wwPDB X-ray Structure Validation Summary Report (i)

Sep 22, 2026 – 03:59 PM EDT

PDB ID	:	1L0L / pdb_00001l0l
Title	:	structure of bovine mitochondrial cytochrome bc1 complex with a bound fungicide famoxadone
Authors	:	Gao, X.; Wen, X.; Yu, C.A.; Esser, L.; Tsao, S.; Quinn, B.; Zhang, L.; Yu, L.; Xia, D.
Deposited on	:	2002-02-11
Resolution	:	2.35 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:

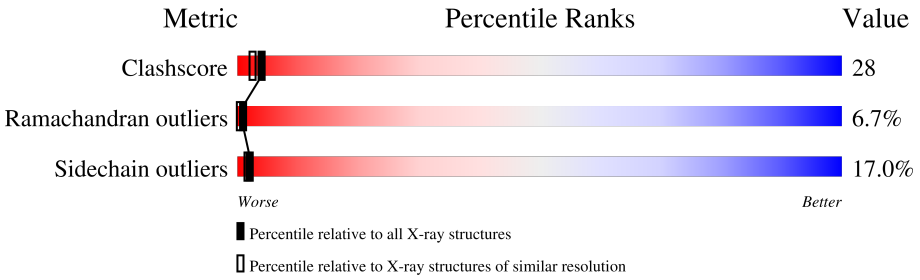
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.35 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	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)

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	A	446	61% 30% 8%
2	B	439	60% 28% 8%
3	C	379	61% 28% 9%
4	D	241	42% 31% 19% 7%
5	E	196	34% 40% 18% 8%
6	F	110	66% 22% 8%
7	G	81	52% 25% 17%
8	H	78	31% 38% 24% 6%

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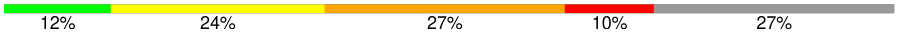
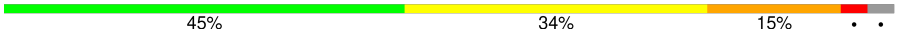
Mol	Chain	Length	Quality of chain
9	I	78	
10	J	62	
11	K	56	

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	HEC	D	242	X	-	-	-
15	FES	E	197	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 16795 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 UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3458	2161	609	668	20	0	0	0

- Molecule 2 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	423	3172	1993	562	610	7	0	0	0

- Molecule 3 is a protein called Cytochrome B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	377	2995	2009	470	498	18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	240	1909	1219	328	347	15	0	0	0

- Molecule 5 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	196	1519	957	263	291	8	0	0	0

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	109	Total	C	N	O	S	0	0	0
			938	592	172	172	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	79	Total	C	N	O	S	0	0	0
			662	431	123	107	1			

- Molecule 8 is a protein called Ubiquinol-cytochrome C reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	78	Total	C	N	O	S	0	0	0
			639	384	111	139	5			

- Molecule 9 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE 8 KDA PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	57	Total	C	N	O	S	0	0	0
			406	253	77	74	2			

- Molecule 10 is a protein called Ubiquinol-cytochrome C reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	60	Total	C	N	O	0	0	0
			495	324	86	85			

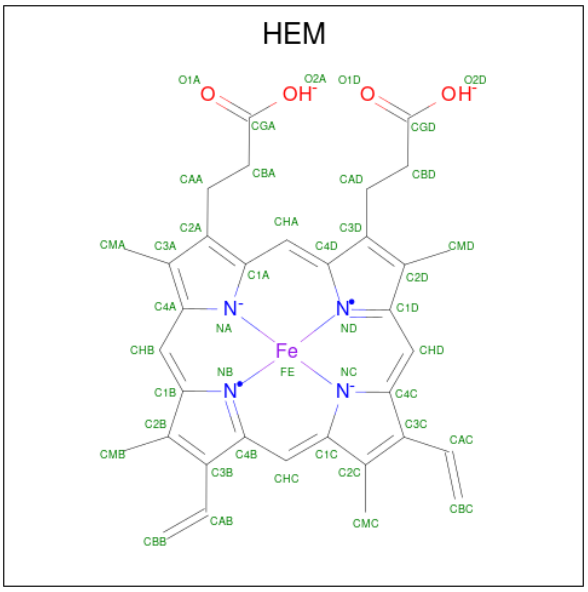
- Molecule 11 is a protein called Ubiquinol-cytochrome C reductase complex 6.4 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	53	Total	C	N	O	S	0	0	0
			441	295	79	66	1			

There is a discrepancy between the modelled and reference sequences:

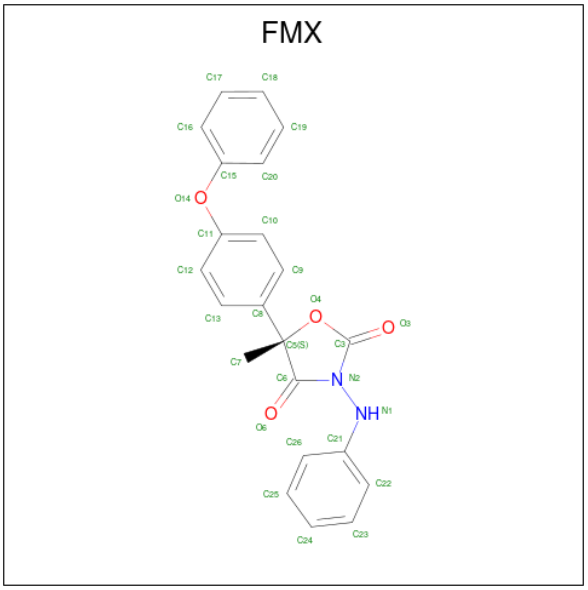
Chain	Residue	Modelled	Actual	Comment	Reference
K	22	GLN	SER	conflict	UNP P07552

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



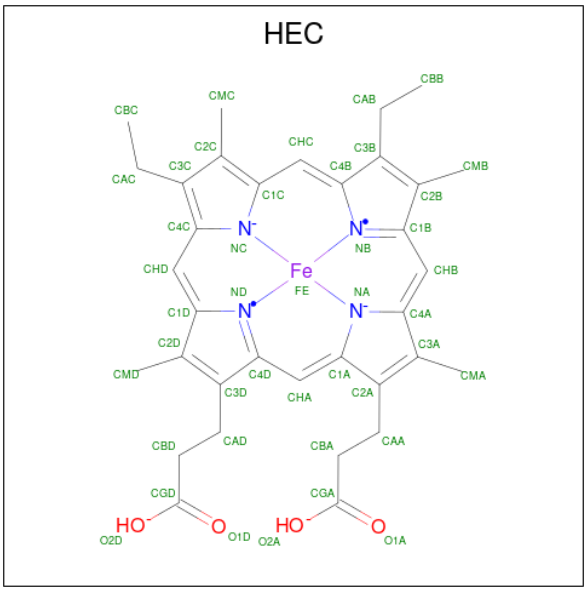
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is FAMOXADONE (CCD ID: FMX) (formula: $C_{22}H_{18}N_2O_4$).



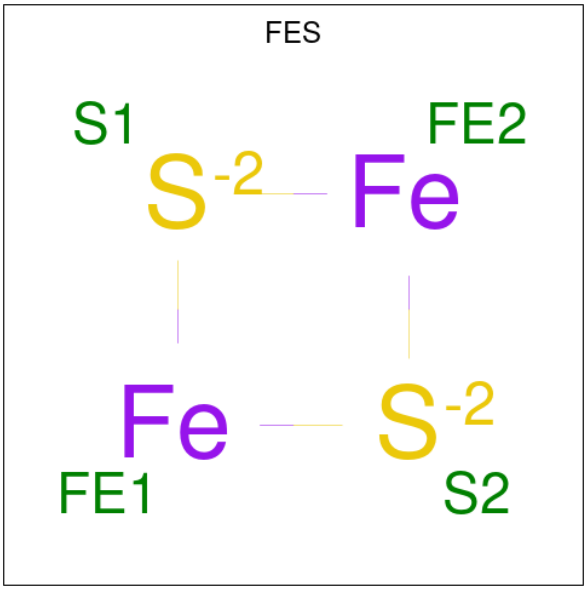
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	N	O	0	0
			28	22	2	4		

- Molecule 14 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

3 Residue-property plots (i)

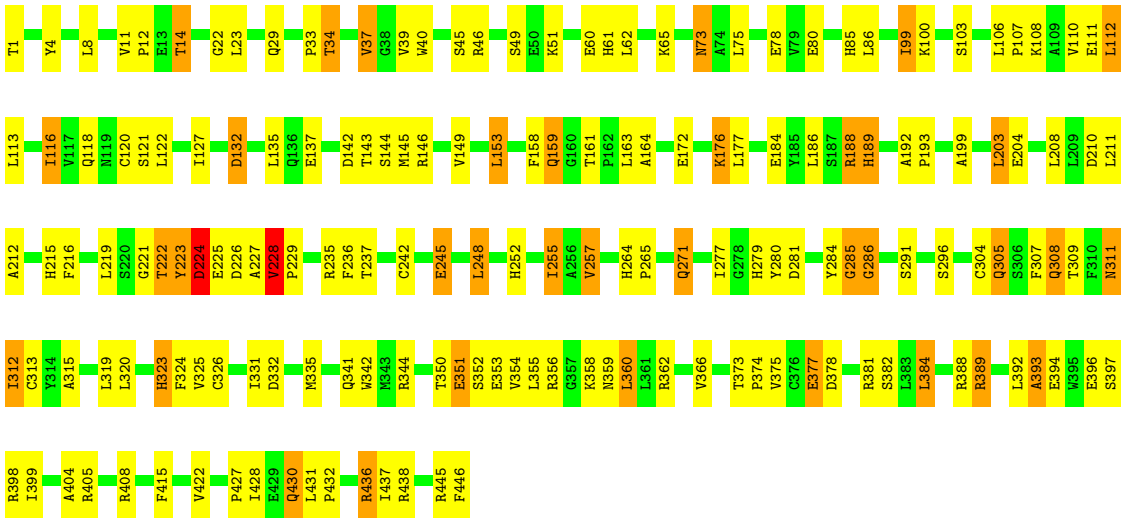
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Chain A:

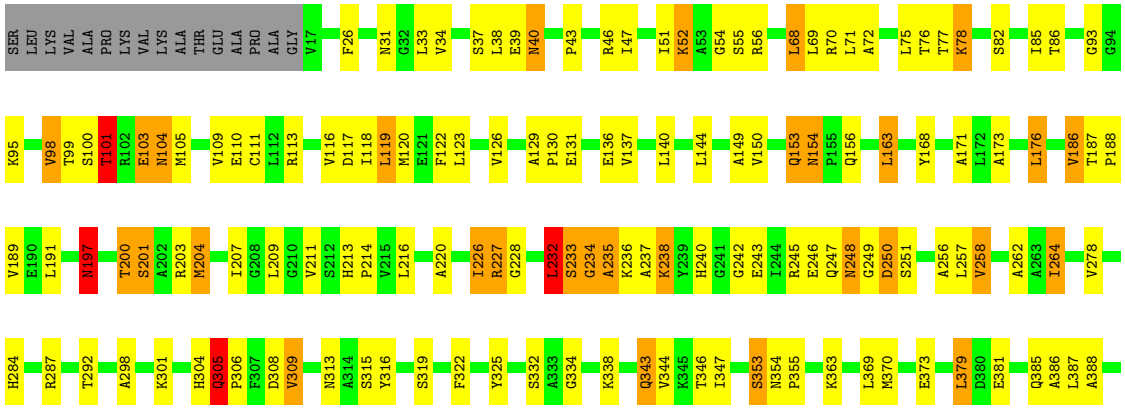


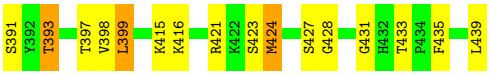


• Molecule 2: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2

Chain B:



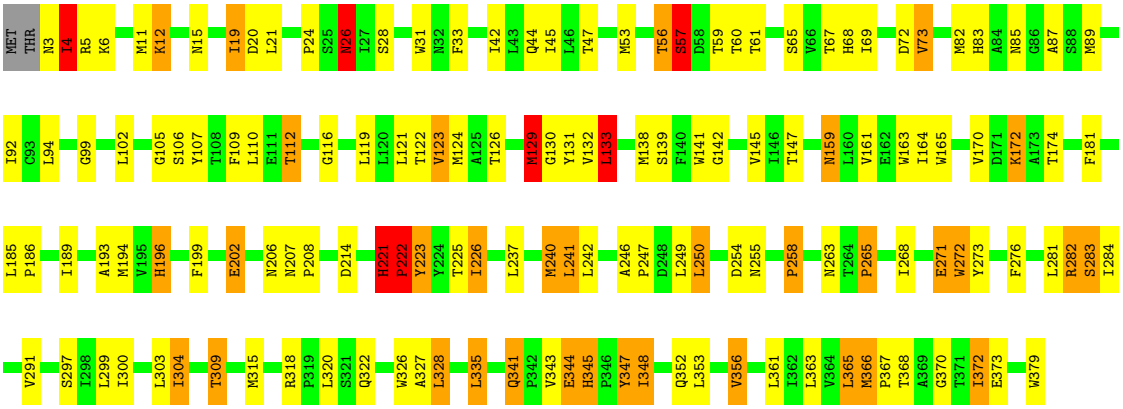




• Molecule 3: Cytochrome B

Chain C:

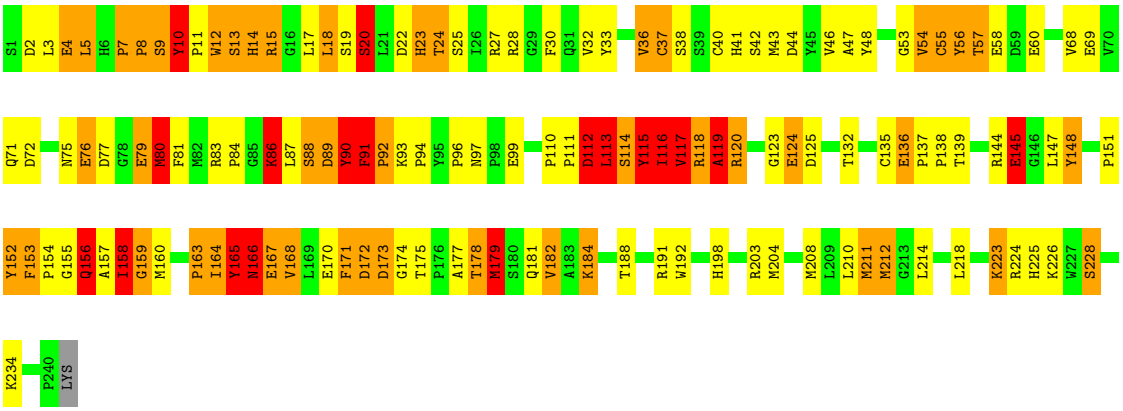




• Molecule 4: Cytochrome c1, heme protein

Chain D:

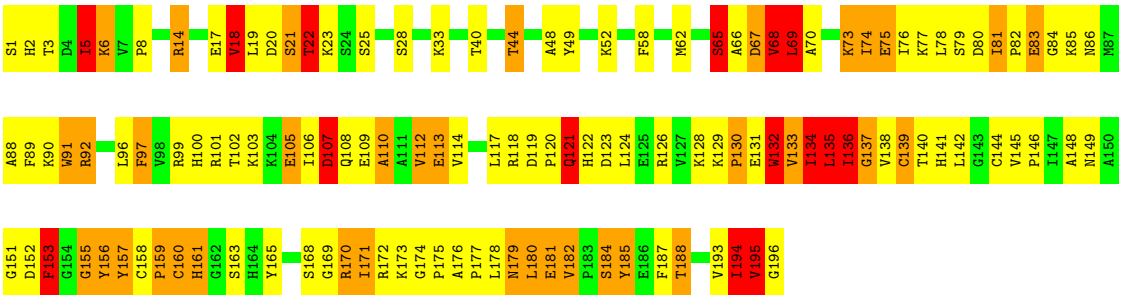




• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT

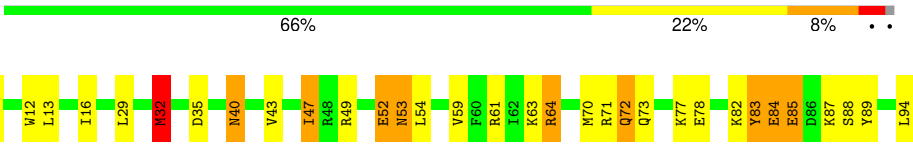
Chain E:





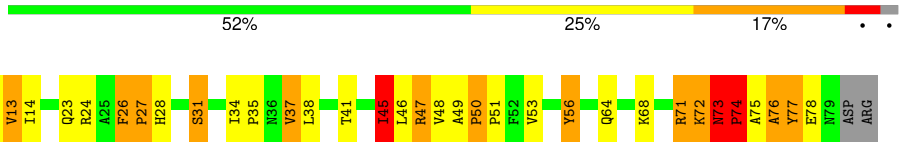
• Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain F:



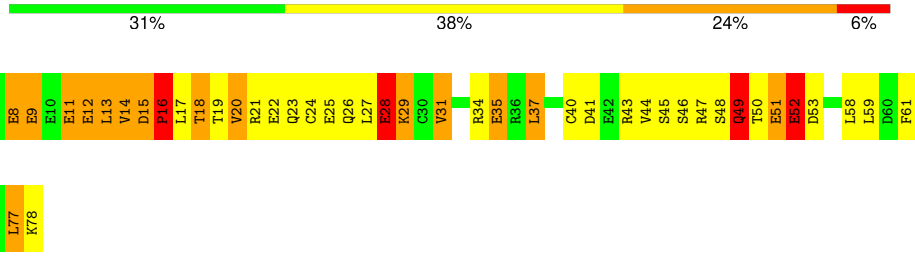
• Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain G:



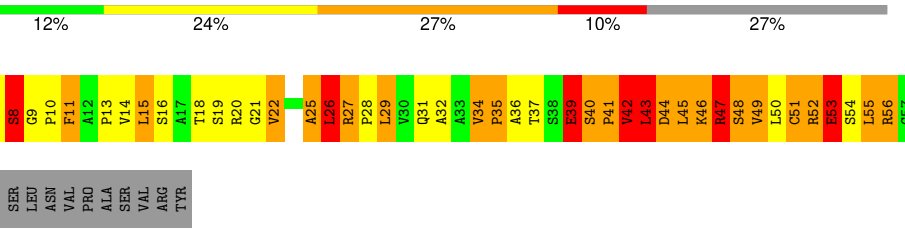
• Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain H:



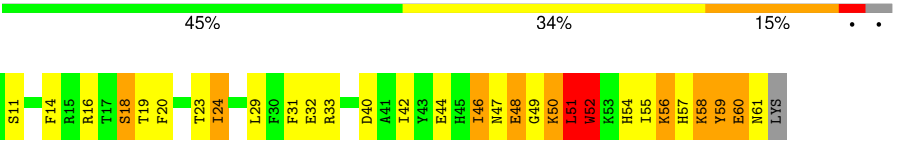
• Molecule 9: UBIQUINOL-CYTOCHROME C REDUCTASE 8 KDA PROTEIN

Chain I:



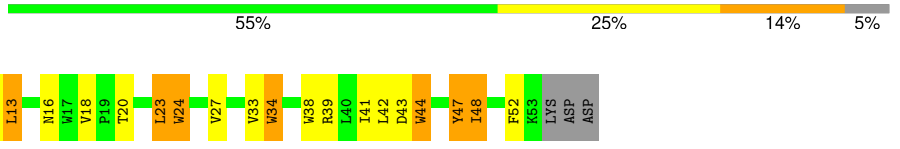
• Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain J:



• Molecule 11: Ubiquinol-cytochrome C reductase complex 6.4 kDa protein

Chain K:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	154.09Å 154.09Å 591.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.35	Depositor
% Data completeness (in resolution range)	96.0 (40.00-2.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.259 , 0.306	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16795	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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: HEM, FES, FMX, HEC

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	1.11	3/3531 (0.1%)	1.14	16/4792 (0.3%)
2	B	1.44	16/3232 (0.5%)	1.29	23/4386 (0.5%)
3	C	1.11	5/3092 (0.2%)	1.24	33/4232 (0.8%)
4	D	0.96	4/1968 (0.2%)	1.26	23/2673 (0.9%)
5	E	1.01	2/1553 (0.1%)	1.37	21/2100 (1.0%)
6	F	1.27	3/958 (0.3%)	1.19	7/1284 (0.5%)
7	G	1.12	0/684	1.23	7/926 (0.8%)
8	H	0.84	0/645	1.41	7/864 (0.8%)
9	I	1.39	5/411 (1.2%)	1.85	12/558 (2.2%)
10	J	0.90	1/508 (0.2%)	1.19	5/686 (0.7%)
11	K	0.99	0/457	1.14	1/625 (0.2%)
All	All	1.16	39/17039 (0.2%)	1.26	155/23126 (0.7%)

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
3	C	0	2

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	424	MET	SD-CE	-16.77	1.37	1.79
4	D	211	MET	SD-CE	-10.21	1.54	1.79
3	C	129	MET	SD-CE	-9.66	1.55	1.79
9	I	43	LEU	N-CA	-8.34	1.35	1.46
4	D	119	ALA	CA-C	-7.92	1.42	1.52

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	233	SER	N-CA-C	-14.19	92.88	110.61
9	I	42	VAL	O-C-N	14.04	140.12	122.57
3	C	221	HIS	CA-C-N	12.36	135.29	119.84
3	C	221	HIS	C-N-CA	12.36	135.29	119.84
4	D	118	ARG	N-CA-C	12.09	125.85	111.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	221	HIS	Peptide,Mainchain

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	3458	0	3356	152	0
2	B	3172	0	3152	123	0
3	C	2995	0	3058	125	0
4	D	1909	0	1857	176	0
5	E	1519	0	1503	182	0
6	F	938	0	932	28	0
7	G	662	0	662	34	0
8	H	639	0	604	50	0
9	I	406	0	437	99	0
10	J	495	0	493	69	0
11	K	441	0	450	27	0
12	C	86	0	60	22	0
13	C	28	0	18	0	0
14	D	43	0	32	8	0
15	E	4	0	0	2	0
All	All	16795	0	16614	935	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 28.

The worst 5 of 935 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:J:49:GLY:C	10:J:54:HIS:HE1	1.40	1.28
4:D:40:CYS:SG	14:D:242:HEC:HAC	1.76	1.26
10:J:51:LEU:O	10:J:55:ILE:HG13	1.43	1.18
3:C:129:MET:CE	3:C:181:PHE:HB2	1.75	1.17
9:I:47:ARG:HG2	9:I:48:SER:H	1.09	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 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	A	444/446 (100%)	408 (92%)	28 (6%)	8 (2%)	6	5
2	B	421/439 (96%)	397 (94%)	17 (4%)	7 (2%)	7	6
3	C	375/379 (99%)	352 (94%)	16 (4%)	7 (2%)	6	5
4	D	238/241 (99%)	164 (69%)	35 (15%)	39 (16%)	0	0
5	E	194/196 (99%)	123 (63%)	35 (18%)	36 (19%)	0	0
6	F	107/110 (97%)	96 (90%)	8 (8%)	3 (3%)	4	2
7	G	77/81 (95%)	64 (83%)	7 (9%)	6 (8%)	1	0
8	H	76/78 (97%)	57 (75%)	7 (9%)	12 (16%)	0	0
9	I	55/78 (70%)	28 (51%)	11 (20%)	16 (29%)	0	0
10	J	58/62 (94%)	46 (79%)	9 (16%)	3 (5%)	1	0
11	K	51/56 (91%)	43 (84%)	4 (8%)	4 (8%)	1	0
All	All	2096/2166 (97%)	1778 (85%)	177 (8%)	141 (7%)	1	0

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	VAL
2	B	232	LEU

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Mol	Chain	Res	Type
2	B	234	GLY
2	B	305	GLN
3	C	172	LYS

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	A	370/370 (100%)	315 (85%)	55 (15%)	3	2
2	B	332/343 (97%)	288 (87%)	44 (13%)	4	3
3	C	325/327 (99%)	279 (86%)	46 (14%)	3	3
4	D	205/206 (100%)	159 (78%)	46 (22%)	1	1
5	E	168/168 (100%)	139 (83%)	29 (17%)	2	1
6	F	98/98 (100%)	80 (82%)	18 (18%)	1	1
7	G	69/71 (97%)	53 (77%)	16 (23%)	1	0
8	H	74/74 (100%)	56 (76%)	18 (24%)	1	0
9	I	44/60 (73%)	30 (68%)	14 (32%)	0	0
10	J	50/52 (96%)	42 (84%)	8 (16%)	2	2
11	K	43/46 (94%)	35 (81%)	8 (19%)	1	1
All	All	1778/1815 (98%)	1476 (83%)	302 (17%)	2	2

5 of 302 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	77	LYS
10	J	5	LEU
7	G	2	ARG
8	H	18	THR
11	K	34	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	116	GLN
11	K	12	GLN
5	E	161	HIS
6	F	73	GLN
2	B	162	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)

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)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	FMX	C	611	-	30,31,31	0.94	2 (6%)	36,44,44	1.23	4 (11%)
14	HEC	D	242	4	50,50,50	1.91	6 (12%)	68,82,82	1.60	15 (22%)
15	FES	E	197	5	0,4,4	-	-	-		
12	HEM	C	609	3	50,50,50	3.56	28 (56%)	67,82,82	2.63	32 (47%)
12	HEM	C	610	3	50,50,50	3.40	28 (56%)	67,82,82	2.67	30 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FMX	C	611	-	-	2/14/33/33	0/4/4/4
14	HEC	D	242	4	1/1/3/7	6/14/54/54	-
15	FES	E	197	5	-	-	0/1/1/1
12	HEM	C	609	3	-	9/14/54/54	-
12	HEM	C	610	3	-	7/14/54/54	-

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	610	HEM	C3C-C4C	-7.50	1.32	1.46
12	C	609	HEM	C3B-C4B	-7.22	1.30	1.44
14	D	242	HEC	C3D-C2D	7.14	1.52	1.36
12	C	609	HEM	CHA-C4D	6.80	1.52	1.38
12	C	609	HEM	CHD-C4C	6.54	1.51	1.38

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	610	HEM	C4C-CHD-C1D	-6.73	111.72	126.02
12	C	609	HEM	C4C-CHD-C1D	-6.33	112.57	126.02
12	C	609	HEM	C1C-CHC-C4B	-6.08	113.09	126.02
12	C	610	HEM	C1C-CHC-C4B	-6.05	113.15	126.02
12	C	609	HEM	CHB-C4A-NA	5.16	133.22	123.86

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	D	242	HEC	NA

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	609	HEM	C2D-C3D-CAD-CBD
12	C	609	HEM	C4D-C3D-CAD-CBD
12	C	610	HEM	C2B-C3B-CAB-CBB
12	C	610	HEM	C2C-C3C-CAC-CBC
12	C	610	HEM	C4C-C3C-CAC-CBC

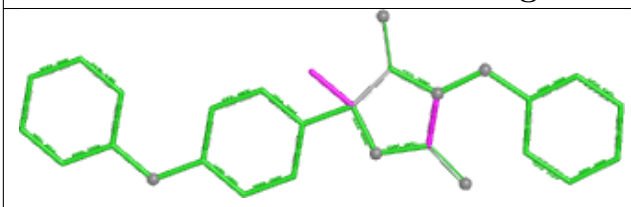
There are no ring outliers.

4 monomers are involved in 32 short contacts:

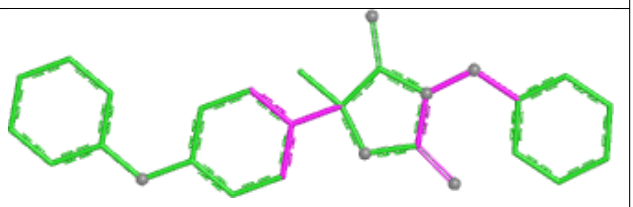
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	D	242	HEC	8	0
15	E	197	FES	2	0
12	C	609	HEM	11	0
12	C	610	HEM	11	0

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.

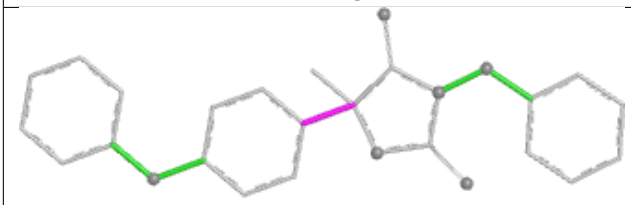
Ligand FMX C 611



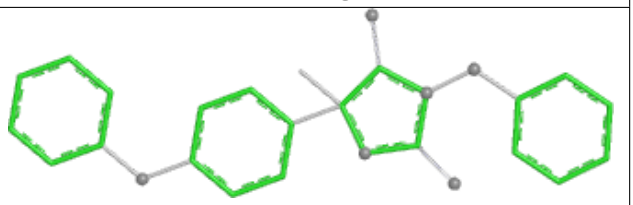
Bond lengths



Bond angles

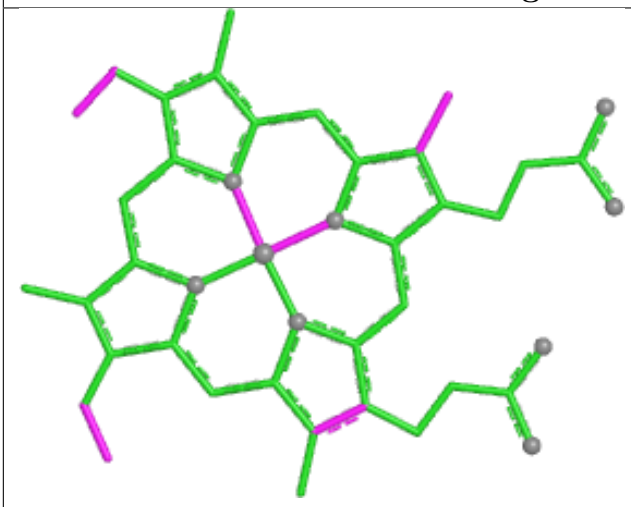


Torsions

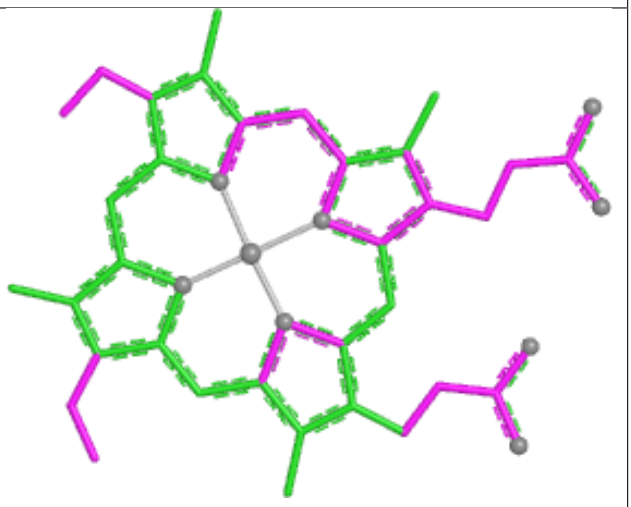


Rings

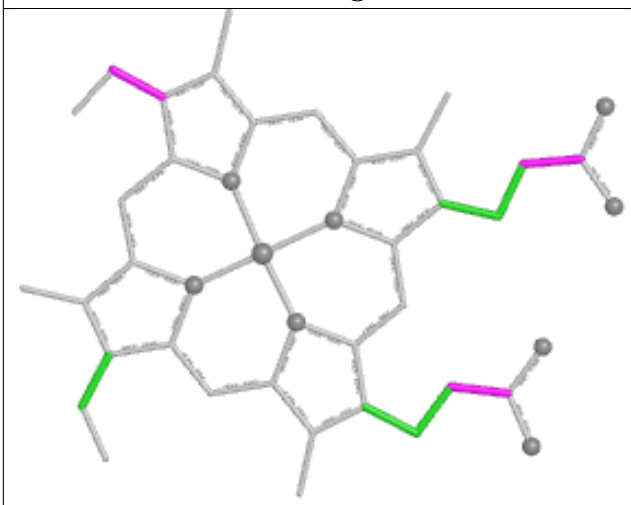
Ligand HEC D 242



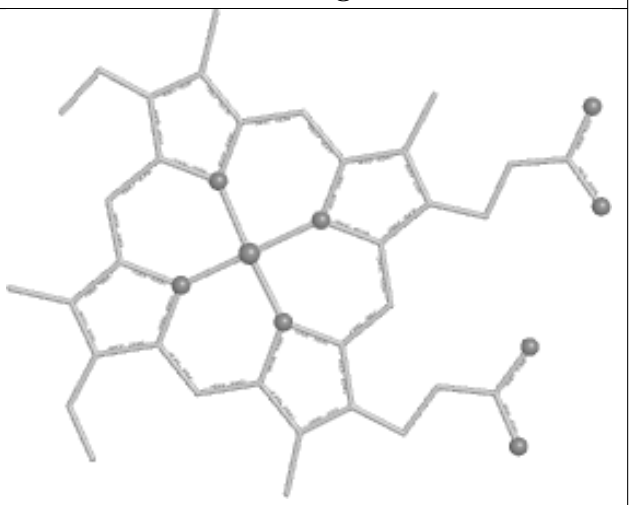
Bond lengths



Bond angles

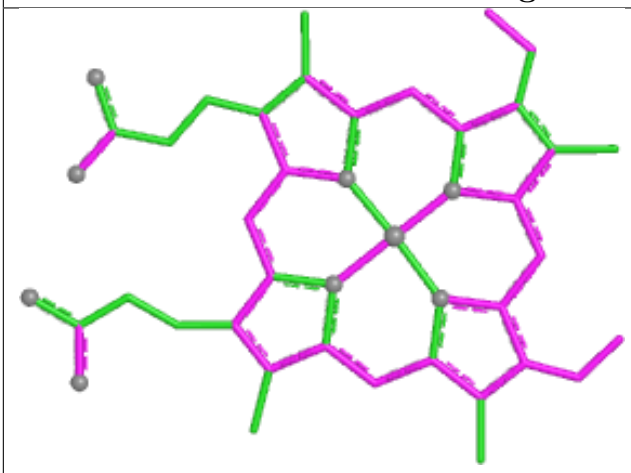


Torsions

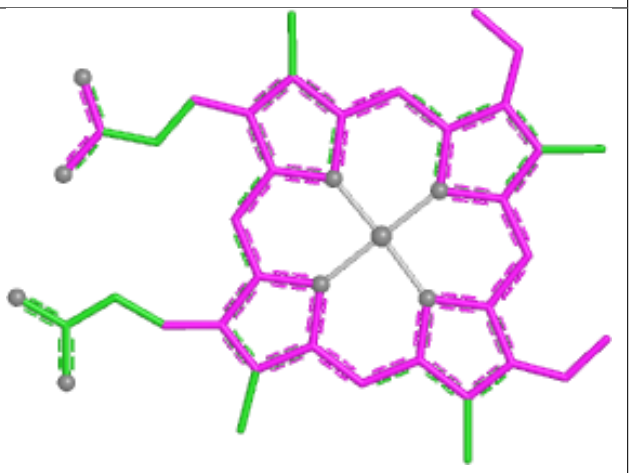


Rings

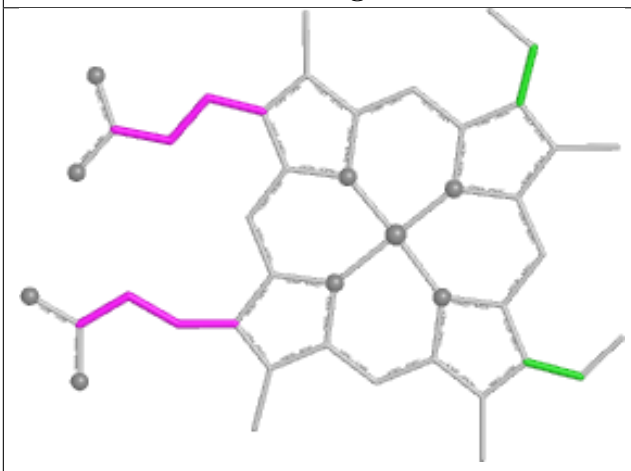
Ligand HEM C 609



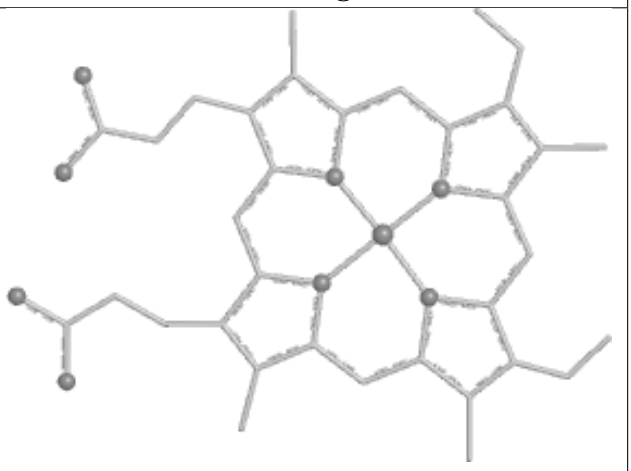
Bond lengths



Bond angles

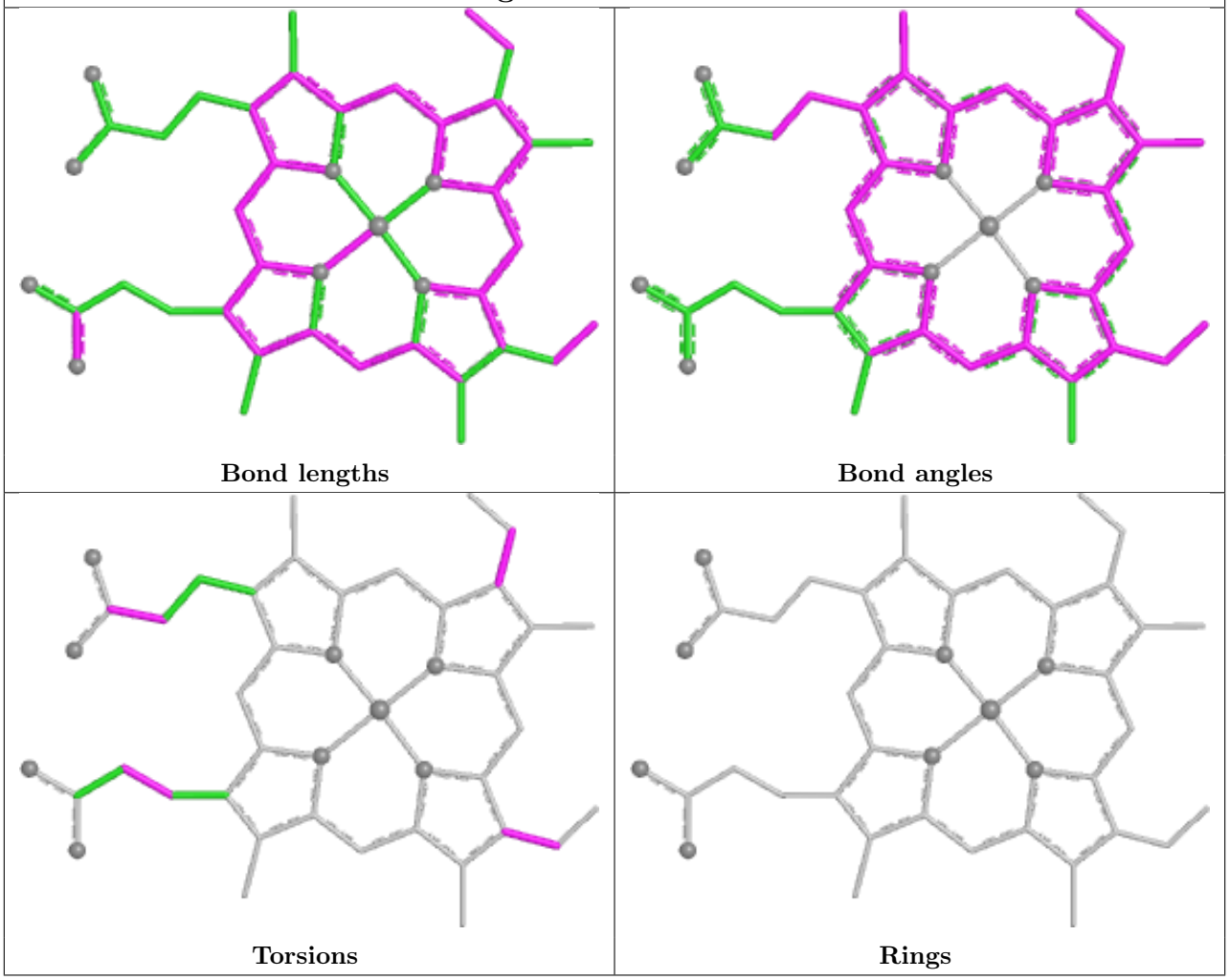


Torsions



Rings

Ligand HEM C 610



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.