



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:13 am BST

PDB ID : 2CP4
Title : CRYSTAL STRUCTURE OF THE CYTOCHROME P450-CAM ACTIVE
SITE MUTANT THR252ALA
Authors : Raag, R.; Poulos, T.L.
Deposited on : 1991-06-04
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) 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) : 2.11

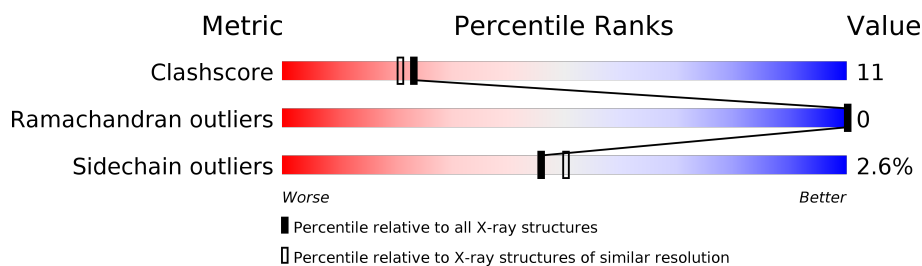
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 on 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	 62% 30% 5% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3519 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.

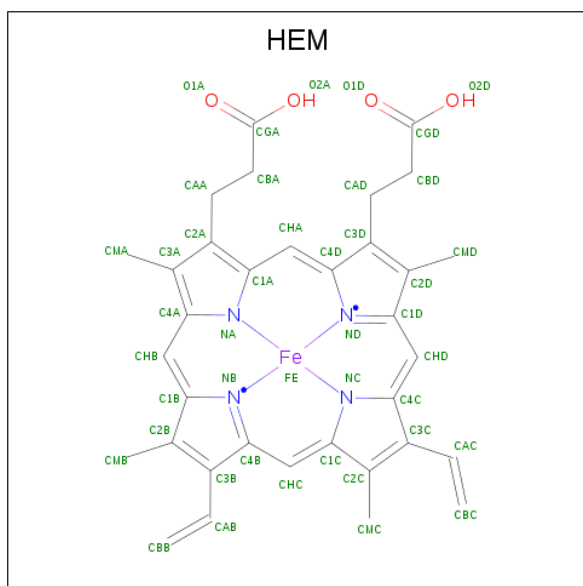
- Molecule 1 is a protein called CYTOCHROME P450-CAM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	405	3233	2054	561	600	18	0	7	0

There is a discrepancy between the modelled and reference sequences:

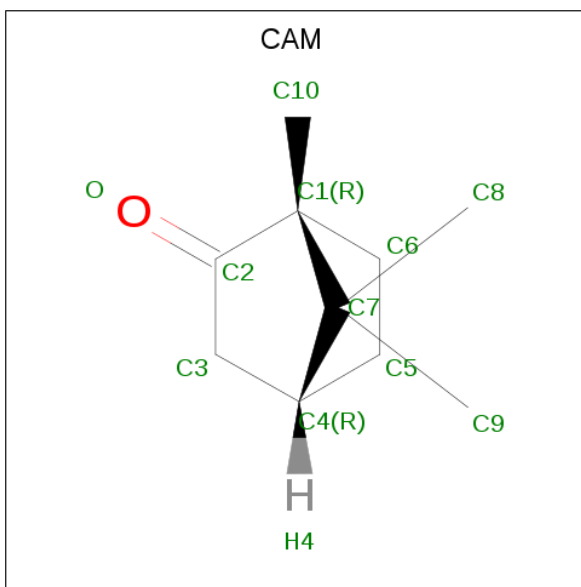
Chain	Residue	Modelled	Actual	Comment	Reference
A	252	ALA	THR	CONFLICT	UNP P00183

- 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 CAMPHOR (three-letter code: CAM) (formula: $C_{10}H_{16}O$).



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

- Molecule 4 is water.

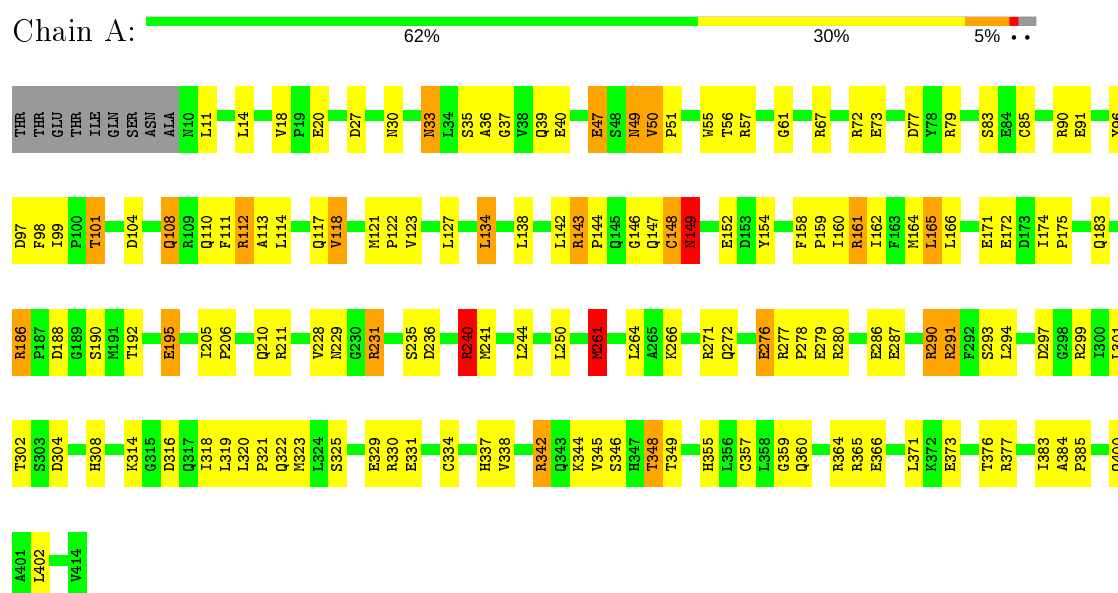
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	232	Total	O	0	0
			232	232		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 P450-CAM



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	108.67Å 103.90Å 36.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3519	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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, CAM

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	2/3340 (0.1%)	1.85	75/4538 (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	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	GLU	CD-OE1	7.78	1.34	1.25
1	A	37	GLY	N-CA	5.50	1.54	1.46

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	CD-NE-CZ	21.66	153.92	123.60
1	A	112	ARG	NE-CZ-NH1	14.41	127.50	120.30
1	A	290	ARG	NE-CZ-NH1	13.65	127.12	120.30
1	A	211	ARG	NE-CZ-NH2	13.25	126.92	120.30
1	A	365	ARG	NE-CZ-NH1	12.41	126.51	120.30
1	A	72	ARG	NE-CZ-NH2	-12.07	114.27	120.30
1	A	271	ARG	NE-CZ-NH1	11.84	126.22	120.30
1	A	210	GLN	CA-CB-CG	11.55	138.81	113.40
1	A	365	ARG	CD-NE-CZ	11.43	139.60	123.60
1	A	290	ARG	CD-NE-CZ	11.40	139.56	123.60
1	A	299	ARG	NE-CZ-NH2	-10.87	114.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ARG	CD-NE-CZ	9.86	137.40	123.60
1	A	67	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	A	280	ARG	NE-CZ-NH2	-9.45	115.58	120.30
1	A	148	CYS	C-N-CA	9.36	145.10	121.70
1	A	279	GLU	CA-CB-CG	9.07	133.35	113.40
1	A	27	ASP	CB-CG-OD1	8.83	126.25	118.30
1	A	79	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	A	271	ARG	CD-NE-CZ	8.47	135.46	123.60
1	A	33	ASN	CB-CA-C	8.43	127.25	110.40
1	A	186	ARG	NE-CZ-NH2	8.18	124.39	120.30
1	A	240	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	A	161	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	A	236	ASP	CB-CG-OD1	-7.64	111.42	118.30
1	A	90	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	A	231	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	67	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	277	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	A	79	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	280	ARG	CD-NE-CZ	6.35	132.50	123.60
1	A	342	ARG	CD-NE-CZ	6.32	132.44	123.60
1	A	90	ARG	CD-NE-CZ	6.29	132.41	123.60
1	A	400	GLN	CA-CB-CG	6.26	127.18	113.40
1	A	104	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	373	GLU	OE1-CD-OE2	-6.11	115.97	123.30
1	A	195	GLU	CA-CB-CG	5.96	126.52	113.40
1	A	291	ARG	CD-NE-CZ	5.96	131.94	123.60
1	A	330	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	364	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	261	MET	CG-SD-CE	5.85	109.55	100.20
1	A	161	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	57	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	366	GLU	OE1-CD-OE2	-5.76	116.39	123.30
1	A	11	LEU	CB-CA-C	5.74	121.10	110.20
1	A	152	GLU	CA-CB-CG	5.74	126.02	113.40
1	A	149	ASN	N-CA-CB	5.73	120.92	110.60
1	A	297	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	113	ALA	CB-CA-C	5.66	118.59	110.10
1	A	20	GLU	CA-CB-CG	5.66	125.85	113.40
1	A	172[A]	GLU	N-CA-CB	5.61	120.69	110.60
1	A	172[B]	GLU	N-CA-CB	5.61	120.69	110.60
1	A	47	GLU	CG-CD-OE1	5.59	129.49	118.30
1	A	85	CYS	N-CA-CB	-5.57	100.58	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	LEU	CA-CB-CG	5.49	127.94	115.30
1	A	348	THR	CA-CB-CG2	5.45	120.03	112.40
1	A	118	VAL	CA-CB-CG2	5.42	119.03	110.90
1	A	165[A]	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	165[B]	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	47	GLU	CG-CD-OE2	-5.40	107.50	118.30
1	A	149	ASN	CB-CA-C	5.40	121.20	110.40
1	A	286	GLU	CG-CD-OE2	-5.37	107.56	118.30
1	A	290	ARG	NH1-CZ-NH2	-5.32	113.55	119.40
1	A	142	LEU	C-N-CA	5.29	134.93	121.70
1	A	304	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	376	THR	CA-CB-CG2	5.21	119.69	112.40
1	A	301	LEU	CB-CA-C	5.21	120.09	110.20
1	A	149	ASN	O-C-N	-5.18	114.40	122.70
1	A	316	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	279	GLU	CB-CG-CD	5.15	128.10	114.20
1	A	123	VAL	CA-CB-CG1	5.09	118.54	110.90
1	A	50	VAL	CA-CB-CG2	5.09	118.53	110.90
1	A	329	GLU	CA-CB-CG	5.06	124.52	113.40
1	A	55	TRP	O-C-N	5.03	130.74	122.70
1	A	349	THR	CA-CB-CG2	5.03	119.44	112.40
1	A	40	GLU	OE1-CD-OE2	-5.02	117.28	123.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	VAL	Mainchain
1	A	143	ARG	Sidechain
1	A	148	CYS	Mainchain
1	A	149	ASN	Mainchain
1	A	154	TYR	Mainchain
1	A	186	ARG	Sidechain
1	A	240	ARG	Sidechain
1	A	250	LEU	Mainchain
1	A	377	ARG	Sidechain
1	A	77	ASP	Mainchain
1	A	96	TYR	Mainchain

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	3233	0	3186	73	0
2	A	43	0	30	3	0
3	A	11	0	16	1	0
4	A	232	0	0	3	0
All	All	3519	0	3232	74	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 11.

All (74) 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:110:GLN:HB3	1:A:228[A]:VAL:HG13	1.51	0.90
1:A:183:GLN:HE22	1:A:188:ASP:HB2	1.34	0.90
1:A:261:MET:HA	1:A:261:MET:HE2	1.71	0.73
1:A:127:LEU:HD11	1:A:166:LEU:HD13	1.72	0.72
1:A:110:GLN:HG3	1:A:229[A]:ASN:HB3	1.73	0.70
1:A:143:ARG:HB3	1:A:144:PRO:HD3	1.73	0.69
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.75	0.69
1:A:110:GLN:HG3	1:A:229[B]:ASN:HB2	1.74	0.68
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.77	0.65
1:A:261:MET:HE2	1:A:264:LEU:HD12	1.80	0.62
1:A:158:PHE:CE1	1:A:162[B]:ILE:HD11	2.36	0.61
1:A:261:MET:CE	1:A:264:LEU:HD12	2.31	0.61
1:A:134:LEU:HD22	1:A:138:LEU:HD22	1.83	0.60
1:A:112:ARG:NH1	2:A:415:HEM:O1D	2.32	0.59
1:A:183:GLN:NE2	1:A:188:ASP:HB2	2.13	0.58
1:A:146:GLY:O	1:A:147:GLN:HB3	2.04	0.57
1:A:160:ILE:O	1:A:164:MET:HG2	2.05	0.56
1:A:192:THR:OG1	1:A:195:GLU:HG2	2.06	0.54
1:A:276:GLU:C	1:A:278:PRO:HD3	2.30	0.52
1:A:33:ASN:O	1:A:36:ALA:HB3	2.10	0.51
1:A:30:ASN:HB2	4:A:730:HOH:O	2.10	0.51
2:A:415:HEM:HMB2	2:A:415:HEM:HBB2	1.93	0.50
1:A:291:ARG:HG2	1:A:338:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LYS:HD2	1:A:383:ILE:HD12	1.93	0.50
1:A:73:GLU:OE1	1:A:308:HIS:NE2	2.39	0.49
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.95	0.49
1:A:108:GLN:HG3	1:A:355:HIS:CE1	2.48	0.49
1:A:344:LYS:HE3	1:A:346:SER:HB2	1.94	0.48
1:A:359:GLY:HA3	2:A:415:HEM:C3C	2.49	0.48
1:A:56:THR:O	1:A:61:GLY:HA2	2.13	0.48
1:A:325:SER:O	1:A:331:GLU:HG3	2.13	0.48
1:A:97:ASP:O	1:A:240:ARG:HD2	2.14	0.47
1:A:110:GLN:HB2	4:A:707:HOH:O	2.13	0.47
1:A:134:LEU:HD12	1:A:162[A]:ILE:HG12	1.97	0.47
1:A:30:ASN:ND2	4:A:555:HOH:O	2.47	0.47
1:A:290:ARG:HD3	1:A:345:VAL:HG13	1.98	0.46
1:A:158:PHE:O	1:A:162[B]:ILE:HG13	2.16	0.46
1:A:111:PHE:HD1	1:A:241:MET:HE2	1.81	0.45
1:A:174:ILE:HB	1:A:175:PRO:HD3	1.98	0.45
1:A:319:LEU:HG	1:A:321:PRO:HG3	1.97	0.45
1:A:98:PHE:HB3	1:A:244:LEU:HB2	1.97	0.45
1:A:261:MET:HA	1:A:261:MET:CE	2.45	0.45
1:A:318:ILE:HD13	1:A:320:LEU:HD21	1.97	0.45
1:A:99:ILE:HG13	1:A:240:ARG:HB3	1.99	0.45
1:A:302:THR:O	1:A:314:LYS:HG3	2.16	0.45
1:A:110:GLN:CB	1:A:228[A]:VAL:HG13	2.36	0.45
1:A:384:ALA:HA	1:A:385:PRO:HD3	1.79	0.45
1:A:114:LEU:HD23	1:A:241:MET:HE3	2.00	0.44
1:A:127:LEU:CD1	1:A:166:LEU:HD13	2.43	0.44
1:A:114:LEU:HD23	1:A:241:MET:CE	2.47	0.44
1:A:334:CYS:O	1:A:337:HIS:HB3	2.16	0.44
1:A:101[B]:THR:HG21	3:A:416:CAM:H31	2.00	0.44
1:A:114:LEU:O	1:A:117:GLN:HB2	2.18	0.43
1:A:188:ASP:HB3	1:A:190:SER:H	1.83	0.43
1:A:14:LEU:HD11	1:A:18:VAL:CG1	2.47	0.43
1:A:50:VAL:HA	1:A:51:PRO:HD3	1.90	0.43
1:A:121:MET:CB	1:A:122:PRO:HD3	2.41	0.43
1:A:322:GLN:HB3	1:A:348:THR:O	2.18	0.43
1:A:294:LEU:HD23	1:A:294:LEU:H	1.84	0.42
1:A:293:SER:O	1:A:323:MET:HG3	2.20	0.42
1:A:266:LYS:HD2	1:A:383:ILE:CD1	2.49	0.42
1:A:47:GLU:HB2	1:A:49:ASN:ND2	2.34	0.42
1:A:287:GLU:OE1	1:A:342:ARG:HD2	2.20	0.42
1:A:149:ASN:ND2	1:A:402:LEU:H	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ARG:HD3	1:A:171:GLU:OE2	2.19	0.42
1:A:111:PHE:HB3	1:A:241:MET:HE2	2.02	0.42
1:A:91:GLU:H	1:A:91:GLU:CD	2.24	0.41
1:A:357:CYS:HB3	1:A:360:GLN:HB3	2.02	0.41
1:A:39:GLN:NE2	1:A:39:GLN:H	2.19	0.41
1:A:231:ARG:HG3	1:A:231:ARG:H	1.75	0.41
1:A:134:LEU:O	1:A:138:LEU:HB2	2.21	0.40
1:A:272:GLN:NE2	1:A:276:GLU:OE2	2.52	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	410/414 (99%)	392 (96%)	18 (4%)	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	356/357 (100%)	344 (97%)	12 (3%)	37	39

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

Mol	Chain	Res	Type
1	A	35	SER
1	A	49	ASN
1	A	101[A]	THR
1	A	101[B]	THR
1	A	108	GLN
1	A	134	LEU
1	A	165[A]	LEU
1	A	165[B]	LEU
1	A	235	SER
1	A	261	MET
1	A	371[A]	LEU
1	A	371[B]	LEU

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

Mol	Chain	Res	Type
1	A	30	ASN
1	A	39	GLN
1	A	49	ASN
1	A	69	GLN
1	A	108	GLN
1	A	149	ASN
1	A	213	GLN
1	A	225	ASN
1	A	337	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

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	HEM	A	415	1	27,50,50	2.15	7 (25%)	17,82,82	1.72	6 (35%)
3	CAM	A	416	-	12,12,12	1.59	3 (25%)	20,21,21	1.51	4 (20%)

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	415	1	-	0/6/54/54	-
3	CAM	A	416	-	-	-	0/3/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	415	HEM	C3C-C2C	-5.26	1.33	1.40
2	A	415	HEM	C3B-C2B	-4.48	1.34	1.40
2	A	415	HEM	C3C-CAC	4.22	1.56	1.47
2	A	415	HEM	C3B-CAB	3.58	1.55	1.47
3	A	416	CAM	C1-C2	3.47	1.57	1.52
2	A	415	HEM	C4B-NB	2.53	1.41	1.36
2	A	415	HEM	CMC-C2C	2.47	1.57	1.51
2	A	415	HEM	CAA-C2A	2.35	1.55	1.52
3	A	416	CAM	C7-C4	2.22	1.61	1.54
3	A	416	CAM	C3-C4	2.17	1.58	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	416	CAM	C9-C7-C8	-4.28	96.81	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	415	HEM	CBD-CAD-C3D	3.69	119.28	112.48
2	A	415	HEM	CMA-C3A-C4A	-3.03	123.81	128.46
3	A	416	CAM	C8-C7-C1	2.77	119.33	113.06
3	A	416	CAM	C9-C7-C1	2.49	118.70	113.06
2	A	415	HEM	CMD-C2D-C1D	-2.43	124.73	128.46
2	A	415	HEM	CMA-C3A-C2A	2.17	129.04	124.94
2	A	415	HEM	CMC-C2C-C3C	2.15	128.69	124.68
2	A	415	HEM	C4C-C3C-C2C	2.03	108.31	106.90
3	A	416	CAM	C5-C4-C3	2.01	111.94	106.40

There are no chirality outliers.

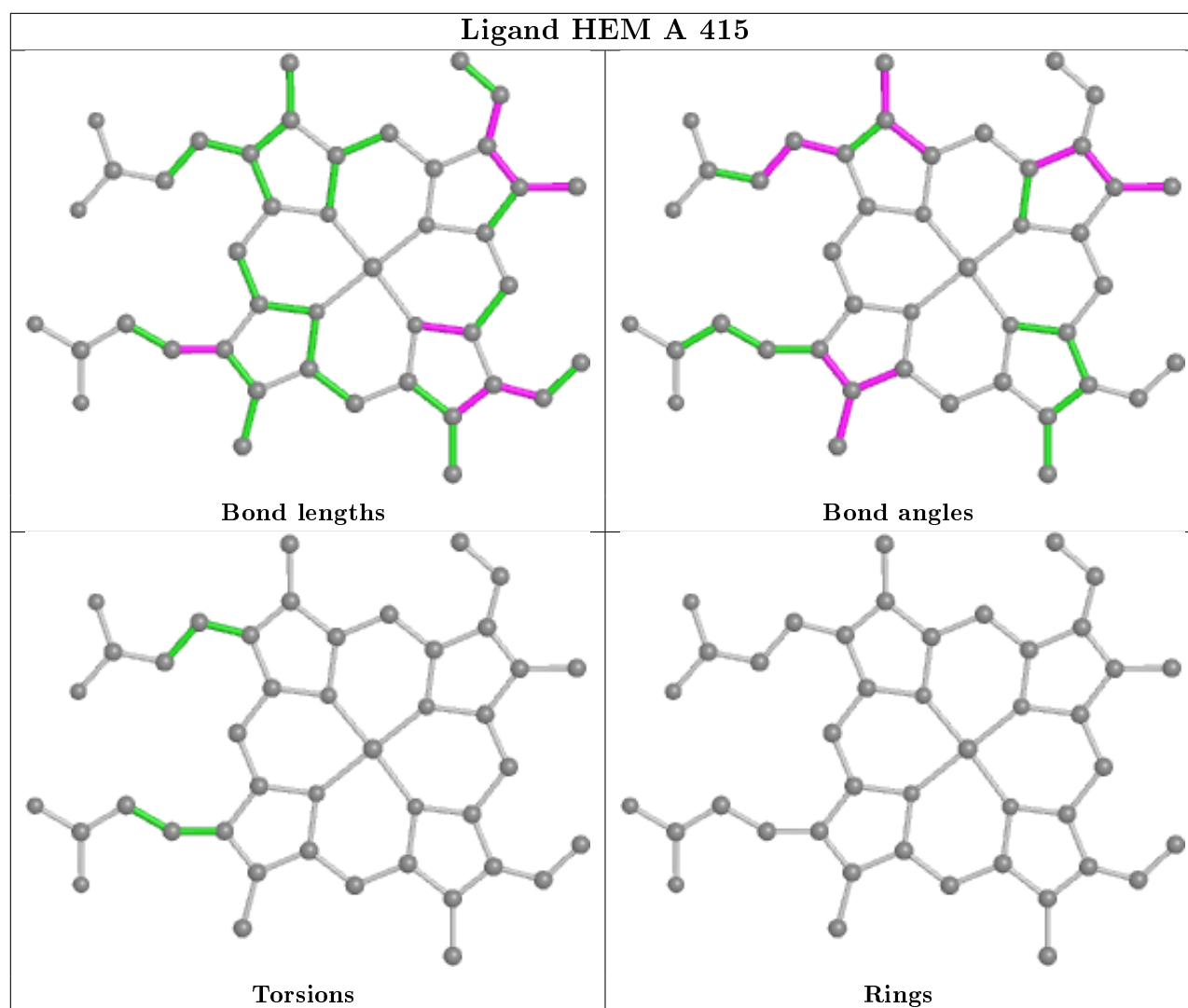
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	415	HEM	3	0
3	A	416	CAM	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.