



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:34 PM GMT

PDB ID : 4CP4
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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

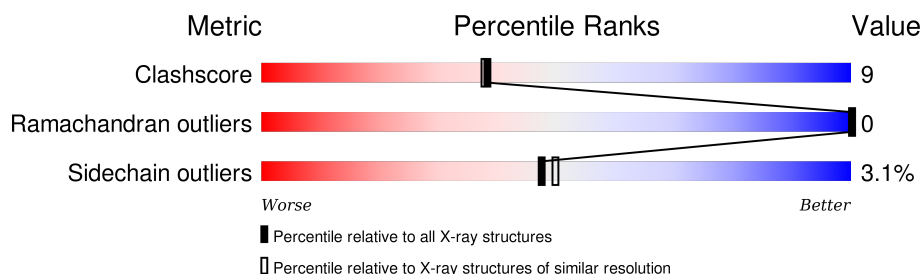
1 Overall quality at a glance

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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	414	 63% 28% 6% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3466 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.

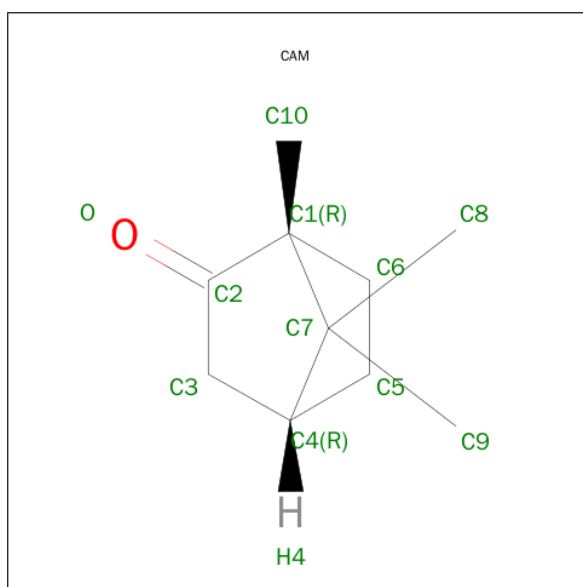
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3208	2033	560	597	18			

- 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
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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.

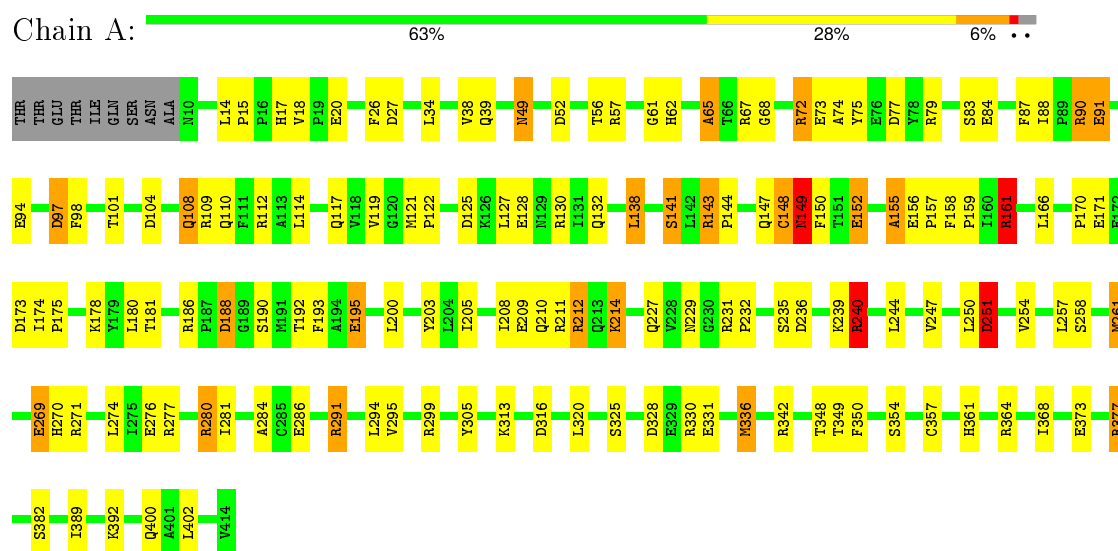
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	204	Total	O	0	0
			204	204		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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 will therefore be 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}	0.164 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3466	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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	1.28	3/3287 (0.1%)	1.97	86/4465 (1.9%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	ARG	NE-CZ	-6.33	1.24	1.33
1	A	286	GLU	CD-OE1	-5.08	1.20	1.25
1	A	373	GLU	CD-OE1	-5.02	1.20	1.25

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	CD-NE-CZ	30.17	165.84	123.60
1	A	67	ARG	NE-CZ-NH2	-20.27	110.16	120.30
1	A	67	ARG	NE-CZ-NH1	15.93	128.26	120.30
1	A	212	ARG	CD-NE-CZ	14.60	144.03	123.60
1	A	214	LYS	CB-CA-C	12.93	136.25	110.40
1	A	79	ARG	NE-CZ-NH1	11.88	126.24	120.30
1	A	211	ARG	NE-CZ-NH2	11.44	126.02	120.30
1	A	143	ARG	NE-CZ-NH2	-11.30	114.65	120.30
1	A	280	ARG	NE-CZ-NH1	11.17	125.89	120.30
1	A	79	ARG	NE-CZ-NH2	-10.73	114.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	ARG	CD-NE-CZ	10.45	138.22	123.60
1	A	72	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	A	20	GLU	CA-CB-CG	9.46	134.21	113.40
1	A	186	ARG	NE-CZ-NH2	9.40	125.00	120.30
1	A	195	GLU	CA-CB-CG	9.05	133.32	113.40
1	A	148	CYS	C-N-CA	8.95	144.07	121.70
1	A	330	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	A	74	ALA	CB-CA-C	8.68	123.12	110.10
1	A	299	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	271	ARG	CD-NE-CZ	8.40	135.37	123.60
1	A	316	ASP	CB-CG-OD2	8.40	125.86	118.30
1	A	104	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	A	377	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	A	109	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	209	GLU	CA-CB-CG	7.59	130.11	113.40
1	A	348	THR	CA-CB-CG2	7.43	122.80	112.40
1	A	112	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	299	ARG	CD-NE-CZ	7.17	133.64	123.60
1	A	104	ASP	CB-CG-OD1	7.12	124.71	118.30
1	A	392	LYS	CA-CB-CG	7.09	129.00	113.40
1	A	373	GLU	OE1-CD-OE2	-7.08	114.80	123.30
1	A	149	ASN	N-CA-CB	7.08	123.34	110.60
1	A	97	ASP	CB-CG-OD1	7.00	124.59	118.30
1	A	349	THR	CA-CB-CG2	6.90	122.06	112.40
1	A	342	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	A	280	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	295	VAL	CG1-CB-CG2	-6.55	100.42	110.90
1	A	286	GLU	N-CA-CB	6.43	122.18	110.60
1	A	143	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	A	84	GLU	CA-CB-CG	6.40	127.48	113.40
1	A	128	GLU	N-CA-CB	6.36	122.05	110.60
1	A	72	ARG	NH1-CZ-NH2	6.35	126.39	119.40
1	A	73	GLU	OE1-CD-OE2	6.34	130.91	123.30
1	A	280	ARG	CD-NE-CZ	6.34	132.47	123.60
1	A	155	ALA	CB-CA-C	6.31	119.56	110.10
1	A	138	LEU	CB-CA-C	6.30	122.17	110.20
1	A	91	GLU	CB-CA-C	-6.30	97.81	110.40
1	A	132	GLN	N-CA-CB	-6.17	99.50	110.60
1	A	65	ALA	CB-CA-C	6.07	119.20	110.10
1	A	336	MET	CA-CB-CG	6.00	123.51	113.30
1	A	26	PHE	CB-CG-CD1	-5.94	116.64	120.80
1	A	261	MET	CA-CB-CG	-5.89	103.28	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	NH1-CZ-NH2	-5.89	112.92	119.40
1	A	52	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	210	GLN	CA-CB-CG	5.79	126.15	113.40
1	A	90	ARG	CD-NE-CZ	5.78	131.69	123.60
1	A	400	GLN	CA-CB-CG	5.73	126.02	113.40
1	A	141	SER	CB-CA-C	5.68	120.89	110.10
1	A	161	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	152	GLU	OE1-CD-OE2	5.64	130.07	123.30
1	A	188	ASP	N-CA-CB	-5.56	100.59	110.60
1	A	27	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	109	ARG	CD-NE-CZ	5.51	131.31	123.60
1	A	38	VAL	CA-CB-CG2	5.47	119.10	110.90
1	A	251	ASP	O-C-N	-5.43	114.02	122.70
1	A	38	VAL	CG1-CB-CG2	-5.42	102.23	110.90
1	A	161	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	87	PHE	CB-CG-CD1	5.39	124.57	120.80
1	A	138	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	305	TYR	O-C-N	5.31	131.20	122.70
1	A	130	ARG	N-CA-CB	5.30	120.14	110.60
1	A	291	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	258	SER	CB-CA-C	5.21	120.00	110.10
1	A	178	LYS	CB-CA-C	5.20	120.81	110.40
1	A	156	GLU	CA-CB-CG	5.20	124.83	113.40
1	A	125	ASP	CB-CG-OD2	5.20	122.97	118.30
1	A	276	GLU	N-CA-CB	5.19	119.94	110.60
1	A	79	ARG	CD-NE-CZ	5.11	130.75	123.60
1	A	269	GLU	CG-CD-OE2	-5.09	108.12	118.30
1	A	34	LEU	CB-CA-C	5.08	119.84	110.20
1	A	270	HIS	N-CA-CB	5.08	119.74	110.60
1	A	257	LEU	CA-CB-CG	5.07	126.97	115.30
1	A	75	TYR	CB-CG-CD2	5.02	124.01	121.00
1	A	240	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	A	193	PHE	O-C-N	5.01	130.72	122.70
1	A	180	LEU	CB-CA-C	5.01	119.71	110.20

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	VAL	Mainchain
1	A	147	GLN	Mainchain
1	A	148	CYS	Mainchain

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Mol	Chain	Res	Type	Group
1	A	149	ASN	Mainchain
1	A	161	ARG	Sidechain
1	A	240	ARG	Sidechain
1	A	250	LEU	Mainchain
1	A	251	ASP	Mainchain
1	A	280	ARG	Sidechain
1	A	377	ARG	Sidechain
1	A	77	ASP	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	3208	0	3155	56	0
2	A	43	0	30	3	0
3	A	11	0	16	1	0
4	A	204	0	0	8	0
All	All	3466	0	3201	59	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 9.

All (59) 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:127:LEU:HD11	1:A:166:LEU:HD13	1.59	0.81
1:A:208:ILE:O	1:A:212:ARG:HG3	1.94	0.67
1:A:328:ASP:HB3	1:A:331:GLU:HG3	1.79	0.65
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.80	0.63
2:A:415:HEM:HMB2	2:A:415:HEM:HBB2	1.84	0.58
1:A:68:GLY:O	1:A:72:ARG:HG3	2.02	0.58
1:A:62:HIS:CG	1:A:88:ILE:HD13	2.38	0.58
1:A:149:ASN:ND2	1:A:402:LEU:H	2.02	0.57
1:A:281:ILE:HG22	1:A:368:ILE:HG23	1.87	0.56
1:A:188:ASP:HB3	1:A:190:SER:H	1.72	0.55
1:A:181:THR:CG2	1:A:251:ASP:HB2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ARG:HB3	1:A:144:PRO:HD3	1.89	0.54
1:A:149:ASN:HD21	1:A:402:LEU:H	1.54	0.54
1:A:254:VAL:HG23	4:A:687:HOH:O	2.07	0.54
1:A:281:ILE:CG2	1:A:368:ILE:HG23	2.37	0.53
1:A:192:THR:OG1	1:A:195:GLU:HG2	2.07	0.53
2:A:415:HEM:C1A	3:A:416:CAM:H4	2.43	0.53
1:A:181:THR:HG22	1:A:251:ASP:HB2	1.90	0.53
1:A:110:GLN:NE2	1:A:229:ASN:HA	2.24	0.53
1:A:49:ASN:H	1:A:49:ASN:HD22	1.57	0.53
1:A:389:ILE:HA	4:A:659:HOH:O	2.09	0.52
1:A:170:PRO:HG2	1:A:173:ASP:OD2	2.09	0.52
1:A:108:GLN:HE22	1:A:354:SER:HB2	1.74	0.52
1:A:150:PHE:CE2	1:A:155:ALA:HB2	2.45	0.51
1:A:200:LEU:O	1:A:203:TYR:HB3	2.11	0.50
1:A:274:LEU:HD21	1:A:284:ALA:HB2	1.94	0.49
1:A:294:LEU:HD23	1:A:294:LEU:N	2.28	0.48
1:A:361:HIS:HB2	4:A:560:HOH:O	2.12	0.48
1:A:97:ASP:O	1:A:240:ARG:HD2	2.13	0.48
1:A:158:PHE:CB	1:A:159:PRO:HD3	2.42	0.47
1:A:56:THR:HG21	1:A:62:HIS:CE1	2.49	0.47
1:A:291:ARG:CZ	1:A:336:MET:HE3	2.45	0.47
1:A:121:MET:HB2	1:A:122:PRO:HD3	1.97	0.46
1:A:205:ILE:HD11	1:A:239:LYS:HD2	1.95	0.46
1:A:14:LEU:HA	1:A:15:PRO:HD3	1.82	0.46
1:A:152:GLU:HB3	4:A:563:HOH:O	2.15	0.46
1:A:56:THR:O	1:A:61:GLY:HA2	2.16	0.46
1:A:382:SER:HB2	4:A:608:HOH:O	2.16	0.45
1:A:91:GLU:H	1:A:91:GLU:CD	2.20	0.45
1:A:65:ALA:HB3	1:A:320:LEU:HD23	1.97	0.45
1:A:161:ARG:HD3	1:A:171:GLU:OE2	2.16	0.45
1:A:17:HIS:CD2	1:A:313:LYS:HG3	2.52	0.45
1:A:138:LEU:HD21	1:A:157:PRO:HB2	1.99	0.45
1:A:236:ASP:O	1:A:240:ARG:HG3	2.16	0.45
1:A:57:ARG:HG2	4:A:508:HOH:O	2.16	0.45
1:A:181:THR:HG23	1:A:247:VAL:HG13	1.98	0.44
1:A:174:ILE:HB	1:A:175:PRO:HD3	1.99	0.44
1:A:98:PHE:HB3	1:A:244:LEU:HB2	1.98	0.44
1:A:350:PHE:HB3	1:A:357:CYS:HB3	1.99	0.44
1:A:114:LEU:O	1:A:117:GLN:HB2	2.18	0.44
1:A:231:ARG:HB2	1:A:232:PRO:CD	2.49	0.43
1:A:328:ASP:HB3	1:A:331:GLU:CG	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:415:HEM:HBB2	2:A:415:HEM:CMB	2.50	0.42
1:A:294:LEU:HD23	1:A:294:LEU:H	1.85	0.42
1:A:14:LEU:HD11	1:A:18:VAL:CG1	2.49	0.42
1:A:101:THR:HB	4:A:652:HOH:O	2.20	0.41
1:A:269:GLU:H	1:A:269:GLU:CD	2.23	0.41
1:A:122:PRO:HD2	4:A:701:HOH:O	2.20	0.41
1:A:90:ARG:O	1:A:94:GLU:HG3	2.21	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	403/414 (97%)	388 (96%)	15 (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	350/358 (98%)	339 (97%)	11 (3%)	47	50

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	49	ASN
1	A	83	SER
1	A	108	GLN
1	A	141	SER
1	A	214	LYS
1	A	227	GLN
1	A	235	SER
1	A	261	MET
1	A	277	ARG
1	A	325	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	46	GLN
1	A	49	ASN
1	A	59	ASN
1	A	69	GLN
1	A	108	GLN
1	A	110	GLN
1	A	149	ASN
1	A	213	GLN
1	A	225	ASN
1	A	388	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 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	30,50,50	2.79	8 (26%)	24,82,82	2.93	12 (50%)
3	CAM	A	416	-	12,12,12	1.83	2 (16%)	21,21,21	1.94	4 (19%)

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	-	0/10/54/54	0/0/8/8
3	CAM	A	416	-	-	0/0/31/31	0/0/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	415	HEM	C3B-C4B	-10.92	1.42	1.51
2	A	415	HEM	C2D-C3D	-6.71	1.34	1.54
2	A	415	HEM	C3D-C4D	-4.78	1.45	1.51
2	A	415	HEM	C2B-C1B	-2.69	1.43	1.51
2	A	415	HEM	C2D-C1D	-2.66	1.43	1.51
2	A	415	HEM	C2C-C1C	-2.51	1.47	1.52
3	A	416	CAM	C3-C2	2.37	1.58	1.51
2	A	415	HEM	FE-NC	2.39	2.05	1.95
2	A	415	HEM	C3C-CAC	2.46	1.55	1.51
3	A	416	CAM	C1-C2	4.99	1.59	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	416	CAM	C9-C7-C8	-5.97	93.73	107.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	415	HEM	CMA-C3A-C4A	-4.57	120.80	128.36
2	A	415	HEM	C3C-CAC-CBC	-4.32	117.83	124.46
2	A	415	HEM	CAA-C2A-C1A	-4.13	122.52	127.01
3	A	416	CAM	C9-C7-C4	2.34	119.27	113.53
2	A	415	HEM	CBD-CAD-C3D	2.46	120.70	113.55
2	A	415	HEM	CMA-C3A-C2A	2.75	130.99	125.24
2	A	415	HEM	CMD-C2D-C3D	2.83	126.88	114.35
3	A	416	CAM	C8-C7-C1	2.85	119.98	113.01
2	A	415	HEM	CAD-C3D-C4D	3.04	123.19	112.47
2	A	415	HEM	C3B-C4B-CHC	3.32	127.83	123.16
3	A	416	CAM	C6-C1-C2	3.41	108.72	102.93
2	A	415	HEM	C2D-C3D-C4D	3.64	107.66	101.50
2	A	415	HEM	CMC-C2C-C3C	4.81	128.53	116.53
2	A	415	HEM	CMB-C2B-C3B	5.32	129.82	116.53
2	A	415	HEM	CAD-C3D-C2D	5.53	129.12	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	415	HEM	3	0
3	A	416	CAM	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.