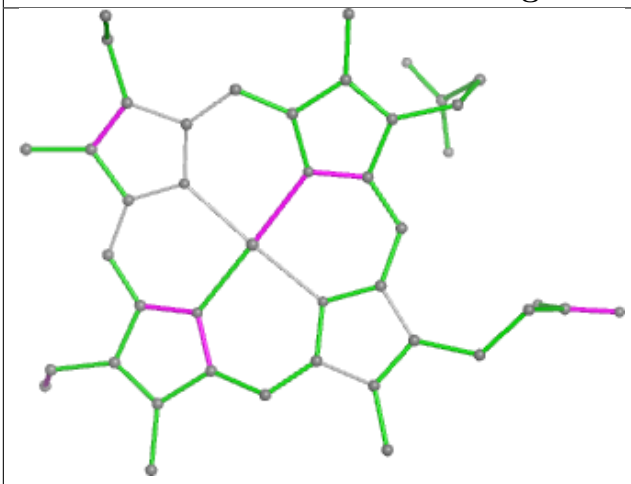


Torsions

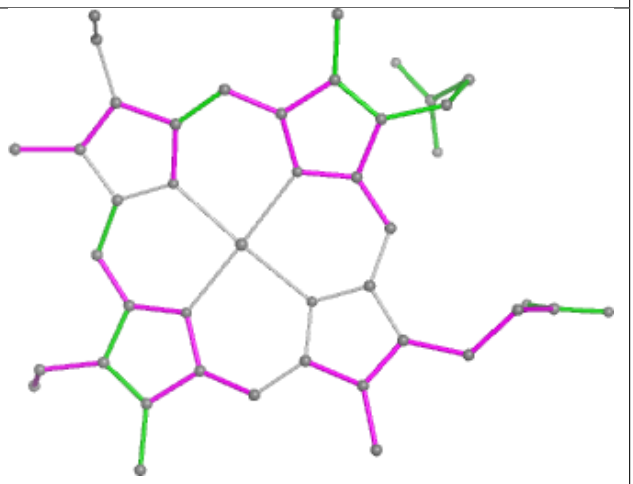


Rings

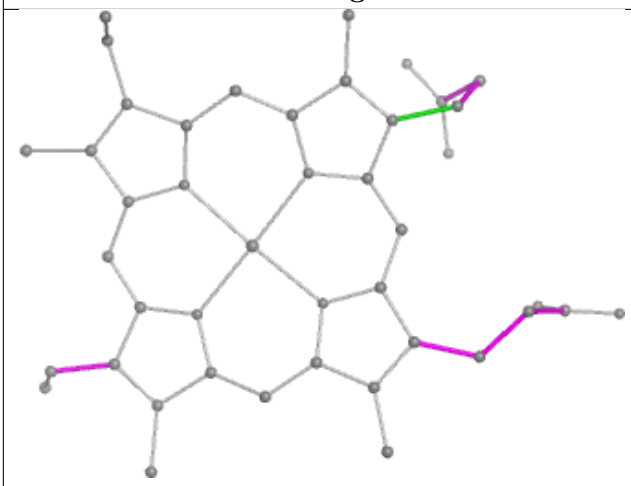
Ligand HEM b 601



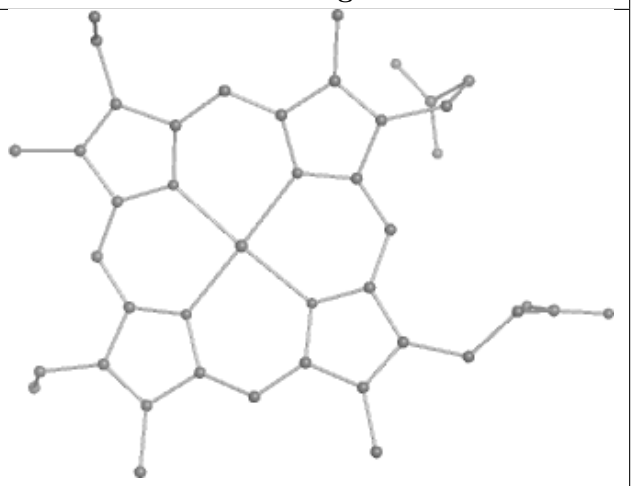
Bond lengths



Bond angles

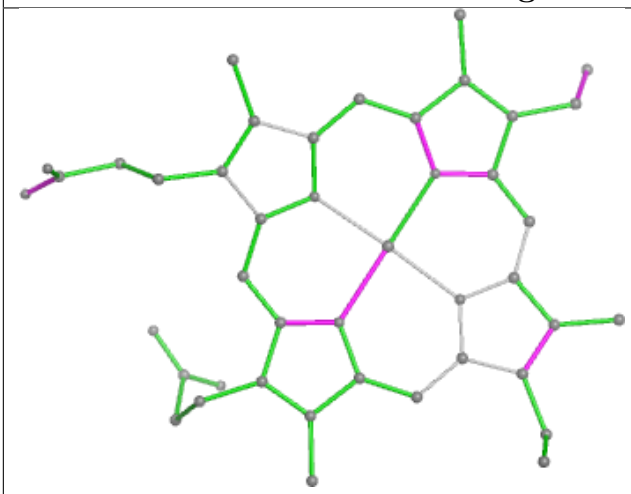


Torsions



Rings

Ligand HEM Y 602



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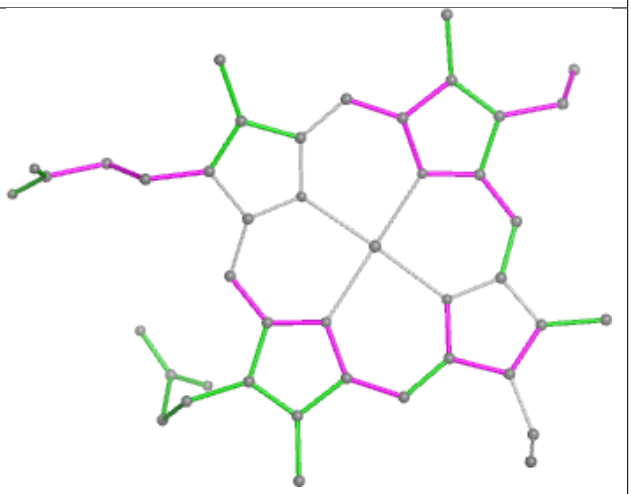
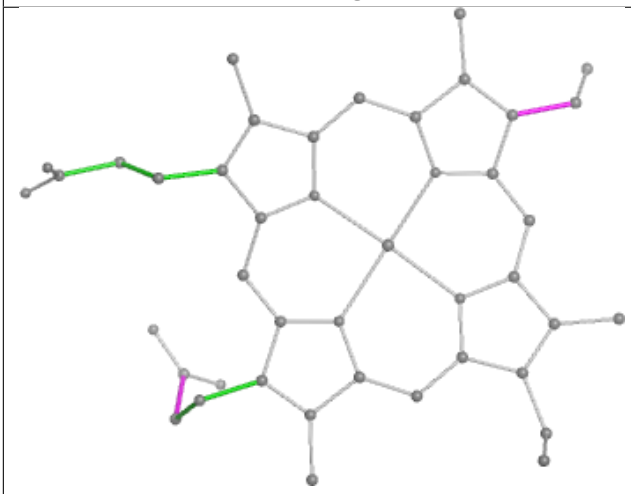


Bond angles



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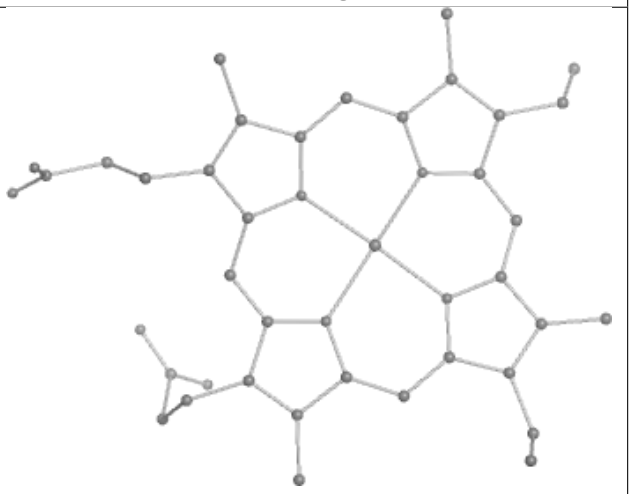
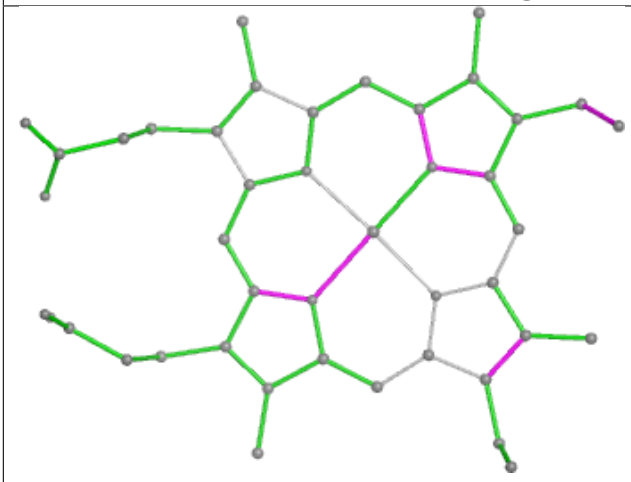
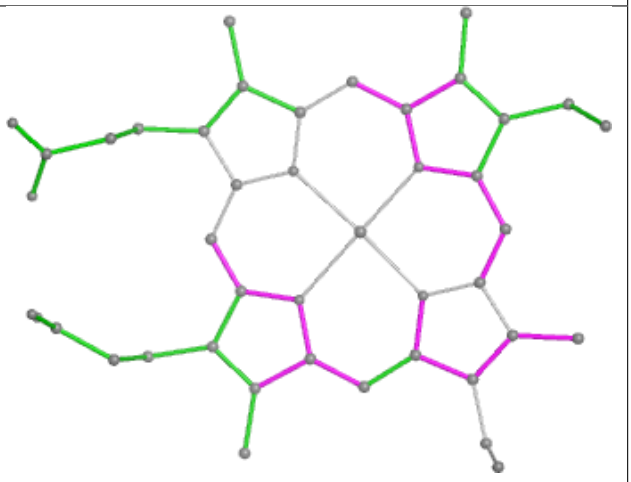


Rings

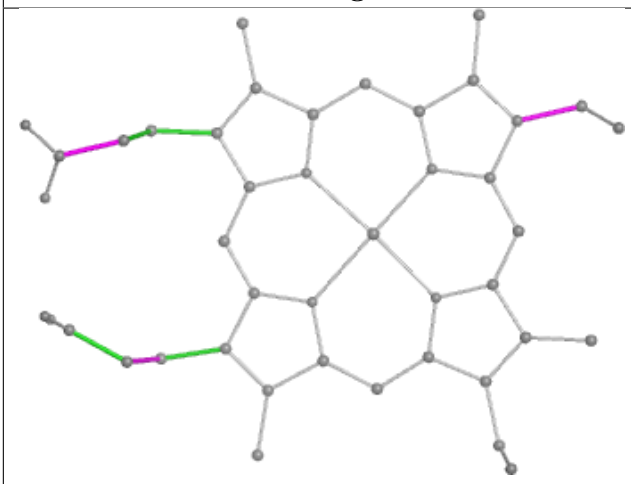
Ligand HEM Y 601



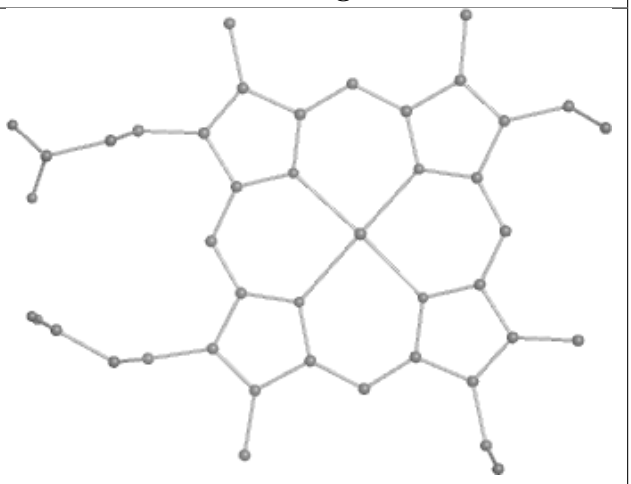
Bond lengths



Bond angles

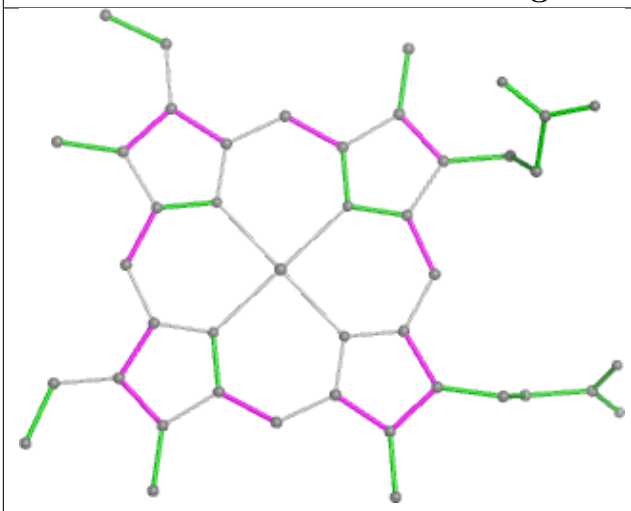


Torsions

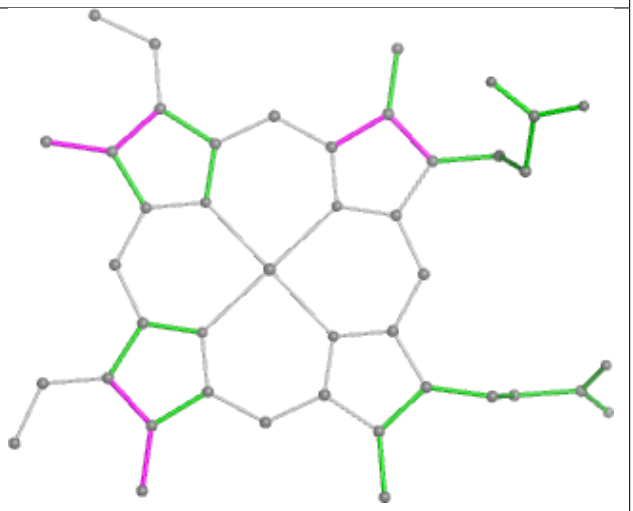


Rings

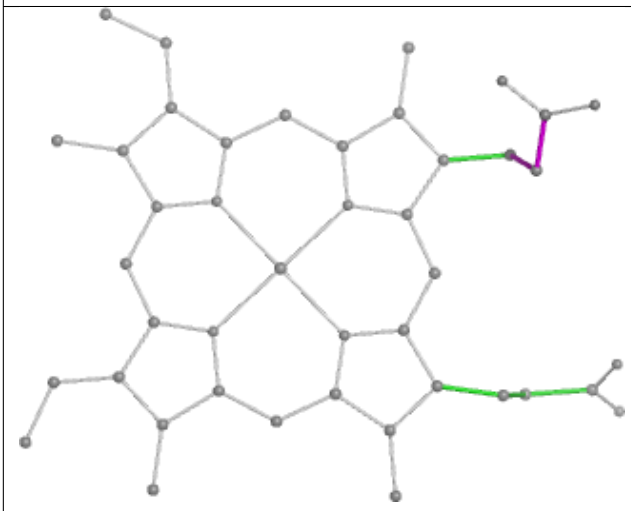
Ligand HEC i 301



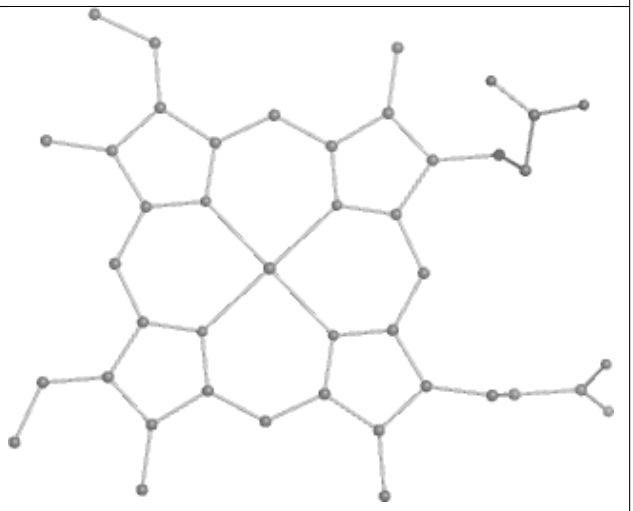
Bond lengths



Bond angles

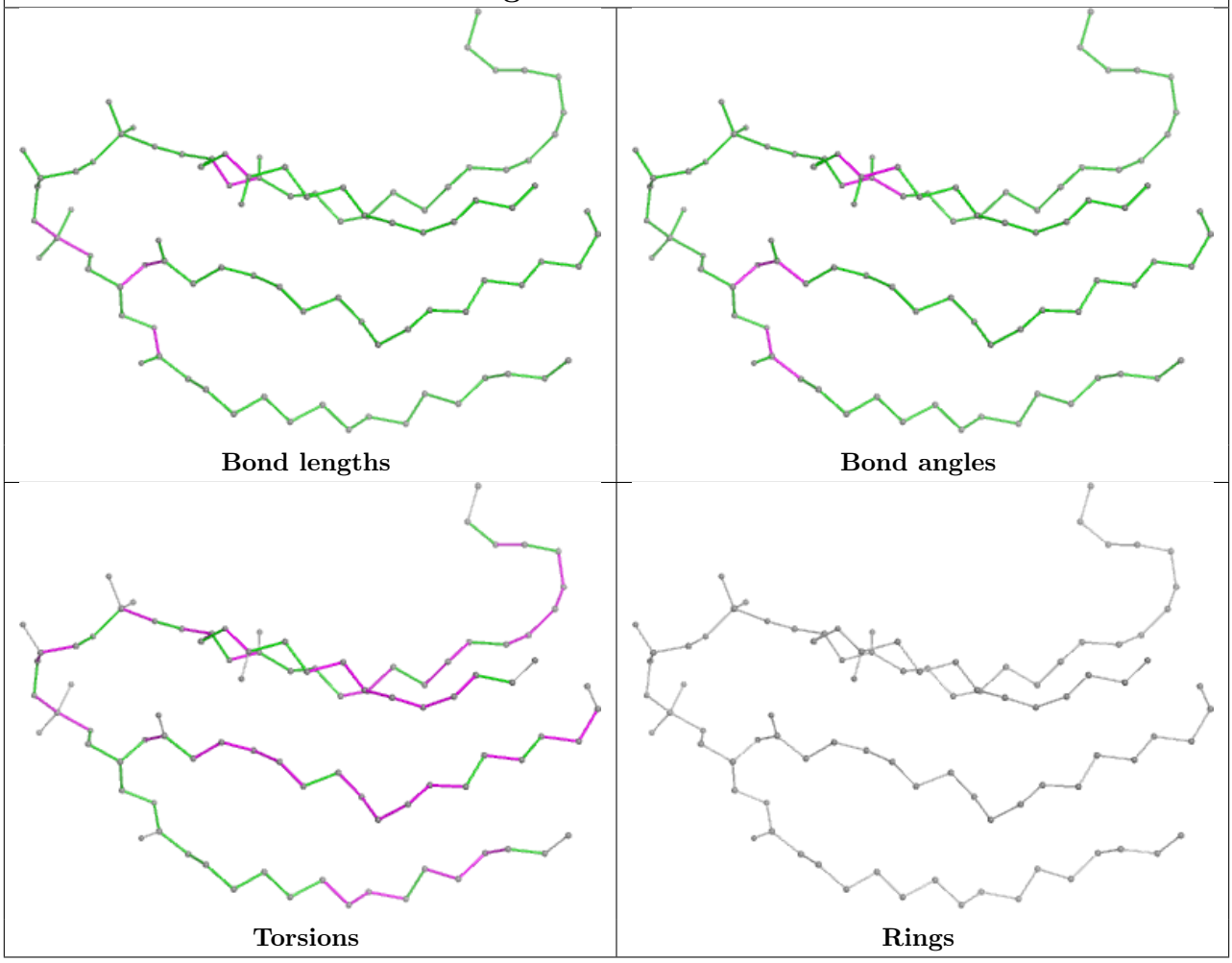


Torsions

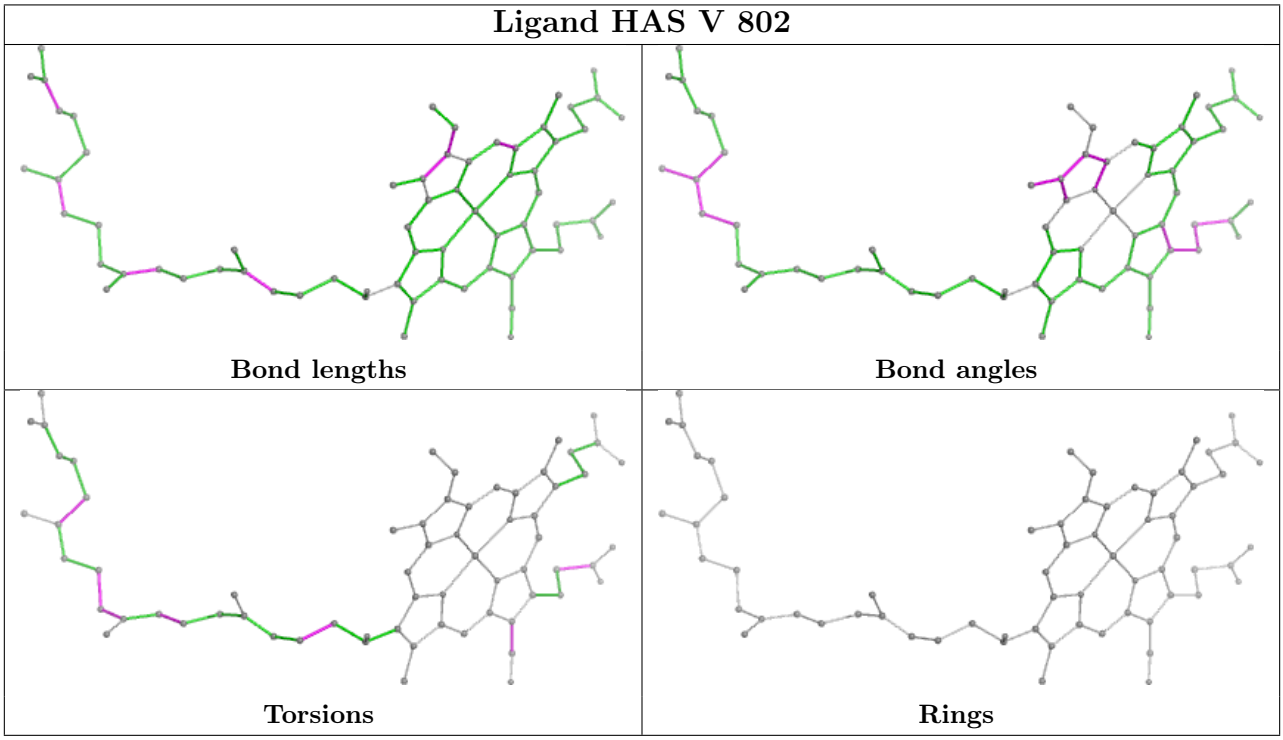


Rings

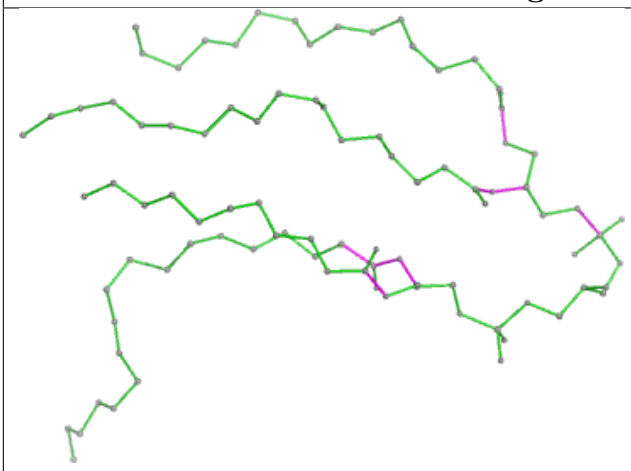
Ligand CDL Y 603



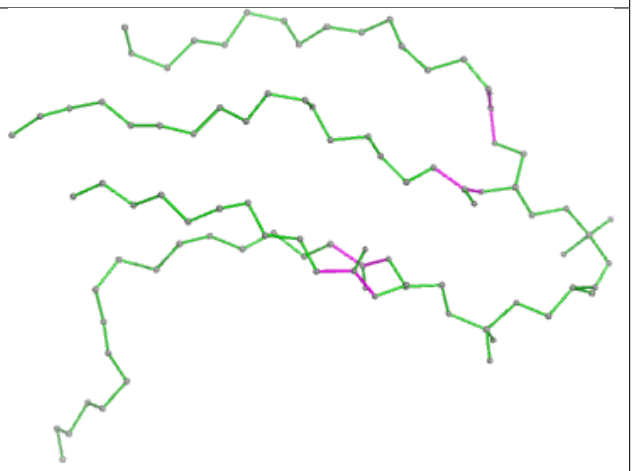
Ligand HAS V 802



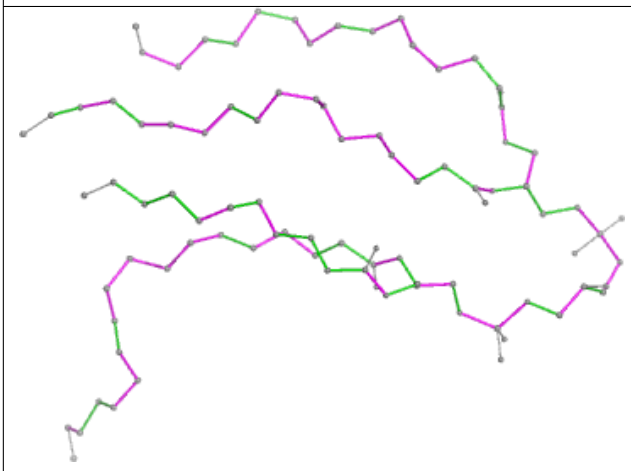
Ligand CDL b 604



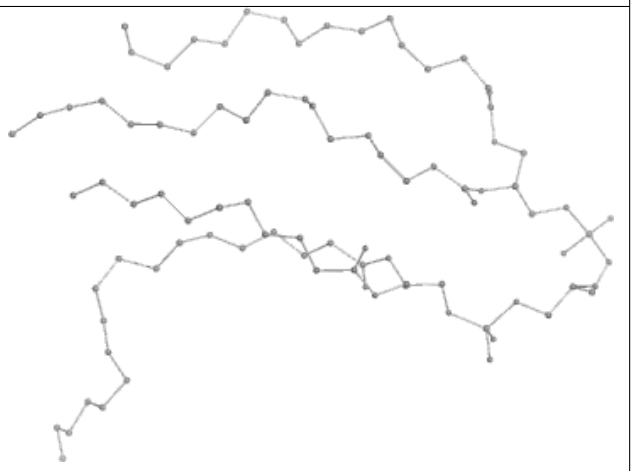
Bond lengths



Bond angles

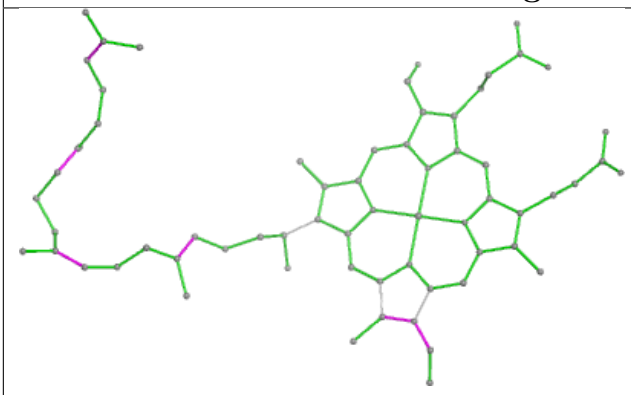


Torsions

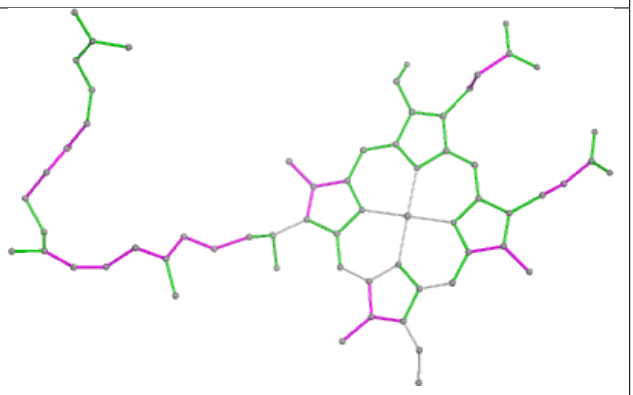


Rings

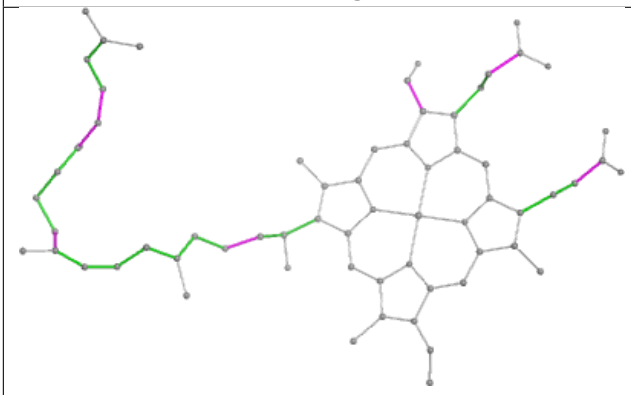
Ligand HAS V 801



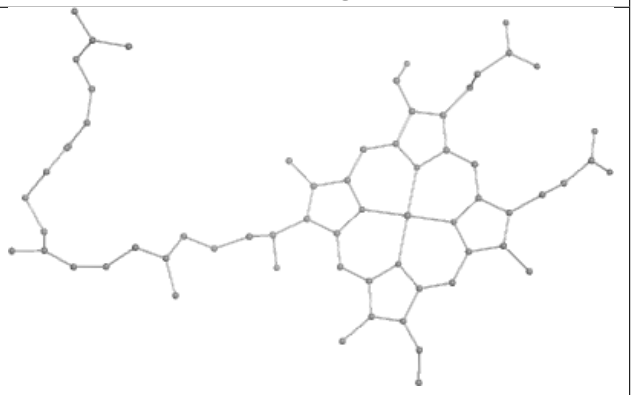
Bond lengths



Bond angles

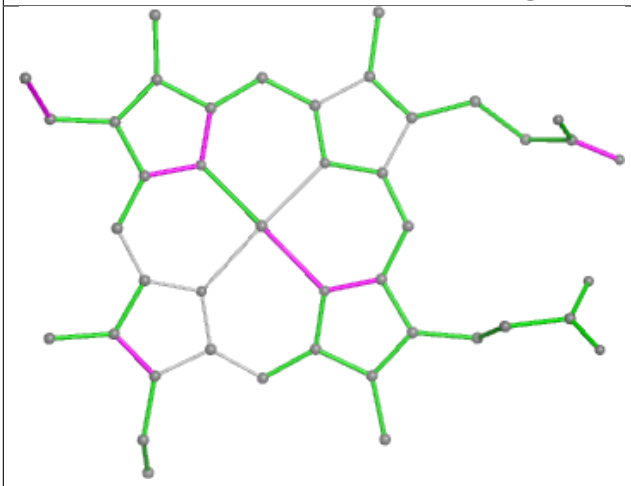


Torsions

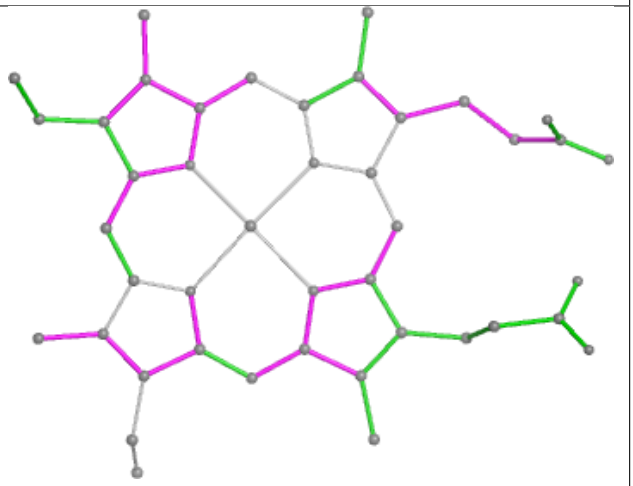


Rings

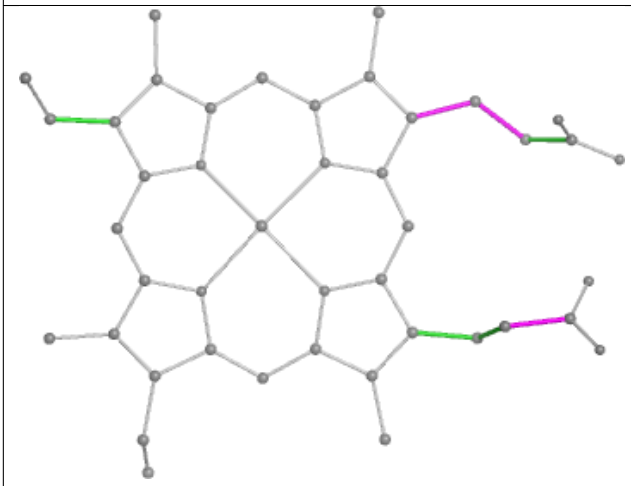
Ligand HEM b 602



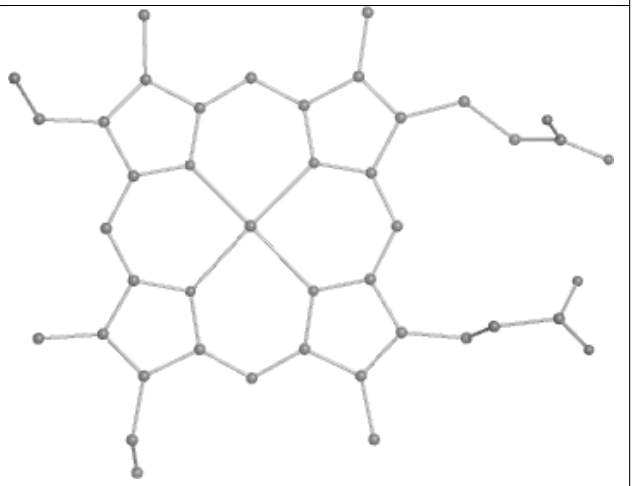
Bond lengths



Bond angles

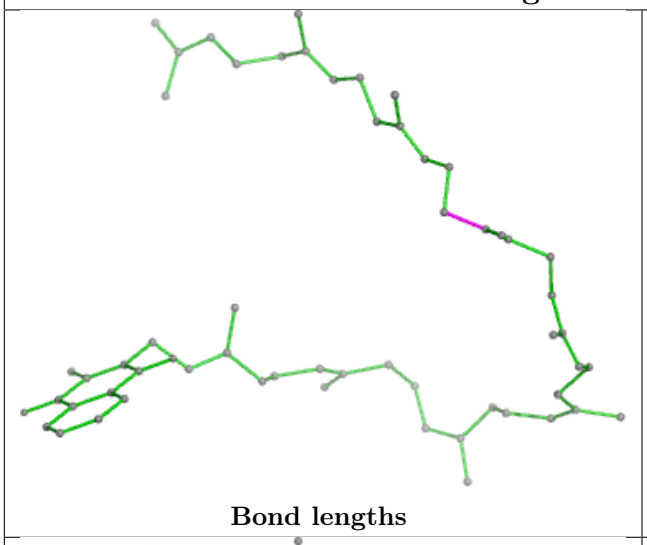


Torsions

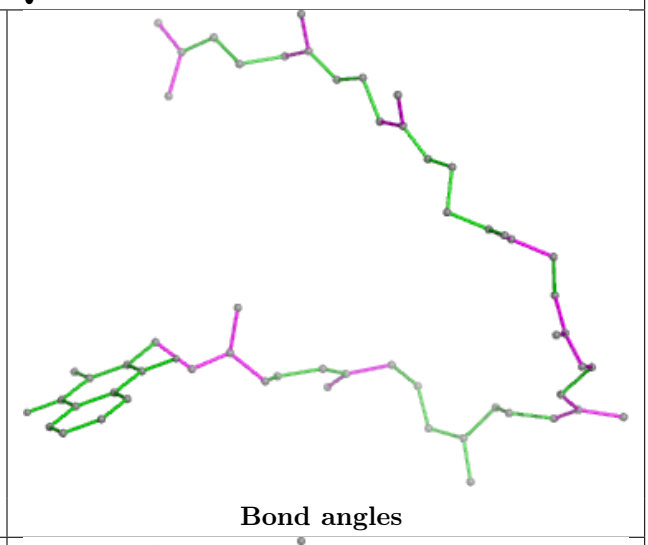


Rings

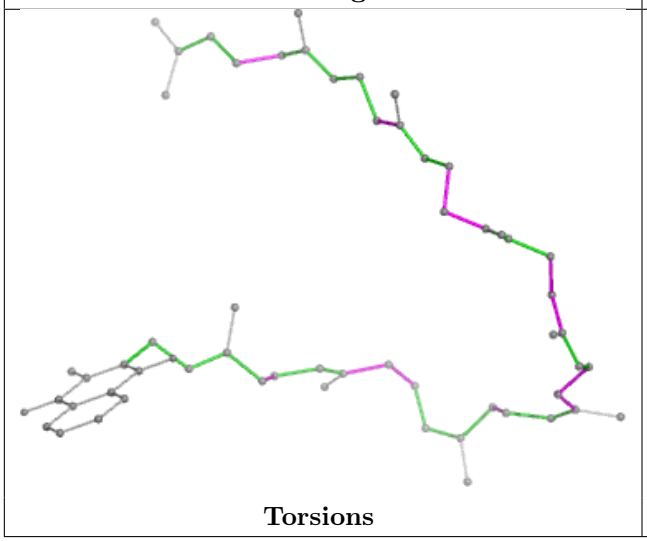
Ligand MQ9 Y 605



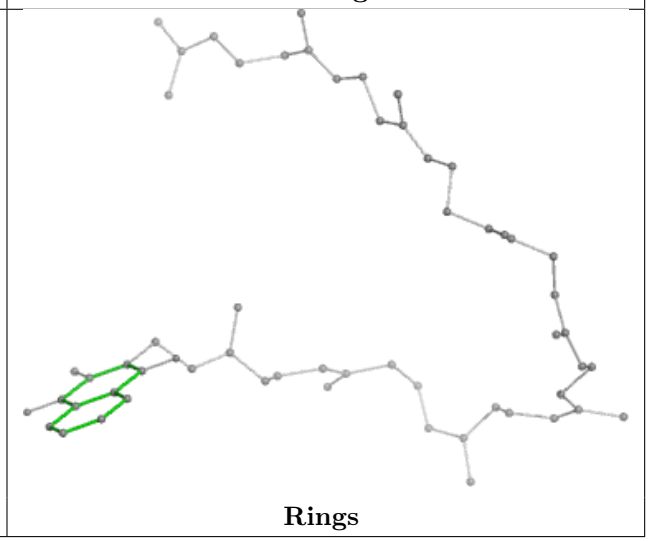
Bond lengths



Bond angles

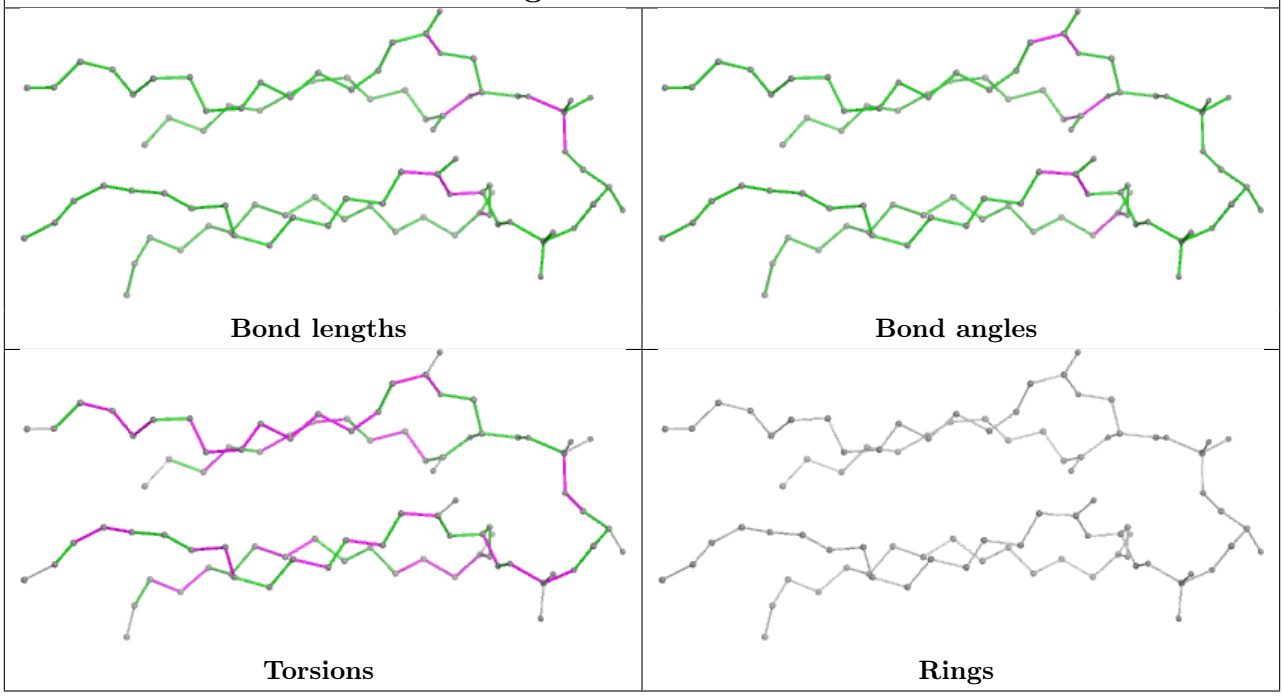


Torsions

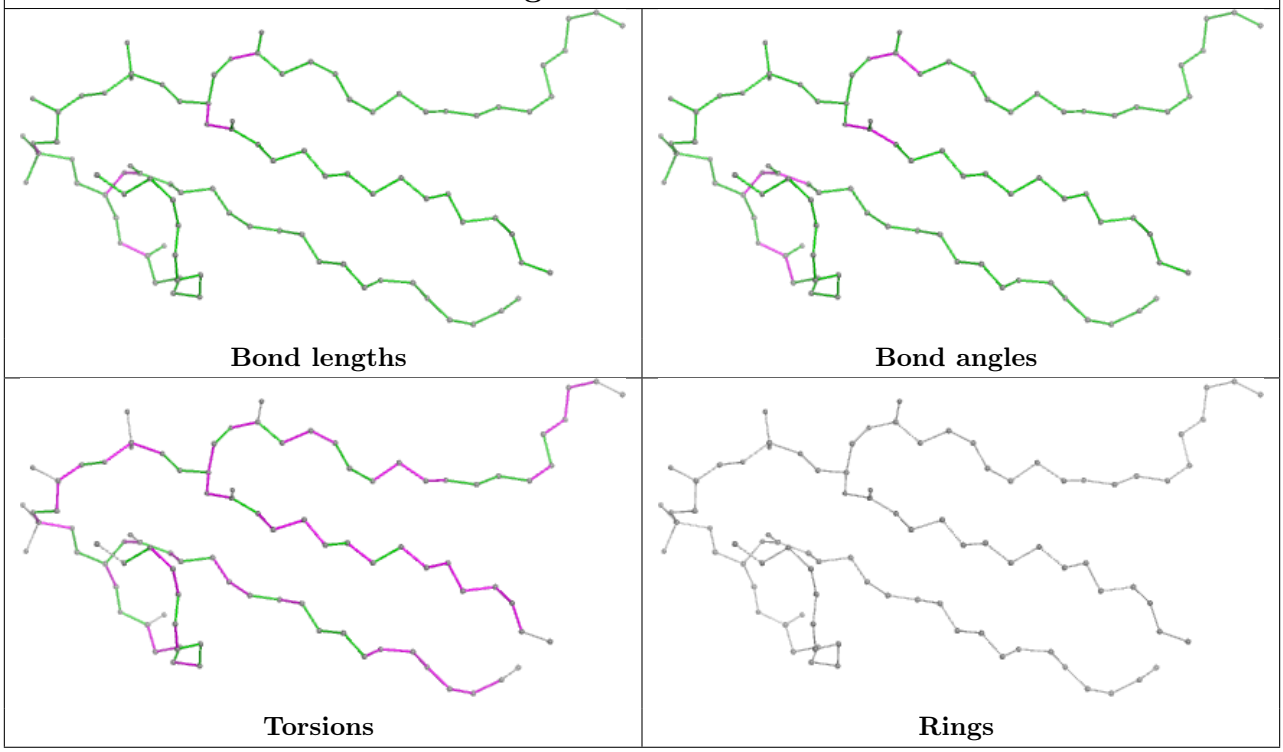


Rings

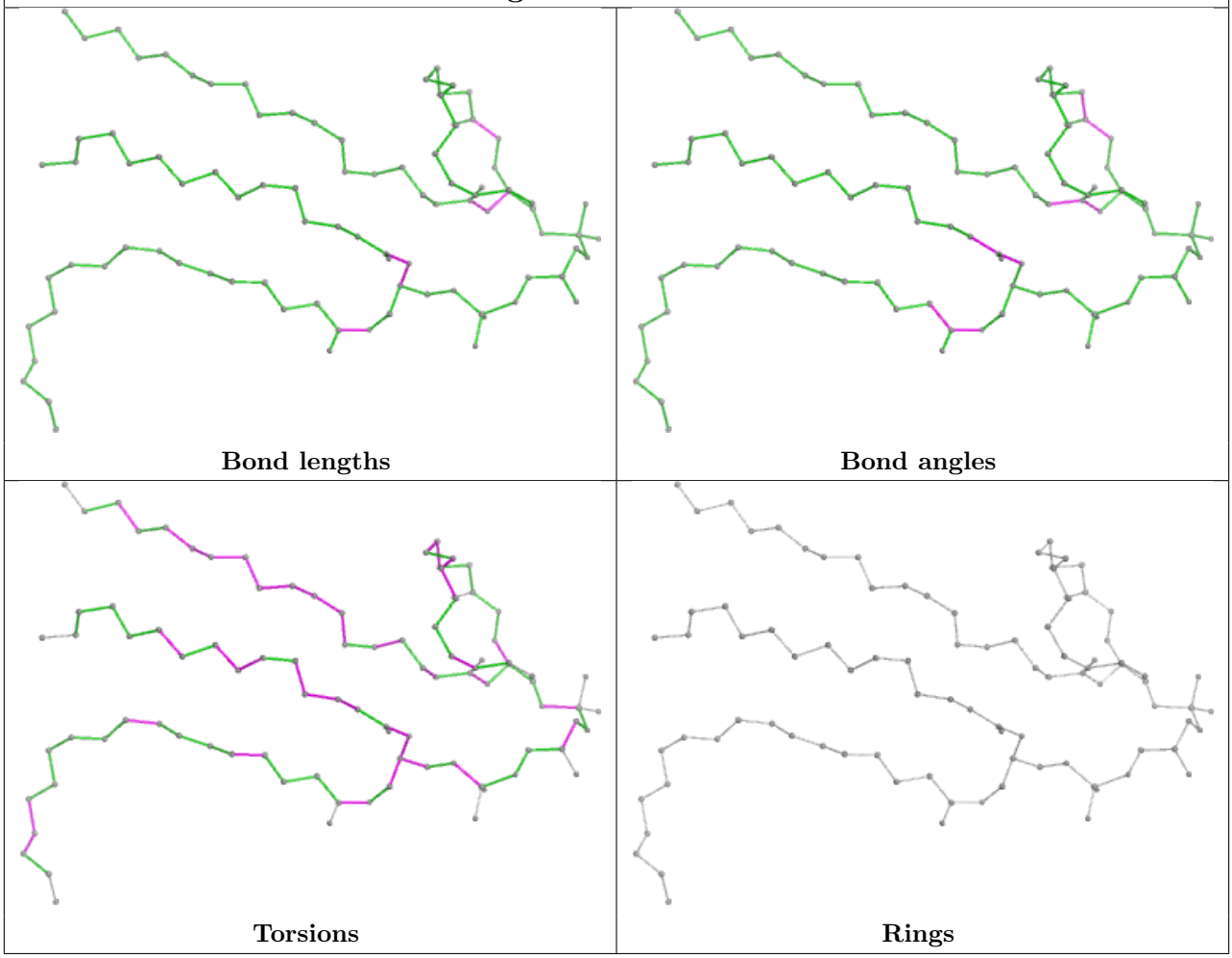
Ligand CDL V 805



Ligand CDL Y 604



Ligand CDL b 603



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 Map visualisation

This section contains visualisations of the EMDB entry EMD-0289. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.