wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 09:50 PM EDT

PDB ID	:	1BE3
Title	:	CYTOCHROME BC1 COMPLEX FROM BOVINE
Authors	:	Iwata, S.; Lee, J.W.; Okada, K.; Lee, J.K.; Iwata, M.; Ramaswamy, S.; Jap, B.K.
Deposited on	:	1998-05-19
Resolution	:	3.00 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:

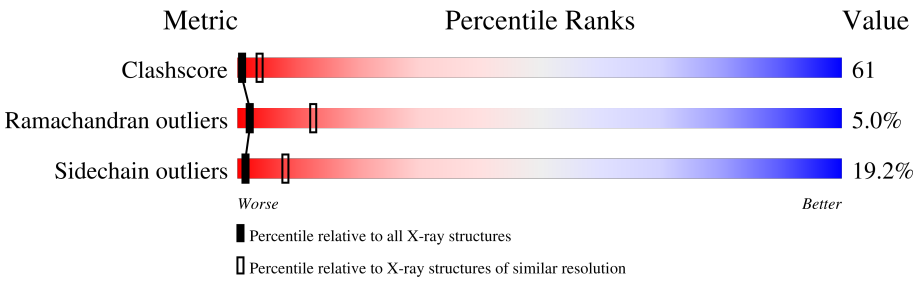
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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	A	446	23% 56% 17% •
2	B	439	23% 55% 15% • 5%
3	C	379	29% 49% 19% •
4	D	241	26% 53% 20% •
5	E	196	25% 51% 22% •
6	F	110	33% 46% 14% • •
7	G	81	21% 58% 16% 5%
8	H	78	24% 41% 17% 18%

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Mol	Chain	Length	Quality of chain
9	I	78	9% 23% 10% 58%
10	J	62	44% 45% 10% •
11	K	56	12% 14% 12% 61%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 16222 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 CYTOCHROME BC1 COMPLEX.

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 CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	419	3141	1972	556	606	7	0	0	0

- Molecule 3 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	379	3011	2018	472	502	19	0	0	0

- Molecule 4 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	241	1919	1225	330	349	15	0	0	0

- Molecule 5 is a protein called CYTOCHROME BC1 COMPLEX.

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 CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	106	916	579	166	169	2	0	0	0

- Molecule 7 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	81	682	441	128	112	1	0	0	0

- Molecule 8 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	64	524	316	96	107	5	0	0	0

- Molecule 9 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	33	248	152	51	44	1	0	0	0

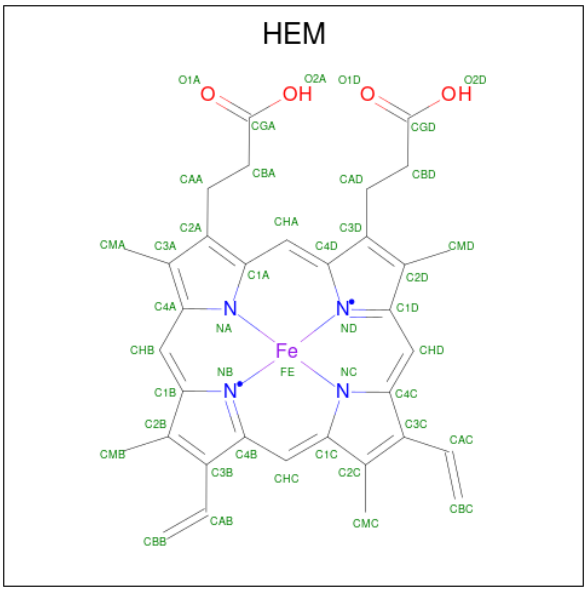
- Molecule 10 is a protein called CYTOCHROME BC1 COMPLEX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	J	62	512	335	89	88	0	0	0

- Molecule 11 is a protein called CYTOCHROME BC1 COMPLEX.

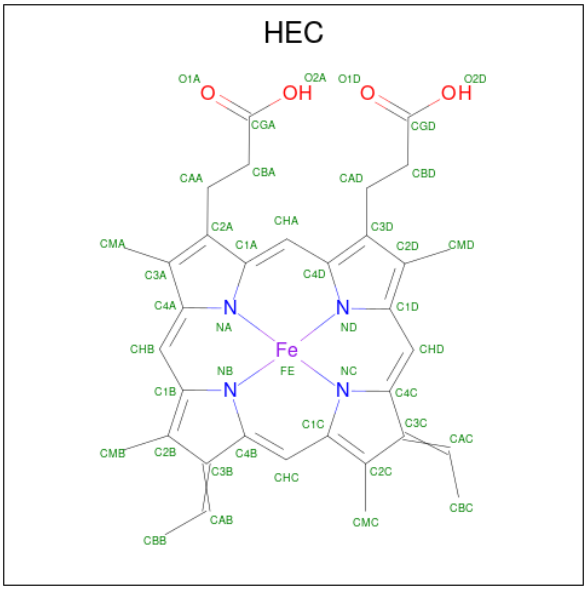
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	K	22	159	103	29	27	0	0	0

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



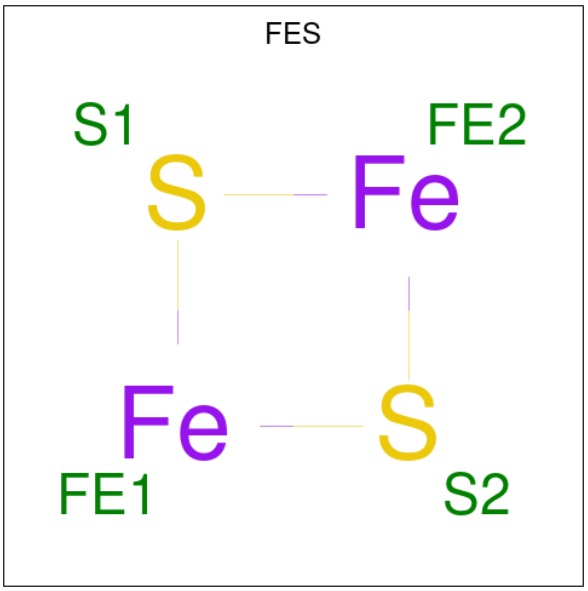
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
12	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
12	C	1	43	34	1	4	4	0	0

- Molecule 13 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

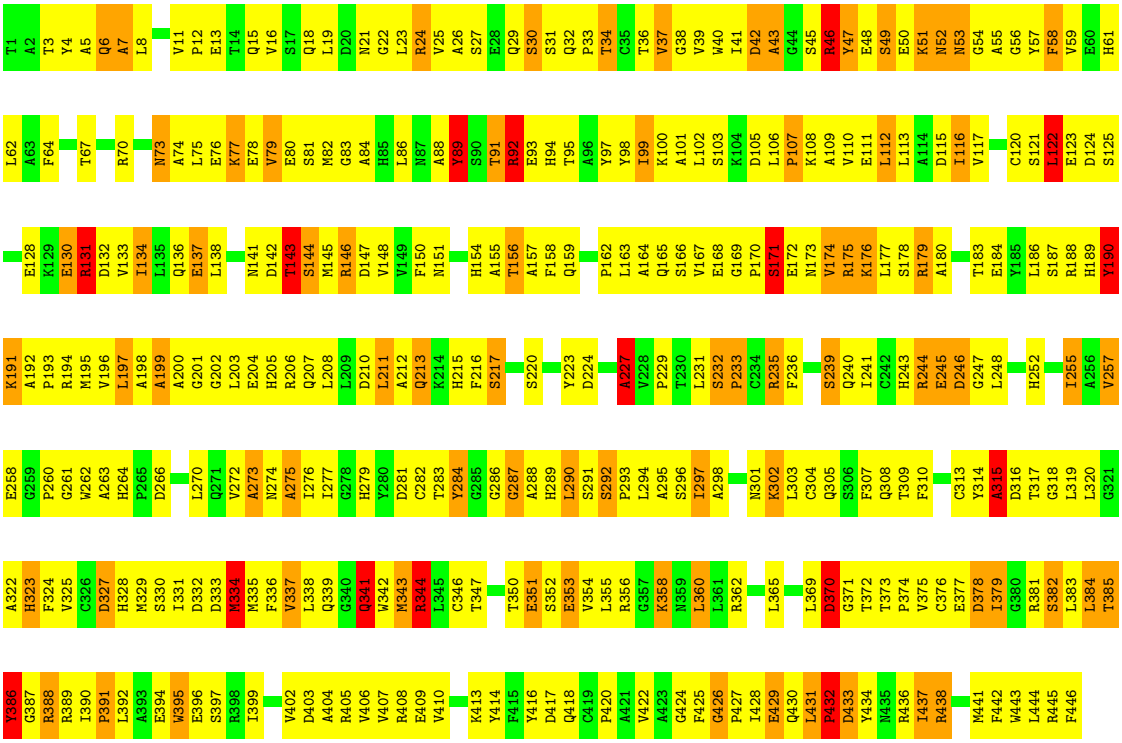
3 Residue-property plots (i)

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.

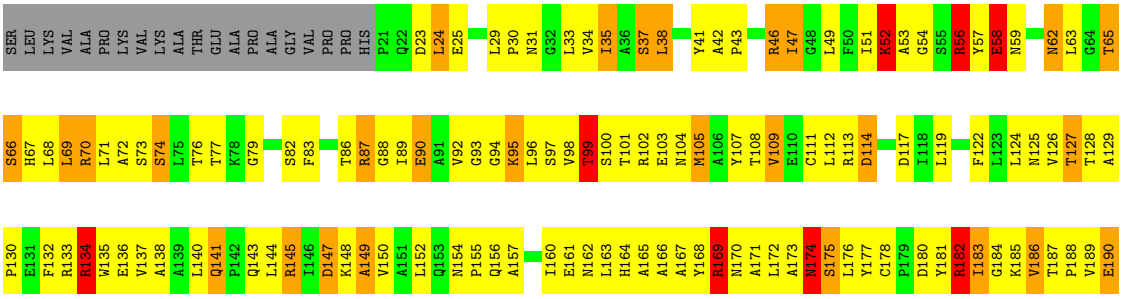
• Molecule 1: CYTOCHROME BC1 COMPLEX

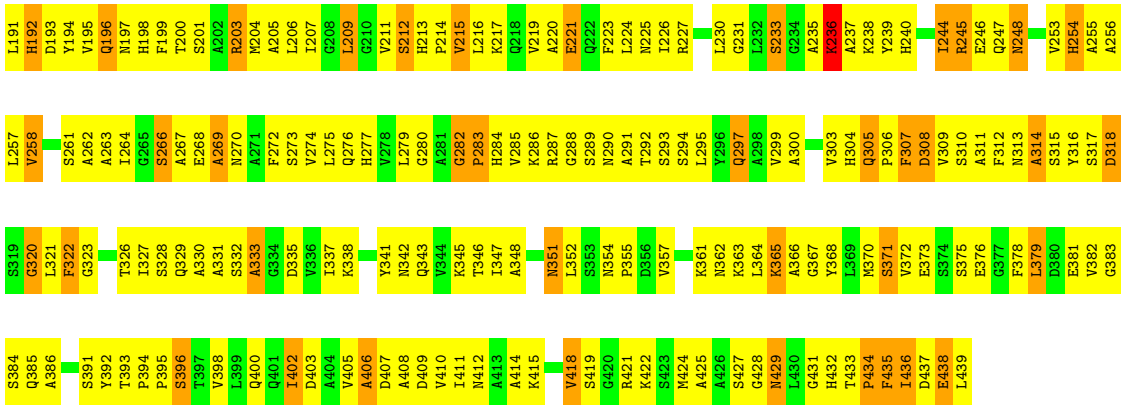
Chain A: 23% 56% 17% •



• Molecule 2: CYTOCHROME BC1 COMPLEX

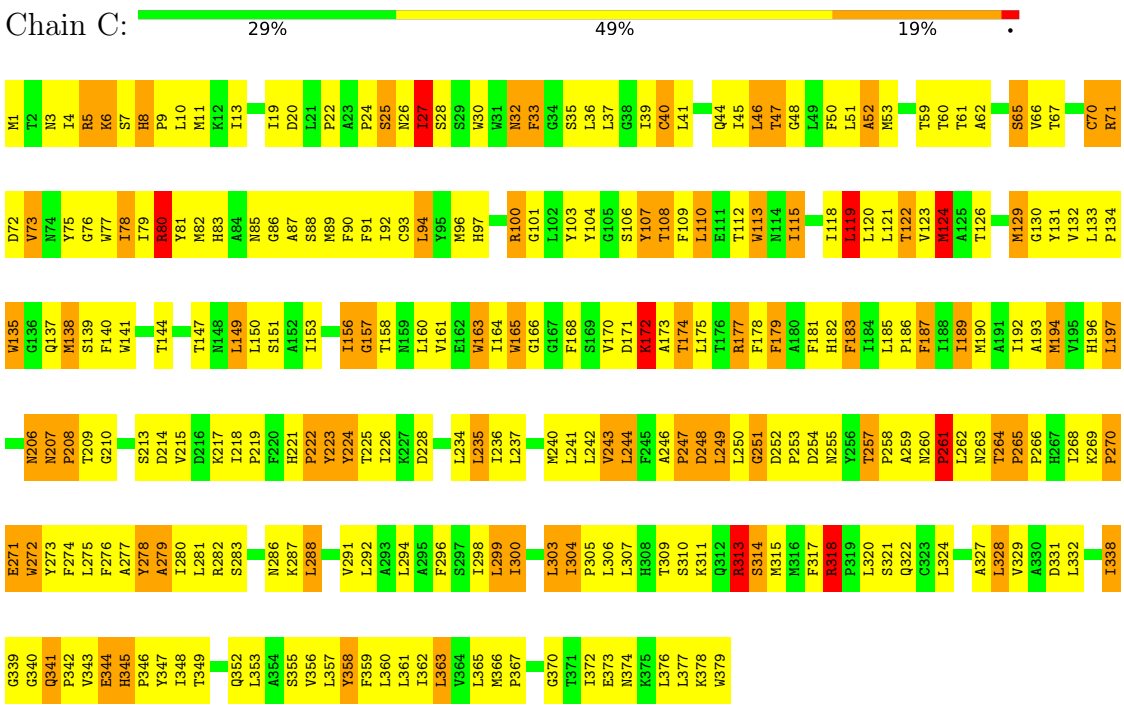
Chain B: 23% 55% 15% • 5%





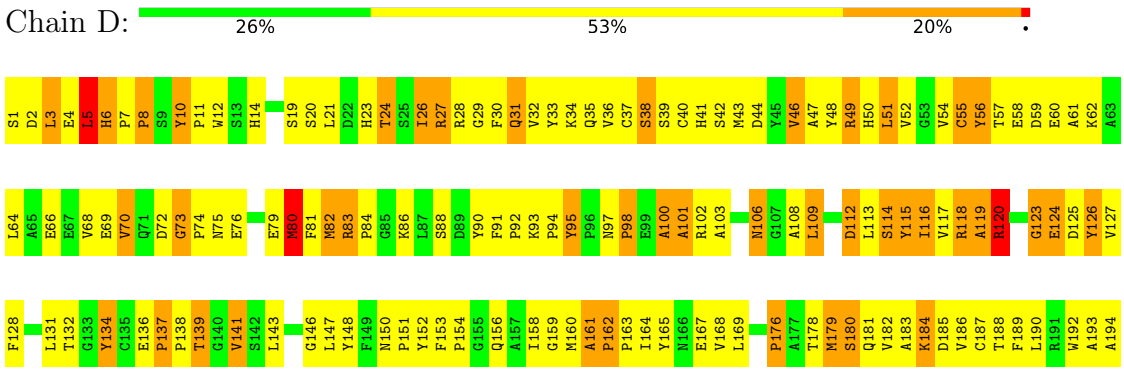
- Molecule 3: CYTOCHROME BC1 COMPLEX

Chain C:



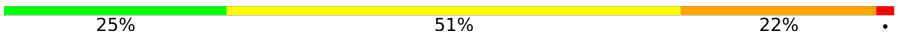
- Molecule 4: CYTOCHROME BC1 COMPLEX

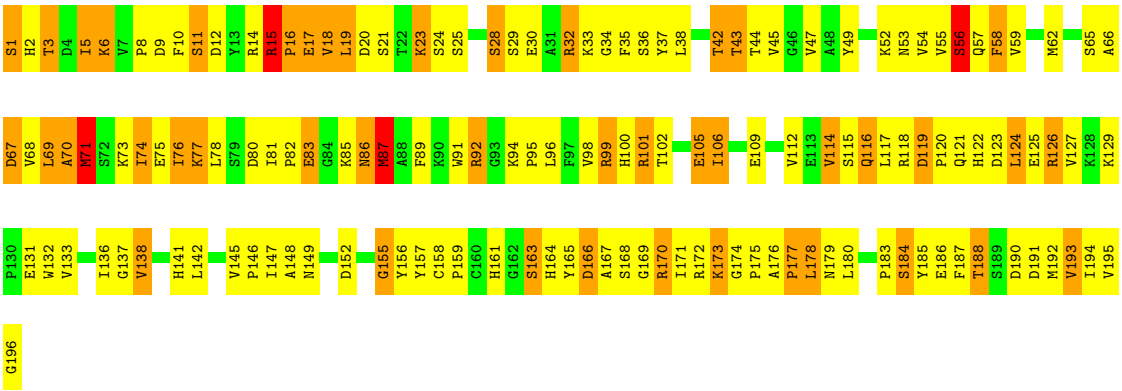
Chain D:



• Molecule 5: CYTOCHROME BC1 COMPLEX

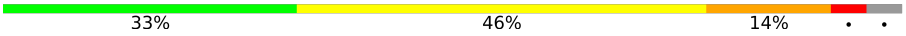
Chain E:

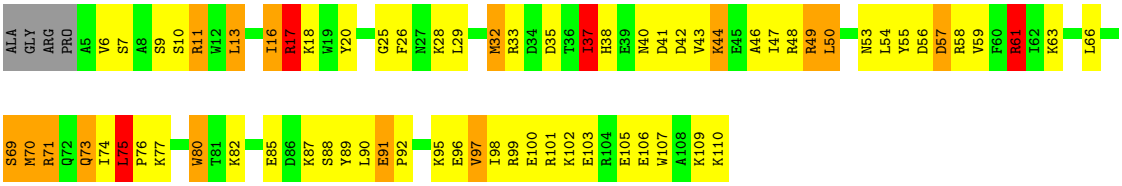




• Molecule 6: CYTOCHROME BC1 COMPLEX

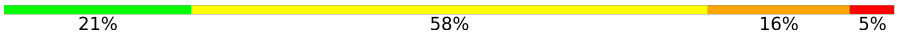
Chain F:

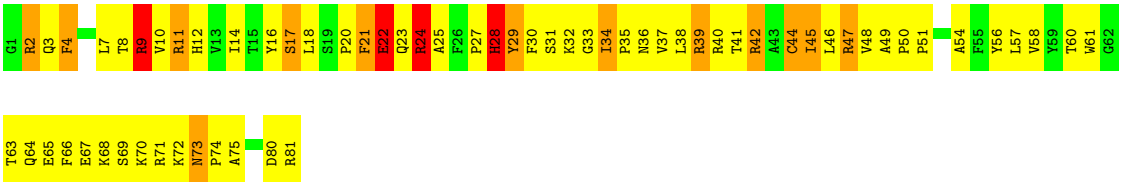




• Molecule 7: CYTOCHROME BC1 COMPLEX

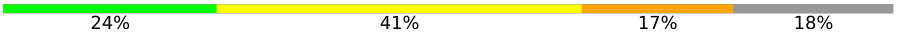
Chain G:

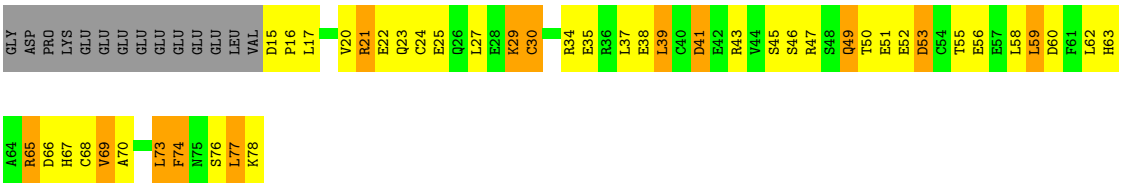




• Molecule 8: CYTOCHROME BC1 COMPLEX

Chain H:





• Molecule 9: CYTOCHROME BC1 COMPLEX

Chain I: 9% 23% 10% 58%

MET LEU SER VAL ALA ALA ARG SER GLY PRO PHE ALA PRO VAL LEU SER ALA THR SER ARG GLY VAL ALA ALA GLY ALA LEU ARG PRO LEU VAL GLN ALA ALA VAL PRO ALA THR SER GLU SER PRO VAL LEU ASP LEU K46 R47 S48 V49 L50 C51 R52 E53 S54 L55 R56 G57 Q58 A59

R62 P63 L64 V65 V68 S69 L70 N71 V72 P73 V76 R77 Y78

- Molecule 10: CYTOCHROME BC1 COMPLEX

Chain J: 44% 45% 10%

V1 A2 P3 T4 L5 T6 A7 R8 L9 Y10 L13 F14 T17 S18 T19 F20 A21 L22 T23 I24 V25 L29 F30 F31 E32 R33 I42 Y43 I46 G49 K50 L51 W52 K53 H54 I55 K56 H57 K58 Y59 E60 N61 K62

- Molecule 11: CYTOCHROME BC1 COMPLEX

Chain K: 12% 14% 12% 61%

MET LEU THR ARG PHE LEU GLY PRO ARG TYR ARG GLN LEU ALA R15 N16 W17 V18 P19 T20 A21 Q22 L23 W24 V30 G31 L32 V33 S34 A35 T36 ASP SER ARG LEU ILE LEU ASP TRP VAL PRO TYR ILE ASN GLY LYS PHE LYS LYS ASP ASP

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	211.20Å 211.20Å 339.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.00	Depositor
% Data completeness (in resolution range)	81.7 (40.00-3.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.260 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16222	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

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: HEM, HEC, FES

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	0.62	1/3531 (0.0%)	1.63	35/4792 (0.7%)
2	B	0.59	0/3198	1.52	25/4336 (0.6%)
3	C	0.67	2/3108 (0.1%)	1.56	34/4252 (0.8%)
4	D	0.55	0/1978	1.41	15/2684 (0.6%)
5	E	0.55	1/1553 (0.1%)	1.47	16/2100 (0.8%)
6	F	0.58	1/935 (0.1%)	1.59	12/1253 (1.0%)
7	G	0.56	0/704	1.54	11/951 (1.2%)
8	H	0.51	0/529	1.14	1/708 (0.1%)
9	I	0.64	0/250	1.48	1/335 (0.3%)
10	J	0.54	0/525	1.29	4/707 (0.6%)
11	K	0.55	0/163	1.22	1/225 (0.4%)
All	All	0.60	5/16474 (0.0%)	1.52	155/22343 (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
1	A	0	14
2	B	0	17
3	C	0	8
4	D	0	5
5	E	0	5
6	F	0	5
7	G	0	2
8	H	0	1
All	All	0	57

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	344	GLU	CD-OE1	7.85	1.34	1.25
6	F	91	GLU	CD-OE1	7.13	1.33	1.25
3	C	261	PRO	N-CD	-6.11	1.39	1.47
1	A	122	LEU	C-O	5.64	1.34	1.23
5	E	56	SER	C-O	5.41	1.33	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	15	ARG	NE-CZ-NH2	15.63	128.11	120.30
3	C	177	ARG	NE-CZ-NH2	-15.12	112.74	120.30
1	A	235	ARG	NE-CZ-NH2	14.30	127.45	120.30
1	A	235	ARG	NE-CZ-NH1	-13.98	113.31	120.30
3	C	80	ARG	NE-CZ-NH1	-13.54	113.53	120.30

There are no chirality outliers.

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	THR	Mainchain
1	A	190	TYR	Mainchain
1	A	197	LEU	Mainchain
1	A	210	ASP	Mainchain
1	A	47	TYR	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	492	0
2	B	3141	0	3123	408	1
3	C	3011	0	3077	382	2
4	D	1919	0	1868	295	0
5	E	1519	0	1503	184	2
6	F	916	0	909	83	0
7	G	682	0	679	104	0
8	H	524	0	504	58	0
9	I	248	0	265	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	512	0	518	60	0
11	K	159	0	159	23	0
12	C	86	0	60	19	0
13	D	43	0	30	2	0
14	E	4	0	0	1	0
All	All	16222	0	16051	1980	3

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 61.

The worst 5 of 1980 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)
1:A:158:PHE:CE1	1:A:317:THR:HG21	1.71	1.26
1:A:21:ASN:CB	1:A:217:SER:HB2	1.70	1.20
1:A:392:LEU:HA	1:A:395:TRP:CD1	1.79	1.17
2:B:29:LEU:HD12	2:B:33:LEU:HD21	1.19	1.15
1:A:158:PHE:HE1	1:A:317:THR:HG21	0.97	1.12

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:264:THR:OG1	5:E:141:HIS:O[10_665]	1.93	0.27
2:B:169:ARG:NH2	2:B:438:GLU:OE2[10_665]	1.99	0.21
3:C:177:ARG:NH2	5:E:62:MET:O[10_665]	2.12	0.08

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%)	359 (81%)	65 (15%)	20 (4%)	2 14
2	B	417/439 (95%)	360 (86%)	43 (10%)	14 (3%)	3 20
3	C	377/379 (100%)	300 (80%)	55 (15%)	22 (6%)	1 10
4	D	239/241 (99%)	188 (79%)	32 (13%)	19 (8%)	1 4
5	E	194/196 (99%)	144 (74%)	40 (21%)	10 (5%)	2 12
6	F	104/110 (94%)	89 (86%)	14 (14%)	1 (1%)	15 53
7	G	79/81 (98%)	57 (72%)	18 (23%)	4 (5%)	2 12
8	H	62/78 (80%)	46 (74%)	11 (18%)	5 (8%)	1 4
9	I	31/78 (40%)	17 (55%)	9 (29%)	5 (16%)	0 1
10	J	60/62 (97%)	47 (78%)	13 (22%)	0	100 100
11	K	20/56 (36%)	15 (75%)	3 (15%)	2 (10%)	0 2
All	All	2027/2166 (94%)	1622 (80%)	303 (15%)	102 (5%)	2 12

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	PRO
1	A	432	PRO
2	B	183	ILE
3	C	8	HIS
3	C	27	ILE

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%)	291 (79%)	79 (21%)	1 5
2	B	328/343 (96%)	265 (81%)	63 (19%)	1 8
3	C	327/327 (100%)	273 (84%)	54 (16%)	2 11
4	D	206/206 (100%)	177 (86%)	29 (14%)	3 16
5	E	168/168 (100%)	124 (74%)	44 (26%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	96/98 (98%)	73 (76%)	23 (24%)	0 3
7	G	71/71 (100%)	59 (83%)	12 (17%)	2 11
8	H	61/74 (82%)	52 (85%)	9 (15%)	3 14
9	I	27/60 (45%)	21 (78%)	6 (22%)	1 4
10	J	52/52 (100%)	45 (86%)	7 (14%)	4 17
11	K	15/46 (33%)	11 (73%)	4 (27%)	0 2
All	All	1721/1815 (95%)	1391 (81%)	330 (19%)	1 8

5 of 330 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	17	GLU
6	F	82	LYS
5	E	52	LYS
5	E	163	SER
7	G	42	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	206	ASN
4	D	106	ASN
11	K	16	ASN
3	C	267	HIS
3	C	374	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	HEC	D	242	4	32,50,50	2.26	5 (15%)	24,82,82	2.26	11 (45%)
12	HEM	C	380	3	41,50,50	1.56	4 (9%)	45,82,82	1.53	9 (20%)
12	HEM	C	381	3	41,50,50	1.41	4 (9%)	45,82,82	1.72	12 (26%)
14	FES	E	197	5	0,4,4	-	-	-		

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
13	HEC	D	242	4	-	7/10/54/54	-
12	HEM	C	380	3	-	5/12/54/54	-
12	HEM	C	381	3	-	5/12/54/54	-
14	FES	E	197	5	-	-	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	242	HEC	C2B-C3B	-7.23	1.33	1.40
13	D	242	HEC	C3C-C2C	-6.61	1.33	1.40
12	C	380	HEM	C3C-C2C	-5.23	1.33	1.40
12	C	381	HEM	C3C-C2C	-4.84	1.33	1.40
13	D	242	HEC	CBB-CAB	-4.01	1.34	1.49

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	380	HEM	CMA-C3A-C4A	-4.97	120.83	128.46
12	C	381	HEM	C2C-C3C-C4C	4.23	109.85	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	380	HEM	CMA-C3A-C2A	4.02	132.53	124.94
12	C	380	HEM	CBD-CAD-C3D	3.92	123.52	112.63
13	D	242	HEC	CMD-C2D-C1D	-3.60	122.94	128.46

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	D	242	HEC	C2A-CAA-CBA-CGA
12	C	380	HEM	C2A-CAA-CBA-CGA
13	D	242	HEC	C1A-C2A-CAA-CBA
13	D	242	HEC	C3A-C2A-CAA-CBA
12	C	381	HEM	C2D-C3D-CAD-CBD

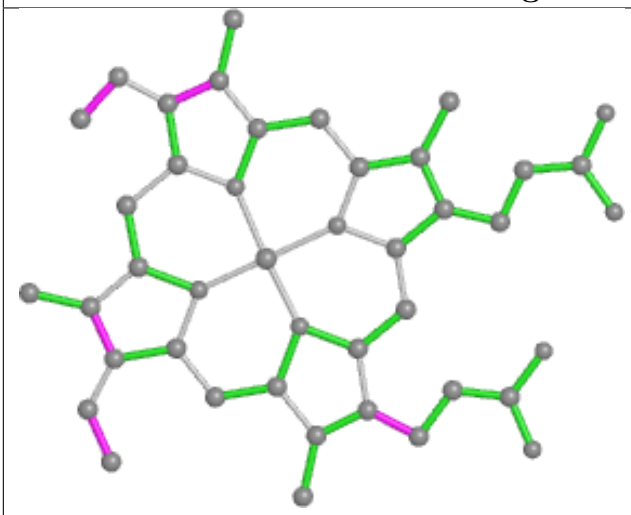
There are no ring outliers.

4 monomers are involved in 22 short contacts:

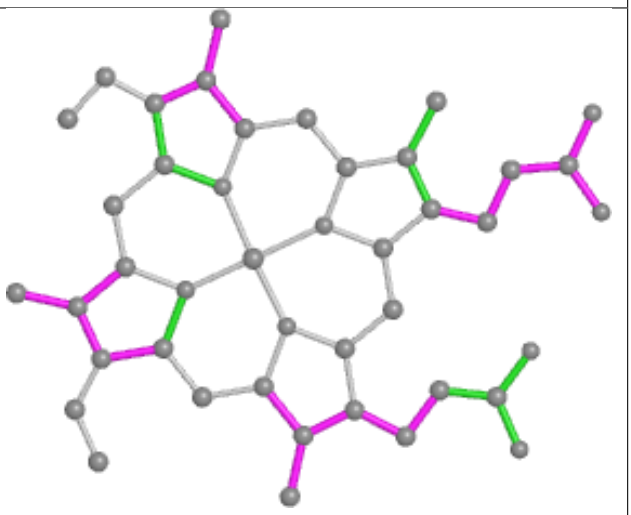
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	D	242	HEC	2	0
12	C	380	HEM	10	0
12	C	381	HEM	9	0
14	E	197	FES	1	0

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.

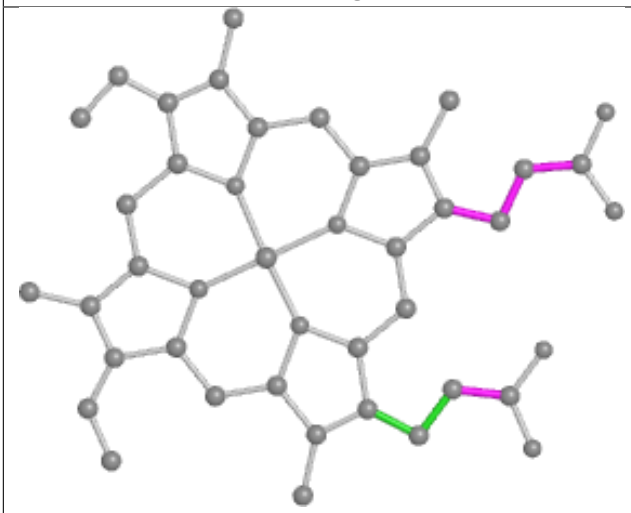
Ligand HEC D 242



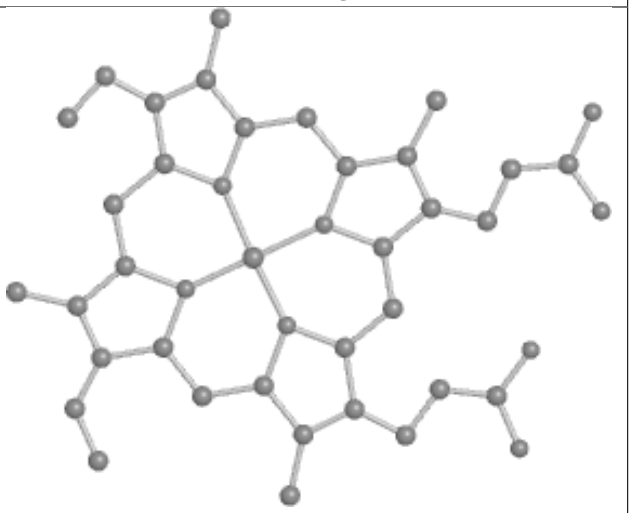
Bond lengths



Bond angles

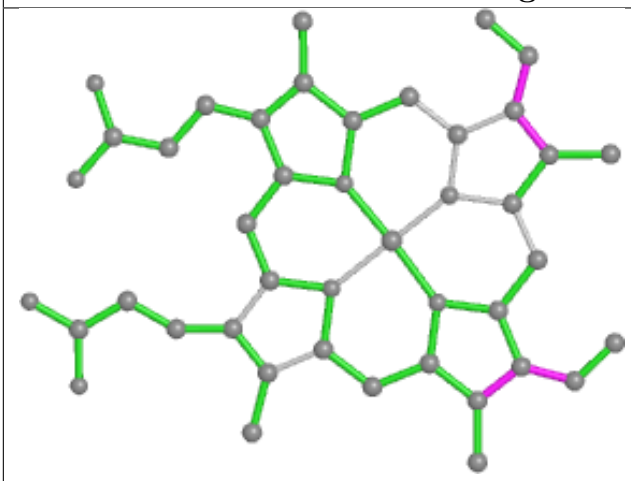


Torsions

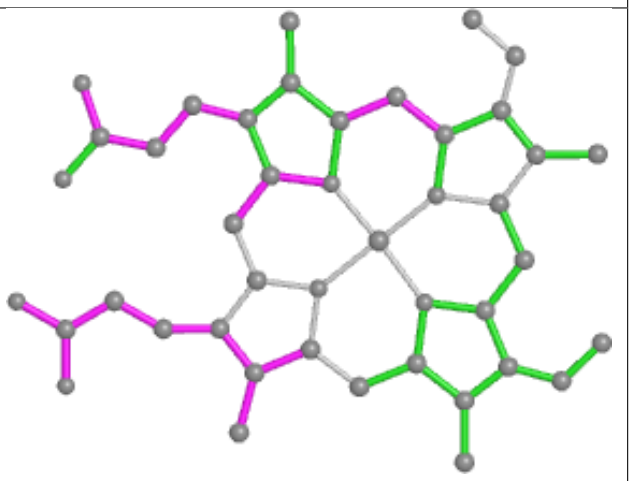


Rings

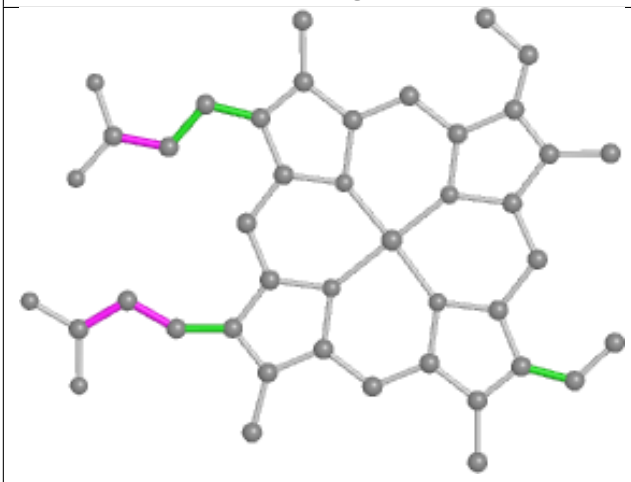
Ligand HEM C 380



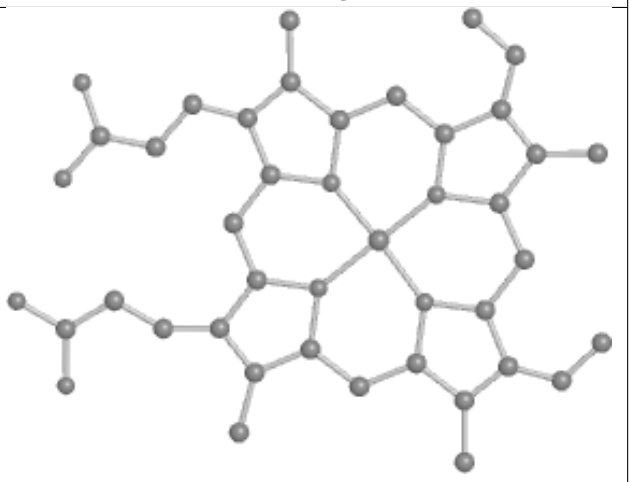
Bond lengths



Bond angles

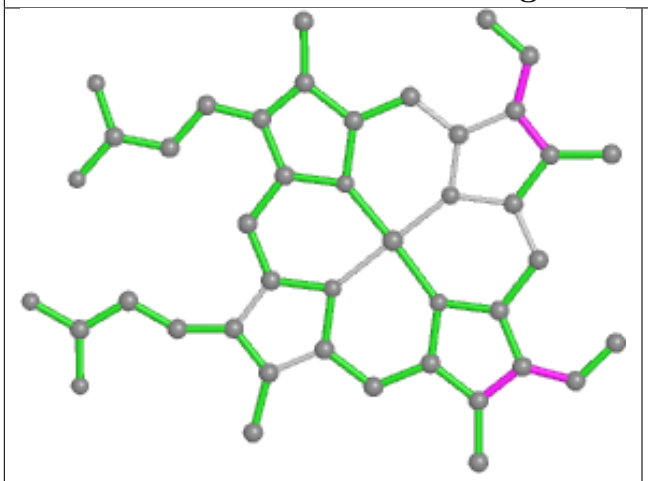


Torsions

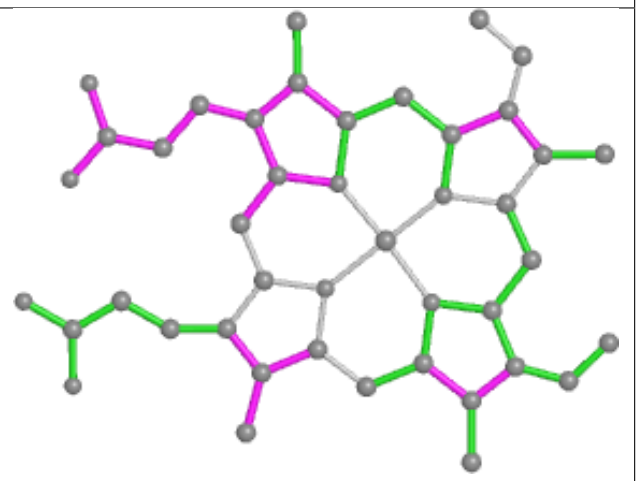


Rings

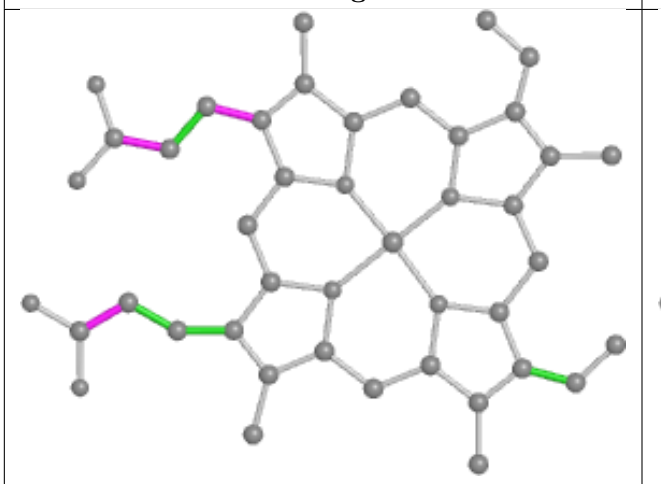
Ligand HEM C 381



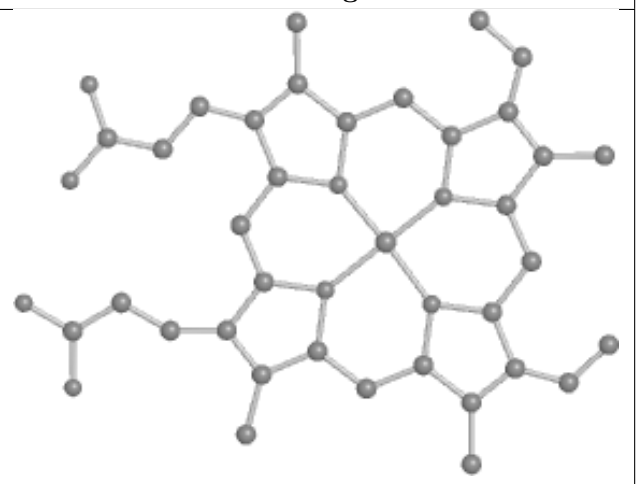
Bond lengths



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.