wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2021 – 05:56 AM EDT

PDB ID	:	1MG2
Title	:	MUTATION OF ALPHA PHE55 OF METHYLAMINE DEHYDROGENASE ALTERS THE REORGANIZATION ENERGY AND ELECTRONIC COUPLING FOR ITS ELECTRON TRANSFER REACTION WITH AMICYANIN
Authors	:	Sun, D.; Chen, Z.W.; Mathews, F.S.; Davidson, V.L.
Deposited on	:	2002-08-14
Resolution	:	2.25 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 following versions of software and data (see references (i)) were used in the production of this report:

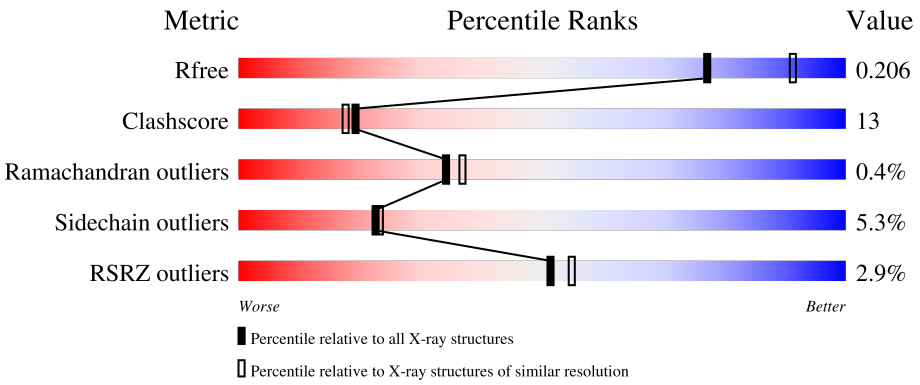
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.25 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))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	390	2% 73% 23% • •
1	E	390	2% 73% 23% • •
1	I	390	2% 75% 21% • •
1	M	390	2% 74% 22% • •
2	B	131	% 70% 22% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	131	%, 71%, 21%, 5%
2	J	131	%, 73%, 19%, 5%
2	N	131	%, 72%, 21%, 5%
3	C	105	8%, 77%, 23%
3	G	105	3%, 90%, 8%
3	K	105	2%, 80%, 20%
3	O	105	6%, 87%, 11%
4	D	155	%, 68%, 24%, 5%
4	H	155	7%, 73%, 19%, 5%
4	L	155	6%, 65%, 27%, 5%
4	P	155	6%, 66%, 26%, 5%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 25377 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 Methylamine dehydrogenase, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	382	2961	1872	509	572	8	0	0	0
1	E	382	2961	1872	509	572	8	0	0	0
1	I	382	2961	1872	509	572	8	0	0	0
1	M	382	2961	1872	509	572	8	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	ALA	PHE	engineered mutation	UNP P29894
A	312	PHE	LEU	SEE REMARK 999	UNP P29894
A	313	VAL	LEU	SEE REMARK 999	UNP P29894
E	55	ALA	PHE	engineered mutation	UNP P29894
E	312	PHE	LEU	SEE REMARK 999	UNP P29894
E	313	VAL	LEU	SEE REMARK 999	UNP P29894
I	55	ALA	PHE	engineered mutation	UNP P29894
I	312	PHE	LEU	SEE REMARK 999	UNP P29894
I	313	VAL	LEU	SEE REMARK 999	UNP P29894
M	55	ALA	PHE	engineered mutation	UNP P29894
M	312	PHE	LEU	SEE REMARK 999	UNP P29894
M	313	VAL	LEU	SEE REMARK 999	UNP P29894

- Molecule 2 is a protein called Methylamine dehydrogenase, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	125	956	590	161	192	13	0	0	0
2	F	125	956	590	161	192	13	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	J	125	956	590	161	192	13	0	0	0
2	N	125	956	590	161	192	13	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	57	TRQ	TRP	modified residue	UNP P22619
F	57	TRQ	TRP	modified residue	UNP P22619
J	57	TRQ	TRP	modified residue	UNP P22619
N	57	TRQ	TRP	modified residue	UNP P22619

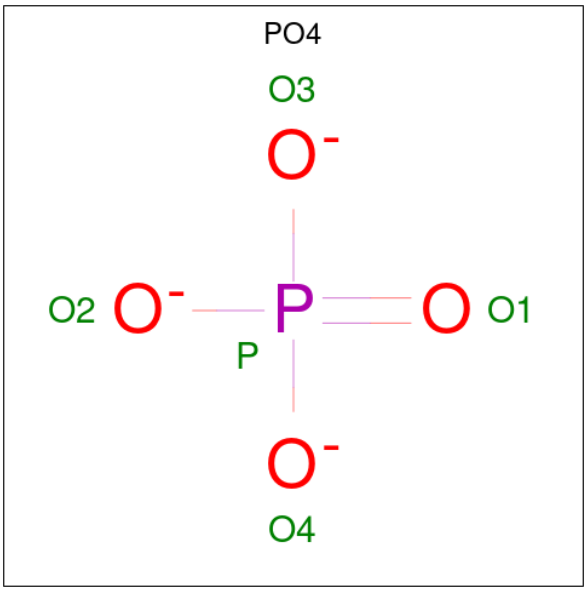
- Molecule 3 is a protein called Amicyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	105	807	516	133	152	6	0	0	0
3	G	105	807	516	133	152	6	0	0	0
3	K	105	807	516	133	152	6	0	0	0
3	O	105	807	516	133	152	6	0	0	0

- Molecule 4 is a protein called CYTOCHROME C-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	147	1144	724	182	230	8	0	0	0
4	H	147	1144	724	182	230	8	0	0	0
4	L	147	1144	724	182	230	8	0	0	0
4	P	147	1144	724	182	230	8	0	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	E	1	Total O P 5 4 1	0	0
5	F	1	Total O P 5 4 1	0	0
5	I	1	Total O P 5 4 1	0	0
5	J	1	Total O P 5 4 1	0	0
5	M	1	Total O P 5 4 1	0	0
5	N	1	Total O P 5 4 1	0	0

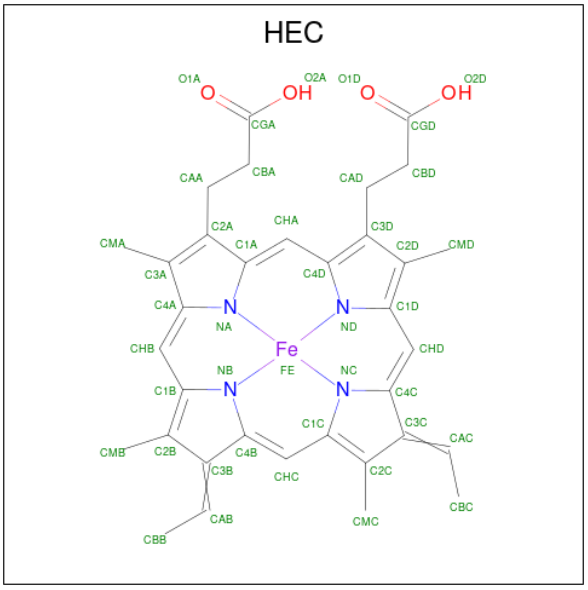
- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Cu 1 1	0	0
6	G	1	Total Cu 1 1	0	0
6	K	1	Total Cu 1 1	0	0
6	O	1	Total Cu 1 1	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total Na 1 1	0	0
7	H	1	Total Na 1 1	0	0
7	L	1	Total Na 1 1	0	0
7	P	1	Total Na 1 1	0	0

- Molecule 8 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total C Fe N O 43 34 1 4 4	0	0
8	H	1	Total C Fe N O 43 34 1 4 4	0	0
8	L	1	Total C Fe N O 43 34 1 4 4	0	0
8	P	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	218	Total O 218 218	0	0

Continued on next page...

Continued from previous page...

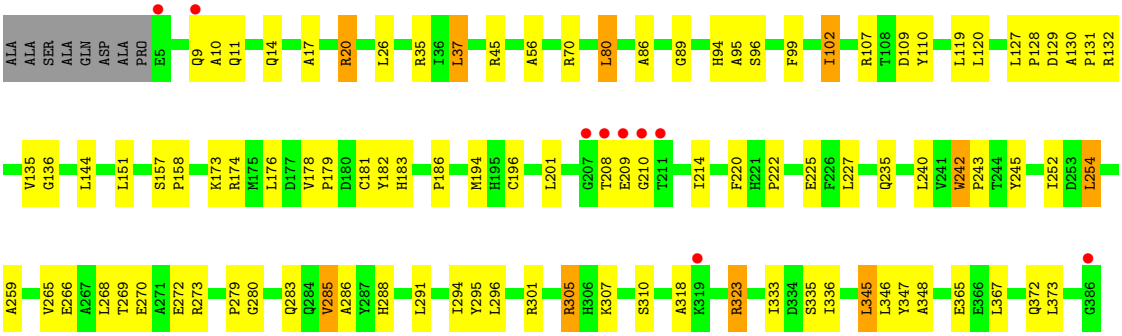
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	74	Total O 74 74	0	0
9	C	46	Total O 46 46	0	0
9	D	78	Total O 78 78	0	0
9	E	223	Total O 223 223	0	0
9	F	97	Total O 97 97	0	0
9	G	57	Total O 57 57	0	0
9	H	55	Total O 55 55	0	0
9	I	224	Total O 224 224	0	0
9	J	93	Total O 93 93	0	0
9	K	56	Total O 56 56	0	0
9	L	52	Total O 52 52	0	0
9	M	245	Total O 245 245	0	0
9	N	78	Total O 78 78	0	0
9	O	34	Total O 34 34	0	0
9	P	55	Total O 55 55	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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

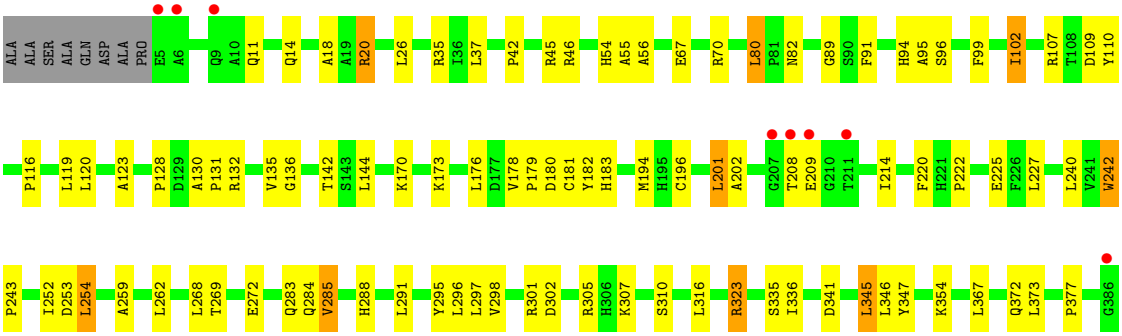
• Molecule 1: Methylamine dehydrogenase, heavy chain

Chain A:



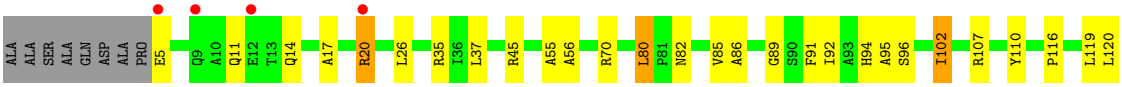
• Molecule 1: Methylamine dehydrogenase, heavy chain

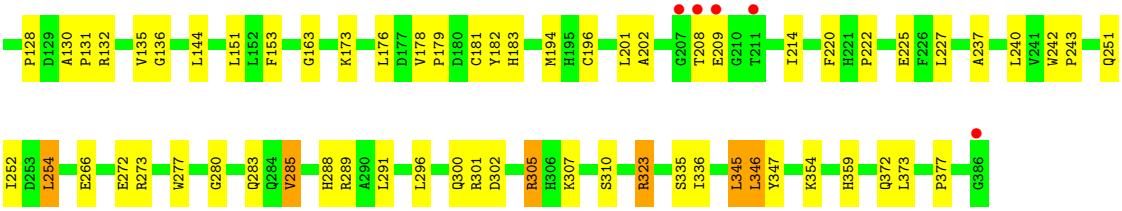
Chain E:



• Molecule 1: Methylamine dehydrogenase, heavy chain

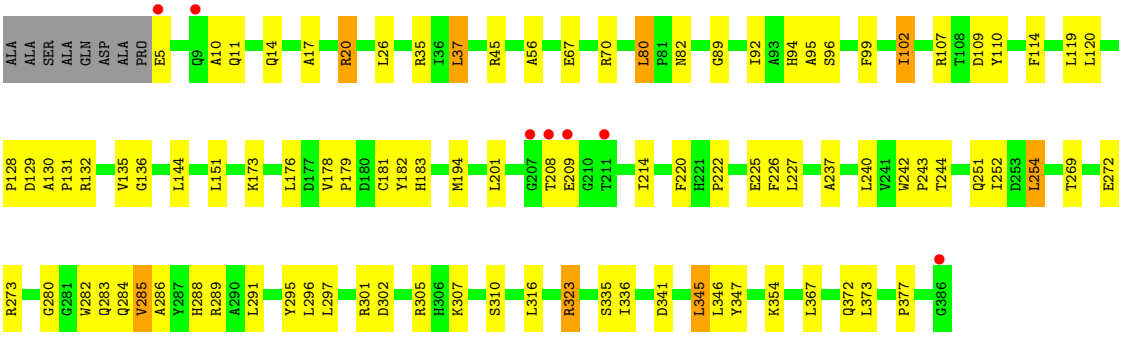
Chain I:





• Molecule 1: Methylamine dehydrogenase, heavy chain

Chain M:

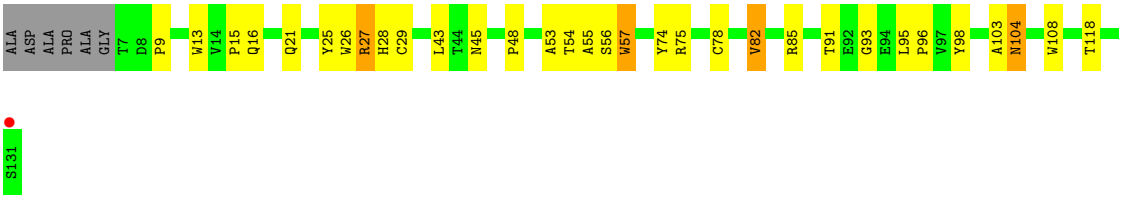


• Molecule 2: Methylamine dehydrogenase, light chain

Chain B:

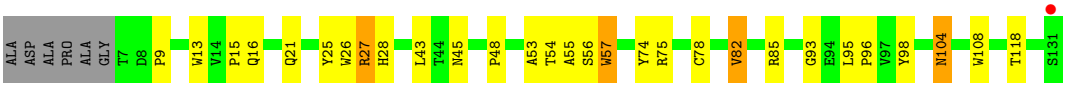
• Molecule 2: Methylamine dehydrogenase, light chain

Chain F:



• Molecule 2: Methylamine dehydrogenase, light chain

Chain J:



• Molecule 2: Methylamine dehydrogenase, light chain

Chain N: %
72% 21% • 5%

ALA ASP ALA PRO ALA GLY T7 D8 P9 R10 A11 K12 W13 V14 P15 Q16 Q21 Y25 W26 R27 H28 C29 L43 T44 N45 P48 A53 T54 A55 S56 W57 Y74 R75 C78 V82 R85 G93 E94 L95 P96 W97 Y98 N104 W108 T118 S131

• Molecule 3: Amicyanin

Chain C: 8%
77% 23%

D1 K2 A3 T4 I5 P6 S7 E8 V16 A17 D18 K27 L35 H36 V37 K38 D41 I46 A59 G60 G63 E64 A65 A66 N71 N72 K73 Q76 S79 L80 T81 E84 D89 P94 E105

• Molecule 3: Amicyanin

Chain G: 3%
90% 8% •

D1 E8 P33 E34 L35 K38 V61 E64 P94 R99 G100 K101 E105

• Molecule 3: Amicyanin

Chain K: 2%
80% 20%

D1 K2 I5 E8 K27 M28 E31 T32 P33 E34 L35 V39 M51 L62 G63 E64 L67 K68 M71 E84 T93 P94 H95 P96 F97 N98 R99 E105

• Molecule 3: Amicyanin

Chain O: 6%
87% 11% •

D1 K2 A3 T4 I5 E8 D18 L35 H36 V37 K38 I46 N47 R48 A59 G60 E64 A65 A66 K73 Q76 T93 P94 K101 E105

• Molecule 4: CYTOCHROME C-L

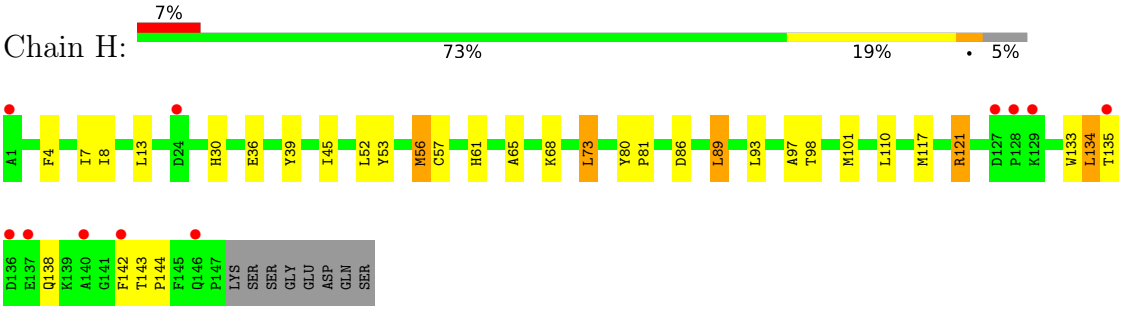
Chain D: %
68% 24% • 5%

A1 F4 L13 R23 D24 T25 V28 Y39 N40 E41 D42 P43 E44 I45 L46 P47 E48 A49 L52 Y53 C57 H61 K68 I69 L73 A76 Y80 P81 D86 L89 L93 T109 L110 D111 E112 M113 L114 R115 T116 M117 A118 W119 V120 R121

D127 P128 K129 D130 A131 S132 W133 L134 T135 K139 F142 P147 LYS SER SER GLY GLU ASP GLN SER

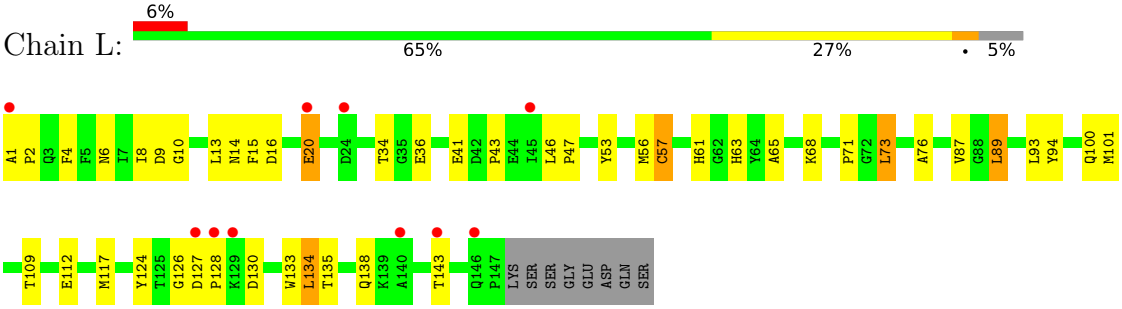
• Molecule 4: CYTOCHROME C-L

Chain H:



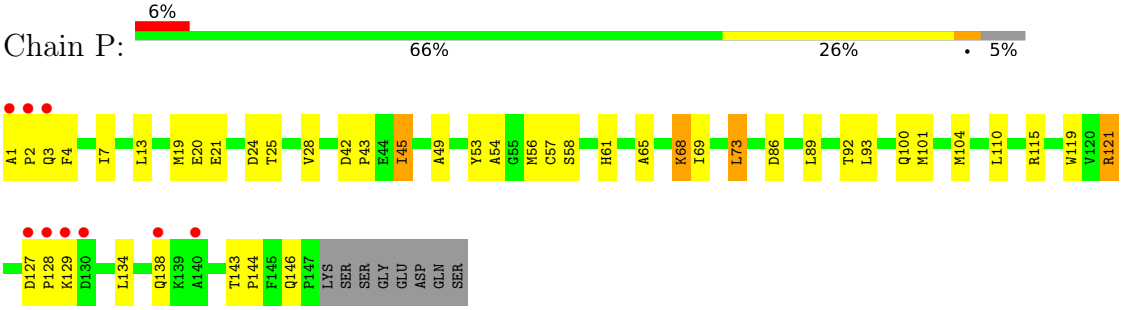
- Molecule 4: CYTOCHROME C-L

Chain L:



- Molecule 4: CYTOCHROME C-L

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.12Å 188.20Å 127.10Å 90.00° 99.24° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 48.91 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.9 (50.00-2.25) 83.5 (48.91-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.67 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.173 , 0.210 0.169 , 0.206	Depositor DCC
R_{free} test set	15487 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å^2)	17.8	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	25377	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: PO4, NA, HEC, TRQ, 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	0.32	0/3037	0.64	0/4139
1	E	0.32	0/3037	0.64	0/4139
1	I	0.34	0/3037	0.65	0/4139
1	M	0.33	0/3037	0.65	0/4139
2	B	0.34	0/964	0.61	0/1315
2	F	0.34	0/964	0.61	0/1315
2	J	0.34	0/964	0.61	0/1315
2	N	0.35	0/964	0.61	0/1315
3	C	0.33	0/828	0.56	0/1124
3	G	0.33	0/828	0.59	0/1124
3	K	0.34	0/828	0.61	0/1124
3	O	0.32	0/828	0.59	0/1124
4	D	0.37	0/1179	0.65	1/1605 (0.1%)
4	H	0.36	0/1179	0.67	1/1605 (0.1%)
4	L	0.35	1/1179 (0.1%)	0.63	1/1605 (0.1%)
4	P	0.35	1/1179 (0.1%)	0.63	1/1605 (0.1%)
All	All	0.34	2/24032 (0.0%)	0.63	4/32732 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	61	HIS	CE1-NE2	5.49	1.45	1.32
4	L	61	HIS	CE1-NE2	5.26	1.44	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	61	HIS	ND1-CG-CD2	8.07	120.10	108.80
4	P	61	HIS	ND1-CG-CD2	8.07	120.09	108.80
4	D	61	HIS	ND1-CG-CD2	8.03	120.03	108.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	61	HIS	ND1-CG-CD2	7.95	119.93	108.80

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	2961	0	2843	90	0
1	E	2961	0	2843	82	0
1	I	2961	0	2843	78	0
1	M	2961	0	2843	89	0
2	B	956	0	869	35	0
2	F	956	0	869	33	0
2	J	956	0	869	32	0
2	N	956	0	869	34	0
3	C	807	0	794	15	0
3	G	807	0	794	7	0
3	K	807	0	794	16	0
3	O	807	0	794	11	0
4	D	1144	0	1038	26	0
4	H	1144	0	1038	23	0
4	L	1144	0	1038	31	0
4	P	1144	0	1038	29	0
5	A	5	0	0	1	0
5	B	5	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
5	I	5	0	0	1	0
5	J	5	0	0	1	0
5	M	5	0	0	0	0
5	N	5	0	0	0	0
6	C	1	0	0	0	0
6	G	1	0	0	0	0
6	K	1	0	0	0	0
6	O	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1	0	0	0	0
7	H	1	0	0	0	0
7	L	1	0	0	0	0
7	P	1	0	0	0	0
8	D	43	0	30	1	0
8	H	43	0	30	4	0
8	L	43	0	30	2	0
8	P	43	0	30	4	0
9	A	218	0	0	8	0
9	B	74	0	0	2	0
9	C	46	0	0	0	0
9	D	78	0	0	0	0
9	E	223	0	0	5	0
9	F	97	0	0	2	0
9	G	57	0	0	1	0
9	H	55	0	0	2	0
9	I	224	0	0	6	0
9	J	93	0	0	2	0
9	K	56	0	0	2	0
9	L	52	0	0	2	0
9	M	245	0	0	4	0
9	N	78	0	0	2	0
9	O	34	0	0	0	0
9	P	55	0	0	0	0
All	All	25377	0	22296	564	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 13.

The worst 5 of 564 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:I:20:ARG:HB2	1:I:20:ARG:HH21	1.20	1.05
4:H:7:ILE:HG13	4:H:8:ILE:HD12	1.38	1.03
1:A:20:ARG:HB2	1:A:20:ARG:HH21	1.20	1.00
2:J:21:GLN:HE22	1:M:11:GLN:HG3	1.22	1.00
2:N:25:TYR:CE2	2:N:27:ARG:HG3	2.00	0.96

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	380/390 (97%)	364 (96%)	15 (4%)	1 (0%)	41	46
1	E	380/390 (97%)	365 (96%)	14 (4%)	1 (0%)	41	46
1	I	380/390 (97%)	365 (96%)	14 (4%)	1 (0%)	41	46
1	M	380/390 (97%)	367 (97%)	12 (3%)	1 (0%)	41	46
2	B	122/131 (93%)	118 (97%)	4 (3%)	0	100	100
2	F	122/131 (93%)	118 (97%)	4 (3%)	0	100	100
2	J	122/131 (93%)	118 (97%)	4 (3%)	0	100	100
2	N	122/131 (93%)	116 (95%)	6 (5%)	0	100	100
3	C	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
3	G	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
3	K	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
3	O	103/105 (98%)	97 (94%)	5 (5%)	1 (1%)	15	13
4	D	145/155 (94%)	139 (96%)	5 (3%)	1 (1%)	22	21
4	H	145/155 (94%)	133 (92%)	11 (8%)	1 (1%)	22	21
4	L	145/155 (94%)	136 (94%)	7 (5%)	2 (1%)	11	7
4	P	145/155 (94%)	134 (92%)	9 (6%)	2 (1%)	11	7
All	All	3000/3124 (96%)	2872 (96%)	117 (4%)	11 (0%)	34	37

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	68	LYS
4	H	68	LYS
4	L	10	GLY
4	P	68	LYS
1	A	102	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	307/311 (99%)	290 (94%)	17 (6%)	21	21
1	E	307/311 (99%)	289 (94%)	18 (6%)	19	19
1	I	307/311 (99%)	292 (95%)	15 (5%)	25	27
1	M	307/311 (99%)	291 (95%)	16 (5%)	23	24
2	B	104/106 (98%)	98 (94%)	6 (6%)	20	20
2	F	104/106 (98%)	98 (94%)	6 (6%)	20	20
2	J	104/106 (98%)	99 (95%)	5 (5%)	25	28
2	N	104/106 (98%)	98 (94%)	6 (6%)	20	20
3	C	85/85 (100%)	81 (95%)	4 (5%)	26	29
3	G	85/85 (100%)	81 (95%)	4 (5%)	26	29
3	K	85/85 (100%)	83 (98%)	2 (2%)	49	58
3	O	85/85 (100%)	82 (96%)	3 (4%)	36	43
4	D	118/125 (94%)	111 (94%)	7 (6%)	19	19
4	H	118/125 (94%)	111 (94%)	7 (6%)	19	19
4	L	118/125 (94%)	110 (93%)	8 (7%)	16	14
4	P	118/125 (94%)	111 (94%)	7 (6%)	19	19
All	All	2456/2508 (98%)	2325 (95%)	131 (5%)	22	23

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	16	GLN
2	N	82	VAL
4	P	121	ARG
1	E	345	LEU
1	E	323	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	82	ASN
4	L	3	GLN
4	P	30	HIS
1	I	284	GLN
2	J	34	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)

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
2	TRQ	F	57	2	13,17,18	4.64	3 (23%)	14,24,26	2.26	5 (35%)
2	TRQ	B	57	2	13,17,18	4.64	3 (23%)	14,24,26	2.28	5 (35%)
2	TRQ	J	57	2	13,17,18	4.64	3 (23%)	14,24,26	2.27	5 (35%)
2	TRQ	N	57	2	13,17,18	4.72	3 (23%)	14,24,26	2.25	4 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRQ	F	57	2	-	0/4/19/21	0/2/2/2
2	TRQ	B	57	2	-	0/4/19/21	0/2/2/2
2	TRQ	J	57	2	-	0/4/19/21	0/2/2/2
2	TRQ	N	57	2	-	0/4/19/21	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	57	TRQ	CH2-CZ2	-14.70	1.37	1.54
2	B	57	TRQ	CH2-CZ2	-14.54	1.37	1.54
2	J	57	TRQ	CH2-CZ2	-14.53	1.37	1.54
2	F	57	TRQ	CH2-CZ2	-14.47	1.37	1.54
2	N	57	TRQ	CE2-CZ2	-7.46	1.40	1.50

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	57	TRQ	CZ2-CE2-NE1	5.75	129.13	119.94
2	F	57	TRQ	CZ2-CE2-NE1	5.70	129.05	119.94
2	B	57	TRQ	CZ2-CE2-NE1	5.68	129.01	119.94
2	N	57	TRQ	CZ2-CE2-NE1	5.68	129.00	119.94
2	N	57	TRQ	O7-CZ2-CH2	3.84	123.52	119.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	57	TRQ	2	0
2	B	57	TRQ	3	0
2	J	57	TRQ	3	0
2	N	57	TRQ	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
5	PO4	J	403	-	4,4,4	1.69	1 (25%)	6,6,6	0.43	0
5	PO4	E	406	-	4,4,4	1.65	0	6,6,6	0.43	0
8	HEC	P	200	4	26,50,50	1.94	2 (7%)	18,82,82	1.76	7 (38%)
5	PO4	N	404	-	4,4,4	1.68	0	6,6,6	0.43	0
5	PO4	I	405	-	4,4,4	1.68	0	6,6,6	0.42	0
5	PO4	B	402	-	4,4,4	1.71	0	6,6,6	0.43	0
5	PO4	F	401	-	4,4,4	1.66	0	6,6,6	0.44	0
8	HEC	D	200	4	26,50,50	1.96	2 (7%)	18,82,82	1.93	7 (38%)
8	HEC	H	200	4	26,50,50	2.00	2 (7%)	18,82,82	1.69	7 (38%)
8	HEC	L	200	4	26,50,50	1.98	3 (11%)	18,82,82	1.88	7 (38%)
5	PO4	M	407	-	4,4,4	1.65	0	6,6,6	0.43	0
5	PO4	A	408	-	4,4,4	1.88	3 (75%)	6,6,6	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	HEC	P	200	4	-	0/6/54/54	-
8	HEC	D	200	4	-	0/6/54/54	-
8	HEC	H	200	4	-	0/6/54/54	-
8	HEC	L	200	4	-	0/6/54/54	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	200	HEC	C3C-C2C	-6.58	1.33	1.40
8	L	200	HEC	C3C-C2C	-6.46	1.34	1.40
8	P	200	HEC	C3C-C2C	-6.31	1.34	1.40
8	D	200	HEC	C3C-C2C	-6.17	1.34	1.40
8	D	200	HEC	C3B-C2B	-4.54	1.36	1.40

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	200	HEC	CBD-CAD-C3D	-4.14	104.84	112.49
8	L	200	HEC	CBD-CAD-C3D	-3.52	106.00	112.49
8	H	200	HEC	CMC-C2C-C3C	3.02	129.37	125.82
8	L	200	HEC	CAD-CBD-CGD	2.97	117.66	112.67
8	L	200	HEC	CMC-C2C-C3C	2.92	129.25	125.82

There are no chirality outliers.

There are no torsion outliers.

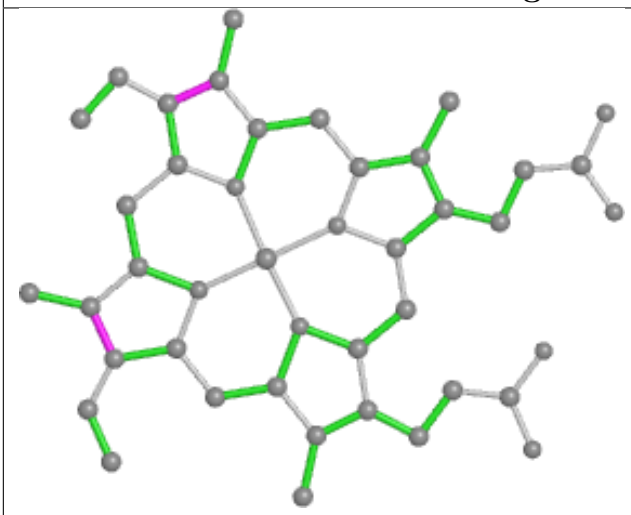
There are no ring outliers.

7 monomers are involved in 14 short contacts:

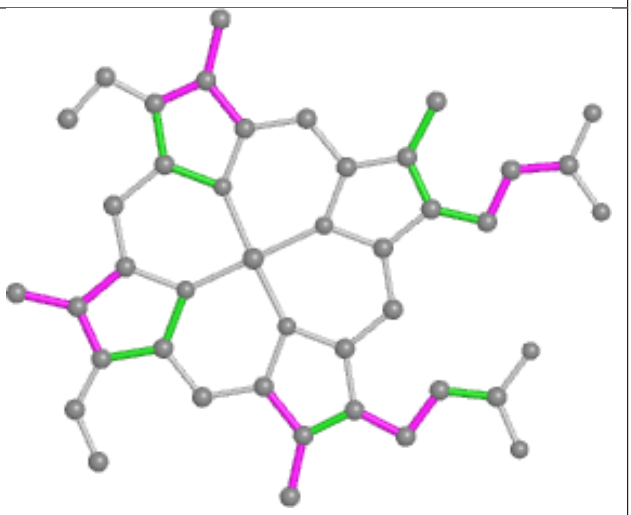
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	403	PO4	1	0
8	P	200	HEC	4	0
5	I	405	PO4	1	0
8	D	200	HEC	1	0
8	H	200	HEC	4	0
8	L	200	HEC	2	0
5	A	408	PO4	1	0

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.

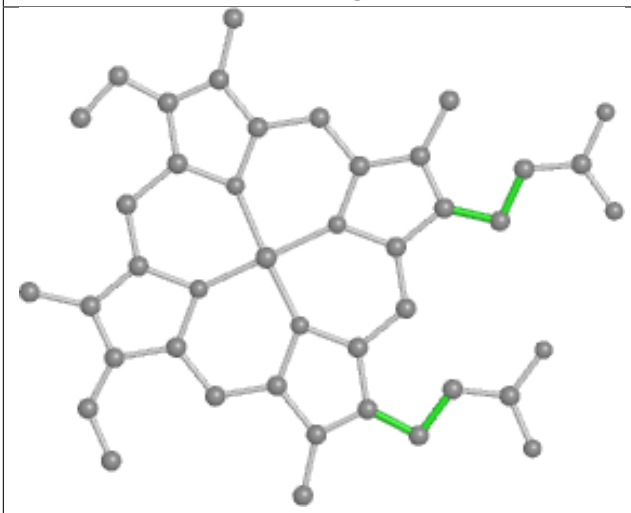
Ligand HEC P 200



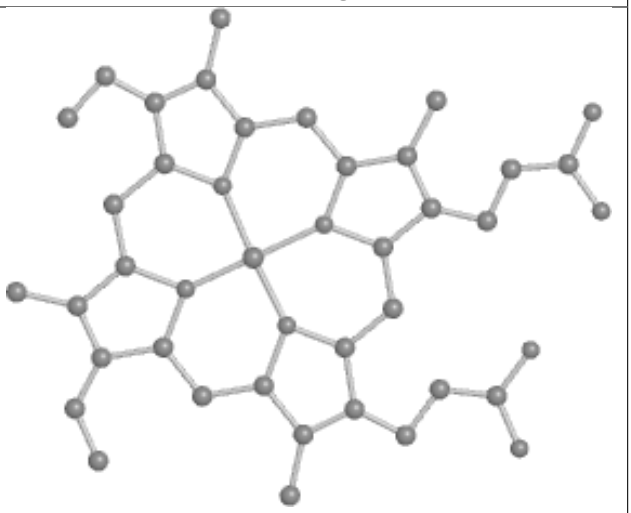
Bond lengths



Bond angles

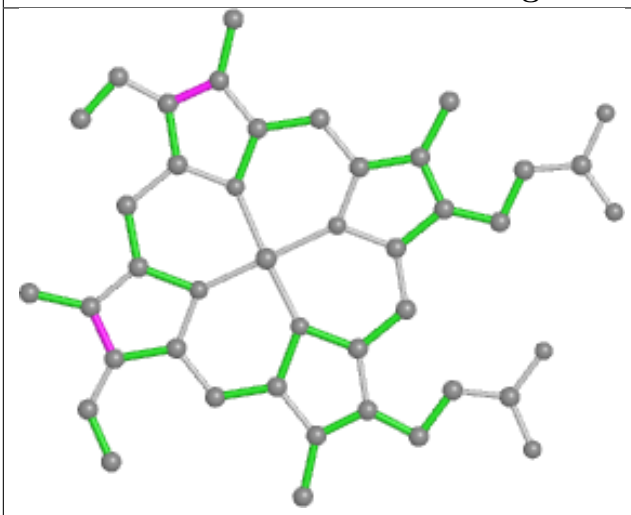


Torsions

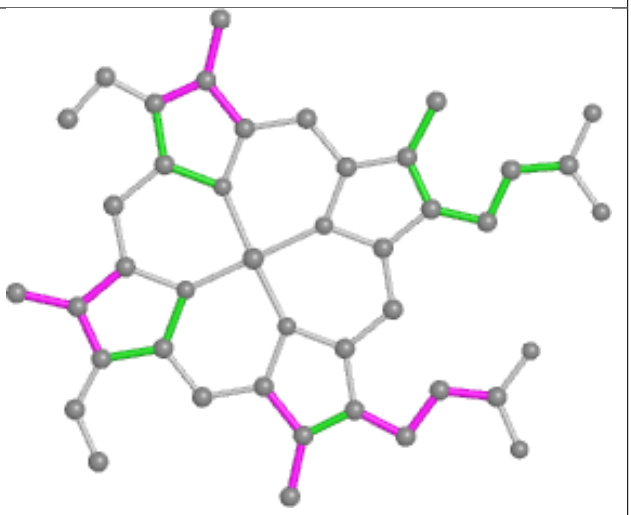


Rings

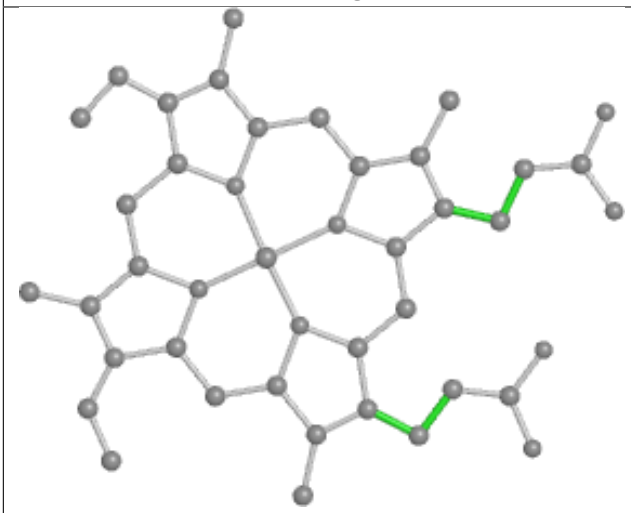
Ligand HEC D 200



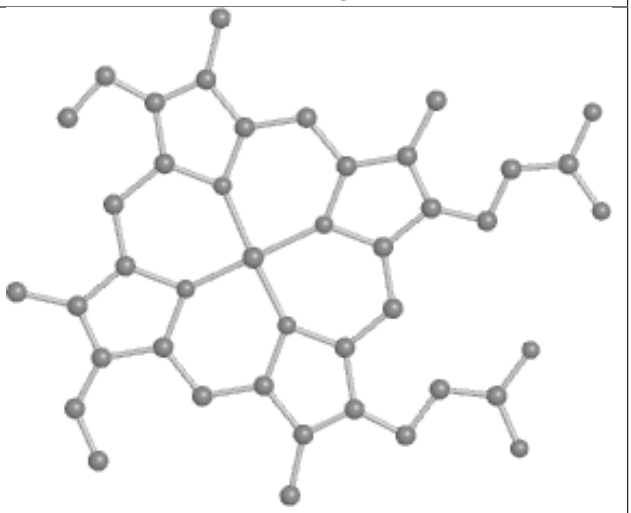
Bond lengths



Bond angles

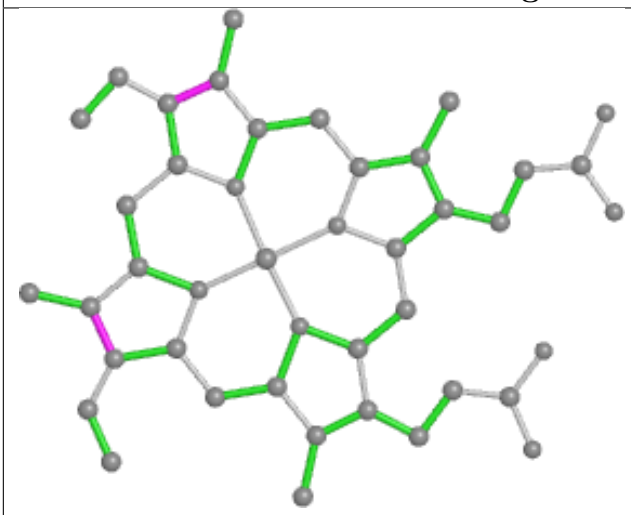


Torsions

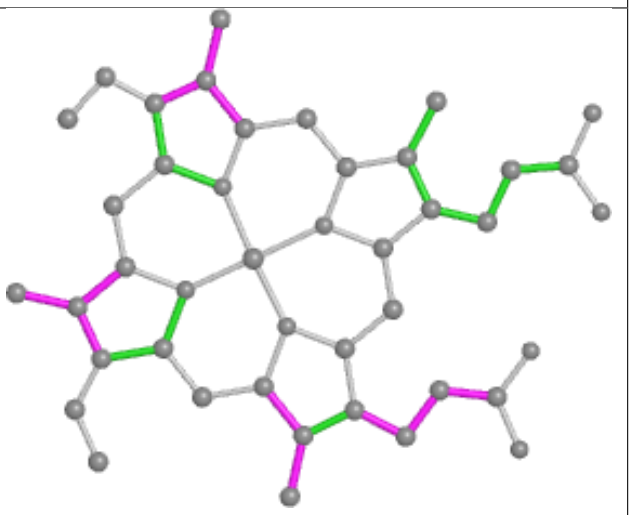


Rings

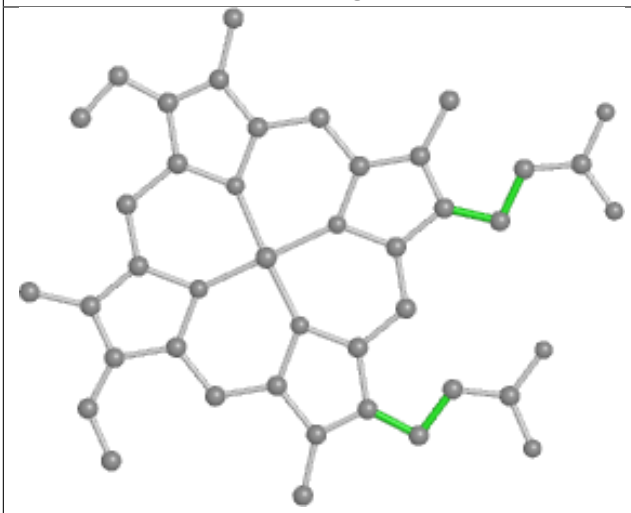
Ligand HEC H 200



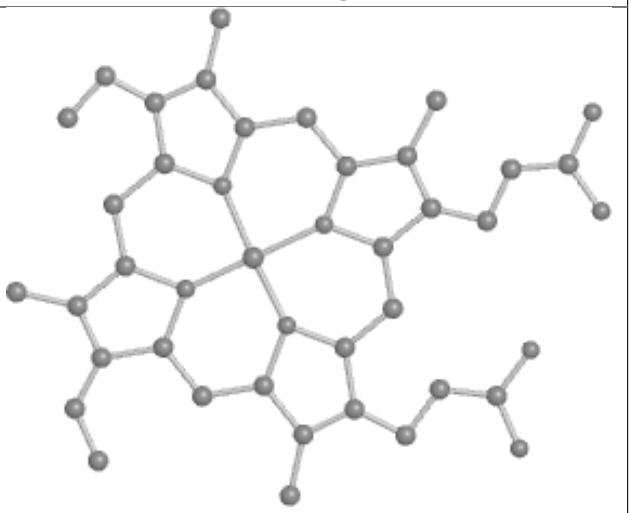
Bond lengths



Bond angles

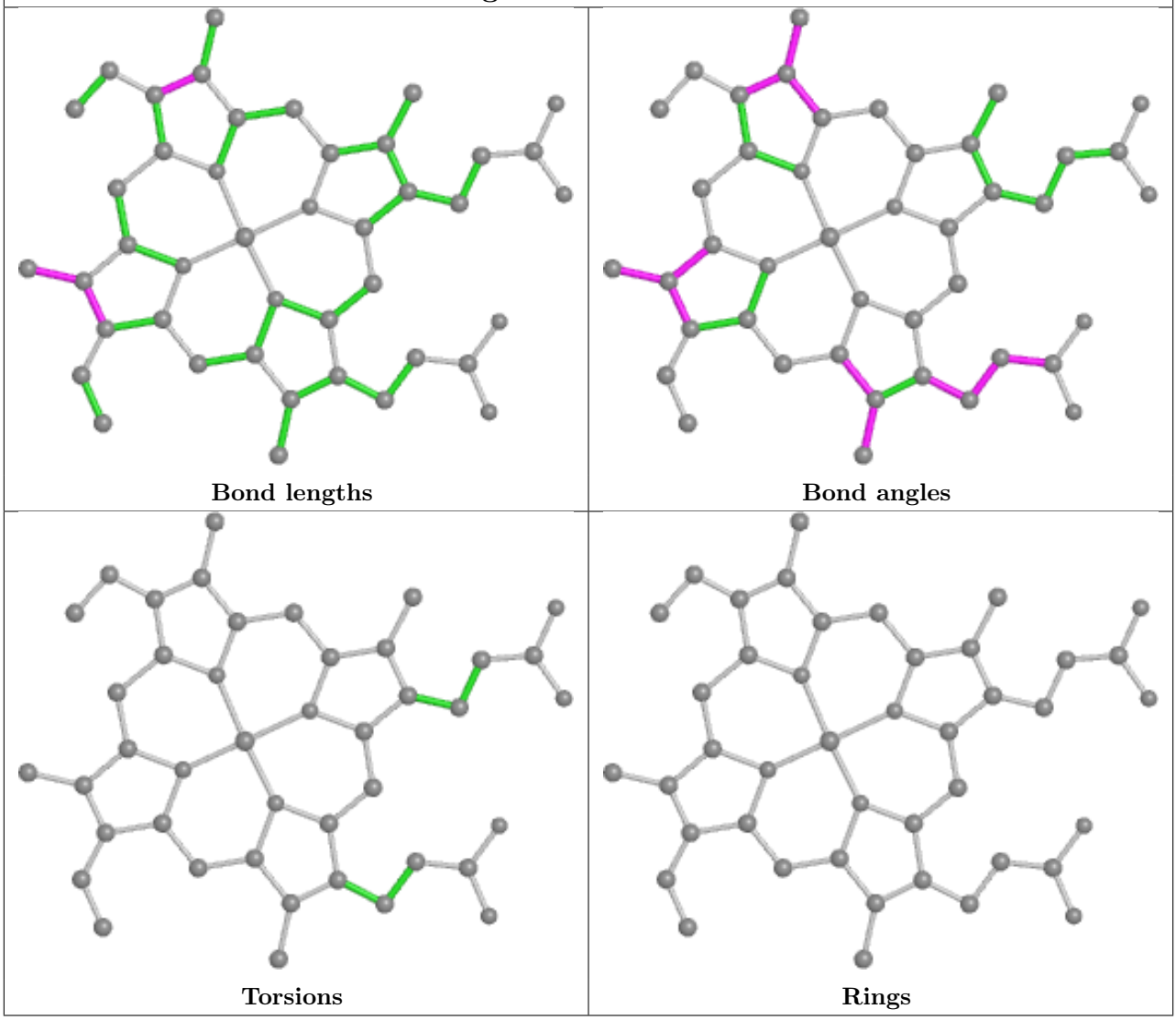


Torsions



Rings

Ligand HEC L 200



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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	382/390 (97%)	-0.19	9 (2%)	59	62	9, 19, 40, 77	0
1	E	382/390 (97%)	-0.17	8 (2%)	63	66	9, 19, 38, 74	0
1	I	382/390 (97%)	-0.26	9 (2%)	59	62	6, 17, 38, 74	0
1	M	382/390 (97%)	-0.24	7 (1%)	68	71	8, 18, 36, 74	0
2	B	124/131 (94%)	-0.23	1 (0%)	86	87	11, 17, 30, 68	0
2	F	124/131 (94%)	-0.25	1 (0%)	86	87	10, 15, 27, 69	0
2	J	124/131 (94%)	-0.23	1 (0%)	86	87	7, 15, 27, 68	0
2	N	124/131 (94%)	-0.25	1 (0%)	86	87	11, 18, 29, 68	0
3	C	105/105 (100%)	0.24	8 (7%)	13	15	16, 28, 52, 61	0
3	G	105/105 (100%)	-0.27	3 (2%)	51	55	12, 21, 32, 51	0
3	K	105/105 (100%)	-0.28	2 (1%)	66	69	10, 20, 33, 51	0
3	O	105/105 (100%)	0.14	6 (5%)	23	25	16, 28, 53, 66	0
4	D	147/155 (94%)	-0.28	2 (1%)	75	77	13, 22, 47, 59	0
4	H	147/155 (94%)	-0.02	11 (7%)	14	15	15, 26, 57, 70	0
4	L	147/155 (94%)	0.07	10 (6%)	17	18	15, 31, 50, 58	0
4	P	147/155 (94%)	0.07	9 (6%)	21	23	14, 28, 61, 82	0
All	All	3032/3124 (97%)	-0.16	88 (2%)	51	55	6, 20, 45, 82	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	131	SER	7.8
4	P	129	LYS	7.5
2	F	131	SER	6.2
1	E	386	GLY	6.1
1	E	5	GLU	5.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TRQ	B	57	16/17	0.96	0.11	14,16,19,23	0
2	TRQ	F	57	16/17	0.97	0.11	9,13,16,17	0
2	TRQ	J	57	16/17	0.97	0.10	10,13,15,18	0
2	TRQ	N	57	16/17	0.98	0.09	13,14,18,19	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PO4	M	407	5/5	0.73	0.35	76,76,79,81	0
5	PO4	A	408	5/5	0.76	0.25	51,54,57,58	0
5	PO4	N	404	5/5	0.81	0.28	78,78,81,81	0
5	PO4	J	403	5/5	0.88	0.22	63,64,66,66	0
5	PO4	E	406	5/5	0.88	0.24	69,70,72,73	0
5	PO4	I	405	5/5	0.88	0.23	65,68,69,70	0
5	PO4	F	401	5/5	0.93	0.22	66,67,68,68	0
5	PO4	B	402	5/5	0.97	0.15	51,52,53,54	0
7	NA	H	603	1/1	0.97	0.15	14,14,14,14	0
8	HEC	H	200	43/43	0.97	0.12	12,19,23,29	0
8	HEC	L	200	43/43	0.97	0.12	15,18,22,27	0
8	HEC	P	200	43/43	0.97	0.13	16,25,29,32	0
8	HEC	D	200	43/43	0.98	0.12	6,14,19,25	0
7	NA	L	601	1/1	0.99	0.14	13,13,13,13	0
7	NA	P	602	1/1	0.99	0.10	8,8,8,8	0
7	NA	D	604	1/1	0.99	0.09	22,22,22,22	0
6	CU	C	107	1/1	1.00	0.05	26,26,26,26	0
6	CU	G	107	1/1	1.00	0.07	19,19,19,19	0

Continued on next page...

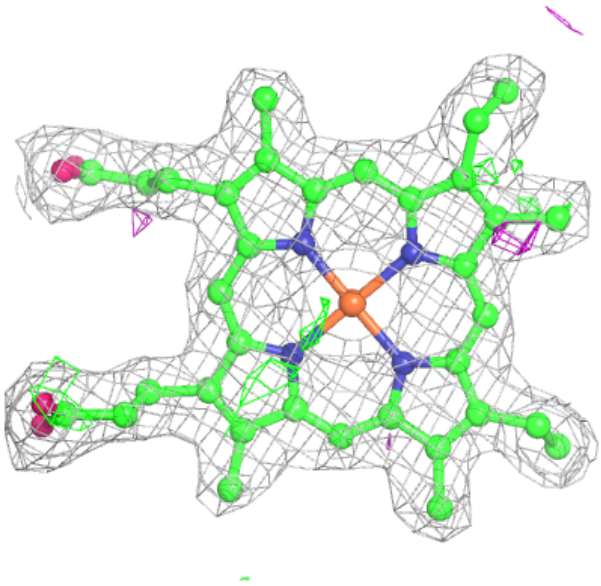
Continued from previous page...

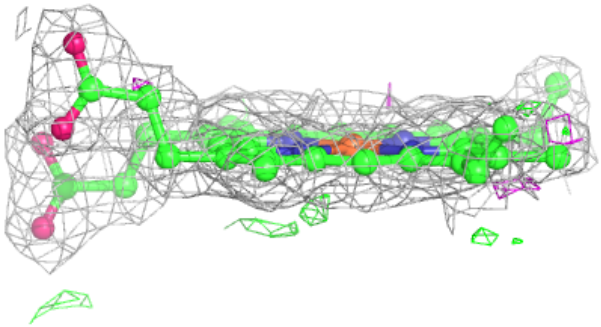
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CU	K	107	1/1	1.00	0.09	18,18,18,18	0
6	CU	O	107	1/1	1.00	0.06	29,29,29,29	0

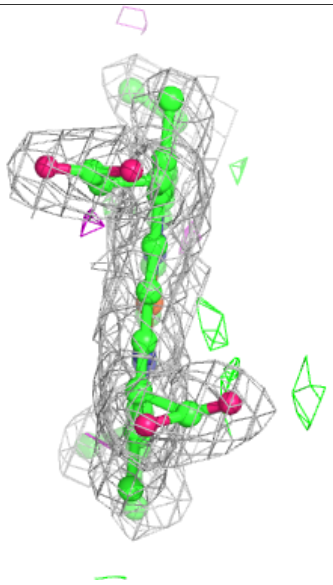
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEC H 200:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

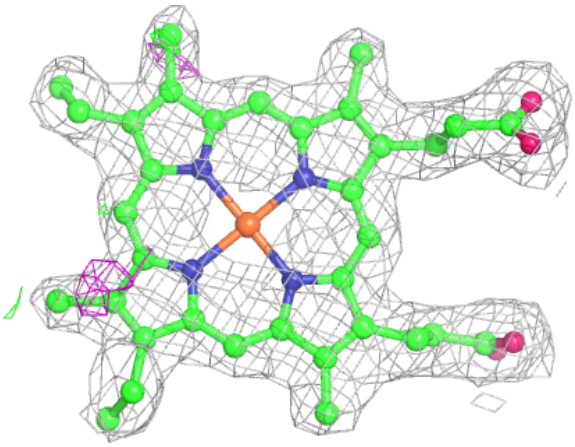


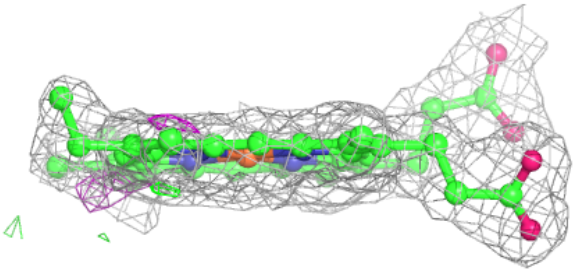


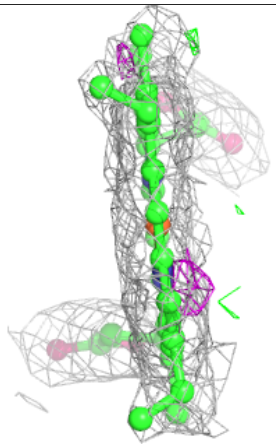


Electron density around HEC L 200:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

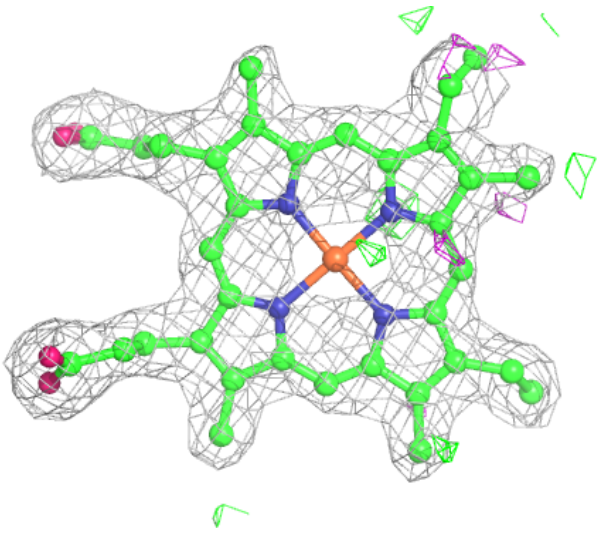


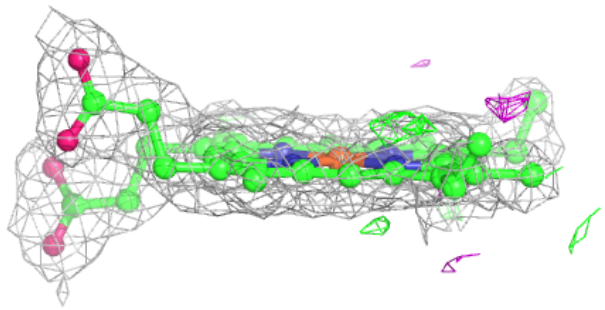




Electron density around HEC P 200:

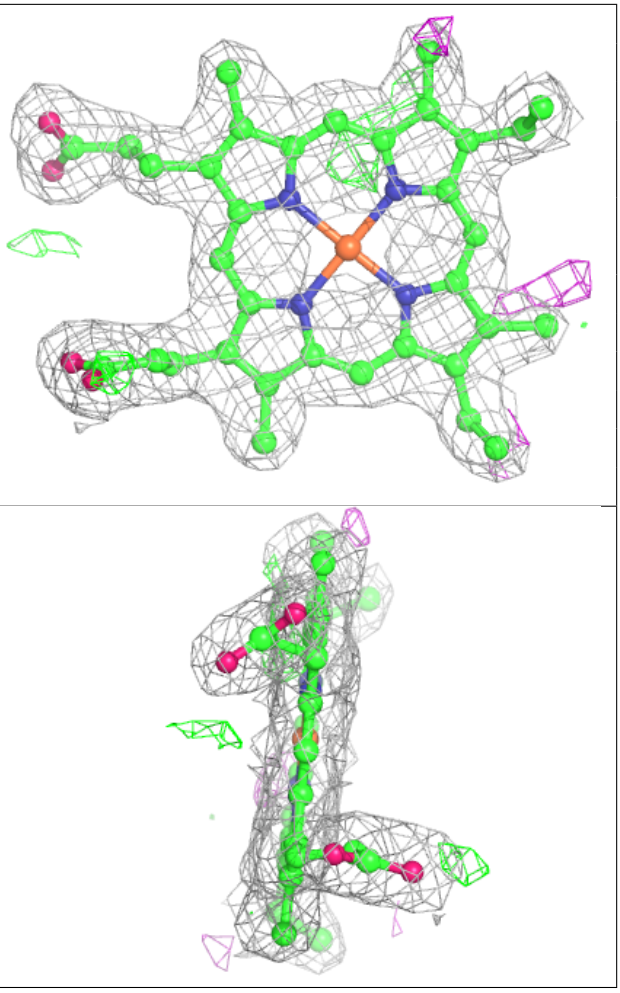
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around HEC D 200:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.