



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:03 PM UTC

PDB ID : 3CCP / pdb_00003ccp
Title : X-RAY STRUCTURES OF RECOMBINANT YEAST CYTOCHROME C
PEROXIDASE AND THREE HEME-CLEFT MUTANTS PREPARED BY
SITE-DIRECTED MUTAGENESIS
Authors : Wang, J.; Mauro, J.M.; Edwards, S.L.; Oatley, S.J.; Fishel, L.A.; Ashford,
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Deposited on : 1990-02-28
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 ⓘ 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)
Xtrriage (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

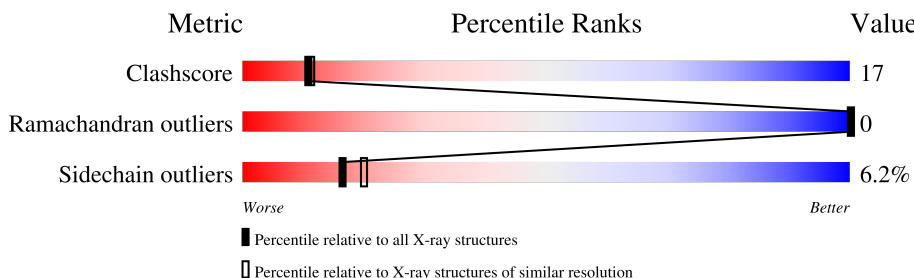
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (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 $\leq 5\%$.

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 2578 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 YEAST CYTOCHROME C PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2336	1494	385	451	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ILE	THR	variant	UNP P00431
A	152	GLY	ASP	variant	UNP P00431
A	191	PHE	TRP	engineered mutation	UNP P00431

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



- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	199	Total 199	O 199	0	0

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	104.57Å 74.38Å 45.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.165 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2578	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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	1.12	1/2402 (0.0%)	2.05	89/3257 (2.7%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	THR	N-CA	5.13	1.55	1.46

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ASN	CA-CB-CG	12.94	125.54	112.60
1	A	93	GLU	CA-CB-CG	9.98	134.06	114.10
1	A	48	ARG	NE-CZ-NH2	9.45	127.71	119.20
1	A	67	TYR	N-CA-C	9.11	122.14	111.02
1	A	256	ASP	CA-CB-CG	-8.98	103.62	112.60
1	A	38	ASN	CA-CB-CG	-8.97	103.63	112.60
1	A	162	ASN	OD1-CG-ND2	8.90	131.50	122.60
1	A	162	ASN	CA-CB-CG	-8.73	103.87	112.60
1	A	127	ARG	CD-NE-CZ	8.53	136.34	124.40
1	A	195	ASN	CB-CG-ND2	7.91	128.27	116.40
1	A	7	VAL	O-C-N	7.69	131.08	122.93
1	A	157	PHE	CA-CB-CG	-7.68	106.12	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	ALA	N-CA-C	-7.47	104.17	113.28
1	A	194	ALA	CA-C-O	-7.40	113.86	122.37
1	A	56	THR	CA-CB-OG1	-7.33	98.60	109.60
1	A	191	PHE	CA-CB-CG	7.22	121.02	113.80
1	A	96	HIS	CA-CB-CG	-7.10	106.70	113.80
1	A	176	ALA	N-CA-C	-6.87	104.37	112.89
1	A	208	ASN	N-CA-C	6.75	121.51	113.28
1	A	38	ASN	CA-C-O	-6.68	113.33	121.28
1	A	262	PHE	CA-C-O	6.64	127.79	120.82
1	A	141	ASN	CA-CB-CG	6.50	119.10	112.60
1	A	239	ILE	O-C-N	6.44	128.64	122.20
1	A	45	VAL	O-C-N	6.44	128.37	121.87
1	A	58	ASP	CA-CB-CG	-6.42	106.18	112.60
1	A	136	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	195	ASN	N-CA-C	6.34	120.70	113.15
1	A	114	THR	CA-CB-OG1	-6.30	100.15	109.60
1	A	144	LEU	CB-CA-C	6.28	117.90	108.86
1	A	251	TYR	O-C-N	6.26	129.97	122.27
1	A	166	ARG	NE-CZ-NH1	6.16	127.66	121.50
1	A	162	ASN	N-CA-CB	-6.13	103.15	112.47
1	A	156	THR	CA-CB-OG1	-6.11	100.44	109.60
1	A	99	PHE	CA-CB-CG	5.93	119.73	113.80
1	A	217	ASP	CA-CB-CG	-5.90	106.70	112.60
1	A	177	LEU	N-CA-C	5.89	119.42	109.76
1	A	6	HIS	O-C-N	5.87	130.86	123.12
1	A	158	PHE	CA-CB-CG	-5.81	107.99	113.80
1	A	210	ASP	CA-C-N	5.81	130.38	122.19
1	A	210	ASP	C-N-CA	5.81	130.38	122.19
1	A	114	THR	O-C-N	5.79	128.04	122.07
1	A	5	VAL	CA-C-O	-5.77	114.33	120.39
1	A	256	ASP	CB-CA-C	5.73	119.88	110.88
1	A	258	PHE	O-C-N	5.66	127.90	122.07
1	A	149	LYS	O-C-N	5.66	130.11	122.59
1	A	255	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	A	236	TYR	O-C-N	5.55	128.00	122.12
1	A	38	ASN	OD1-CG-ND2	5.54	128.14	122.60
1	A	162	ASN	CA-C-O	-5.53	113.94	120.57
1	A	155	ARG	CA-C-N	5.50	127.59	120.44
1	A	155	ARG	C-N-CA	5.50	127.59	120.44
1	A	155	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	A	45	VAL	CA-C-O	-5.45	114.74	120.57
1	A	252	ALA	N-CA-C	-5.43	105.52	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	PHE	O-C-N	5.40	127.65	122.03
1	A	220	ASN	CA-C-N	-5.39	114.11	122.09
1	A	220	ASN	C-N-CA	-5.39	114.11	122.09
1	A	33	ASP	CB-CA-C	-5.37	104.31	111.88
1	A	274	ILE	O-C-N	5.35	128.59	123.14
1	A	21	LYS	CA-C-O	-5.33	114.77	120.42
1	A	125	PRO	CB-CA-C	5.30	118.30	111.46
1	A	206	LEU	CA-C-O	-5.30	115.25	120.82
1	A	21	LYS	O-C-N	5.30	128.19	122.15
1	A	33	ASP	CA-C-O	-5.30	114.49	122.38
1	A	32	GLU	N-CA-C	5.29	118.20	111.69
1	A	20	GLN	CA-C-N	5.29	127.80	120.29
1	A	20	GLN	C-N-CA	5.29	127.80	120.29
1	A	124	ILE	CA-C-O	5.27	125.63	119.89
1	A	231	MET	N-CA-CB	5.24	120.50	111.13
1	A	46	LEU	O-C-N	5.23	128.12	122.15
1	A	195	ASN	CB-CA-C	5.22	120.02	110.36
1	A	150	ASP	CA-C-N	5.15	127.44	120.38
1	A	150	ASP	C-N-CA	5.15	127.44	120.38
1	A	272	ASN	CA-CB-CG	5.15	117.75	112.60
1	A	214	GLU	O-C-N	5.14	129.11	123.25
1	A	186	GLY	N-CA-C	-5.13	107.73	115.32
1	A	253	ASN	CA-CB-CG	-5.10	107.50	112.60
1	A	284	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	39	TYR	CA-CB-CG	-5.07	104.78	113.90
1	A	202	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	174	ALA	N-CA-C	-5.06	107.06	113.18
1	A	210	ASP	CB-CA-C	5.04	120.11	111.68
1	A	273	GLY	CA-C-N	-5.04	116.60	123.10
1	A	273	GLY	C-N-CA	-5.04	116.60	123.10
1	A	166	ARG	NE-CZ-NH2	-5.03	114.67	119.20
1	A	146	ASP	CA-CB-CG	5.03	117.62	112.60
1	A	162	ASN	CB-CA-C	-5.02	103.61	111.39
1	A	264	LYS	O-C-N	5.01	127.23	122.07
1	A	161	LEU	O-C-N	5.01	128.21	122.25

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	ARG	Sidechain

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	2336	0	2171	73	0
2	A	43	0	30	3	0
3	A	199	0	0	10	0
All	All	2578	0	2201	76	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 17.

All (76) 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:86:GLN:H	1:A:86:GLN:NE2	1.67	0.93
1:A:255:GLN:HG2	3:A:556:HOH:O	1.70	0.88
1:A:20:GLN:HE22	1:A:287:LYS:H	1.25	0.84
1:A:216:ASN:HD22	1:A:222:GLN:HE21	1.23	0.84
1:A:216:ASN:HD22	1:A:222:GLN:NE2	1.77	0.82
1:A:4:LEU:H	1:A:4:LEU:CD2	1.93	0.81
1:A:84:GLY:C	1:A:86:GLN:HE21	1.93	0.76
1:A:84:GLY:C	1:A:86:GLN:NE2	2.48	0.70
1:A:4:LEU:H	1:A:4:LEU:HD22	1.58	0.68
1:A:84:GLY:N	1:A:86:GLN:HE22	1.91	0.68
1:A:288:THR:OG1	1:A:291:GLU:HG3	1.93	0.67
1:A:195:ASN:HD22	1:A:195:ASN:H	1.43	0.67
1:A:85:LEU:N	1:A:86:GLN:NE2	2.43	0.65
1:A:123:LYS:HE2	3:A:889:HOH:O	1.97	0.65
1:A:84:GLY:N	1:A:86:GLN:NE2	2.45	0.65
1:A:4:LEU:HD22	1:A:4:LEU:N	2.14	0.63
1:A:213:LEU:HD11	1:A:221:GLU:HB3	1.81	0.62
1:A:123:LYS:CE	3:A:889:HOH:O	2.48	0.62
1:A:4:LEU:HD23	1:A:61:ASP:O	2.02	0.60
1:A:199:THR:HA	1:A:255:GLN:OE1	2.03	0.59
1:A:84:GLY:H	1:A:86:GLN:NE2	2.00	0.59
1:A:195:ASN:HB3	3:A:477:HOH:O	2.01	0.59
1:A:183:LYS:CG	3:A:483:HOH:O	2.51	0.58
1:A:84:GLY:CA	1:A:86:GLN:NE2	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ASN:ND2	1:A:222:GLN:HE21	1.99	0.57
1:A:72:ARG:NH2	1:A:133:THR:O	2.37	0.57
1:A:294:LEU:CD1	1:A:294:LEU:N	2.67	0.56
1:A:23:TYR:CD2	1:A:23:TYR:C	2.84	0.56
1:A:293:GLY:C	1:A:294:LEU:HD12	2.30	0.56
1:A:93:GLU:N	1:A:94:PRO:HD2	2.21	0.55
1:A:218:ALA:O	1:A:219:ASN:HB3	2.05	0.55
2:A:296:HEM:CMC	2:A:296:HEM:HBC2	2.36	0.54
1:A:143:ARG:HB2	3:A:443:HOH:O	2.08	0.54
1:A:73:PHE:CE1	1:A:135:GLU:HA	2.43	0.54
1:A:145:PRO:HD3	1:A:157:PHE:CZ	2.43	0.54
1:A:159:GLN:NE2	1:A:159:GLN:HA	2.23	0.54
1:A:4:LEU:H	1:A:4:LEU:HD23	1.73	0.53
1:A:294:LEU:N	1:A:294:LEU:HD12	2.23	0.53
1:A:188:GLU:H	1:A:222:GLN:HE22	1.57	0.53
1:A:218:ALA:O	1:A:219:ASN:CB	2.56	0.53
1:A:161:LEU:O	1:A:162:ASN:CB	2.56	0.53
1:A:86:GLN:H	1:A:86:GLN:CD	2.17	0.51
1:A:86:GLN:H	1:A:86:GLN:HE21	1.55	0.51
1:A:52:HIS:HE1	1:A:81:SER:O	1.93	0.51
1:A:67:TYR:O	1:A:130:ARG:HB3	2.11	0.50
1:A:163:MET:HA	1:A:167:GLU:OE2	2.11	0.50
2:A:296:HEM:CMB	2:A:296:HEM:HBB2	2.42	0.49
1:A:58:ASP:OD1	1:A:58:ASP:C	2.54	0.49
1:A:98:GLU:C	1:A:100:PRO:HD3	2.38	0.49
1:A:183:LYS:HG3	3:A:483:HOH:O	2.13	0.48
1:A:236:TYR:CE2	1:A:239:ILE:HD11	2.48	0.48
1:A:292:GLN:C	1:A:294:LEU:HD13	2.39	0.48
1:A:133:THR:HB	1:A:134:PRO:CD	2.44	0.48
1:A:236:TYR:O	1:A:239:ILE:HG12	2.14	0.47
1:A:4:LEU:CD2	1:A:4:LEU:N	2.63	0.47
1:A:281:PRO:O	3:A:427:HOH:O	2.20	0.47
1:A:183:LYS:HG2	3:A:483:HOH:O	2.12	0.47
1:A:292:GLN:O	1:A:294:LEU:CD1	2.63	0.47
1:A:245:LEU:O	1:A:249:LYS:HG3	2.14	0.47
1:A:84:GLY:H	1:A:86:GLN:HE22	1.57	0.46
1:A:3:PRO:C	1:A:4:LEU:O	2.58	0.46
1:A:212:LYS:HB3	3:A:812:HOH:O	2.16	0.46
1:A:99:PHE:N	1:A:100:PRO:HD3	2.30	0.45
1:A:86:GLN:NE2	1:A:86:GLN:N	2.50	0.45
1:A:3:PRO:O	1:A:4:LEU:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ILE:HG22	1:A:71:TYR:HB2	2.01	0.43
1:A:79:ASP:OD1	1:A:80:PRO:HD2	2.20	0.42
1:A:292:GLN:O	1:A:294:LEU:HD13	2.19	0.42
1:A:85:LEU:N	1:A:86:GLN:HE22	2.17	0.41
1:A:195:ASN:H	1:A:195:ASN:ND2	2.12	0.41
1:A:38:ASN:O	1:A:39:TYR:HB2	2.20	0.41
1:A:35:GLU:CG	1:A:39:TYR:CE2	3.05	0.40
2:A:296:HEM:HBC2	2:A:296:HEM:HMC1	2.03	0.40
1:A:211:TRP:CH2	1:A:231:MET:HG2	2.56	0.40
1:A:245:LEU:O	1:A:245:LEU:HD12	2.22	0.40
1:A:241:ASP:OD2	1:A:243:LYS:HB2	2.22	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%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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%)	226 (94%)	15 (6%)	16	20

All (15) 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	95	ILE
1	A	124	ILE
1	A	156	THR
1	A	195	ASN
1	A	200	ASN
1	A	215	LYS
1	A	225	SER
1	A	233	PRO
1	A	246	SER
1	A	282	SER
1	A	287	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	24	ASN
1	A	60	HIS
1	A	86	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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	50,50,50	1.43	9 (18%)	67,82,82	1.34	10 (14%)

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	-	2/14/54/54	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	296	HEM	CAC-C3C	3.39	1.56	1.47
2	A	296	HEM	FE-NB	3.13	2.04	1.94
2	A	296	HEM	FE-NC	3.01	2.05	1.95
2	A	296	HEM	FE-ND	2.78	2.03	1.94
2	A	296	HEM	CAB-C3B	2.37	1.53	1.47
2	A	296	HEM	CMA-C3A	2.22	1.55	1.50
2	A	296	HEM	CMB-C2B	2.20	1.55	1.50
2	A	296	HEM	CAD-C3D	2.18	1.56	1.51
2	A	296	HEM	C3D-C2D	-2.09	1.32	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	296	HEM	O1D-CGD-CBD	-3.77	111.13	123.09
2	A	296	HEM	CBC-CAC-C3C	-2.79	113.60	127.53
2	A	296	HEM	C1B-NB-C4B	2.41	108.06	105.21
2	A	296	HEM	C4A-CHB-C1B	-2.38	120.65	126.25
2	A	296	HEM	O2D-CGD-O1D	2.30	129.26	123.33
2	A	296	HEM	CHB-C4A-NA	2.28	127.99	123.86
2	A	296	HEM	CHC-C4B-NB	2.25	126.84	124.42
2	A	296	HEM	CHB-C1B-NB	2.24	127.14	124.37
2	A	296	HEM	CMA-C3A-C2A	2.08	130.05	125.62
2	A	296	HEM	C3B-C4B-NB	-2.06	107.99	109.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

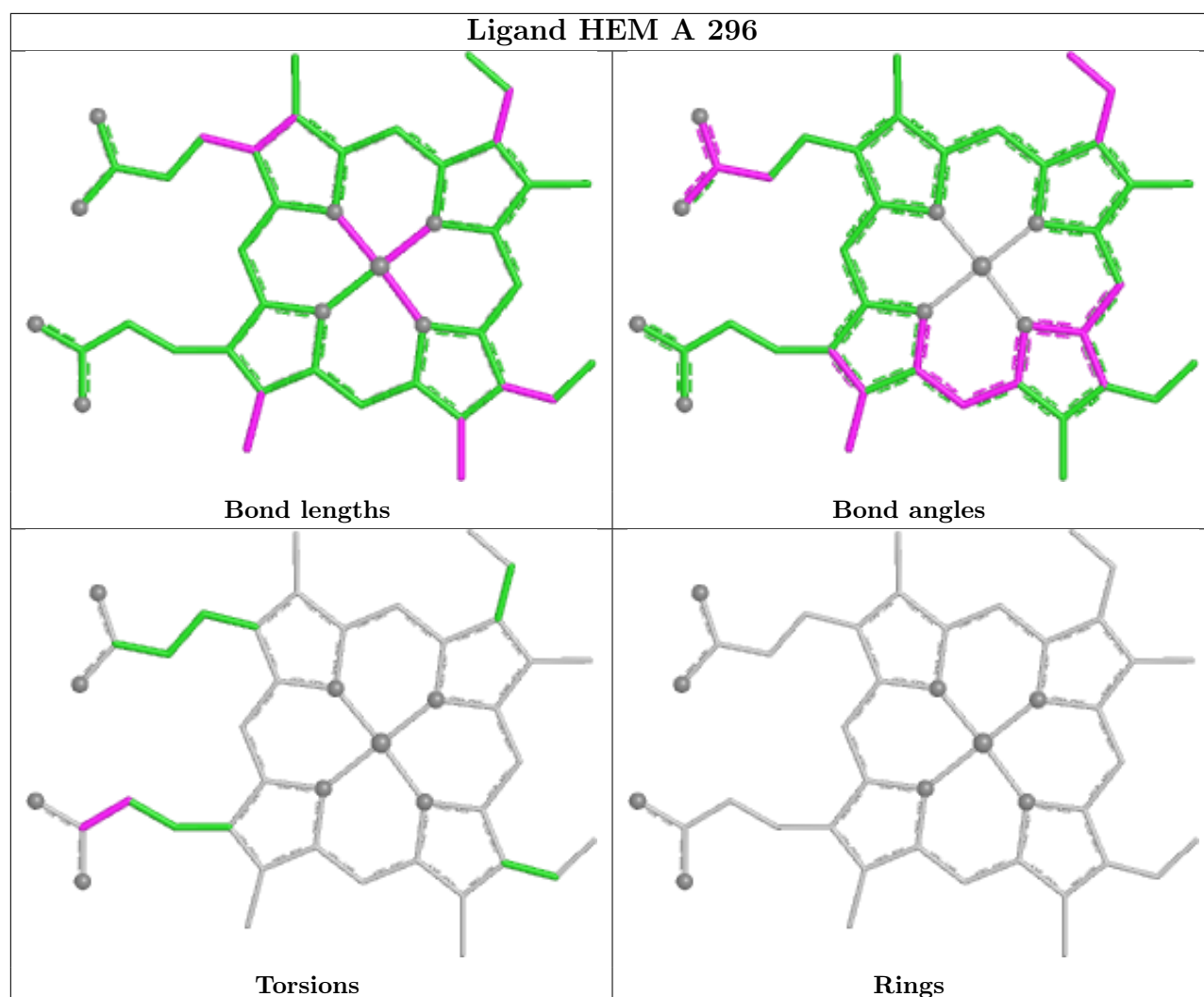
Mol	Chain	Res	Type	Atoms
2	A	296	HEM	CAA-CBA-CGA-O2A
2	A	296	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	296	HEM	3	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.