



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:56 PM UTC

PDB ID : 1CCE / pdb_00001cce
Title : CONSTRUCTION OF A BIS-AQUO HEME ENZYME AND REPLACEMENT WITH EXOGENOUS LIGAND
Authors : Mcree, D.E.; Jensen, G.M.; Fitzgerald, M.M.; Siegel, H.A.; Goodin, D.B.
Deposited on : 1994-05-04
Resolution : 2.30 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 ⓘ 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 ⓘ](#)) 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)	:	2.49

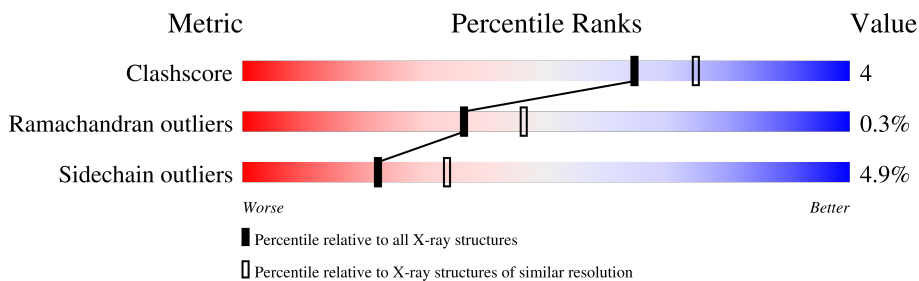
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	291	 70% 24% 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2976 atoms, of which 505 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.

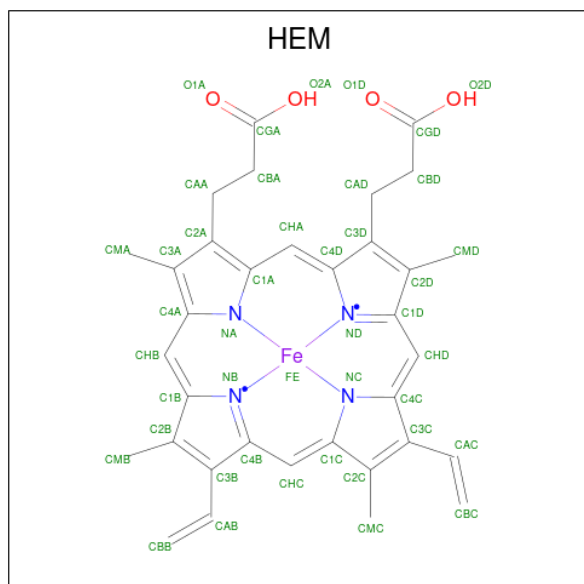
- Molecule 1 is a protein called CYTOCHROME C PEROXIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	291	Total	C	H	N	O	S	0	0	0
			2847	1497	505	388	451	6			

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	175	GLY	HIS	conflict	UNP P00431

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is water.

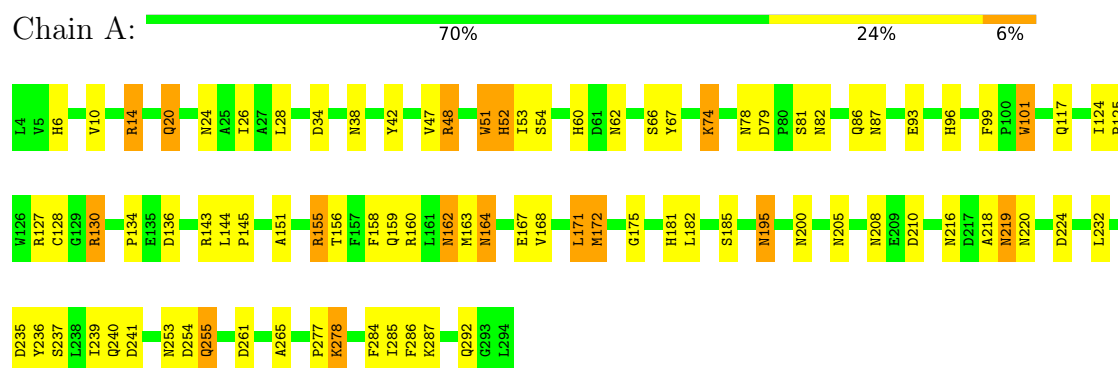
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	86	Total	O	0	0
			86	86		

3 Residue-property plots

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



4 Data and refinement statistics

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	105.20Å 74.30Å 45.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2976	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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

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	1.08	6/2407 (0.2%)	2.01	87/3258 (2.7%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	HIS	CD2-NE2	-7.06	1.30	1.37
1	A	26	ILE	CA-CB	6.84	1.62	1.54
1	A	181	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	60	HIS	CD2-NE2	-6.42	1.30	1.37
1	A	6	HIS	CD2-NE2	-6.30	1.30	1.37
1	A	52	HIS	CD2-NE2	-6.21	1.31	1.37

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	ASN	CA-CB-CG	12.10	124.70	112.60
1	A	78	ASN	OD1-CG-ND2	-11.12	111.48	122.60
1	A	159	GLN	OE1-CD-NE2	-10.55	112.05	122.60
1	A	62	ASN	OD1-CG-ND2	-9.45	113.15	122.60
1	A	210	ASP	CA-CB-CG	9.38	121.98	112.60
1	A	195	ASN	CA-CB-CG	8.92	121.52	112.60
1	A	253	ASN	OD1-CG-ND2	-8.67	113.93	122.60
1	A	195	ASN	N-CA-C	8.52	125.13	113.37
1	A	82	ASN	OD1-CG-ND2	-8.31	114.29	122.60
1	A	278	LYS	CA-CB-CG	-8.20	97.71	114.10
1	A	34	ASP	CA-CB-CG	8.01	120.61	112.60
1	A	124	ILE	O-C-N	-7.90	116.39	121.37
1	A	208	ASN	OD1-CG-ND2	-7.88	114.72	122.60
1	A	265	ALA	N-CA-C	7.86	119.93	111.36
1	A	195	ASN	OD1-CG-ND2	-7.55	115.05	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	GLN	OE1-CD-NE2	-7.31	115.29	122.60
1	A	130	ARG	NE-CZ-NH2	-7.19	112.73	119.20
1	A	155	ARG	NE-CZ-NH2	-7.13	112.78	119.20
1	A	205	ASN	OD1-CG-ND2	-7.01	115.59	122.60
1	A	216	ASN	CA-CB-CG	6.97	119.57	112.60
1	A	52	HIS	N-CA-C	6.67	119.56	111.82
1	A	66	SER	N-CA-C	6.67	121.16	112.89
1	A	175	GLY	O-C-N	-6.66	114.32	122.71
1	A	172	MET	CG-SD-CE	-6.65	86.27	100.90
1	A	155	ARG	NE-CZ-NH1	6.64	128.14	121.50
1	A	78	ASN	CB-CG-ND2	6.50	126.16	116.40
1	A	86	GLN	OE1-CD-NE2	-6.44	116.16	122.60
1	A	20	GLN	OE1-CD-NE2	-6.41	116.19	122.60
1	A	164	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	A	24	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	A	67	TYR	N-CA-C	6.38	118.81	111.02
1	A	240	GLN	OE1-CD-NE2	-6.36	116.24	122.60
1	A	145	PRO	N-CA-C	6.35	122.17	111.32
1	A	195	ASN	CB-CG-ND2	6.24	125.76	116.40
1	A	181	HIS	CB-CG-CD2	-6.14	123.21	131.20
1	A	38	ASN	CA-CB-CG	-6.11	106.49	112.60
1	A	14	ARG	CB-CG-CD	6.10	125.33	111.30
1	A	117	GLN	CG-CD-NE2	6.06	125.48	116.40
1	A	136	ASP	CA-CB-CG	6.05	118.65	112.60
1	A	130	ARG	NE-CZ-NH1	6.03	127.53	121.50
1	A	255	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	A	162	ASN	N-CA-C	5.97	123.52	110.80
1	A	220	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	A	87	ASN	OD1-CG-ND2	-5.86	116.75	122.60
1	A	48	ARG	CB-CG-CD	5.85	124.76	111.30
1	A	99	PHE	CA-C-N	5.84	125.94	119.87
1	A	99	PHE	C-N-CA	5.84	125.94	119.87
1	A	160	ARG	CB-CG-CD	5.82	124.69	111.30
1	A	62	ASN	CB-CG-ND2	5.81	125.11	116.40
1	A	185	SER	N-CA-C	5.80	121.26	113.72
1	A	261	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	130	ARG	CB-CG-CD	5.70	124.41	111.30
1	A	292	GLN	OE1-CD-NE2	-5.67	116.93	122.60
1	A	42	TYR	N-CA-C	5.66	120.19	113.28
1	A	60	HIS	CB-CG-CD2	-5.66	123.85	131.20
1	A	101	TRP	CB-CG-CD1	-5.64	118.44	126.90
1	A	79	ASP	CA-CB-CG	5.64	118.24	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	ARG	NE-CZ-NH1	5.60	127.10	121.50
1	A	208	ASN	CB-CG-ND2	5.56	124.74	116.40
1	A	235	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	286	PHE	N-CA-C	5.55	118.49	110.28
1	A	128	CYS	O-C-N	-5.55	116.19	122.68
1	A	158	PHE	N-CA-C	5.52	119.63	113.01
1	A	224	ASP	O-C-N	-5.47	117.09	123.27
1	A	219	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	A	144	LEU	CA-C-N	5.40	125.82	119.99
1	A	144	LEU	C-N-CA	5.40	125.82	119.99
1	A	93	GLU	CA-C-N	5.40	125.47	119.32
1	A	93	GLU	C-N-CA	5.40	125.47	119.32
1	A	101	TRP	CG-CD2-CE3	5.38	139.28	133.90
1	A	171	LEU	CA-C-O	5.38	126.16	119.97
1	A	277	PRO	CA-C-O	-5.35	115.26	121.95
1	A	54	SER	N-CA-C	5.35	118.97	112.23
1	A	163	MET	CG-SD-CE	-5.30	89.25	100.90
1	A	254	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	101	TRP	CE2-CD2-CG	-5.21	100.95	107.20
1	A	160	ARG	NE-CZ-NH1	5.19	126.69	121.50
1	A	159	GLN	CG-CD-NE2	5.18	124.17	116.40
1	A	96	HIS	CA-C-O	-5.18	114.93	120.42
1	A	10	VAL	CB-CA-C	-5.17	103.53	111.71
1	A	164	ASN	CA-CB-CG	5.14	117.75	112.60
1	A	162	ASN	CA-C-O	5.10	127.81	120.51
1	A	284	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	48	ARG	CA-CB-CG	-5.04	104.03	114.10
1	A	134	PRO	N-CA-C	5.03	119.14	111.34
1	A	38	ASN	N-CA-C	5.02	118.37	111.54
1	A	48	ARG	O-C-N	-5.02	116.80	122.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2342	505	2214	18	0
2	A	43	0	30	1	0
3	A	86	0	0	0	0
All	All	2471	505	2244	18	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 4.

All (18) 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:20:GLN:HE22	1:A:287:LYS:H	1.37	0.72
1:A:125:PRO:HG3	1:A:285:ILE:HD11	1.80	0.63
1:A:200:ASN:H	1:A:255:GLN:HE21	1.45	0.62
1:A:74:LYS:HD2	1:A:74:LYS:H	1.67	0.60
1:A:20:GLN:HE22	1:A:287:LYS:N	2.06	0.53
1:A:168:VAL:O	1:A:172:MET:HB2	2.12	0.50
1:A:51:TRP:CD1	1:A:52:HIS:HD2	2.31	0.48
1:A:167:GLU:O	1:A:171:LEU:HB2	2.15	0.46
1:A:127:ARG:O	1:A:130:ARG:NH2	2.49	0.46
1:A:200:ASN:HB3	1:A:255:GLN:HG3	1.98	0.46
1:A:155:ARG:HH22	1:A:241:ASP:CG	2.24	0.45
1:A:14:ARG:HG3	1:A:101:TRP:CZ3	2.53	0.44
1:A:48:ARG:HD3	2:A:1:HEM:C4D	2.53	0.43
1:A:164:ASN:O	1:A:168:VAL:HG23	2.19	0.42
1:A:218:ALA:O	1:A:219:ASN:HB2	2.19	0.42
1:A:236:TYR:O	1:A:239:ILE:HG12	2.20	0.42
1:A:14:ARG:HG3	1:A:101:TRP:CE3	2.56	0.41
1:A:151:ALA:HB2	1:A:237:SER:HB3	2.03	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	289/291 (99%)	279 (96%)	9 (3%)	1 (0%)	36	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ASN

5.3.2 Protein sidechains ⓘ

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	246/248 (99%)	234 (95%)	12 (5%)	22	34

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	47	VAL
1	A	51	TRP
1	A	53	ILE
1	A	74	LYS
1	A	81	SER
1	A	143	ARG
1	A	156	THR
1	A	182	LEU
1	A	195	ASN
1	A	232	LEU
1	A	278	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	24	ASN
1	A	195	ASN

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Mol	Chain	Res	Type
1	A	220	ASN
1	A	253	ASN
1	A	255	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 oligosaccharides 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	1	3	50,50,50	2.27	25 (50%)	67,82,82	1.40	11 (16%)

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	1	3	-	3/14/54/54	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	HEM	FE-ND	4.59	2.09	1.94
2	A	1	HEM	FE-NB	4.10	2.07	1.94
2	A	1	HEM	C4D-ND	-3.75	1.33	1.40
2	A	1	HEM	C1B-NB	-3.74	1.33	1.40
2	A	1	HEM	C4C-NC	-3.68	1.32	1.39
2	A	1	HEM	C3C-C4C	-3.57	1.39	1.46
2	A	1	HEM	FE-NA	3.23	2.05	1.95
2	A	1	HEM	CBB-CAB	3.20	1.45	1.30
2	A	1	HEM	CBC-CAC	3.12	1.45	1.30
2	A	1	HEM	C4A-NA	-3.09	1.33	1.39
2	A	1	HEM	C4D-C3D	-3.04	1.39	1.45
2	A	1	HEM	C1A-C2A	-2.98	1.38	1.44
2	A	1	HEM	C1A-NA	-2.92	1.34	1.39
2	A	1	HEM	C1D-ND	-2.92	1.33	1.38
2	A	1	HEM	C1C-C2C	-2.82	1.39	1.45
2	A	1	HEM	C1C-NC	-2.71	1.34	1.39
2	A	1	HEM	C1D-C2D	-2.54	1.39	1.44
2	A	1	HEM	CAB-C3B	-2.52	1.40	1.47
2	A	1	HEM	FE-NC	2.48	2.03	1.95
2	A	1	HEM	O2D-CGD	-2.45	1.22	1.30
2	A	1	HEM	CAC-C3C	-2.37	1.41	1.47
2	A	1	HEM	C4B-NB	-2.33	1.34	1.38
2	A	1	HEM	O2A-CGA	-2.29	1.23	1.30
2	A	1	HEM	C3C-C2C	2.21	1.41	1.37
2	A	1	HEM	C3B-C4B	-2.10	1.40	1.44

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	HEM	CMD-C2D-C1D	3.77	130.93	125.03
2	A	1	HEM	C2D-C1D-ND	2.69	113.01	109.90
2	A	1	HEM	CAD-C3D-C4D	2.68	129.37	124.70
2	A	1	HEM	CHD-C1D-ND	-2.66	121.56	124.42
2	A	1	HEM	C3C-C2C-C1C	-2.60	104.59	107.05
2	A	1	HEM	C1D-C2D-C3D	-2.30	104.57	106.98
2	A	1	HEM	C3B-C4B-NB	2.22	111.06	109.47
2	A	1	HEM	O2A-CGA-CBA	2.18	120.88	114.00
2	A	1	HEM	C3B-C2B-C1B	-2.15	104.80	106.41
2	A	1	HEM	CAA-C2A-C3A	2.14	131.86	127.07
2	A	1	HEM	C4C-CHD-C1D	2.03	130.34	126.02

There are no chirality outliers.

All (3) torsion outliers are listed below:

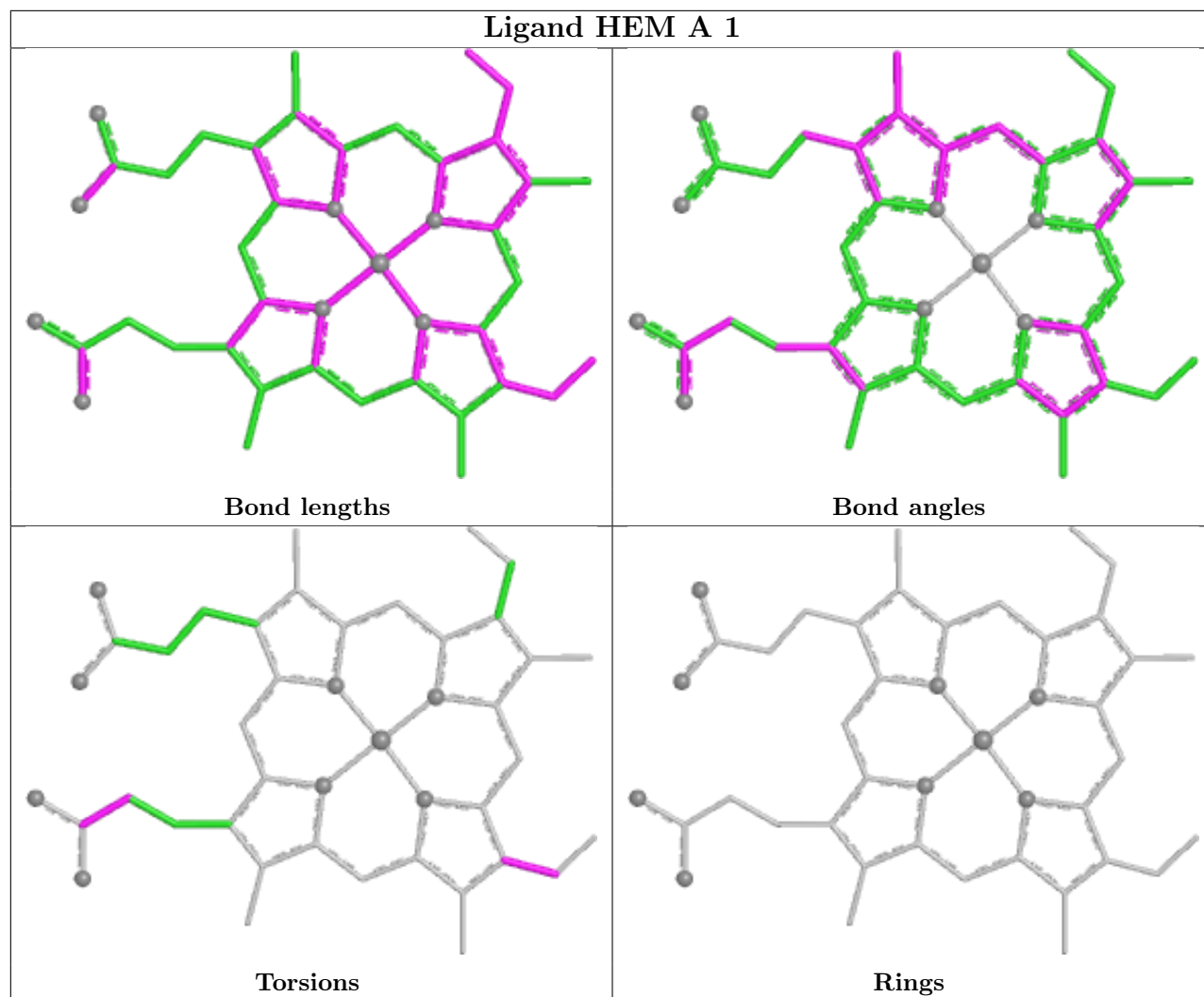
Mol	Chain	Res	Type	Atoms
2	A	1	HEM	CAA-CBA-CGA-O2A
2	A	1	HEM	CAA-CBA-CGA-O1A
2	A	1	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	HEM	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 than 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.



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

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.