



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:11 PM UTC

PDB ID : 1CMP / pdb_00001cmp
Title : SMALL MOLECULE BINDING TO AN ARTIFICIALLY CREATED CAVITY AT THE ACTIVE SITE OF CYTOCHROME C PEROXIDASE
Authors : Fitzgerald, M.M.; Mcree, D.E.; Churchill, M.J.; Goodin, D.B.
Deposited on : 1993-11-23
Resolution : 1.90 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

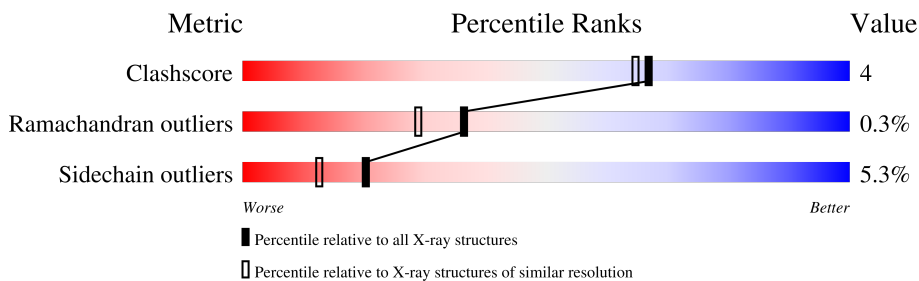
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	294	77% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DMI	A	295	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2942 atoms, of which 504 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.

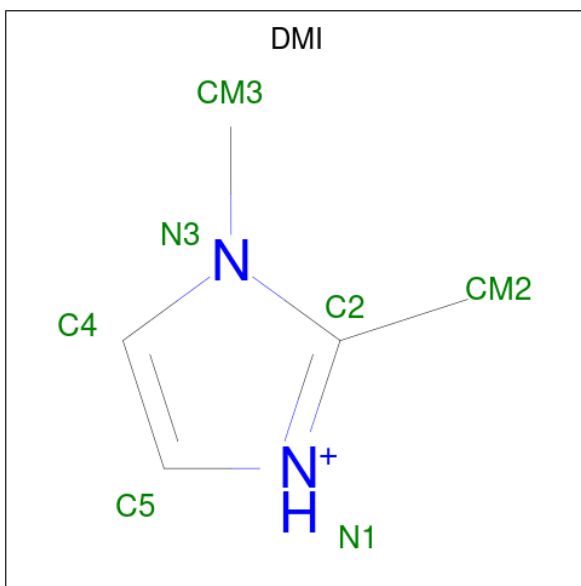
- Molecule 1 is a protein called CYTOCHROME C PEROXIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	291	2841	1492	503	389	451	6	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	191	GLY	TRP	conflict	UNP P00431

- Molecule 2 is 2,3-DIMETHYLIMIDAZOLIUM ION (CCD ID: DMI) (formula: C₅H₉N₂).




Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	N		
2	A	1	8	5	1	2	0	0

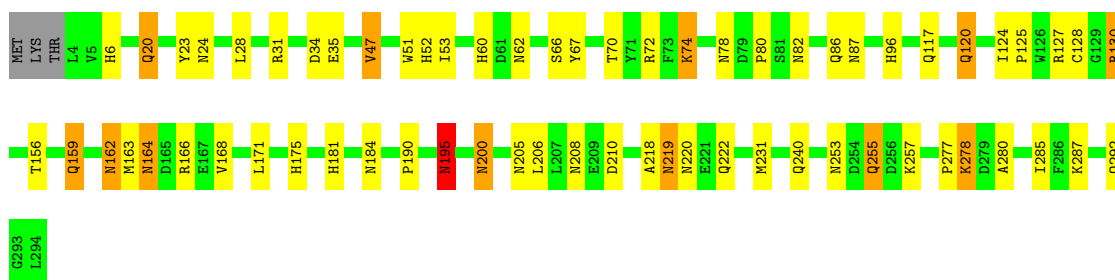
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: CYTOCHROME C PEROXIDASE

Chain A:  77% 18%



4 Data and refinement statistics

Xtrriage (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)	5.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-1.90)	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.	Xtrriage
Total number of atoms	2942	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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, DMI

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	1.04	8/2402 (0.3%)	1.84	56/3250 (1.7%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	HIS	CD2-NE2	-7.00	1.30	1.37
1	A	60	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	96	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	175	HIS	CD2-NE2	-5.87	1.31	1.37
1	A	52	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	47	VAL	CA-CB	5.77	1.62	1.54
1	A	181	HIS	CD2-NE2	-5.53	1.31	1.37
1	A	6	HIS	CG-ND1	-5.24	1.32	1.38

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ASN	OD1-CG-ND2	-9.84	112.76	122.60
1	A	34	ASP	CA-CB-CG	9.58	122.18	112.60
1	A	124	ILE	O-C-N	-9.15	115.61	121.37
1	A	240	GLN	OE1-CD-NE2	-8.64	113.95	122.60
1	A	162	ASN	CA-CB-CG	8.41	121.01	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	LYS	CA-CB-CG	-8.31	97.48	114.10
1	A	292	GLN	OE1-CD-NE2	-8.29	114.31	122.60
1	A	20	GLN	OE1-CD-NE2	-8.20	114.40	122.60
1	A	195	ASN	N-CA-C	8.00	122.62	113.02
1	A	62	ASN	OD1-CG-ND2	-7.99	114.61	122.60
1	A	205	ASN	OD1-CG-ND2	-7.88	114.72	122.60
1	A	220	ASN	OD1-CG-ND2	-7.66	114.94	122.60
1	A	82	ASN	OD1-CG-ND2	-7.41	115.19	122.60
1	A	195	ASN	CA-CB-CG	7.33	119.93	112.60
1	A	164	ASN	OD1-CG-ND2	-7.31	115.29	122.60
1	A	162	ASN	N-CA-C	7.22	126.19	110.80
1	A	277	PRO	CA-C-O	-7.16	113.26	121.56
1	A	255	GLN	OE1-CD-NE2	-7.10	115.50	122.60
1	A	184	ASN	OD1-CG-ND2	-7.01	115.59	122.60
1	A	67	TYR	N-CA-C	6.81	119.29	111.11
1	A	117	GLN	OE1-CD-NE2	-6.64	115.96	122.60
1	A	162	ASN	CA-C-O	6.60	129.95	120.51
1	A	219	ASN	OD1-CG-ND2	-6.53	116.07	122.60
1	A	159	GLN	OE1-CD-NE2	-6.53	116.07	122.60
1	A	78	ASN	OD1-CG-ND2	-6.53	116.07	122.60
1	A	219	ASN	CB-CG-ND2	6.46	126.09	116.40
1	A	51	TRP	CB-CG-CD1	-6.39	117.32	126.90
1	A	52	HIS	N-CA-C	6.25	118.18	111.36
1	A	86	GLN	OE1-CD-NE2	-6.21	116.39	122.60
1	A	128	CYS	O-C-N	-6.20	115.42	122.68
1	A	130	ARG	CG-CD-NE	-6.18	98.40	112.00
1	A	253	ASN	CA-CB-CG	-6.18	106.42	112.60
1	A	195	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	A	280	ALA	N-CA-C	6.10	116.61	109.60
1	A	31	ARG	NE-CZ-NH2	-5.99	113.81	119.20
1	A	66	SER	N-CA-C	5.95	119.80	112.54
1	A	181	HIS	CB-CG-CD2	-5.94	123.48	131.20
1	A	51	TRP	CG-CD2-CE3	5.93	139.83	133.90
1	A	127	ARG	NE-CZ-NH2	-5.80	113.98	119.20
1	A	87	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	A	253	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	A	222	GLN	OE1-CD-NE2	-5.67	116.93	122.60
1	A	163	MET	CG-SD-CE	-5.66	88.45	100.90
1	A	24	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	A	210	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	200	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	70	THR	N-CA-C	5.38	119.46	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ASN	CB-CG-ND2	5.37	124.46	116.40
1	A	51	TRP	CE2-CD2-CG	-5.37	100.76	107.20
1	A	117	GLN	CG-CD-NE2	5.19	124.19	116.40
1	A	277	PRO	O-C-N	-5.17	116.61	123.01
1	A	120	GLN	CA-CB-CG	5.16	124.42	114.10
1	A	52	HIS	CB-CG-CD2	-5.14	124.51	131.20
1	A	127	ARG	NE-CZ-NH1	5.11	126.61	121.50
1	A	200	ASN	CB-CG-ND2	5.11	124.07	116.40
1	A	240	GLN	CG-CD-NE2	5.02	123.93	116.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	ARG	Sidechain

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	2338	503	2211	17	0
2	A	7	1	9	0	0
3	A	43	0	30	0	0
4	A	50	0	0	3	0
All	All	2438	504	2250	17	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 (17) 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:74:LYS:HD2	1:A:74:LYS:H	1.53	0.71
1:A:20:GLN:HE22	1:A:287:LYS:H	1.41	0.68
1:A:200:ASN:H	1:A:255:GLN:HE21	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ASN:HD22	1:A:195:ASN:H	1.55	0.55
1:A:166:ARG:HH21	1:A:257:LYS:HZ2	1.54	0.54
1:A:130:ARG:NE	4:A:326:HOH:O	2.39	0.54
1:A:20:GLN:HE22	1:A:287:LYS:N	2.04	0.53
1:A:125:PRO:HG3	1:A:285:ILE:CD1	2.42	0.50
1:A:206:LEU:HD13	1:A:231:MET:SD	2.53	0.49
1:A:218:ALA:O	1:A:219:ASN:HB2	2.15	0.46
1:A:164:ASN:O	1:A:168:VAL:HG23	2.15	0.46
1:A:166:ARG:HH21	1:A:257:LYS:NZ	2.12	0.46
1:A:125:PRO:HG3	1:A:285:ILE:HD11	1.98	0.44
1:A:130:ARG:CZ	4:A:326:HOH:O	2.66	0.44
1:A:130:ARG:NH2	4:A:326:HOH:O	2.53	0.41
1:A:23:TYR:CD1	1:A:23:TYR:C	2.98	0.41
1:A:20:GLN:NE2	1:A:287:LYS:H	2.13	0.41

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	289/294 (98%)	283 (98%)	5 (2%)	1 (0%)	36 29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ASN

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	246/251 (98%)	233 (95%)	13 (5%)	20	12

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	35	GLU
1	A	47	VAL
1	A	53	ILE
1	A	74	LYS
1	A	80	PRO
1	A	120	GLN
1	A	156	THR
1	A	159	GLN
1	A	171	LEU
1	A	190	PRO
1	A	195	ASN
1	A	278	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	24	ASN
1	A	87	ASN
1	A	159	GLN
1	A	195	ASN
1	A	220	ASN
1	A	255	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 [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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMI	A	295	-	7,7,7	2.71	3 (42%)	8,9,9	4.39	5 (62%)
3	HEM	A	296	4,1	50,50,50	2.30	23 (46%)	67,82,82	1.09	2 (2%)

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	DMI	A	295	-	-	-	0/1/1/1
3	HEM	A	296	4,1	-	3/14/54/54	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	296	HEM	FE-NB	4.81	2.09	1.94
3	A	296	HEM	FE-NA	3.97	2.08	1.95
3	A	296	HEM	FE-ND	3.92	2.07	1.94
2	A	295	DMI	C4-N3	-3.85	1.30	1.37
3	A	296	HEM	C4D-ND	-3.85	1.33	1.40
2	A	295	DMI	C5-N1	-3.80	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	296	HEM	C4C-NC	-3.71	1.32	1.39
2	A	295	DMI	C2-N3	-3.60	1.30	1.38
3	A	296	HEM	C3C-C4C	-3.57	1.39	1.46
3	A	296	HEM	C1D-ND	-3.29	1.32	1.38
3	A	296	HEM	FE-NC	3.27	2.06	1.95
3	A	296	HEM	C1C-C2C	-3.22	1.39	1.45
3	A	296	HEM	C1A-C2A	-3.02	1.38	1.44
3	A	296	HEM	C4D-C3D	-2.97	1.40	1.45
3	A	296	HEM	CAB-C3B	-2.95	1.39	1.47
3	A	296	HEM	CBB-CAB	2.95	1.44	1.30
3	A	296	HEM	C1D-C2D	-2.86	1.38	1.44
3	A	296	HEM	C1C-NC	-2.82	1.34	1.39
3	A	296	HEM	C1B-NB	-2.79	1.35	1.40
3	A	296	HEM	CBC-CAC	2.72	1.43	1.30
3	A	296	HEM	C1A-NA	-2.67	1.34	1.39
3	A	296	HEM	O2A-CGA	-2.54	1.22	1.30
3	A	296	HEM	CAC-C3C	-2.47	1.40	1.47
3	A	296	HEM	C4B-NB	-2.44	1.34	1.38
3	A	296	HEM	O2D-CGD	-2.40	1.22	1.30
3	A	296	HEM	C4A-NA	-2.26	1.35	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	295	DMI	C4-N3-C2	8.71	112.52	106.83
2	A	295	DMI	C5-N1-C2	5.09	112.71	105.86
2	A	295	DMI	C4-C5-N1	-4.44	104.93	110.74
2	A	295	DMI	CM2-C2-N3	4.29	128.97	122.25
2	A	295	DMI	CM3-N3-C2	-2.64	125.45	127.64
3	A	296	HEM	C3C-C2C-C1C	-2.49	104.69	107.05
3	A	296	HEM	CMA-C3A-C4A	2.24	128.84	125.42

There are no chirality outliers.

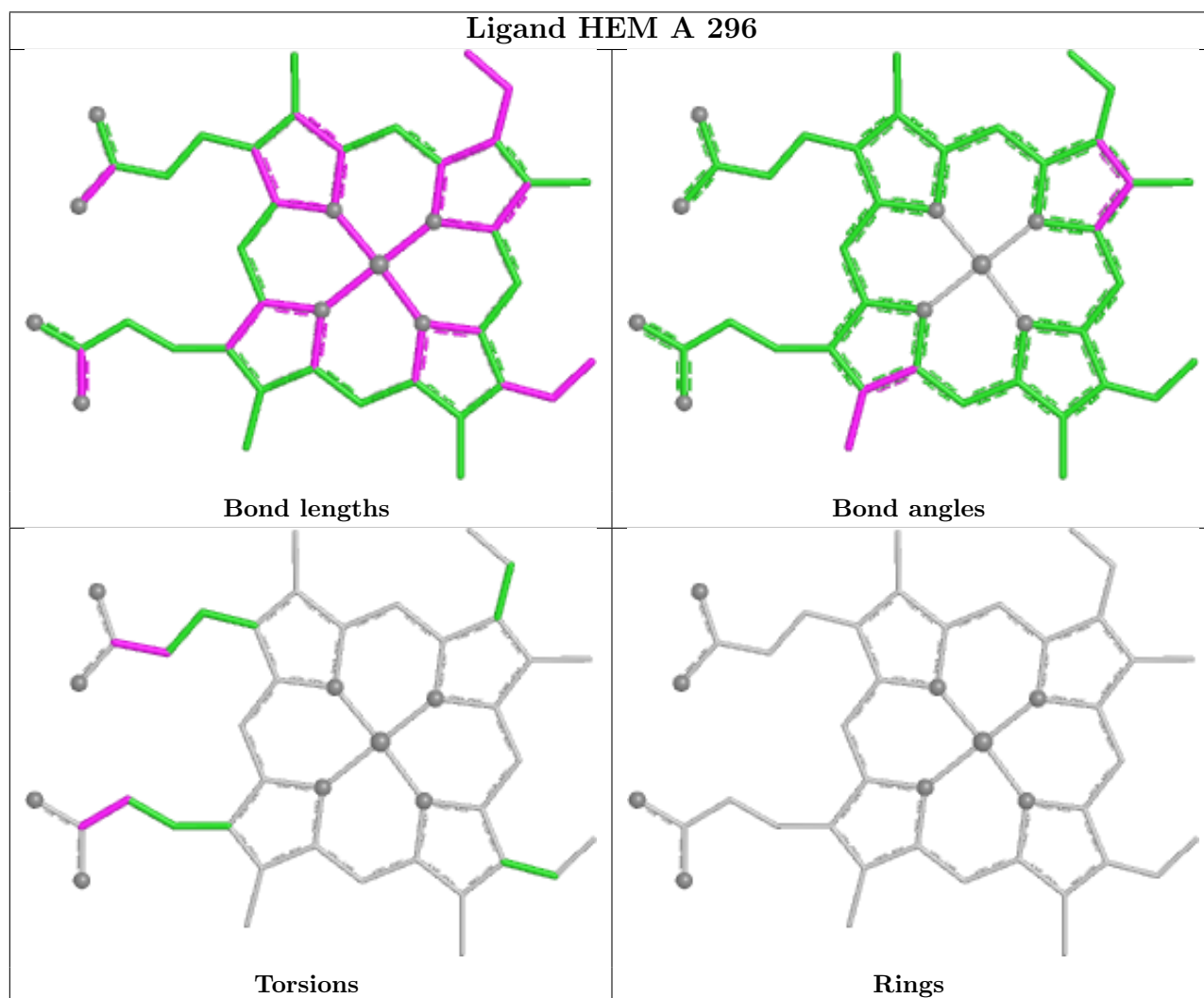
All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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

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.