Full wwPDB X-ray Structure Validation Report (i)

Feb 6, 2024 – 09:54 AM EST

PDB ID	:	2CEP
Title	:	ROLE OF MET-230 IN INTRAMOLECULAR ELECTRON TRANSFER BETWEEN THE OXYFERRYL HEME AND TRP 191 IN CYTOCHROME C PEROXIDASE COMPOUND II
Authors	:	Han, G.W.; Miller, M.A.; Kraut, J.
Deposited on	:	1994-05-31
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

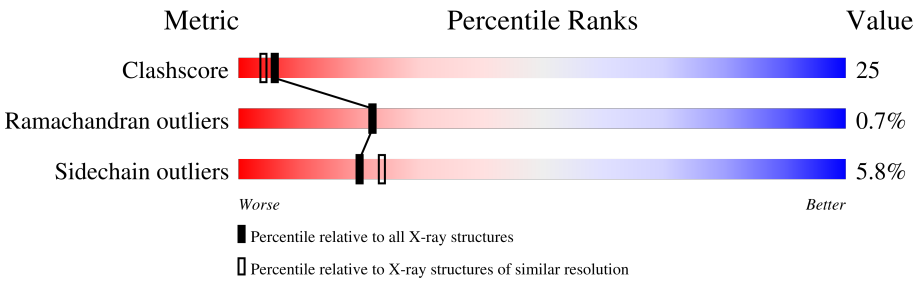
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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	296	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2607 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.

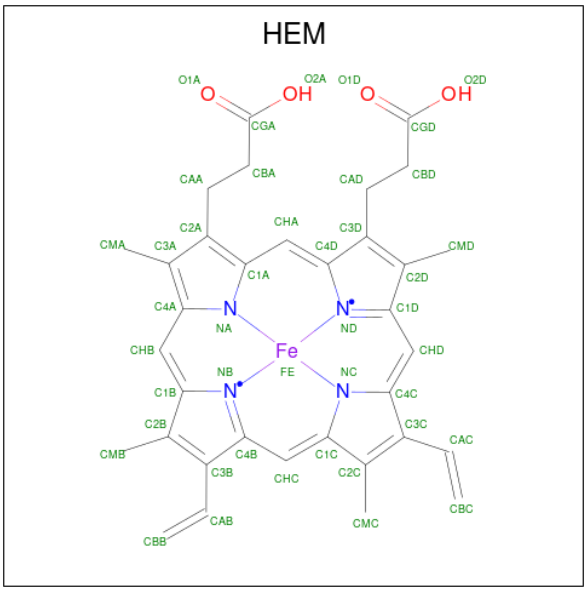
- Molecule 1 is a protein called CYTOCHROME C PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	293	2339	1497	386	451	5	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ILE	THR	conflict	UNP P00431
A	152	GLY	ASP	conflict	UNP P00431
A	230	ILE	MET	conflict	UNP P00431

- Molecule 2 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		
2	A	1	43	34	1	4	4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	225	225	225	0	0

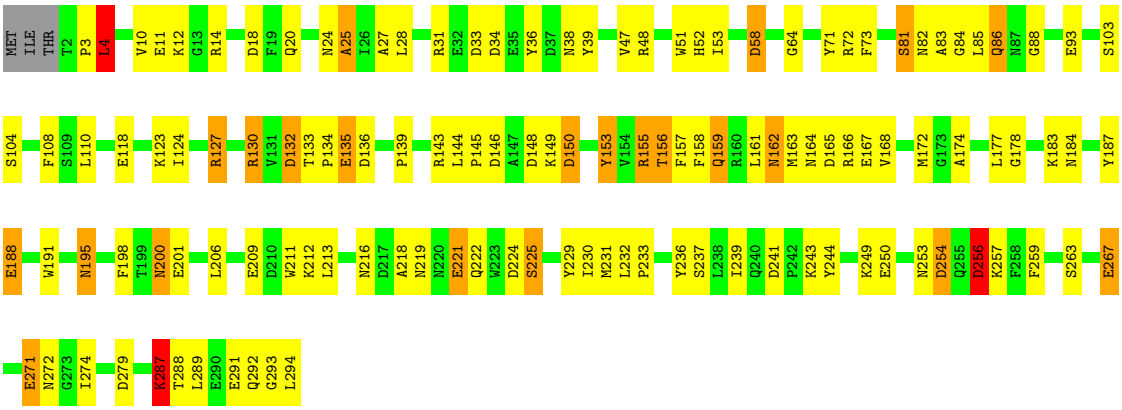
3 Residue-property plots (i)

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 C PEROXIDASE

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.00Å 74.20Å 45.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2607	wwPDB-VP
Average B, all atoms ($Å^2$)	27.0	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

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	1.12	1/2406 (0.0%)	2.04	66/3265 (2.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	GLU	CD-OE1	5.37	1.31	1.25

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	48	ARG	CD-NE-CZ	15.11	144.76	123.60
1	A	166	ARG	NE-CZ-NH1	14.81	127.70	120.30
1	A	143	ARG	NE-CZ-NH2	-14.25	113.17	120.30
1	A	48	ARG	NE-CZ-NH1	13.97	127.29	120.30
1	A	155	ARG	NE-CZ-NH2	12.93	126.77	120.30
1	A	14	ARG	NE-CZ-NH2	-11.63	114.48	120.30
1	A	136	ASP	CB-CG-OD1	11.33	128.49	118.30
1	A	155	ARG	NE-CZ-NH1	-11.25	114.67	120.30
1	A	165	ASP	CB-CG-OD1	11.20	128.38	118.30
1	A	132	ASP	CB-CG-OD1	11.13	128.32	118.30
1	A	165	ASP	CB-CG-OD2	-10.47	108.88	118.30
1	A	93	GLU	CA-CB-CG	9.94	135.26	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	130	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	A	14	ARG	NH1-CZ-NH2	8.88	129.17	119.40
1	A	143	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	A	14	ARG	NE-CZ-NH1	-8.47	116.06	120.30
1	A	256	ASP	CB-CG-OD2	-8.24	110.88	118.30
1	A	127	ARG	CD-NE-CZ	8.22	135.10	123.60
1	A	156	THR	CA-CB-CG2	8.02	123.63	112.40
1	A	279	ASP	CB-CG-OD1	7.57	125.11	118.30
1	A	18	ASP	CB-CG-OD2	7.24	124.81	118.30
1	A	130	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	136	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	A	132	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	A	224	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	4	LEU	CA-CB-CG	6.66	130.61	115.30
1	A	127	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	108	PHE	CB-CG-CD2	-6.37	116.34	120.80
1	A	153	TYR	CB-CG-CD2	-6.36	117.18	121.00
1	A	153	TYR	CB-CG-CD1	6.25	124.75	121.00
1	A	33	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	72	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	221	GLU	OE1-CD-OE2	6.14	130.66	123.30
1	A	254	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	231	MET	N-CA-CB	5.94	121.30	110.60
1	A	188	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	A	31	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	A	58	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	201	GLU	N-CA-CB	5.71	120.87	110.60
1	A	146	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	271	GLU	OE1-CD-OE2	-5.66	116.51	123.30
1	A	250	GLU	OE1-CD-OE2	5.66	130.09	123.30
1	A	36	TYR	CB-CG-CD2	-5.59	117.64	121.00
1	A	187	TYR	N-CA-CB	5.58	120.65	110.60
1	A	162	ASN	OD1-CG-ND2	5.57	134.72	121.90
1	A	225	SER	N-CA-CB	5.56	118.84	110.50
1	A	48	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	156	THR	CA-CB-OG1	-5.53	97.39	109.00
1	A	166	ARG	CD-NE-CZ	5.44	131.22	123.60
1	A	144	LEU	CB-CA-C	5.44	120.53	110.20
1	A	191	TRP	CB-CG-CD2	5.44	133.67	126.60
1	A	104	SER	N-CA-CB	-5.42	102.37	110.50
1	A	279	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	A	244	TYR	CB-CG-CD2	-5.36	117.78	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	31	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	287	LYS	CB-CA-C	-5.19	100.02	110.40
1	A	25	ALA	O-C-N	-5.17	114.43	122.70
1	A	110	LEU	CB-CG-CD2	-5.16	102.23	111.00
1	A	267	GLU	CA-CB-CG	-5.16	102.06	113.40
1	A	259	PHE	CB-CG-CD1	5.14	124.40	120.80
1	A	287	LYS	CD-CE-NZ	-5.07	100.04	111.70
1	A	47	VAL	CA-CB-CG2	-5.06	103.31	110.90
1	A	274	ILE	O-C-N	5.05	130.78	122.70
1	A	158	PHE	CA-C-N	-5.04	106.10	117.20
1	A	229	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	A	150	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	ALA	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	2339	0	2174	108	0
2	A	43	0	30	8	0
3	A	225	0	0	16	0
All	All	2607	0	2204	114	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 25.

All (114) 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:216:ASN:HD22	1:A:222:GLN:HE21	1.07	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLN:H	1:A:86:GLN:NE2	1.74	0.86
1:A:195:ASN:HD22	1:A:195:ASN:H	1.19	0.84
1:A:294:LEU:HB3	3:A:717:HOH:O	1.78	0.82
1:A:216:ASN:HD22	1:A:222:GLN:NE2	1.77	0.81
1:A:84:GLY:N	1:A:86:GLN:HE22	1.79	0.79
1:A:292:GLN:O	1:A:294:LEU:CD1	2.35	0.75
1:A:133:THR:HB	1:A:134:PRO:HD2	1.69	0.75
1:A:294:LEU:N	1:A:294:LEU:HD12	2.02	0.75
1:A:34:ASP:OD2	3:A:700:HOH:O	2.03	0.75
1:A:86:GLN:CG	3:A:708:HOH:O	2.38	0.71
1:A:73:PHE:CE2	1:A:135:GLU:HA	2.27	0.70
1:A:287:LYS:HZ2	1:A:287:LYS:CA	2.04	0.70
1:A:20:GLN:HE22	1:A:287:LYS:H	1.39	0.69
1:A:287:LYS:HZ2	1:A:287:LYS:HA	1.57	0.68
1:A:123:LYS:HE3	3:A:889:HOH:O	1.92	0.68
1:A:287:LYS:HZ2	1:A:287:LYS:CB	2.03	0.68
2:A:296:HEM:CMC	2:A:296:HEM:HBC2	2.23	0.67
1:A:293:GLY:C	1:A:294:LEU:HD12	2.16	0.67
1:A:294:LEU:CB	3:A:717:HOH:O	2.42	0.66
1:A:287:LYS:CA	1:A:287:LYS:NZ	2.59	0.65
1:A:294:LEU:CD1	1:A:294:LEU:N	2.59	0.65
1:A:195:ASN:HD22	1:A:195:ASN:N	1.93	0.65
1:A:294:LEU:CA	3:A:717:HOH:O	2.45	0.64
1:A:84:GLY:H	1:A:86:GLN:HE22	1.44	0.64
1:A:24:ASN:ND2	1:A:292:GLN:OE1	2.29	0.64
1:A:38:ASN:O	3:A:719:HOH:O	2.15	0.63
1:A:287:LYS:HA	1:A:287:LYS:NZ	2.15	0.62
1:A:86:GLN:HG2	3:A:708:HOH:O	1.99	0.61
1:A:159:GLN:NE2	1:A:159:GLN:HA	2.15	0.61
1:A:10:VAL:HG12	1:A:11:GLU:O	2.00	0.61
1:A:288:THR:OG1	1:A:291:GLU:HG3	2.01	0.60
1:A:84:GLY:N	1:A:86:GLN:NE2	2.50	0.60
1:A:287:LYS:CB	1:A:287:LYS:NZ	2.55	0.59
1:A:216:ASN:ND2	1:A:222:GLN:HE21	1.88	0.58
1:A:218:ALA:O	1:A:219:ASN:HB3	2.03	0.58
1:A:103:SER:HB2	1:A:132:ASP:OD1	2.03	0.58
1:A:164:ASN:O	1:A:168:VAL:HG23	2.03	0.58
1:A:86:GLN:H	1:A:86:GLN:HE21	1.51	0.57
1:A:213:LEU:HD11	1:A:221:GLU:HB3	1.87	0.57
1:A:267:GLU:OE2	1:A:271:GLU:OE2	2.21	0.57
1:A:86:GLN:CD	3:A:708:HOH:O	2.43	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLY:C	1:A:86:GLN:NE2	2.58	0.57
1:A:188:GLU:H	1:A:222:GLN:HE22	1.52	0.56
2:A:296:HEM:CBC	2:A:296:HEM:HMC1	2.34	0.56
1:A:200:ASN:HD22	1:A:200:ASN:N	2.04	0.56
1:A:156:THR:HG22	3:A:456:HOH:O	2.07	0.55
1:A:84:GLY:H	1:A:86:GLN:NE2	2.04	0.54
1:A:148:ASP:OD1	1:A:149:LYS:HE2	2.07	0.54
1:A:243:LYS:HD3	3:A:947:HOH:O	2.07	0.53
1:A:73:PHE:CD2	1:A:135:GLU:HA	2.44	0.53
1:A:292:GLN:CB	1:A:294:LEU:HD13	2.39	0.53
2:A:296:HEM:HBC2	2:A:296:HEM:HMC1	1.90	0.53
1:A:161:LEU:O	1:A:162:ASN:CB	2.57	0.52
2:A:296:HEM:CMC	2:A:296:HEM:CBC	2.87	0.52
1:A:127:ARG:O	1:A:130:ARG:NH1	2.37	0.52
2:A:296:HEM:HBB2	2:A:296:HEM:HMB1	1.92	0.51
1:A:85:LEU:N	1:A:86:GLN:NE2	2.58	0.51
1:A:218:ALA:O	1:A:219:ASN:CB	2.58	0.51
1:A:177:LEU:HD11	1:A:198:PHE:HD2	1.76	0.51
1:A:84:GLY:C	1:A:86:GLN:HE21	2.14	0.50
1:A:236:TYR:O	1:A:239:ILE:HG12	2.12	0.50
1:A:249:LYS:O	1:A:253:ASN:HB2	2.12	0.49
1:A:4:LEU:HD22	1:A:4:LEU:H	1.78	0.49
1:A:84:GLY:CA	1:A:86:GLN:NE2	2.76	0.49
1:A:123:LYS:CD	3:A:889:HOH:O	2.61	0.49
1:A:123:LYS:CE	3:A:889:HOH:O	2.56	0.48
1:A:241:ASP:OD1	1:A:243:LYS:HB2	2.13	0.48
1:A:3:PRO:O	1:A:4:LEU:C	2.52	0.48
1:A:53:ILE:HG22	1:A:71:TYR:HB2	1.94	0.48
1:A:287:LYS:HA	1:A:291:GLU:OE1	2.14	0.48
1:A:288:THR:N	1:A:291:GLU:OE1	2.43	0.48
1:A:58:ASP:OD1	1:A:58:ASP:C	2.50	0.47
1:A:232:LEU:HB3	1:A:233:PRO:HD2	1.97	0.47
1:A:27:ALA:HB1	1:A:289:LEU:HG	1.97	0.47
1:A:183:LYS:CG	3:A:483:HOH:O	2.62	0.46
1:A:86:GLN:NE2	1:A:86:GLN:N	2.54	0.46
1:A:150:ASP:O	1:A:153:TYR:HB3	2.16	0.46
1:A:145:PRO:HD3	1:A:157:PHE:CZ	2.51	0.46
1:A:85:LEU:O	1:A:88:GLY:N	2.44	0.46
1:A:195:ASN:H	1:A:195:ASN:ND2	2.00	0.45
1:A:177:LEU:HD11	1:A:198:PHE:CD2	2.52	0.45
1:A:52:HIS:HE1	1:A:81:SER:O	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLN:HE21	1:A:86:GLN:N	2.14	0.45
1:A:212:LYS:CB	3:A:812:HOH:O	2.64	0.45
1:A:10:VAL:HG12	1:A:11:GLU:N	2.32	0.45
1:A:124:ILE:CD1	1:A:263:SER:HA	2.47	0.44
2:A:296:HEM:HBB2	2:A:296:HEM:CMB	2.48	0.44
1:A:148:ASP:HA	1:A:233:PRO:HG2	1.99	0.44
1:A:163:MET:HA	1:A:167:GLU:OE1	2.17	0.44
1:A:10:VAL:CG1	1:A:11:GLU:N	2.81	0.44
1:A:292:GLN:O	1:A:294:LEU:HD11	2.18	0.44
1:A:178:GLY:HA3	2:A:296:HEM:O2D	2.18	0.43
1:A:200:ASN:C	1:A:200:ASN:ND2	2.72	0.43
1:A:209:GLU:HB2	1:A:211:TRP:CE2	2.54	0.43
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.69	0.43
1:A:292:GLN:C	1:A:294:LEU:HD13	2.38	0.43
1:A:271:GLU:O	1:A:272:ASN:C	2.57	0.43
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.76	0.43
1:A:212:LYS:HA	1:A:212:LYS:HD3	1.85	0.43
1:A:155:ARG:HH11	1:A:155:ARG:HD2	1.68	0.42
1:A:287:LYS:HZ3	1:A:287:LYS:HG2	1.07	0.42
1:A:172:MET:C	1:A:174:ALA:H	2.23	0.42
1:A:200:ASN:HD22	1:A:200:ASN:H	1.66	0.41
1:A:3:PRO:C	1:A:4:LEU:O	2.58	0.41
1:A:38:ASN:O	1:A:39:TYR:HB2	2.19	0.41
1:A:254:ASP:OD1	1:A:256:ASP:HB2	2.21	0.41
1:A:164:ASN:OD1	1:A:167:GLU:HG3	2.20	0.41
1:A:292:GLN:C	1:A:294:LEU:CD1	2.89	0.41
1:A:64:GLY:HA2	1:A:139:PRO:HG3	2.02	0.41
1:A:82:ASN:O	1:A:83:ALA:C	2.58	0.41
1:A:184:ASN:HB2	2:A:296:HEM:O1A	2.20	0.41
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.94	0.41
1:A:12:LYS:HB2	3:A:312:HOH:O	2.21	0.40

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	291/296 (98%)	284 (98%)	5 (2%)	2 (1%)	22 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	135	GLU

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	241/254 (95%)	227 (94%)	14 (6%)	20 23

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	51	TRP
1	A	81	SER
1	A	86	GLN
1	A	159	GLN
1	A	195	ASN
1	A	200	ASN
1	A	206	LEU
1	A	225	SER
1	A	230	ILE
1	A	237	SER
1	A	256	ASP
1	A	257	LYS
1	A	287	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	24	ASN
1	A	86	GLN
1	A	87	ASN
1	A	159	GLN
1	A	195	ASN
1	A	200	ASN
1	A	208	ASN
1	A	222	GLN
1	A	292	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	296	1,3	41,50,50	1.90	11 (26%)	45,82,82	2.05	15 (33%)

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	HEM	A	296	1,3	-	3/12/54/54	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	296	HEM	C3C-CAC	4.91	1.57	1.47
2	A	296	HEM	C3C-C2C	-4.01	1.34	1.40
2	A	296	HEM	CAA-C2A	3.28	1.56	1.52
2	A	296	HEM	C4A-NA	2.89	1.42	1.36
2	A	296	HEM	CMA-C3A	2.69	1.57	1.51
2	A	296	HEM	CMC-C2C	2.66	1.57	1.51
2	A	296	HEM	C1A-NA	2.58	1.41	1.36
2	A	296	HEM	CAB-C3B	2.56	1.54	1.47
2	A	296	HEM	C3B-C2B	-2.45	1.32	1.37
2	A	296	HEM	CMB-C2B	2.44	1.56	1.50
2	A	296	HEM	C1B-C2B	2.02	1.48	1.44

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	296	HEM	O1D-CGD-CBD	-5.36	105.87	123.08
2	A	296	HEM	O2D-CGD-O1D	4.95	135.63	123.30
2	A	296	HEM	C4B-CHC-C1C	3.50	127.18	122.56
2	A	296	HEM	CBA-CAA-C2A	3.23	118.13	112.62
2	A	296	HEM	CHB-C1B-NB	3.17	128.29	124.38
2	A	296	HEM	CHD-C1D-ND	3.09	127.79	124.43
2	A	296	HEM	CMA-C3A-C4A	-3.05	123.78	128.46
2	A	296	HEM	C2C-C3C-C4C	3.03	109.01	106.90
2	A	296	HEM	C1B-NB-C4B	2.84	108.00	105.07
2	A	296	HEM	C4D-ND-C1D	2.78	107.95	105.07
2	A	296	HEM	CMB-C2B-C1B	-2.64	121.02	125.04
2	A	296	HEM	C4C-CHD-C1D	-2.44	119.34	122.56
2	A	296	HEM	CMD-C2D-C1D	-2.18	121.72	125.04
2	A	296	HEM	CMD-C2D-C3D	2.08	131.75	126.12
2	A	296	HEM	CHC-C4B-NB	2.04	126.64	124.43

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	296	HEM	CAA-CBA-CGA-O1A
2	A	296	HEM	CAA-CBA-CGA-O2A
2	A	296	HEM	CAD-CBD-CGD-O2D

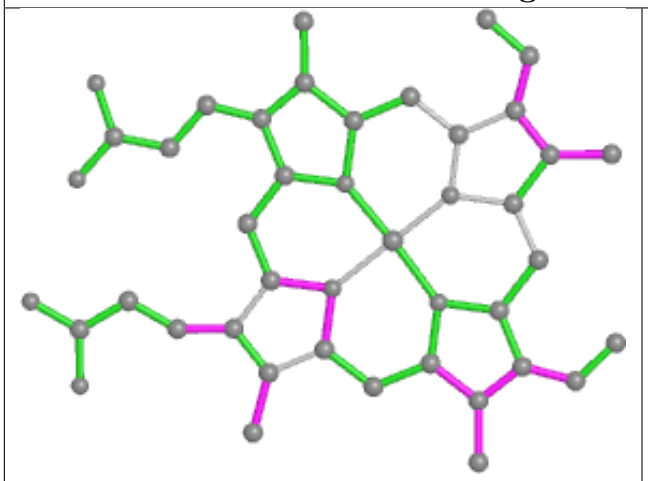
There are no ring outliers.

1 monomer is involved in 8 short contacts:

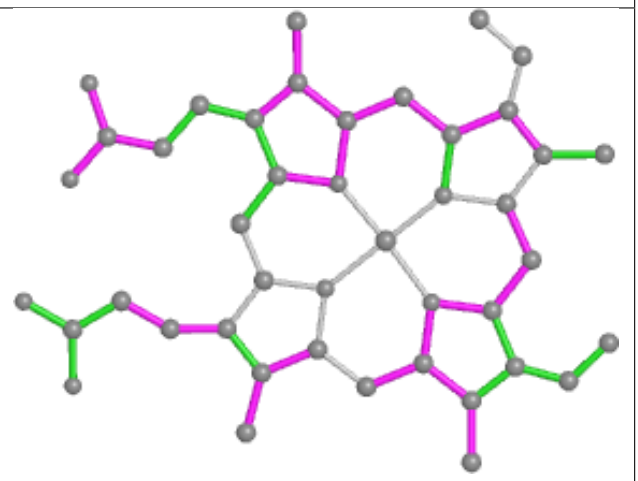
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	296	HEM	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

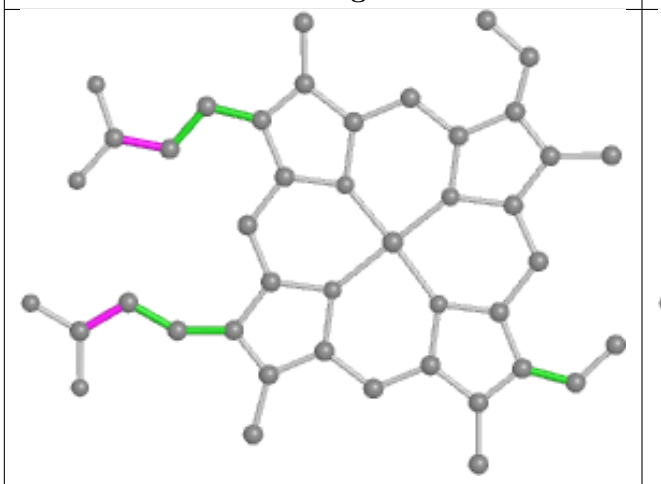
Ligand HEM A 296



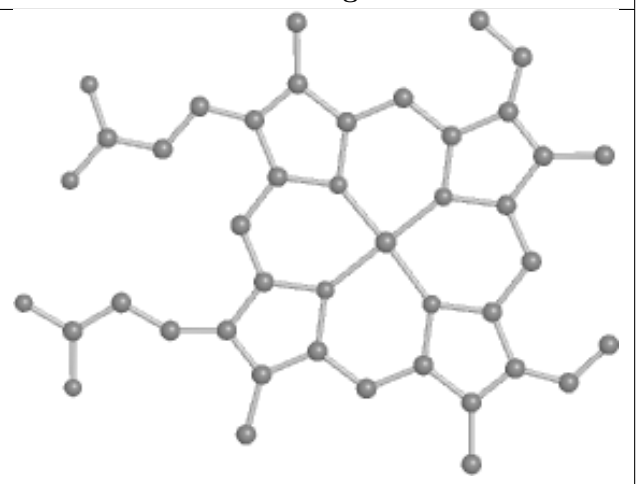
Bond lengths



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.