



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:46 AM UTC

PDB ID : 6CP4 / pdb_00006cp4
Title : P450CAM D251N MUTANT
Authors : Li, H.; Poulos, T.L.
Deposited on : 1998-05-28
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)
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

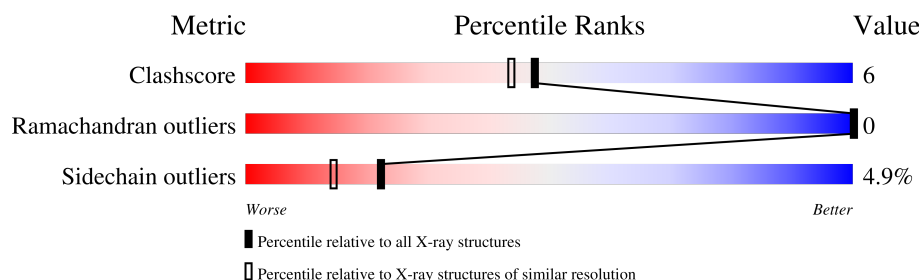
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	414	 79% 18% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5076 atoms, of which 1437 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 P450CAM.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	C	H	N	O	S	0	0	0
			3898	2033	690	561	596	18			

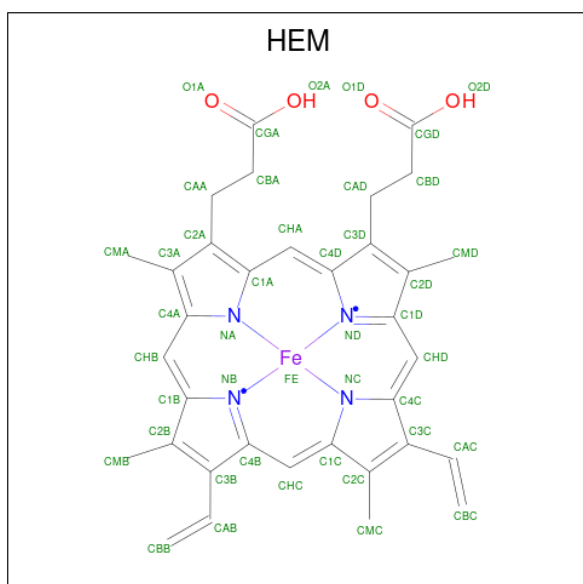
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	251	ASN	ASP	engineered mutation	UNP P00183

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

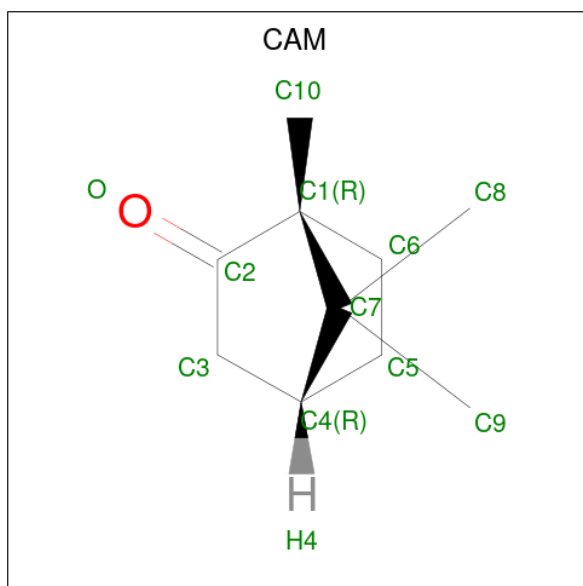
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



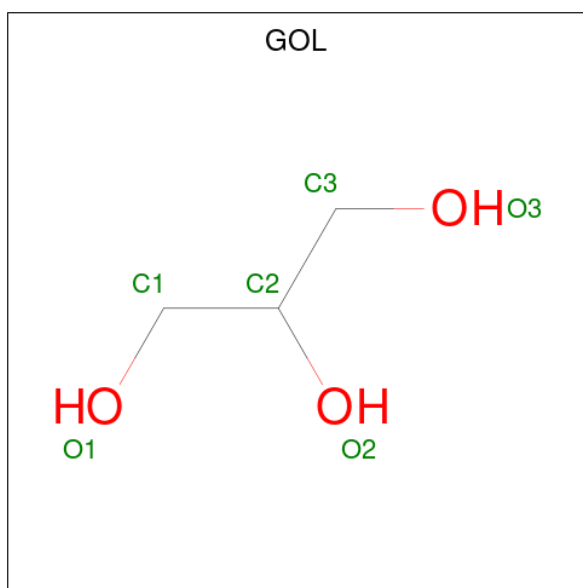
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Fe	H	N	O	0	0
			47	34	1	4	4	4		

- Molecule 4 is CAMPHOR (CCD ID: CAM) (formula: $C_{10}H_{16}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	10	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



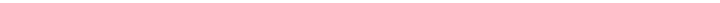
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			9	3	3	3		

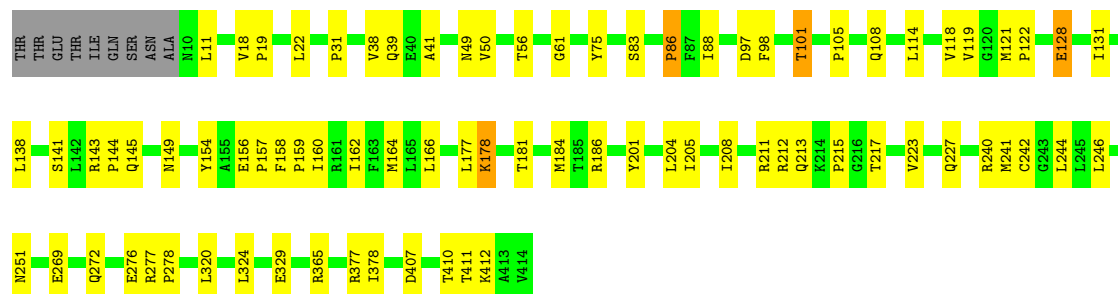
- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	370	Total	H	O	0	0
			1110	740	370		

Note EDS was not executed.

- Molecule 1: CYTOCHROME P450CAM

Chain A:  79% 18% ..



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	106.60Å 103.20Å 36.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90	Depositor
% Data completeness (in resolution range)	95.0 (10.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.200 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5076	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: K, CAM, HEM, GOL

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	0.53	0/3287	0.99	11/4465 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	251	ASN	N-CA-C	6.79	119.57	110.88
1	A	18	VAL	N-CA-C	6.69	113.65	107.56
1	A	38	VAL	N-CA-C	6.62	116.78	110.42
1	A	186	ARG	CA-C-N	6.60	126.99	119.93
1	A	186	ARG	C-N-CA	6.60	126.99	119.93
1	A	324	LEU	N-CA-C	6.59	119.46	111.82
1	A	378	ILE	CA-C-N	6.24	126.15	119.28
1	A	378	ILE	C-N-CA	6.24	126.15	119.28
1	A	101	THR	N-CA-C	5.83	118.41	111.71
1	A	50	VAL	N-CA-C	5.82	114.36	107.73
1	A	204	LEU	N-CA-C	5.74	117.34	111.14

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	3208	690	3158	34	2
2	A	1	0	0	0	0
3	A	43	4	30	2	0
4	A	11	0	16	1	0
5	A	6	3	8	0	0
6	A	370	740	0	1	3
All	All	3639	1437	3212	36	3

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 6.

All (36) 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:407:ASP:O	1:A:410:THR:HG22	1.83	0.79
1:A:114:LEU:HD23	1:A:241:MET:HE1	1.65	0.78
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.73	0.69
1:A:208:ILE:O	1:A:212:ARG:HG3	1.95	0.66
1:A:97:ASP:O	1:A:240:ARG:HD2	2.00	0.62
1:A:131:ILE:HG12	1:A:162:ILE:HD13	1.82	0.61
1:A:181:THR:HA	1:A:184:MET:HE2	1.85	0.59
1:A:272:GLN:HE21	1:A:276:GLU:HG3	1.68	0.58
1:A:118:VAL:HG23	1:A:119:VAL:HG13	1.87	0.57
1:A:242:CYS:O	1:A:246:LEU:HD23	2.05	0.57
1:A:19:PRO:HG2	1:A:22:LEU:HD12	1.86	0.56
1:A:118:VAL:HG11	1:A:223:VAL:HG23	1.88	0.56
1:A:128:GLU:OE1	1:A:365:ARG:HD3	2.07	0.54
1:A:181:THR:HA	1:A:184:MET:CE	2.40	0.52
1:A:49:ASN:HD22	1:A:49:ASN:H	1.57	0.52
1:A:410:THR:HG23	6:A:546:HOH:O	2.12	0.50
1:A:83:SER:HB3	1:A:101:THR:O	2.12	0.49
1:A:141:SER:O	1:A:144:PRO:HD2	2.11	0.49
1:A:156:GLU:HB2	1:A:157:PRO:HD3	1.94	0.49
1:A:143:ARG:HB3	1:A:144:PRO:HD3	1.97	0.47
1:A:98:PHE:HB3	1:A:244:LEU:HB2	1.97	0.46
1:A:49:ASN:H	1:A:49:ASN:ND2	2.14	0.46
1:A:31:PRO:HB2	1:A:41:ALA:HB1	1.98	0.46
1:A:213:GLN:C	1:A:215:PRO:HD3	2.42	0.45
1:A:121:MET:HB3	1:A:122:PRO:HD3	1.97	0.44
3:A:417:HEM:HMB1	3:A:417:HEM:HBB2	1.99	0.44
1:A:164:MET:HE1	1:A:177:LEU:HD12	2.00	0.43
1:A:377:ARG:O	1:A:411:THR:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:SER:O	1:A:86:PRO:HD3	2.18	0.42
3:A:417:HEM:C1A	4:A:422:CAM:H4	2.55	0.42
1:A:201:TYR:O	1:A:205:ILE:HG13	2.20	0.42
1:A:56:THR:O	1:A:61:GLY:HA2	2.20	0.41
1:A:160:ILE:HD11	1:A:178:LYS:HD2	2.02	0.41
1:A:154:TYR:C	1:A:157:PRO:HD2	2.45	0.41
1:A:276:GLU:C	1:A:278:PRO:HD3	2.45	0.41
1:A:75:TYR:CZ	1:A:320:LEU:HB2	2.56	0.41

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LYS:HZ1	6:A:548:HOH:H2[2_454]	1.33	0.27
1:A:145:GLN:O	6:A:628:HOH:H1[2_455]	1.57	0.03
6:A:639:HOH:O	6:A:770:HOH:H2[3_555]	1.59	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	403/414 (97%)	390 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	350/358 (98%)	333 (95%)	17 (5%)	22	14

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	39	GLN
1	A	86	PRO
1	A	88	ILE
1	A	105	PRO
1	A	108	GLN
1	A	128	GLU
1	A	138	LEU
1	A	149	ASN
1	A	166	LEU
1	A	178	LYS
1	A	211	ARG
1	A	217	THR
1	A	227	GLN
1	A	269	GLU
1	A	277	ARG
1	A	329	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	39	GLN
1	A	46	GLN
1	A	49	ASN
1	A	69	GLN
1	A	129	ASN
1	A	149	ASN
1	A	176	HIS
1	A	210	GLN
1	A	213	GLN
1	A	225	ASN
1	A	272	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 ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
4	CAM	A	422	-	12,12,12	0.91	0	20,21,21	1.67	6 (30%)
5	GOL	A	491	-	5,5,5	0.35	0	5,5,5	0.40	0
3	HEM	A	417	1	50,50,50	1.29	7 (14%)	67,82,82	1.12	3 (4%)

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
4	CAM	A	422	-	-	-	0/3/2/2
5	GOL	A	491	-	-	2/4/4/4	-
3	HEM	A	417	1	-	2/14/54/54	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	417	HEM	CAB-C3B	-3.27	1.38	1.47
3	A	417	HEM	CAC-C3C	-2.71	1.40	1.47
3	A	417	HEM	FE-NA	2.55	2.03	1.95
3	A	417	HEM	C4A-C3A	2.35	1.48	1.43
3	A	417	HEM	C1A-C2A	2.33	1.49	1.44
3	A	417	HEM	C4D-C3D	2.23	1.48	1.45
3	A	417	HEM	FE-NC	2.00	2.01	1.95

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	417	HEM	C3B-C4B-NB	4.19	112.48	109.47
4	A	422	CAM	C4-C3-C2	-3.06	96.68	102.05
4	A	422	CAM	C7-C1-C2	-2.97	95.27	100.33
3	A	417	HEM	C4B-C3B-C2B	-2.92	104.59	107.28
4	A	422	CAM	C5-C6-C1	-2.57	99.56	104.73
3	A	417	HEM	C3B-C2B-C1B	2.34	108.17	106.41
4	A	422	CAM	C3-C2-C1	2.33	112.98	107.43
4	A	422	CAM	C9-C7-C8	2.30	113.50	107.67
4	A	422	CAM	C6-C5-C4	2.09	106.42	103.16

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	417	HEM	C2C-C3C-CAC-CBC
3	A	417	HEM	C4C-C3C-CAC-CBC
5	A	491	GOL	O1-C1-C2-C3
5	A	491	GOL	O1-C1-C2-O2

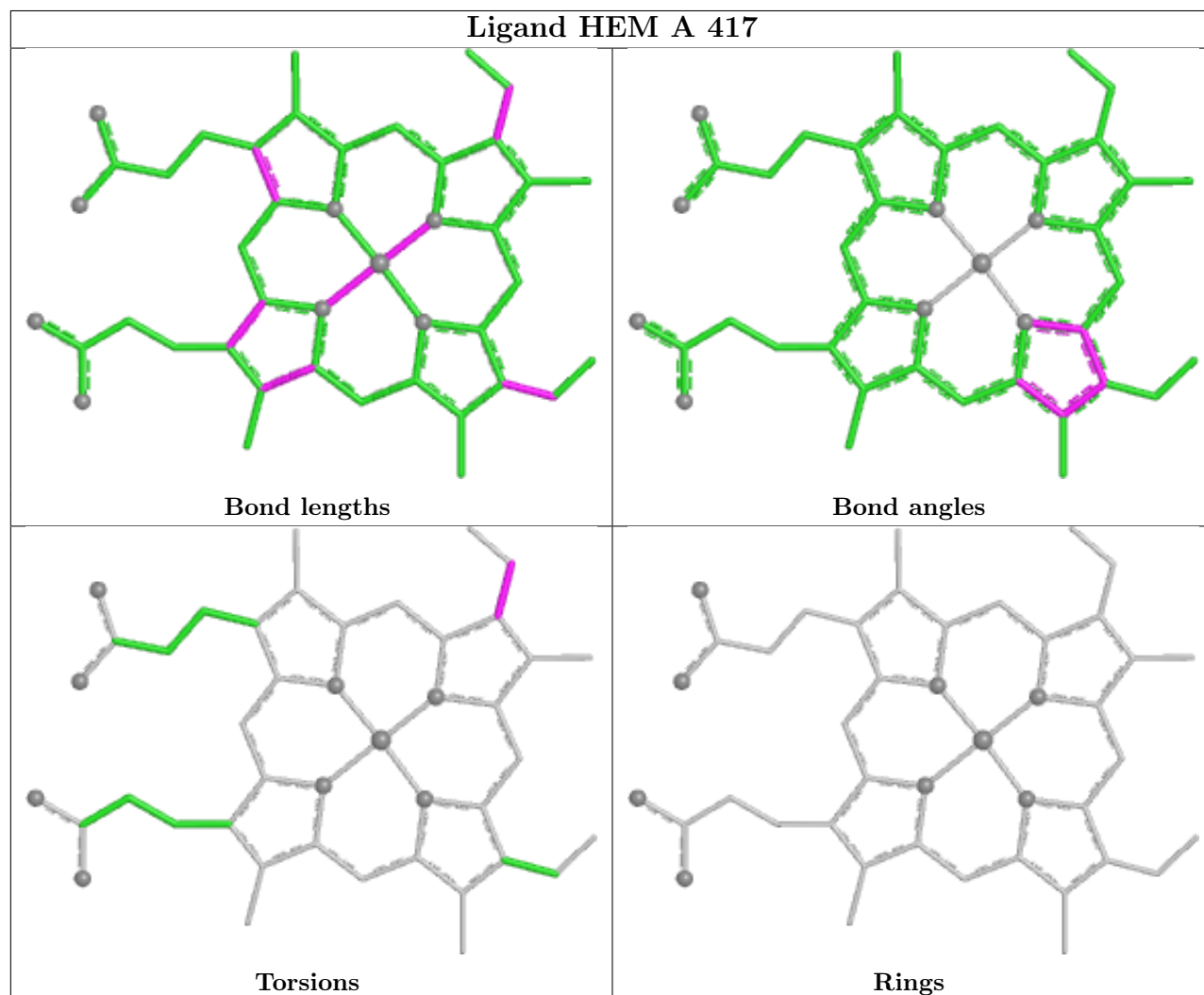
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	422	CAM	1	0
3	A	417	HEM	2	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.